Homogenisierung in finiter Thermo-Viskoplastizität
Homogenization in finite thermo-viscoplasticity
Zusammenfassung


Schlagworte: große Deformationen, Thermo-Plastizität, Thermo-Viskoelastizität, asymptotische Erweiterung, Homogenisierung.
Abstract

This dissertation mainly presents a two-scale thermo-viscoplastic analysis for heterogeneous compressible rubber-like materials at finite strains in a fully transient setting. This work consists of three major parts: first, material modeling is performed to present the governing equations of the problem, second, an asymptotic expansion approach is employed to build up the homogenization procedure, and finally these results are applied to consistently perform the first-order classical/computational homogenization technique. On the material modeling side, two (kinematically) different constitutive theories are developed to model a combination of thermo-plastoelastic and thermo-viscoelastic material behaviors. These finite deformation models have been motivated by simple rheological models and lead to decoupled (first model) and coupled (second model) interactions of the plastic and viscous intermediate configurations. Assuming a general internal variable vector which induces a total dissipation function, a thermoinelastic material in the most general case is considered from the outset for the asymptotic expansion analysis. Within this framework, two microscopically uncoupled cell problems (a purely mechanical problem is followed by a purely thermal one) with the explicit enforcement of macroscopic temperature are obtained as in the thermoelastic problems. Assuming this temperature enforcement on the computational homogenization side, the two mechanical and thermal cell problems together with their consistent macroscopic governing equations are analyzed for the problem at hand. The micro-to-macro transition is based on the appropriate identification of the macroscopic density, internal energy, elastic entropy and total dissipation function which guarantees the thermodynamic consistency among various macroscopic quantities. Details of the algorithmic treatment and consistent linearization are provided in the monolithic way for the macroscopic boundary value problems as well as the material modeling part. It is shown that in a fully transient setting the macroscopic solution scheme can be completed in the monolithic manner as well as the staggering methods without any knowledge of higher-order sensitivity terms. Moreover, the macroscopic entropy production rate and its individual constituents are explicitly identified. Numerical examples are provided to demonstrate some aspects of the problem.

Keywords: Finite deformations, thermo-plasticity, thermo-viscoelasticity, asymptotic expansion, homogenization.
Acknowledgments

I would like to express my special appreciation and thanks to my advisor Prof. Dr.-Ing. habil. Dr. h.c. mult. Peter Wriggers, for supporting me during these past four years. He is a tremendous mentor and one of the smartest and nicest people I know. I hope that I could be as lively, enthusiastic, and energetic as him and to someday be able to command an audience as well as he can. He has been really supportive and gave me the freedom to find my PhD topic without any objection. I would like to thank him for encouraging my research and for allowing me to grow as a research scientist. His advice on my project has been priceless.

Besides my advisor, I would like to thank Dr. Ilker Temizer for his scientific advice and many insightful discussions and suggestions. He has been my primary resource for getting my science questions answered. He has also provided insightful discussions about the research and his perceptive questions about the details of the work led me to daily progress and really encouraged me to see my PhD topic deeper and deeper. His friendly welcome and support during my stay in Ankara is also appreciated.

I would also like to thank my colleagues at IKM for their brilliant comments, suggestions, and instrumental personalities. In particular, I am grateful to Dr. Stefan Löhner (the person who I learnt a lot of things from him because of his permanent astute discussions during the institute seminars), Dip.-Ing. Nasim Hajibeik, Dipl.-Math. Mohammadreza Safiei, Dip.-Ing. Tao Wu and Dip.-Ing. Chao Zhang for the daily discussions and enjoyable moments at IKM. My sincere thanks also go to Vera Halfar for her help and support throughout my time here.

Furthermore, I also thank my friends (too many to list here but you know who you are!) for providing support and friendship that I needed. I would especially like to thank Dr. Marco Paggi, Dr. Laura de Lorenzis, Dr. Tymofiy Gerasimov and Dr. Juan Ma for being supportive and their comments on choosing my PhD topic.

Finally, I especially thank my mom and dad. My hard-working parents have sacrificed their lives for me and provided unconditional love and care. Although they are not alive, they are in my heart forever. Special thanks to my sisters and brothers for their care and support. I love them so much, and I would not have made it this far without them.

Hannover, March 2014

Shahab Sahraee
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Chapter 1
Introduction

1.1 Motivation

Polymer-based micro-heterogeneous solids span a wide range of technologically relevant applications, from tires (Rattanasom et al., 2007), foams (Mills, 2007; Wu et al., 2013) and composites (Dang et al., 2012) to flexible electronics (Lee et al., 2012; Xu and Zhu, 2012), electro-active materials (Bar-Cohen, 2004, Kil et al., 2013) and hydrogels (Choi et al., 2013; Vashist et al., 2013; Yu et al., 2013). With rubber-like materials as a prime example, such solids are highly deformable and exhibit a strong rate- and temperature-sensitivity that is additionally accompanied by damage and plasticity effects. Having in mind the high deformability of polymers, applying the large deformation mechanics, i.e. geometrical nonlinearities makes sense. When combined with the multiscale nature of the material, this complex constitutive behavior poses a challenge in the characterization of the macroscopic response. The development and investigation of a homogenization-based multiscale approach in order to address this challenge within a computationally efficient and theoretically robust framework is the main goal of this thesis.

1.2 Background and state of the art

A firm mathematical foundation for homogenization has been established in 1970s and early 1980s based on the asymptotic expansion (AE) analysis. Pioneered by Babuska (1976), Sanchez-Palencia (1980) and Bakhvalov and Panasenko (1989), among others, the AE analysis naturally addresses the distinct scales within a heterogeneous domain and leads to a coupled set of boundary value problems which describes the macroscopic response based on the microscopic physics. Recent applications include interface mechanics (Lebon and Rizzoni, 2011), structural elements such as beams (Lee and Yu, 2011), the inelastic behavior of composites (Teng et al., 2012; Fish et al., 2012) and thermomechanical modeling (Terada et al., 2010; Tang et al., 2012). The advantage of AE is its ability to predict an exact macroscopic response once the microstructural
topography and the microscopic constitutive models are chosen. In particular for linear problems, exact or approximate macroscopic descriptions may also be obtained through effective medium theories which can significantly decrease the cost associated with the solution of the macroscopic problem – see Sevostianov and Giraud (2013), Manoylov et al. (2013), Fleischmann et al. (2013a), Fleischmann et al. (2013b) and To et al. (2013) for recent examples. However, kinematic nonlinearities pose significant limitations in pursuing effective medium theories (Ponte Castañeda and Galipeau, 2011; Ponte Castañeda and Siboni, 2012).

While the structure of the AE description of the multiscale problem is amenable to a direct computational implementation (Guedes and Kikuchi, 1990; Terada et al., 2003; Yu and Fish, 2002; Zhang et al., 2007), in an algorithmically equivalent fashion to the so-called FE² method (Feyel and Chaboche, 2000; Miehe et al., 1999; Kouznetsova et al., 2001; Linder et al., 2011); physically-based homogenization schemes can alternatively be pursued. These computational micromechanics approaches take energetic arguments such as the Hill-Mandel condition (Hill, 1965; Hill, 1984) as the starting point in order to link the macroscopic kinematic and kinetic variables to their microscopic counterparts (Zohdi and Wriggers, 2005; Gross and Seelig, 2011; Maugin, 1999). A shortcoming of this approach is the obscured link between the boundary value problems at the two scales. In particular, the identification of the macroscopic tangents for nonlinear problems requires additional effort (Geers et al., 2007; Miehe et al., 2002; Temizer and Wriggers, 2008b). One advantage, on the other hand, is the direct focus of the approach on macroscopic quantities of interest, such as stresses and fluxes, based on the efficient identification of a statistically representative sample (Moussaddy et al., 2013; Giraldi et al., 2013; Yvonnet, 2012). Recent example applications include the multiscale degradation of concrete (Nguyen et al., 2012), viscoelasticity (Miehe et al., 2004; Tang et al., 2006; Schüler et al., 2013), elasto-plasticity (Yvonnet et al., 2005; Nezamabadi et al., 2010; Poh et al., 2013; Khdir et al., 2013; Fritzen et al., 2012; Harthong et al., 2012), transformation-induced plasticity (Turteltaub and Suiker, 2006a; Yadegari et al., 2014), dynamic excitation problems (Chen and Ghosh, 2012; Srivastava and Nemat-Nasser, 2012; Gonella et al., 2011), interface inelasticity (Reina-Romo and Sanz-Herrera, 2011; Sacco and Lebon, 2012) and electrodynamics (Kim, 2011; Schröder and Keip, 2012; Zohdi, 2012; Zohdi, 2014).

Another advantage of micromechanical approaches is the ability to generalize the computational basis for homogenization towards higher-order continuum formulations (Kouznetsova et al., 2004; Jänicke and Steeb, 2012) which can describe size effects that are not accessible once scale separation is enforced as in most AE approaches. Size effects are inherent to modeling multiscale plates (Lebée and Sab, 2012), shells (Larsson and Landervik, 2013) and surfaces (Javili et al., 2013) as well as micromorphic continua (Jänicke et al., 2009; Jänicke and Diebels, 2009). It is noted that, while often ignored, stability of heterogeneous media may be a dominant factor in the macroscopic response exhibited – see Bertoldi and Gei (2011), Rudykh and Bertoldi (2013) and references therein for recent studies.

Either through AE analysis or a micromechanical approach, kinematically and materially nonlinear problems pose additional challenges, specifically due to the absence of an explicit macroscopic material model. The study of purely mechanical finite deformation
problems have been initiated in Terada and Kikuchi (1996), Miehe et al. (1999) and Takano et al. (2000); see Nguyen et al. (2013), Schröder et al. (2011) and Larsson et al. (2011) for recent examples, and nonlinear thermal problems have been addressed in Laschet (2002), Özdemir et al. (2008a) and Teng et al. (2012). Studies of coupled thermomechanical problems at finite deformations are significantly more limited. Miehe et al. (1999) have made a pioneering contribution in the context of crystal plasticity by linking the scales in a transient setting where microscopic dissipation is reflected onto the macroscale as a heating term within an adiabatic assumption. Among others, Aboudi (2002) addressed the thermoelastic behavior of multiphase composites that involve rubber-like phases and Turteltaub and Suiker (2006b) developed a multiscale thermomechanical model to analyze martensitic phase transformations from a cubic crystalline lattice to a tetragonal crystalline lattice. The thermodynamic consistency of the scale transition for homogenization in finite thermo-elastoplasticity (TE) has been investigated in Temizer and Wriggers (2011), the conclusions of which were supported by an AE analysis in Temizer (2012). Recently, with applications to modeling damage and plasticity in crystalline microstructures, Mandadapu et al. (2012) and Sengupta et al. (2012) have proposed an alternative approach with the additional capability of incorporating inelastic effects based on the computational framework that was advocated in Özdemir et al. (2008b). The present work aims to build on these recent contributions by further investigating the thermodynamic assumptions underlying homogenization in finite thermo-inelasticity and establishing a general framework that is motivated by the finite thermo-viscoplastic response of micro-heterogeneous polymeric materials.

1.3 Structure of this work

This work contains three main chapters presenting 1- material modeling, 2- AE analysis, and 3- computational homogenization approach as well as numerical examples and conclusions presented in chapters 4 and 5, respectively. The first chapter deals with the development of two (kinematically) distinct constitutive theories which accounts for combinations of finite thermo-viscoelasticity (TVE) and thermo-plasticity for compressible rubber-like materials. Throughout this work, the both constitutive theories are distinguished by "first formulation" and "second formulation". For the thermo-viscoelastic part, the procedure developed by Reese and Govindjee (1998a) is followed and for the thermo-plastoelastic behavior, it is mainly focused on the work of Simo and Miehe (1992) based on the $J_2$-plasticity theory. Throughout the developments, some aspects of endochronic plasticity are also partly addressed for completeness. For the first formulation, dual decompositions of the deformation gradient as $F = F_{ep}F_p = F_{ev}F_v$ are taken whereas for the second formulation a decomposition of the form $F = F_{ev}F_pF_v$ is presumed at the outset. This leads to the associated thermo-viscoelastic and thermo-plastoelastic formulations decoupled from each other in the first formulation whereas interaction between viscous and plastic intermediate configurations in the second formulation becomes unavoidable. The class of compressible Ogden materials (Ogden, 1972a; Ogden, 1972b) is taken throughout the work as an application for the developed
constitutive formulations. An outline of the reminder of this chapter is as follows. In subsections 2.1 and 2.2, two distinct simple one-dimensional rheological models and subsequently their generalization to the three-dimensional geometrically linear theory are presented which motivates the two classes of the finite thermo-viscoelastic-plastic formulations presented in this work. The generalization of the developed linear formulations to the finite deformation regime is carried out in subsection 2.3 in a thermodynamically consistent framework. Suitable for finite element implementation, the algorithmic treatment and linearization of the both thermo-viscoelastic-plastic models using the well-known product formula and exponential mapping algorithms are represented in details in subsections 2.3.5-2.3.6 as well as Appendixes A-C.

To provide a clear mathematical basis for practical homogenization methods, AE approach is presented in chapter 3. In this chapter, the procedure developed by Temizer (2012) is mainly followed and extended to a general thermoinelastic material. At the beginning of this chapter, AEs of primal and dual variables are presented and at the end, two-scale (micro and macro) forms of developed mechanical and thermal governing equations are represented. The developed constitutive formulations in one hand and a consistent mathematical framework for homogenization analysis on the other hand, help in providing a consistent and robust classical first-order homogenization approach. This is done in chapter 4 with an outline as follows. First, the macroscopic governing equations are reviewed in 4.1 and then the identifications of some fundamental thermodynamic quantities are discussed in 4.2. These identifications are thoroughly examined and consistently verified in 4.3.3. At the end, macroscale solution is considered which consists of mechanical and thermal tangent computations. Appendixes D and E are related to this part.

In chapter 5, numerical examples are provided to demonstrate the applicability and robustness of the methodology developed in the chapters 2-4. At the end, chapter 6 discusses the results of this work by comparing the different models and indicates the possible future extensions.
Chapter 2
Material modeling

Rubber-like materials have gained much attention in technical industries due to the low weight, machinability and high deformability properties. Some important technical applications are vehicle tires (68%), footwear (5%), engineering devices (7.8%), latex products (8%), adhesives (3.2%) and pharmaceutical articles (Saccomandi and Ogden, 2004). Due to the wide and increasing applications of these materials in industry, a large number of research studies have been undertaken on the description of their elastic and inelastic (viscoelastic, plastoelastic, damage, etc) - typically not coupled with thermal - effects. To characterize the complex physics of inelastic deformation of the rubber-like polymers from the continuum and material science point of views, typically, two methodologies have been followed in the literature. They are based on the molecular network or phenomenological approaches. In the first approach and based on the transient network theory which is relied on the statistical mechanics approaches, a time-dependent energy function is presented - taking into account debonding and reformation of rubber molecule chains from the micromechanics point of view - to characterize constitutive equations of the problem. For more details on this approach see e.g. Treloar (1943, 1975), James and Guth (1949), Arruda and Boyce (1993), Bergström and Boyce (1998, 2000), Reese (2003), and Nguyen et al. (2008) among others. In the second approach, the phenomenological models of viscoelastic and/or plastoelastic solids in the realm of irreversible continuum thermodynamics with the so-called history variables are often employed. The constitutive relations for these models are supplemented with (the so-called evolution equations for the internal variables) some linear and/or nonlinear differential equations. The latter procedure is followed in this work.

One of the common features observed in this approach (for the finite deformation analysis) is utilizing the multiplicative decomposition of the deformation gradient (this is also employed in molecular network theories). To consider equilibrium hysteresis effects, this is based on the so-called Kröner-Lee decomposition (Kröner, 1960; Lee, 1969; Lee and Liu, 1967) as \( F = F_e F_p \) and to represent the non-equilibrium rate dependent behavior Sidoroff (1974) assumed the same deformation gradient as \( F = F_e F_v \) for the first time. The crucial point in developing phenomenological constitutive theories in (thermo-) viscoelasticity, is the choice of linear or nonlinear evolution equations. Based
on this classification Reese and Govindjee (1998a) called the theories with linear evolution equations as finite linear viscoelasticity theories which are valid when small perturbations away from equilibrium states are assumed while they termed finite viscoelasticity theories based on the utilizing nonlinear evolution equations account for large deviations away from thermodynamic equilibrium. For finite linear viscoelasticity theories it is referenced to Coleman and Noll (1961), Lubliner (1985), Le Tallec et al. (1993) and Holzapfel (1996); and for finite viscoelasticity theories see e.g. Koh and Eringen (1963), Sidoroff (1974), Haupt (1993), Reese and Govindjee (1998a), and Huber and Tsakmakis (2000) among others. Since rubber-like materials such as polymeric foams in reality exhibit a range of plasticity together with viscoelastic effects at macroscopic level, some research studies have been done on viscoplasticity effects of rubbers such as Miehe and Keck (2000), Nedjar (2002a and 2002b) and Lin et al., (2006). Miehe and Keck (2000) also considered damage effects and assuming the endochronic plasticity (Valanis, 1971); they fitted their results with experimental data while Nedjar (2002a) followed the work of Reese and Govindjee (1998a) for the viscoelastic part and assumed the \( J_2 \)-flow theory for the plastic part. Lin et al. (2006) considered four different internal dissipation inequalities and compared them with each other from theoretical and computational point of view using the endochronic plasticity and \( J_2 \) flow theory for the plastic part. From experience it is clear that when the materials are loaded by inelastic deformations heat up and from thermodynamical point of view an amount of stress power is dissipated into heat. This motivated the scientists to consider the thermomechanical behavior of rubber-like materials with inelastic effects. See Lion (1997a), Lion (1997b), Reese and Govindjee (1998b), and Holzapfel and Simo (1996a) (it can be considered as the finite linear viscoelasticity theory) for this thermomechanical point of view. It is also referenced to the valuable work of Simo and Miehe (1992) on associative coupled thermo-plasticity accounts for metal plasticity.

In order to account for energy storage mechanisms associated with plastic flow, Lion (2000) introduced further multiplicative decomposition in a way that inelastic part of deformation gradient (in Lion's notation \( F = F_e F_{in} \)) can be written as \( F_{in} = F_{ine} F_{inp} \). As a result of this additional multiplicative decomposition an additional intermediate configuration appears which Lion called it intermediate configuration of kinematic hardening. This Lion-type constitutive theory was followed by the other researchers such as Nedjar (2002a), Dettmer and Reese (2004), Menzel et al. (2005), Håkansson et al. (2005), Wallin and Ristinmaa (2005), Shutov and Kreißig (2008), Vladimirov et al. (2008), and Henann and Anand (2009).

To consider the thermal effects of elastic - possibly inelastic - continuum solids there is a well-known procedure originally proposed by Lu and Pister (1975). This is based on a separation of thermal and mechanical deformations in such way that deformation gradient is multiplicatively decomposed into mechanical and thermal parts as \( F = F_{e} F_{\theta} \) and this establishes a new (thermal) intermediate configuration. This idea was further developed in order to account for inelastic deformations. Some research works pertaining to this procedure are as follows. Boyce et al. (1992) proposed a decomposition of deformation gradient into elastic, thermal and plastic parts \( (F = F_e F_{\theta} F_p) \) - see also
Kamlah and Tsakmakis (1999) - whereas Yu et al. (1997) introduced a decomposition of deformation gradient into thermal, elastic and plastic parts \( F = F_\theta F_e F_p \).

The purpose of this chapter is to extend existing three-dimensional frameworks for finite TVE and thermo-plasticity to two unified thermo-viscoplastic material models. The development of these models will additionally help establish the continuum thermodynamics basis for the homogenization theory and provide the particular constitutive choices to be employed in the numerical investigations. The aim is to keep the approach sufficiently general so as to render it applicable to soft, finitely deformable materials, although the particular motivation is rubber-like materials which span a wide range of technological applications. To this end, the viscoelastic constituent of the theory represents rate-dependent effects which do not induce permanent microstructural changes or deformations while the plasticity constituent induces rate-independent effects that cause permanent microstructural changes and deformations. Damage effects, which induce permanent microstructural changes but no permanent deformations, are conceptually spanned by these two choices and hence are excluded.

Following the work of Reese and Govindjee (1998a) for modeling TVE and relying on the work of Simo and Miehe (1992) to characterize thermo-plasticity help in developing two (kinematically) distinct constitutive theories which are distinguished by the names "first formulation" and "second formulation" throughout this chapter. The deformation gradient \( F \) is assumed as the total one and therefore the work of Lu and Pister (1975) is not followed. Assuming additively decomposition of local free energy (and hence internal energy), the class of compressible Ogden materials (Ogden, 1972a; Ogden, 1972b) is presumed to specify the behavior of rubber-like materials.

### 2.1 Rheological model 1

**One-dimensional constitutive model for motivation**

In order to formulate the constitutive theory of materials with thermo-viscoelastic-plastic effects, let’s start with design of a one-dimensional rheological model depicted in figure 2.1 as the first model (Nedjar, 2002a). As shown, this model is based on the introduction of two springs (elasticity), a dashpot (viscosity) and a friction element (plasticity). This model consists of a frictional devise presenting rate-independent thermo-elastoplasticity (the spring of Hookean type with temperature dependent Young’s moduli \( E_{ep}(\theta) \) in series with a friction element with \( \sigma_y(\theta) > 0 \)) in parallel with a Maxwell element (the spring with \( E_{ev}(\theta) \) in series with a damper of Newtonian type with temperature dependent shear viscosity \( \zeta(\theta) \)). It is assumed that the rheological model has a unit area and unit length and in the context of thermodynamic this is called thermomechanical devise (Mauglin, 1999; Holzapfel, 2001). It should be noted that utilizing of the frictional element with initial temperature dependent yield stress \( \sigma_y(\theta) \)
is in the framework of the $J_2$-flow theory whereas for endochronic plasticity the yield condition does not exist anymore. As motivated by figure 2.1, the total stress $\sigma$ decomposes into an equilibrium stress and an overstress. The overstress is attributed to the Maxwell element, whose dashpot depends linearly on the deformation rate and on temperature. The equilibrium stress is due to the spring in the rate-independent friction element at the top. Now, the total stress is

$$\sigma = \sigma_{\text{eq}} + \sigma_{\text{neq}}.$$  \hspace{1cm} (2.1)

Since the strains at the top and bottom springs are $(\varepsilon - \varepsilon^p)$ and $(\varepsilon - \alpha)$, respectively; the equilibrium and non-equilibrium parts of the stress are as follow

$$\sigma_{\text{eq}} = E_{ep}(\theta)(\varepsilon - \varepsilon^p),$$ \hspace{1cm} (2.2a)

$$\sigma_{\text{neq}} = E_{ev}(\theta)(\varepsilon - \alpha) = \zeta(\theta)\dot{\alpha},$$ \hspace{1cm} (2.2b)

where from Eq. (2.2b) one can obtain the evolution equation for the internal variable $\alpha$

$$\dot{\alpha} + \frac{1}{\hat{\tau}}\alpha = \frac{1}{\hat{\tau}}\varepsilon,$$  \hspace{1cm} (2.3)

where $\hat{\tau}$ denotes the relaxation time and dot above the quantity denotes its time derivative.

### 2.1.1 Three-dimensional linearized model and continuum thermodynamic

Here the preceding simple uniaxial model is extended to the three-dimensional geometrically linear - with possibly materially nonlinear - theory. Motivated by the rheological model 1, one can assume the following free energy function of the form

$$\psi = \psi(\varepsilon, \varepsilon^p, \xi, \alpha, \theta) = \psi_{\text{eq}}(\varepsilon - \varepsilon^p, \xi, \theta) + \psi_{\text{ev}}(\varepsilon - \alpha, \theta),$$  \hspace{1cm} (2.4)
where $\varepsilon$ denotes the total infinitesimal strain tensor; $\varepsilon^p$ and $\alpha$ refer to the plastic and viscous strain tensors; and $\xi$ is vector of strain-like variables characterizing the hardening mechanism of the material. $\psi^{ep}$ presents the time-independent or equilibrium part of the free energy and $\psi^{ev}$ characterizes the time-dependent or non-equilibrium part of it. Please note that with a slight abuse of notation, in Eq. (2.4) and what follows, the same symbol has been used to denote the function and its value.

Let the dissipation principle in the form of the Clausius-Plank inequality to derive the constitutive equations

$$D_{int} = \sigma : \dot{\varepsilon} - \dot{\varepsilon} + \theta \dot{\eta} \geq 0,$$

where $\eta$ denotes the total entropy; two dots : denotes the double contraction between two tensors; and $e$ is the internal energy obtained by the Legendre transformation

$$e = \psi + \eta^e \theta,$$

where $\eta^e = \eta - \eta^p$ denotes the elastic part of the total entropy employed in above equation for two reasons; first it is consistent with the structure of free and internal energies which are functions of elastic deformation and then it is consistent with the temperature dependence property of the yield criterion $\phi$ if for example the maximum dissipation principle has to be used to derive the evolution equations of the problem.

From Eqs. (2.4), (2.5) and (2.6), one can obtain

$$[\sigma - \frac{\partial \psi^{ep}}{\partial (\varepsilon - \varepsilon^p)} - \frac{\partial \psi^{ev}}{\partial (\varepsilon - \alpha)}] : \dot{\varepsilon} + \frac{\partial \psi^{ep}}{\partial (\varepsilon - \varepsilon^p)} : \dot{\varepsilon}^p + \frac{\partial \psi^{ev}}{\partial (\varepsilon - \alpha)} : \dot{\alpha} - \frac{\partial \psi^{ep}}{\partial \xi} : \dot{\xi}

- (\frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta}) \dot{\theta} - \eta^e \dot{\theta} + \theta \dot{\eta}^p \geq 0.$$

By requiring that Eq. (2.7) must hold for all admissible processes, a standard argument (Truesdell and Noll, 1965) yields the following constitutive equations

$$\sigma = \frac{\partial \psi^{ep}}{\partial (\varepsilon - \varepsilon^p)} + \frac{\partial \psi^{ev}}{\partial (\varepsilon - \alpha)} = \sigma^{eq}_p + \sigma^{neq}_v, \quad (2.8a)$$

$$\eta^e = - \left( \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} \right). \quad (2.8b)$$

Furthermore, setting the stress-like vector $\beta = -\partial \psi^{ep} / \partial \xi$, the reduced dissipation inequality takes the form

$$D_{int} = D^p + D^\nu \geq 0,$$

where

$$D^p = \sigma^{eq}_p : \dot{\varepsilon}^p + \beta : \dot{\xi} + \theta \dot{\eta}^p \geq 0, \quad (2.10a)$$

$$D^\nu = \sigma^{neq}_v : \dot{\alpha} \geq 0. \quad (2.10b)$$

Note that the term $\beta : \dot{\xi}$ is small for rubber-like materials and can be ignored since it is not dominant as in the metal plasticity. Throughout this work, the terms $\theta \dot{\eta}^p$ and $\beta : \dot{\xi}$ evolve based on the $J_2$-flow theory in a consistent manner.
2.1.2 Evolution equations: thermo-plastoelastic part

In order to complete the present linearized constitutive theory of thermo-elastoviscoplasticity, it just remains to obtain the suitable evolution equations. To do this, first, one can assume a thermoelastic domain $\mathbb{E}$ (exist only for $J_2$-flow theory) and then take the principle of maximum plastic dissipation (Ciarlet, 1989) as

$$
\mathbb{E} = \{ (\sigma_p^{eq}, \beta, \theta) \mid \phi(\sigma_p^{eq}, \beta, \theta) \leq 0 \},
$$

(2.11)

where $\phi$ is a smooth possibly multi-surface yield criterion and the evolution equations are given by

$$
\dot{\varepsilon}^p = \gamma \frac{\partial \phi}{\partial \sigma_p^{eq}},
$$

(2.12a)

$$
\dot{\xi} = \gamma \frac{\partial \phi}{\partial \beta},
$$

(2.12b)

$$
\dot{\eta}^p = \gamma \frac{\partial \phi}{\partial \theta},
$$

(2.12c)

where $\gamma \geq 0$ is the consistency parameter satisfying the Kuhn-Tucker loading and unloading conditions

$$
\gamma \geq 0, \quad \phi(\sigma_p^{eq}, \beta, \theta) \leq 0, \quad \gamma \phi(\sigma_p^{eq}, \beta, \theta) = 0.
$$

(2.13)

2.1.3 Evolution equations: thermo-viscoelastic part

In order to satisfy the viscous part of internal dissipation, the same procedure as in Reese and Govindjee (1998a) is followed. They have proposed the existence of a convex creep-like potential $\varphi_v$ with the following property

$$
\varphi_v(\sigma_v^{neq}) = 0 \iff \sigma_v^{neq} = 0.
$$

(2.14)

Eq. (2.10b) and existence of the potential $\varphi_v$ leads to evolution of the internal variable $\alpha$

$$
\dot{\alpha} = \frac{\partial \varphi_v(\sigma_v^{neq})}{\partial \sigma_v^{neq}},
$$

(2.15)

which ensures that always $\mathcal{D}^\nu \geq 0$. 
2.2 Rheological model 2

One-dimensional constitutive model for motivation

In what follows, we proceed with design of the second one-dimensional rheological model as depicted in figure 2.2. Since the procedure is similar to the rheological model 1, common details mentioned in the preceding subsections are omitted. This time, this model consists of a frictional devise with $\sigma_y(\theta) > 0$ in series with a standard solid or the so called Zener model (Lejeunes et al., 2011) (the spring with $E_{ep}(\theta)$ in parallel with the Maxwell element). Motivated by figure 2.2, the total stress $\sigma$ decomposes into an equilibrium stress and an overstress. Since the strains at the top and bottom springs are $(\varepsilon - \varepsilon^p)$ and $(\varepsilon - \varepsilon^p - \alpha)$, respectively; the equilibrium and non-equilibrium parts of the stress are

$$\sigma_p^{eq} = E_{ep}(\theta)(\varepsilon - \varepsilon^p),$$  \hspace{1cm} (2.16a) \\
$$\sigma_v^{neq} = E_{ev}(\theta)(\varepsilon - \varepsilon^p - \alpha) = \zeta(\theta)\dot{\alpha}. \hspace{1cm} (2.16b)$$

Eq. (2.16b) yields the evolution equation for the internal variable $\alpha$

$$\dot{\alpha} + \frac{1}{\hat{\tau}} \alpha = \frac{1}{\hat{\tau}} (\varepsilon - \varepsilon^p), \hspace{1cm} (2.17)$$

with $\hat{\tau}$ denoting the relaxation time as before.

2.2.1 Three-dimensional generalization

As for the rheological model 1, the preceding uniaxial model 2 is extended to the 3D geometrically linear theory. The free energy function for this model can be written in the following decomposable form.
2.2. RHEOLOGICAL MODEL 2

\[ \psi = \psi(\epsilon, \epsilon^p, \xi, \alpha, \theta) = \psi^{ep}(\epsilon - \epsilon^p, \xi, \theta) + \psi^{ev}(\epsilon - \epsilon^p - \alpha, \theta). \]  

(2.18)

Using the time derivative of Eq. (2.18), the Clausius-Plank inequality (2.5), the Legendre transformation (2.6) and taking into account the additively decomposition of the total entropy, one can obtain

\[ \begin{align*}
\sigma - \frac{\partial \psi^{ep}}{\partial (\epsilon - \epsilon^p)} &\cdot \dot{\epsilon} + \left[ \frac{\partial \psi^{ep}}{\partial (\epsilon - \epsilon^p)} + \frac{\partial \psi^{ev}}{\partial (\epsilon - \epsilon^p - \alpha)} \right] \cdot \dot{\epsilon}^p \\
+ \frac{\partial \psi^{ev}}{\partial (\epsilon - \epsilon^p - \alpha)} &\cdot \dot{\alpha} - \frac{\partial \psi^{ep}}{\partial \xi} \cdot \dot{\xi} - \left( \eta^e + \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} \right) \dot{\theta} + \theta \dot{\eta}^p &\geq 0.
\end{align*} \]

(2.19)

Since this inequality has to be satisfied for arbitrary values of the rates of \( \epsilon \) and \( \theta \), the following potential relations for the stress and elastic entropy can be obtained as the necessary condition for the compatibility with the second law of thermodynamics as follows

\[ \sigma = \frac{\partial \psi^{ep}}{\partial (\epsilon - \epsilon^p)} + \frac{\partial \psi^{ev}}{\partial (\epsilon - \epsilon^p - \alpha)} = \sigma^{eq} + \sigma^{neq}, \]

\[ \eta^e = - \left( \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} \right), \]

(2.20)

(2.21)

such that by setting the stress-like vector \( \beta = -\frac{\partial \psi^{ep}}{\partial \xi} \) as before, the reduced dissipation inequality takes the form

\[ \mathcal{D}_{int} = \mathcal{D}^p + \mathcal{D}^\nu \geq 0, \]

(2.22)

where

\[ \begin{align*}
\mathcal{D}^p &= \sigma : \dot{\epsilon}^p + \beta : \dot{\xi} + \theta \dot{\eta}^p \geq 0, \\
\mathcal{D}^\nu &= \sigma^{neq} : \dot{\alpha} \geq 0.
\end{align*} \]

(2.23a)

(2.23b)

Now the reader should distinguish between the plastic dissipation given in Eq. (2.23a) for the case of \( J_2 \)-flow theory and its equivalent form for endochronic plasticity which should be \( \mathcal{D}^p = \sigma : \dot{\epsilon}^p \).

2.2.2 Evolution equations: thermo-plastoelastic part

Now, it only remains to define the thermoelastic domain for \( J_2 \)-flow theory in order to obtain suitable evolution equations using the principle of maximum plastic dissipation. This is given by

\[ \mathcal{E} = \{(\sigma, \beta, \theta) \mid \hat{\phi}(\sigma, \beta, \theta) \leq 0\}, \]

(2.24)

where this time the thermoelastic domain is a function of the total stress \( \sigma \) and the evolution equations are
\[ \dot{\varepsilon}^p = \gamma \frac{\partial \hat{\varphi}}{\partial \sigma} \quad (2.25a) \]

\[ \dot{\xi} = \gamma \frac{\partial \hat{\varphi}}{\partial \beta} \quad (2.25b) \]

\[ \dot{\eta}^p = \gamma \frac{\partial \hat{\varphi}}{\partial \theta} \quad (2.25c) \]

where the consistency parameter \( \gamma \) should satisfy the Kuhn-Tucker conditions

\[ \gamma \geq 0, \quad \hat{\varphi}(\sigma, \beta, \theta) \leq 0, \quad \gamma \hat{\varphi}(\sigma, \beta, \theta) = 0. \quad (2.26) \]

### 2.2.3 Evolution equations: thermo-viscoelastic part

Let the following form of the evolution equation for the internal variable \( \alpha \) as for the Rheological model 1

\[ \dot{\alpha} = \frac{\partial \varphi_\nu(\sigma^{neq}_\nu)}{\partial \sigma^{neq}_\nu}. \quad (2.27) \]

### 2.3 Thermo-viscoplasticity at finite strains

In this subsection, the basic ideas associated with the rheological models presented in subsections 2.1-2.2 are generalized to the finite three-dimensional theory of thermo-viscoplasticity. Recall that the linearized theory relied on the additively decomposition of stress and free energy and hence entropy and internal energy functions to model the equilibrium and non-equilibrium effects (based on the extension of the developed 1D rheological models), and one of the key ideas was the additively decomposition of the total strain tensor. The latter idea cannot be generalized to the finite deformation since infinitesimal strain tensor is not an invariant under the superposed rigid body motions. There are various possible choices to formulate the constitutive equations for the finite deformation problems. This leads to the well-known difficulty associated with the definition of a suitable strain and stress measures for the development of finite deformation models. This has been matter of many different research efforts especially in view of numerical algorithms for finite element analysis, see e.g., Hencky (1928), Hill (1970), Alturi (1984), Haupt and Tsakmakis (1989), Miehe (1994), Argyris and Kleiber (1997), Peric and Owen (1997), Simo and Hughes (1998), Xiao et al. (1998), Holzapfel and Böck (2004) and Naghdabadi et al. (2005) among others.
2.3.1 Fundamental assumptions: 1st formulation

Kinematics

Here the continuum approach is employed to consider the deformation and motion of the body. Let $\mathcal{B} \subset \mathbb{R}^3$ be an open set defining a body. The one-to-one map $\varphi: \mathcal{B} \rightarrow \mathbb{R}^3$ is the configuration of body which places the particles of $\mathcal{B}$ in $\mathbb{R}^3$. The motion of the body in the time interval $[0, T]$ is given by the configurations $x = \varphi(X, t)$. The tangent of the map $\varphi$, $3\varphi = F$ well known as the deformation gradient is $F = \partial x/\partial X$ with $J = \det(F)$ and $d\varepsilon = J dV$. The uniaxial model depicted in figure 2.1 motivates the following two local multiplicative decompositions of the deformation gradient

$$F = F_{ep}F_p, \quad (2.28a)$$
$$F = F_{ev}F_v, \quad (2.28b)$$

where $F_p$ is the plastic part of the deformation gradient and $F_{ep}$ is its elastic part at rate-independent equilibrium and $F_v$ is the viscous part of the deformation gradient and $F_{ev}$ is its elastic part at rate-dependent non-equilibrium regime as shown schematically in figure 2.3. In other words, loosely speaking $F_p$ corresponds to the friction element and $F_{ep}$ is related to the spring in the thermoplastic part of figure 2.1 and similarly $F_v$ corresponds to the dashpot and $F_{ev}$ is related to the spring in the Maxwell element. Lee (1969) and Kröner (1960) were the first to employ the plastic decomposition (2.28a) in elastoplasticity (also referred to as Kröner-Lee decomposition) and Sidoroff (1974) seems to be the pioneer to consider the viscous decomposition (2.28b) in the framework of viscoelasticity. This has been deeply investigated by many authors, see e.g., Muller-Hoeppe and Wriggers (1992), Haupt and Lion (1995), Ibrahimbegović and Lotfi (2000), Simo (1985) and Simo (1988) among others. Consistent with the multiplicative decompositions defined in Eqs. (2.28), the total/elastic right and left Cauchy-Green strain tensors and some suitable geometric equations proper for the subsequent developments are given by
2.3. THERMO-VISCOPLASTICITY AT FINITE STRAINS

Figure 2.3: Multiplicative decompositions of deformation gradient (first model).

\[
\begin{align*}
\mathbf{C} &= \mathbf{F}^T \mathbf{F}, \quad \mathbf{b} = \mathbf{F} \mathbf{F}^T, \\
\mathbf{C}_{ep} &= \mathbf{F}_{ep}^T \mathbf{F}_{ep} \quad , \quad \mathbf{b}_{ep} = \mathbf{F}_{ep} \mathbf{F}_{ep}^T, \\
\mathbf{C}_{ev} &= \mathbf{F}_{ev}^T \mathbf{F}_{ev} \quad , \quad \mathbf{b}_{ev} = \mathbf{F}_{ev} \mathbf{F}_{ev}^T, \\
\mathbf{C}_{ep} &= \mathbf{F}_{p}^{-T} \mathbf{C} \mathbf{F}_{ep}^{-1} \quad , \quad \mathbf{C}_{p} = \mathbf{F}^T \mathbf{b}_{ep}^{-1} \mathbf{F}, \\
\mathbf{C}_{ev} &= \mathbf{F}_{v}^{-T} \mathbf{C} \mathbf{F}_{ev}^{-1} \quad , \quad \mathbf{C}_{v} = \mathbf{F}^T \mathbf{b}_{ev}^{-1} \mathbf{F}, \\
\dot{\mathbf{C}}_{ep} &= \mathbf{F}_{p}^{-T} \dot{\mathbf{C}} \mathbf{F}_{p}^{-1} - \mathbf{L}_p \mathbf{C}_{ep} - \mathbf{C}_{ep} \mathbf{L}_p, \\
\dot{\mathbf{C}}_{ev} &= \mathbf{F}_{v}^{-T} \dot{\mathbf{C}} \mathbf{F}_{ev}^{-1} - \mathbf{L}_v \mathbf{C}_{ev} - \mathbf{C}_{ev} \mathbf{L}_v, \\
\dot{\mathbf{b}}_{ep} &= \mathbf{l} \mathbf{b}_{ep} + \mathbf{b}_{ep} \mathbf{l}^T + \mathbf{L}_v \mathbf{b}_{ep}, \\
\dot{\mathbf{b}}_{ev} &= \mathbf{l} \mathbf{b}_{ev} + \mathbf{b}_{ev} \mathbf{l}^T + \mathbf{L}_v \mathbf{b}_{ev}, \\
\mathbf{L}_v \mathbf{b}_{ep} &= \mathbf{F} \dot{\mathbf{C}}_{p}^{-1} \mathbf{F}^T, \quad \mathbf{L}_v \mathbf{b}_{ev} = \mathbf{F} \dot{\mathbf{C}}_{v}^{-1} \mathbf{F}^T,
\end{align*}
\]

where superscript \( ^T \) denotes the transpose of a matrix; \( \mathbf{L}_p \equiv \dot{\mathbf{F}}_p \mathbf{F}_p^{-1} \) and \( \mathbf{L}_v \equiv \dot{\mathbf{F}}_v \mathbf{F}_v^{-1} \) are velocity gradients defined in the intermediate plastic and viscous configurations, respectively; \( \mathbf{l} \equiv \dot{\mathbf{F}} \mathbf{F}^{-1} \) denotes spatial velocity gradient defined in the current configuration and \( \mathbf{L}_v \) stands for the Lie derivative of a spatial tensor. Introduction of the multiplicative decomposition (2.28) into the definition for \( \mathbf{l} \), leads to simultaneously decomposition of the spatial velocity gradient

\[
\mathbf{l} = \mathbf{l}_{ep} + \mathbf{l}_p \quad , \quad \mathbf{l} = \mathbf{l}_{ev} + \mathbf{l}_v,
\]
where \( \mathbf{l}_p \) and \( \mathbf{l}_v \) are the plastic and viscous parts of the spatial velocity gradient and \( \mathbf{l}_{ep} \) and \( \mathbf{l}_{ev} \) are the corresponding elastic parts. They transform as the contra-covariant tensors (Simo, 1998) between the intermediate and current configurations

\[
\mathbf{l}_{ep} = F_{ep} F_{ep}^{-1}, \quad \mathbf{l}_{ev} = F_{ev} F_{ev}^{-1},
\]

(2.36a)

\[
\mathbf{l}_p = F_{ep} L_p F_{ep}^{-1}, \quad \mathbf{l}_v = F_{ev} L_v F_{ev}^{-1}.
\]

(2.36b)

With these notations at hand \( B_0, B^p_t, B^v_t \) and \( B_t \) are, respectively; the initial, intermediate plastic, intermediate viscous, and current configurations of the body at time \( t \) of interest within the time interval \([0,T]\).

**General internal and free energy functions**

Here the general anisotropic case is considered and it is assumed at the outset that internal strain-like variables which describe the inelastic response of the material remain unchanged under superposed rigid body motions. Motivated by the linear case the plastic entropy \( \eta_p \) is introduced as an internal variable (for the case of \( J_2 \)-flow theory) and consistent with the multiplicative decomposition (2.28), let the general functional form of the internal energy

\[
e = e(X, C_{ep}, C_{ev}, \xi, \eta_e),
\]

(2.37)

where the position dependence depicts inhomogeneities within the material and is explicitly investigated in the following chapters; \( \xi \) denotes the plastic hardening variable and for simplicity it is assumed to be a scalar; and \( \eta_e = \eta - \eta_p \) is the elastic part of the entropy. This additively decomposition of the total entropy makes sense to characterize the entropy production within the concept of theory of internal variables as indicated by Coleman and Gurtin (1967) and Simo and Miehe (1992). It is convenient to determine the response of the material with thermo-viscoelastic-plastic behavior by the Helmholtz free energy \( \psi \). To do this the Legendre transformation is employed (Maugin, 1992)

\[
\psi(C_{ep}, C_{ev}, \xi, \theta) = e(C_{ep}, C_{ev}, \xi, \eta_e) - \eta_e \theta,
\]

(2.38)

in which

\[
\eta_e = -\frac{\partial \psi}{\partial \theta}, \quad \theta = \frac{\partial e}{\partial \eta_e},
\]

(2.39)

\[
c = -\theta \frac{\partial^2 \psi}{\partial \theta \partial \theta} = \theta \frac{\partial \eta_e}{\partial \theta} = \frac{\partial e}{\partial \theta},
\]

(2.40)

where \( c \) is the heat capacity at constant deformation and internal variable per unit of the reference volume. From Eq. (2.40) one can obtain
\[ e = e_0 + \int_{\theta_R}^{\theta} c d \hat{\theta}, \quad \eta_e = \eta_{e_0} + \int_{\theta_R}^{\theta} \frac{c}{\hat{\theta}} d \hat{\theta}, \quad (2.41) \]

where \( e_0 \) and \( \eta_{e_0} \) are the internal energy and elastic entropy at the reference temperature \( \theta_R \), respectively. Using Eqs. (2.41) and (2.38), one can obtain

\[ \psi = e_0 - \theta \eta_{e_0} + T(\theta), \quad (2.42) \]

where

\[ T(\theta) = \int_{\theta_R}^{\theta} c (1 - \frac{\theta}{\hat{\theta}}) d \hat{\theta}. \]

Another commonly used alternative form of the thermodynamic potential may be found by considering only the state functions characterizing the elastic and inelastic behavior of the material at the reference temperature. These functions obey the Legendre transformation at \( \theta_R \) and given by

\[ \psi_0 = e_0 - \theta_R \eta_{e_0}, \quad (2.43) \]

\[ \psi = \frac{\theta}{\theta_R} \psi_0 + (1 - \frac{\theta}{\theta_R}) \hat{e}_0 + T(\theta). \quad (2.44) \]

Motivated by the rheological model 1 and considering the multiplicative decomposition (2.28), the following free energy function at the reference temperature \( \theta_R \) is given (Nedjar, 2002a)

\[ \psi_0 = \psi_{0, ep}(C_{ep}, \xi) + \psi_{0, ev}(C_{ev}). \quad (2.45) \]

Eqs. (2.45) and (2.43) motivates the additively decomposition of the internal energy \( e_0 \) into the elastic-plastic and elastic-viscous parts

\[ e_0 = e_{0, ep} + e_{0, ev}. \quad (2.46) \]

From Eqs. (2.44)- (2.46), one can obtain the general Helmholtz free energy function of the form

\[ \psi = \psi_{ep}(C_{ep}, \xi, \theta) + \psi_{ev}(C_{ev}, \theta), \quad (2.47) \]

where

\[ \psi_{ep}(C_{ep}, \xi, \theta) = \frac{\theta}{\theta_R} \psi_{0, ep}(C_{ep}, \xi) + \left(1 - \frac{\theta}{\theta_R}\right) e_{0, ep} + T(\theta), \quad (2.48) \]

\[ \psi_{ev}(C_{ev}, \theta) = \frac{\theta}{\theta_R} \psi_{0, ev}(C_{ev}) + \left(1 - \frac{\theta}{\theta_R}\right) e_{0, ev}. \]
Local dissipation inequality and constitutive equations

As in the linear theory, the Clausius-Plank form of the second law is assumed to derive the constitutive equations

\[ \mathcal{D}_{\text{int}} = \theta \gamma_{\text{loc}} = \frac{1}{2} S : \dot{\mathcal{C}} - \dot{\theta} + \theta \eta \geq 0, \quad (2.49) \]

where \( \gamma_{\text{loc}} \) denotes the local entropy production, \( S \) is the second Piola-Kirchhoff stress tensor and the first term in the right hand of Eq. (2.49) represents the internal power. Inequality (2.49) follows from the Clausius-Duhem inequality form of the second law provided that the thermal dissipation \( \mathcal{D}_t = -q \cdot \nabla (\theta) / \theta \) remains nonnegative for all admissible thermodynamic processes in which \( \nabla (\cdot) \) denotes the spatial gradient operator. To employ the inequality (2.49) for the model at hand the material time derivative of the internal energy is needed first (using Eqs. (2.38) and (2.47))

\[
\dot{e} = \frac{\partial \psi^{ep}}{\partial \theta} \dot{\mathcal{C}}_{ep} + \frac{\partial \psi^{ev}}{\partial \theta} \dot{\mathcal{C}}_{ev} + \left( \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} \right) \dot{\theta} + \frac{\partial \psi^{ep}}{\partial \xi} \dot{\xi} + \eta_e \theta + \eta_v \dot{\theta}. \quad (2.50)
\]

Applying the above equation into Eq. (2.49) gives

\[
\mathcal{D}_{\text{int}} = \left( S - F_p^{-1} \frac{2 \partial \psi^{ep}}{\partial \mathcal{C}_{ep}} F_p^{-T} - F_v^{-1} \frac{2 \partial \psi^{ev}}{\partial \mathcal{C}_{ev}} F_v^{-T} \right) : \frac{1}{2} \mathcal{C}
+ \left( \eta_e \frac{\partial \psi^{ep}}{\partial \theta} + \eta_v \frac{\partial \psi^{ev}}{\partial \theta} \right) \dot{\theta}
+ 2 \frac{\partial \psi^{ep}}{\partial \mathcal{C}_{ep}} C_{ep} L_p + 2 \frac{\partial \psi^{ev}}{\partial \mathcal{C}_{ev}} C_{ev} L_v + \beta \dot{\xi} + \theta \eta_p \geq 0, \quad (2.51)
\]

where \( \beta = -\partial \psi^{ep} / \partial \xi \). Since the above equation must hold for all admissible thermodynamic processes, applying the Coleman-Noll procedure leads to the following constitutive equations

\[
S = S_{p}^{eq} + S_{v}^{neq} = F_p^{-1} \frac{2 \partial \psi^{ep}}{\partial \mathcal{C}_{ep}} F_p^{-T} + F_v^{-1} \frac{2 \partial \psi^{ev}}{\partial \mathcal{C}_{ev}} F_v^{-T}, \quad (2.52a)
\]

\[
\eta_e = -\frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} = -\frac{\partial \psi}{\partial \theta}, \quad (2.52b)
\]

where \( S_{p}^{eq} \) is the equilibrium part of the second Piola-Kirchhoff stress tensor and \( S_{v}^{neq} \) presents its non-equilibrium part; and the elastic entropy is also additively decomposed into elastic-plastic and elastic-viscous parts \( \eta_e^{ep} \) and \( \eta_e^{ev} \), respectively. By push-forward
of the contravariant tensor $\mathbf{S}$ in (2.52a) to the current configuration one can obtain Kirchhoff stress tensor

$$\mathbf{\tau} = F \mathbf{S} F^T = \mathbf{\tau}_p^{eq} + \mathbf{\tau}_v^{neq} = F_{ep} \frac{2 \partial \psi^{ep}}{\partial C_{ep}} \mathbf{F}^T_{ep} + F_{ev} \frac{2 \partial \psi^{ev}}{\partial C_{ev}} \mathbf{F}^T_{ev}, \quad (2.53)$$

where $\mathbf{\tau}_p^{eq}$ denotes the equilibrium part of the Kirchhoff stress tensor whereas $\mathbf{\tau}_v^{neq}$ presents the associative non-equilibrium part. Since the free energy in (2.47) is a function of elastic right Cauchy-Green strain tensors defined in the intermediate configurations, one can define equilibrium and non-equilibrium stress tensors in these configurations. Comparing Eqs. (2.52a) and (2.53) reveals the fact that the equilibrium and non-equilibrium parts of stress tensors $\mathbf{S}$ and $\mathbf{\tau}$ are, respectively, pull-back and push-forward of stress tensors defined by

$$\mathbf{S}_p^{eq} = 2 \frac{\partial \psi^{ep}}{\partial C_{ep}} = F_p \mathbf{S}_p^{eq} \mathbf{F}_p = F_{ep}^{-1} \mathbf{\tau}_p^{eq} \mathbf{F}_ep, \quad (2.54a)$$

$$\mathbf{S}_v^{neq} = 2 \frac{\partial \psi^{ev}}{\partial C_{ev}} = F_v \mathbf{S}_v^{neq} \mathbf{F}_v = F_{ev}^{-1} \mathbf{\tau}_v^{neq} \mathbf{F}_ev, \quad (2.54b)$$

thus

$$\mathbf{S} = F_{ep}^{-1} \mathbf{S}_p^{eq} \mathbf{F}_p^T + F_{ev}^{-1} \mathbf{S}_v^{neq} \mathbf{F}_v^T, \quad (2.55a)$$

$$\mathbf{\tau} = F_{ep} \mathbf{S}_p^{eq} \mathbf{F}_p^T + F_{ev} \mathbf{S}_v^{neq} \mathbf{F}_v^T. \quad (2.55b)$$

Upon these definitions, the dissipation inequality (2.51) takes the following reduced form

$$\mathcal{D}_{int} = \mathcal{M}_p : \mathbf{L}_p + \mathcal{M}_v : \mathbf{L}_v + \beta \dot{\xi} + \theta \dot{\eta}_p$$

$$= \mathbf{S}_p^{eq} : \mathcal{N}_p + \mathbf{S}_v^{neq} : \mathcal{N}_v + \beta \dot{\xi} + \theta \dot{\eta}_p$$

$$= \mathbf{\tau}_p^{eq} : \mathbf{L}_p + \mathbf{\tau}_v^{neq} : \mathbf{L}_v + \beta \dot{\xi} + \theta \dot{\eta}_p \geq 0 \quad (2.56)$$

where $\mathcal{M}_p$ and $\mathcal{M}_v$ are the Mandel stress tensors (Mandel, 1974) defined in the plastic and viscous intermediate configurations, respectively; and $\mathcal{N}_p$ and $\mathcal{N}_v$ are covariant geometric tensors defined in the referential configuration by the pull-back of the covariant tensors $\mathbf{C}_{ep} \mathbf{L}_p$ and $\mathbf{C}_{ev} \mathbf{L}_v$:

$$\mathcal{M}_p = \mathbf{C}_{ep} \mathbf{S}_p^{eq}, \quad \mathcal{M}_v = \mathbf{C}_{ev} \mathbf{S}_v^{neq}, \quad (2.57a)$$

$$\mathcal{N}_p = F_p^T (\mathbf{C}_{ep} \mathbf{L}_p) \mathbf{F}_p, \quad \mathcal{N}_v = F_v^T (\mathbf{C}_{ev} \mathbf{L}_v) \mathbf{F}_v, \quad (2.57b)$$

$$\mathbf{\tau}_p^{eq} : \mathbf{L}_p + \beta \dot{\xi} + \theta \dot{\eta}_p \geq 0 \quad \& \quad \mathbf{\tau}_v^{neq} : \mathbf{L}_v \geq 0. \quad (2.58)$$

Note that in the above equations $\mathbf{C}_{ep}$ and $\mathbf{C}_{ev}$ act as metric or index lowering tensors in the intermediate plastic and viscous configurations, respectively. This completes the derivation of the constitutive equations for the general anisotropic case. In what follows, the alternative results with restriction to the isotropy are derived.
Particularization to isotropy

Of interest for the subsequent developments is consideration of isotropic case. To do this, it is assumed that our model presented in Eq. (2.47) is unaffected by the superposed rigid body motions with respect to the both intermediate configurations. For metallic and polymer glasses this assumption attempts to model the situations in which the material has a completely disordered atomic or molecular structures (Anand and Gurtin, 2003). Recently, Gurtin and Anand (2005) illustrated the notion of material symmetry for a general class of materials that includes, as special cases, isotropic-viscoplastic and amorphous solids. The isotropy assumption changes the elastic Cauchy-Green dependencies of the free energy to the elastic Finger tensor dependencies. Thus, the consistent free energy function and internal dissipation are given by

\[ \psi = \psi^{ep}(b_{ep}, \xi, \theta) + \psi^{ev}(b_{ev}, \theta), \]  
\[ \mathcal{D}_{\text{int}} = \tau : d - \dot{\varepsilon} + \theta \dot{\eta} = \tau : d - \psi - \eta \dot{\theta} + \theta \dot{\eta}_{p} \geq 0, \]  

where \( d \equiv \text{sym}(I) \) is the symmetric rate of deformation tensor. Employing the rate of free energy function in inequality (2.60) and using Eqs. (2.33) leads to

\[ \mathcal{D}_{\text{int}} = (\tau - 2 \frac{\partial \psi^{ep}}{\partial b_{ep}} b_{ep} - 2 \frac{\partial \psi^{ev}}{\partial b_{ev}} b_{ev}) : d - \left( \eta + \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} \right) \dot{\theta} \]  
\[ - \frac{\partial \psi^{ep}}{\partial b_{ep}} : \mathcal{L}_{v} b_{ep} - \frac{\partial \psi^{ev}}{\partial b_{ev}} : \mathcal{L}_{v} b_{ev} + \beta \dot{\xi} + \theta \dot{\eta}_{p} \geq 0, \]  

thus

\[ \tau = \tau_{p}^{eq} + \tau_{v}^{neq} = 2 \frac{\partial \psi^{ep}}{\partial b_{ep}} b_{ep} + 2 \frac{\partial \psi^{ev}}{\partial b_{ev}} b_{ev}, \]  
\[ \eta_{e} = - \frac{\partial \psi^{ep}}{\partial \theta} - \frac{\partial \psi^{ev}}{\partial \theta} = - \frac{\partial \psi}{\partial \theta}, \]  
\[ \mathcal{D}_{\text{int}} = - \frac{\partial \psi^{ep}}{\partial b_{ep}} : \mathcal{L}_{v} b_{ep} + \beta \dot{\xi} + \theta \dot{\eta}_{p} - \frac{\partial \psi^{ev}}{\partial b_{ev}} : \mathcal{L}_{v} b_{ev} \]  
\[ = \tau_{p}^{eq} : \frac{1}{2} b_{ep}^{-1} + \beta \dot{\xi} + \theta \dot{\eta}_{p} + \tau_{v}^{neq} : \frac{1}{2} b_{ev}^{-1} \geq 0. \]  

Remark 2.1:

By comparison of Eqs. (2.56) and (2.62c), one can conclude
2.3. THERMO-VISCOPLASTICITY AT FINITE STRAINS

\[ l_p = \text{sym} \left( \frac{-\mathcal{L}_v b_{ep}}{2} b_{ep}^{-1} \right), \quad l_v = \text{sym} \left( \frac{-\mathcal{L}_v b_{ev}}{2} b_{ev}^{-1} \right). \tag{2.63} \]

The correctness of the above equation can be shown from the definition of the Lie derivative as follows. From Eq. (2.34), one derives

\[ \mathcal{L}_v b_{ep} = F \dot{C}_p^{-1} F^T = -2F_{ep} \text{sym}(L_p) F^T_{ep} = -2\text{sym}(l_p b_{ep}). \tag{2.64} \]

Due to isotropy \( \tau_{peq}^e, b_{ep} \) and \( \mathcal{L}_v b_{ep} \) commute, substitution of \( \mathcal{L}_v b_{ep} \) from Eq. (2.64) in Eq. (2.62c) and taking into account the symmetry of Kirchhoff stress tensor confirms the correctness of Eq. (2.63)\(_1\). The same procedure can be perused to show the correctness of Eq. (2.63)\(_2\).

Satisfaction of the following inequalities

\[ \mathcal{D}_p = \tau_{peq}^e : \frac{-\mathcal{L}_v b_{ep}}{2} b_{ep}^{-1} + \beta \dot{\xi} + \theta \dot{\eta}_p \geq 0, \tag{2.65a} \]

\[ \mathcal{D}_v = \tau_{veq}^n : \frac{-\mathcal{L}_v b_{ev}}{2} b_{ev}^{-1} \geq 0, \tag{2.65b} \]

ensures the satisfaction of the inequality (2.62c). Please note that terms \( \beta \dot{\xi} \) and \( \theta \dot{\eta}_p \) can be ignored for the case of endochronic plasticity.

**Local evolution equations**

- **Thermo-plastoelastic part**

Motivated by the one-dimensional rheological model 1 (Eq. (2.11)) and dictated by inequality (2.65a), the thermoelastic domain \( \mathcal{E} \) is specified in a classical format by means of a smooth single-surface yield criterion expressed in terms of the equilibrium true stresses \( \tau_{peq}^e \)

\[ \mathcal{E} = \{ (\tau_{peq}^e, \beta, \theta) \mid \hat{\phi}(\tau_{peq}^e, \beta, \theta) \leq 0 \}. \tag{2.66} \]

Note that the principle of objectivity restricts the possible forms of \( \hat{\phi} \) in Eq. (2.66) to the isotropic functions

\[ \hat{\phi}(R \tau_{peq}^e R^T, \beta, \theta) = \hat{\phi}(\tau_{peq}^e, \beta, \theta) \quad \forall R \in SO(3), \tag{2.67} \]

which is the condition of isotropy for \( \hat{\phi} \). For the simplest case of associative plasticity, applying the principle of maximum plastic dissipation yields the following evolution Eqs. \( \text{(Simo, 1998)} \)

\[ \mathcal{L}_v b_{ep} = -2\gamma \frac{\partial \hat{\phi}}{\partial \tau_{peq}^e} b_{ep}, \tag{2.68a} \]
\[
\dot{\xi} = \gamma \frac{\partial \hat{\phi}}{\partial \beta'}, \quad \text{(2.68b)}
\]
\[
\dot{\eta}^p = \gamma \frac{\partial \hat{\phi}}{\partial \theta}, \quad \text{(2.68c)}
\]

with \( \gamma \geq 0 \) being the plastic consistency parameter satisfying the Kuhn-Tucker loading and unloading conditions
\[
\gamma \geq 0, \quad \hat{\phi}(\tau_p^{eq}, \beta, \theta) \leq 0, \quad \gamma \hat{\phi}(\tau_p^{eq}, \beta, \theta) = 0. \quad \text{(2.68d)}
\]

\section{Thermo-viscoelastic part}

For the thermo-viscoelastic evolution equation the key ideas of Reese and Govindjee (1998a) is pursued as discussed before. Hence, the existence of pseudo-potential function \( \varphi_v(\tau_v^{neq}) \) is postulated in such a way that
\[
\text{sym}(I_v) = \frac{-L_v b_{ev}}{2} b_{ev}^{-1} \equiv \frac{\partial \varphi_v(\tau_v^{neq})}{\partial \tau_v^{neq}}. \quad \text{(2.69)}
\]

\subsection{2.3.2 Fundamental assumptions: 2\textsuperscript{nd} formulation}

\section*{Kinematics}

Let’s start with a different kinematic assumption rather than the one developed in the previous subsection and present a general finite deformation thermo-viscoelastic-plastic model associated with the rheological model 2. The one-dimensional model depicted in figure 2.2 motivates the following two local multiplicative decompositions of the deformation gradient
\[
F = F_{ep} F_p, \quad \text{(2.70a)}
\]
\[
F = F_{ev} F_i, \quad \text{(2.70a)}
\]

where \( F_p \) is the plastic part of the deformation gradient and \( F_{ep} \) is its elastic part at rate-independent equilibrium as before whereas at the difference with the kinematic assumption (2.28), \( F_i \) denotes the total inelastic part of the deformation gradient and \( F_{ev} \) presents its elastic part at rate-dependent non-equilibrium regime as shown schematically in figure 2.4. Loosely speaking \( F_p \) corresponds to the friction element and \( F_{ep} \) is related to the spring with the \( E_{ep}(\theta) \) and similarly \( F_i \) corresponds to the dashpot and \( F_{ev} \) is related to the spring in the Maxwell element of figure 2.2. It seems that this multiplicative decomposition of deformation gradient was first proposed by Lion (2000) in order to account for energy storage mechanisms associated with the plastic
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Figure 2.4: Multiplicative decompositions of deformation gradient (second model).

Flow. From figure 2.4, one can write

$$F_i = F_v F_p,$$  \hspace{1cm} (2.71)

where $F_v$ is the viscous part of inelastic deformation gradient with respect to the plastic intermediate configuration $B^p_t$. Thus, the total deformation gradient can be written

$$F = F_{ev} F_v F_p.$$  \hspace{1cm} (2.72)

Consistent with the multiplicative decompositions (2.70)-(2.72), the total/plastic/inelastic/viscous/elastic-plastic/elastic-viscous right and left Cauchy-Green strain tensors and some appropriate geometric equations can be derived

$$C = F^T F, \quad C_p = F_p^T F_p, \quad C_i = F_i^T F_i,$$  \hspace{1cm} (2.73a)

$$C_v = F_v^T F_v, \quad C_{ep} = F_{ep}^T F_{ep}, \quad C_{ev} = F_{ev}^T F_{ev},$$  \hspace{1cm} (2.73b)

$$b = F F^T, \quad b_p = F_p F_p^T, \quad b_i = F_i F_i^T,$$  \hspace{1cm} (2.74a)

$$b_v = F_v F_v^T, \quad b_{ep} = F_{ep} F_{ep}^T, \quad b_{ev} = F_{ev} F_{ev}^T,$$  \hspace{1cm} (2.74b)

$$C_{ep} = F_p^T C F_p^{-1}, \quad C_{ev} = F_i^T C F_i^{-1},$$  \hspace{1cm} (2.75a)

$$C_{ev} = F_v^T C_{ep} F_v^{-1}, \quad C_v = F_p^T C_i F_p^{-1},$$  \hspace{1cm} (2.75b)

$$b_{ev} = F C_i^{-1} F^T, \quad b_{ev} = F_{ep} C_{v}^{-1} F_{ep},$$  \hspace{1cm} (2.76a)

$$b_v = F_i C_p^{-1} F_i^T, \quad b_{ep} = F C_p^{-1} F^T,$$  \hspace{1cm} (2.76b)

$$\dot{C}_{ep} = F_p^T \dot{C} F_p^{-1} - L_p^T C_{ep} - C_{ep} L_p,$$  \hspace{1cm} (2.77a)

$$\dot{C}_{ev} = F_i^T \dot{C} F_i^{-1} - L_i^T C_{ev} - C_{ev} L_i,$$  \hspace{1cm} (2.77b)
\[
\dot{\mathbf{C}}_{ev} = F_v^{-T} \dot{C}_{ep} F_v^{-1} - L_v^T C_{ev} - C_{ev} L_v,
\]
\[
\dot{C}_v = F_p^{-T} \dot{C}_i F_p^{-1} - L_p^T C_v - C_v L_p,
\]
\[
\dot{b}_{ep} = l b_{ep} + b_{ep} T^* + L_v b_{ep},
\]
\[
\dot{b}_{ev} = l b_{ev} + b_{ev} T^* + L_v b_{ev},
\]
\[
\dot{l}_p = l_{ep} b_{ep} + b_{ep} L_p^T + L_v b_{ep},
\]
\[
\dot{l}_v = l_{ev} b_{ev} + b_{ev} L_v^T + L_v b_{ev},
\]
\[
\mathcal{L}_v b_{ep} = F \dot{C}_p^{-1} F^* = -2 F_{ep} \text{sym}(L_p) F_{ep}^T,
\]
\[
\mathcal{L}_v b_{ev} = F \dot{C}_i^{-1} F^* = -2 F_{ev} \text{sym}(L_i) F_{ev}^T,
\]
\[
\mathcal{L}_v b_{ev} = F_{ep} \dot{C}_v^{-1} F_{ep}^T = -2 F_{ev} \text{sym}(L_v) F_{ev}^T,
\]
\[
L_i = L_v + F_v L_p F_v^{-1},
\]
\[
(\mathcal{L}_v b_{ev}) b_{ev}^{-1} = (\mathcal{L}_v b_{ev}) b_{ev}^{-1} - (\mathcal{L}_v b_{ep}) b_{ep}^{-1} - F_{ep} L_p^T F_{ep}^{-1} + F_{ev} F_v^{-T} L_p^T F_{ev}^{-1}.
\]

where \( L_p \equiv \dot{F}_p F_p^{-1}, \ L_i \equiv \dot{F}_i F_i^{-1} \) and \( L_v \equiv \dot{F}_v F_v^{-1} \), \( l_{ep} = \dot{F}_{ep} F_{ep}^{-1} \) are velocity gradients defined in the intermediate plastic, total inelastic, intermediate viscous and current configurations, respectively; \( l \equiv \dot{F} F^{-1} \) denotes spatial velocity gradient defined in the current configuration as before and \( \mathcal{L}_v \) stands for the Lie derivative of a spatial tensor whereas \( \mathcal{L}_v b_{ev} \) presents Lie derivative with respect to the intermediate plastic configuration. Introduction of the multiplicative decomposition (2.70) into the definition for the \( l \) leads to simultaneously decomposition of the spatial velocity gradient

\[
l = l_{ep} + l_p, \quad l = l_{el} + l_i.
\]

where \( l_p \) and \( l_i \) denote the plastic and total inelastic parts of the spatial velocity gradient, respectively; and \( l_{ep} \) and \( l_{el} \) present the corresponding elastic-plastic and elastic-inelastic parts. As discussed earlier, they transform as the contra-covariant tensors between their respective configurations

\[
l_p = F_{ep} L_p F_{ep}^{-1}, \quad l_i = F_{ev} L_i F_{ev}^{-1}, \quad l_{el} = \dot{F}_{ev} F_{ev}^{-1}.
\]

### General thermodynamic potentials and local dissipation

As before, the general anisotropic case is assumed here. Motivated by the rheological model 2 and earlier discussions, one can take the following free and internal energy functions of the form

\[
\psi = \psi(C_{ep}, C_{ev}, \xi, \theta) = \psi^{ep}(C_{ep}, \xi, \theta) + \psi^{ev}(C_{ev}, \theta),
\]
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\[ e = e(C_{ep}, C_{ev}, \xi, \eta_e) = \psi(C_{ep}, C_{ev}, \xi, \theta) + \eta_e \theta, \tag{2.84b} \]

where

\[
\begin{align*}
\psi^{ep}(C_{ep}, \xi, \theta) &= \frac{\theta}{\theta_R} \psi^{ep}_0(C_{ep}, \xi) + \left(1 - \frac{\theta}{\theta_R}\right) e^{ep}_0 + T(\theta), \\
\psi^{ev}(C_{ev}, \theta) &= \frac{\theta}{\theta_R} \psi^{ev}_0(C_{ev}) + \left(1 - \frac{\theta}{\theta_R}\right) e^{ev}_0.
\end{align*}
\]

Note that although the above thermodynamics potentials have the same structure as in the first formulation, but essentially yield different results due to the different kinematic assumptions and \( T(\theta) \) is defined in the subsection 2.3.1. Assuming the Clausius-Plank form of the second law

\[
\mathcal{D}_{int} = \frac{1}{2} S : \dot{\mathbf{C}} - \psi - \eta_e \dot{\theta} + \theta \dot{\eta}_p \geq 0, \tag{2.85}
\]

\[
\mathcal{D}_{int} = \left( S - F_p^{-1} 2 \frac{\partial \psi^{ep}}{\partial C_{ep}} F_p^T F_p^{-T} - F_i^{-1} 2 \frac{\partial \psi^{ev}}{\partial C_{ev}} F_i^{T} F_i^{-T} \right) : \frac{1}{2} \dot{C}
\]

\[
- \left( \eta_e + \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi^{ev}}{\partial \theta} \right) \dot{\theta}
\]

\[
+ 2 \frac{\partial \psi^{ep}}{\partial C_{ep}} : C_{ep} L_p + 2 \frac{\partial \psi^{ev}}{\partial C_{ev}} : C_{ev} L_i + \beta \dot{\xi} + \theta \dot{\eta}_p \geq 0,
\tag{2.86}
\]

yields

\[
S = S^{eq}_p + S^{neq}_v = F_p^{-1} 2 \frac{\partial \psi^{ep}}{\partial C_{ep}} F_p^T + F_i^{-1} 2 \frac{\partial \psi^{ev}}{\partial C_{ev}} F_i^{T} F_i^{-T}, \tag{2.87a}
\]

\[
\eta_e = - \frac{\partial \psi^{ep}}{\partial \theta} - \frac{\partial \psi^{ev}}{\partial \theta} = - \frac{\partial \psi}{\partial \theta}. \tag{2.87b}
\]

The Kirchhoff stress tensor can be obtained by push-forward of the above stress tensor \( S \) to the current configuration via

\[
\tau = FSF^T = \tau^{eq}_p + \tau^{neq}_v = F_p \frac{\partial \psi^{ep}}{\partial C_{ep}} F_p^T F_p^{T} + F_e \frac{\partial \psi^{ev}}{\partial C_{ev}} F_e^{T} F_e^{T}. \tag{2.88}
\]

Defining

\[
S^{eq}_p = 2 \frac{\partial \psi^{ep}}{\partial C_{ep}} = F_p S^{eq}_p F_p^T F_p^{-1} \tau^{eq}_p F_p^{-T}, \tag{2.89a}
\]

\[
S^{neq}_v = 2 \frac{\partial \psi^{ev}}{\partial C_{ev}} = F_v S^{neq}_v F_v^T F_v^{-1} \tau^{neq}_v F_v^{-T}, \tag{2.89b}
\]

yields
\[ S_p = F_p S F_p^T = F_p^{-1} \tau F_p^{-T} = S_p^{eq} + F_p^{-1} S_v^{\text{neq}} F_p, \]  
(2.90a)

\[ S_v = F_i S F_i^T = F_{ev}^{-1} \tau F_{ev}^{-T} = F_v S_v^{eq} F_v^T + S_v^{\text{neq}}. \]  
(2.90b)

Note that although the non-equilibrium stress tensor \( S_v^{\text{neq}} \) and the total stress \( S_v \) have been defined with respect to the total inelastic configuration in the above formulations, we did not use the subscript \( i \) in order to simplify the formulations as much as possible from the notational point of view. Upon these definitions the dissipation inequality (2.86) takes the following reduced form as

\[ \mathcal{D}_{int} = M_p : L_p + M_v : L_i + \beta \xi + \theta \eta_p \]
\[ = S_p^{eq} : N_p + S_v^{\text{neq}} : N_v + \beta \xi + \theta \eta_p \]  
(2.91)

where \( M_p, M_v, \) and \( N_p \) are those defined in Eqs. (2.57) and \( N_v \) is a covariant geometric tensor defined in the referential configuration by the pull-back of the covariant tensor \( C_{ev}L_i \)

\[ N_v = F_i^T (C_{ev}L_i)F_i. \]  
(2.92)

Inequality (2.91) can be satisfied if the two following inequalities are satisfied

\[ \tau_p^{eq} : L_p + \beta \xi + \theta \eta_p \geq 0 \quad \& \quad \tau_v^{\text{neq}} : L_i \geq 0. \]  
(2.93)

**Particularization to isotropy**

As for the first formulation, it is assumed that both intermediate configurations defined by \( F_p \) and \( F_i \) are unaffected by the superposed rigid body motions. Thus, the free energy and dissipation function together with constitutive equations are given by

\[ \psi = \psi^{ep}(b_{ep}, \xi, \theta) + \psi^{ev}(b_{ev}, \theta), \]  
(2.94)

\[ \mathcal{D}_{int} = \left( \tau - 2 \frac{\partial \psi^{ep}}{\partial b_{ep}} b_{ep} - 2 \frac{\partial \psi^{ev}}{\partial b_{ev}} b_{ev} \right) \cdot d - \left( \eta_e + \frac{\partial \psi^{ep}}{\partial \theta} + \frac{\partial \psi}{\partial \theta} \right) \dot{\theta} \]
\[ - \frac{\partial \psi^{ep}}{\partial b_{ep}} : L_{uv} b_{ep} - \frac{\partial \psi^{ev}}{\partial b_{ev}} : L_{uv} b_{ev} + \beta \xi + \theta \eta_p \geq 0, \]  
(2.95)

\[ \tau = \tau_p^{eq} + \tau_v^{\text{neq}} = 2 \frac{\partial \psi^{ep}}{\partial b_{ep}} b_{ep} + 2 \frac{\partial \psi^{ev}}{\partial b_{ev}} b_{ev}, \]  
(2.96a)

\[ \eta_e = - \frac{\partial \psi^{ep}}{\partial \theta} - \frac{\partial \psi^{ev}}{\partial \theta} = - \frac{\partial \psi}{\partial \theta}, \]  
(2.96b)
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\[ D_{\text{int}} = - \frac{\partial \psi^{\text{ep}}}{\partial \mathbf{b}^{\text{ep}}} : \mathbf{L}_u \mathbf{b}^{\text{ep}} + \beta \dot{\mathbf{\xi}} + \theta \dot{\mathbf{n}}_p - \frac{\partial \psi^{\text{ev}}}{\partial \mathbf{b}^{\text{ev}}} : \mathbf{L}_u \mathbf{b}^{\text{ev}} \]

\[ = \tau^{\text{eq}}_p : \frac{-\mathbf{L}_u \mathbf{b}^{\text{ev}}}{2} \mathbf{b}^{-1}^{\text{ep}} + \beta \dot{\mathbf{\xi}} + \theta \dot{\mathbf{n}}_p + \tau^{\text{neq}}_v : \frac{-\mathbf{L}_v \mathbf{b}^{\text{ev}}}{2} \mathbf{b}^{-1}^{\text{ev}} \geq 0. \]  

(2.96c)

Apparently Eqs. (2.94)-(2.96) have the same structure as Eqs. (2.59), (2.61) and (2.62) - rewritten here for completeness - but they are different in reality due to the coupling between intermediate configurations and the different definitions for the Lie derivatives.

Remark 2.2:

Comparison of (2.96c) and (2.91) reveals that

\[ \text{sym}(l_i) = \text{sym} \left( \frac{-\mathbf{L}_u \mathbf{b}^{\text{ev}}}{2} \mathbf{b}^{-1}^{\text{ep}} \right), \]  

(2.97)

which can be proved based on the previous discussions given in remark 2.1. To ensure the satisfaction of inequality (2.96c), \( D^p \) and \( D^v \) defined there should be greater than or equal to zero.

Local evolution equations

- Thermo-plastoelastic part

Due to the coupling between TVE and thermo-plasticity observed in the second formulation, the consistent choice of yield and creep functions should be carried out with care. To do this, there are two feasible options discussed shortly in what follows. Using Eq. (2.81), the inequality (2.96c) can be written in an alternative form as

\[ \left( \tau^{\text{eq}}_p + \tau^{\text{neq}}_v \right) : \frac{-\mathbf{L}_u \mathbf{b}^{\text{ev}}}{2} \mathbf{b}^{-1}^{\text{ep}} + \beta \dot{\mathbf{\xi}} + \theta \dot{\mathbf{n}}_p + \tau^{\text{neq}}_v : \frac{-\mathbf{L}_v \mathbf{b}^{\text{ev}}}{2} \mathbf{b}^{-1}^{\text{ev}} \]

\[ + \tau^{\text{neq}}_v : \mathbf{F}^{\text{ep}} \text{skw}[\mathbf{L}_p] \mathbf{F}^{-1}^{\text{ep}} \geq 0. \]  

(2.98)

The above inequality presents the generalization of the inequality (2.22) for the linear case to the finite deformations. Both inequalities have the same structures except for the additional last term in Eq. (2.98). The first possible choice to define a consistent thermoelastic domain for the \( J_2 \)-flow theory is the symmetry assumption for the plastic rate of distortion \( \mathbf{L}_p \). This assumption makes the additional term in Eq. (2.98) disappears and the finite deformation version of thermoelastic domain (2.24) can be considered to
derive the flow rules of the theory\(^1\). Furthermore, this is a typical assumption in metal plasticity (Simo, 1998). Recently, Gurtin and Anand (2005) formally showed that for small elastic stretches $\text{skw}[L_p]$ is small compared to the $\text{sym}[L_p]$. Since we are dealing with rubber-like materials in this work (the Ogden model can predict large elastic stretches accurately), this procedure is not followed. Another feasible option proposed by Nedjar (Nedjar, 2002a) which is pursued here. Motivated by the thermoelastic domain defined for the one-dimensional rheological model 2 and employing the principle of maximum plastic dissipation for the case of associative plasticity, yields the following thermoelastic domain and evolution equations

$$\mathbb{E} = \{ (\tau_p^{\text{eq}}, \tau_v^{\text{neq}}, \beta, \theta) \mid \hat{\varphi}(\tau_p^{\text{eq}}, \tau_v^{\text{neq}}, \beta, \theta) \leq 0 \}, \quad (2.99)$$

$$\mathcal{L}_v b_{ep} = -2\gamma \frac{\partial \hat{\varphi}}{\partial \tau_p^{\text{eq}}} b_{ep}, \quad (2.100a)$$

$$\dot{\xi} = \gamma \frac{\partial \hat{\varphi}}{\partial \beta}, \quad (2.100b)$$

$$\dot{\eta}^p = \gamma \frac{\partial \hat{\varphi}}{\partial \theta}, \quad (2.100c)$$

where the plastic consistency parameter $\gamma$ should satisfy the Kuhn-Tucker loading and unloading conditions

$$\gamma \geq 0, \quad \hat{\varphi}(\tau_p^{\text{eq}}, \tau_v^{\text{neq}}, \beta, \theta) \leq 0, \quad \gamma \hat{\varphi}(\tau_p^{\text{eq}}, \tau_v^{\text{neq}}, \beta, \theta) = 0. \quad (2.100d)$$

**Thermo-viscoelastic part**

For the thermo-viscoelastic part, let

$$\text{sym}(I_i) = \frac{-\mathcal{L}_v b_{ev}}{2} b_{ev}^{-1} = \frac{\partial \varphi_v(\tau_v^{\text{neq}})}{\partial \tau_v^{\text{neq}}}. \quad (2.101)$$

### 2.3.3 The temperature evolution equation

To characterize the thermo-viscoelastic-plastic behavior of rubber-like materials the Clausius-Plank form of second law was used to obtain the constitutive equations and the reduced form of dissipation functions. Beside these equations, the balance equations for

---

\(^1\) By the finite deformation version we mean that the yield function should be a function of the true stress $\tau$. 
energy, mass, linear and angular momenta have to be satisfied. Balance of mass is enforced by \( \rho_0 = \rho J \) where \( \rho_0 \) is the density in the reference configuration whereas \( \rho \) denotes the density at the current configuration. The balance of angular momentum is fulfilled at the outset by requiring that \( \tau = \tau^T \). The well-known equation of linear momentum is given by

\[
\text{Div}(P) + \rho_0 \dddot{f}_b = \rho_0 \dddot{v},
\]

(2.102)

where \( P \equiv FS \) denotes the first Piola-Kirchhoff stress tensor, \( \text{Div}(.) \) is referential divergence operator, \( \dddot{f}_b \) represents the body force per unit mass and \( \rho_0 \dddot{v} \) is the inertia term. In order to obtain the evolution of temperature the local balance of energy is employed

\[
\dot{\varepsilon} = \tau : \dddot{d} - J \text{div}(q) + R,
\]

(2.103)

where \( R \) denotes the heat source, \( q \) is the spatial Cauchy heat flux whose divergence related to the referential Piola-Kirchhoff heat flux \( Q = JF^{-1}q \) by the Piola transformation as \( \text{Div}(Q) = J \text{div}(q) \) in which \( \text{div}(.) \) represents spatial divergence. Using Eqs. (2.60), (2.62c) and (2.65a), Eq. (2.103) can be rewritten

\[
\dot{\varepsilon} = c \dot{\theta} + \mathcal{H},
\]

(2.105)

where \( \mathcal{H} \) is the structural thermo-viscoelastic-plastic heating or cooling (STVPH) defined by

\[
\mathcal{H} = -\theta \frac{\partial}{\partial \theta} \left[ \tau : \dddot{d} - D^P_{\text{mech}} - D^\nu \right] =
\]

\[
- \theta \frac{\partial}{\partial \theta} \left[ \tau : \dddot{d} - D^P_{\text{mech}} \right] + \theta \frac{\partial}{\partial \theta} \left[ \tau : \dddot{d} \right]
\]

(2.106)

\[
\begin{array}{l}
\text{thermo-plastoelastic structural heating} \\
\text{thermoelastic (without dissipation) structural heating} \\
\end{array}
\]

\[
- \theta \frac{\partial}{\partial \theta} \left[ \tau : \dddot{d} - D^\nu \right].
\]

Finally, from Eqs. (2.104) and (2.105) one can obtain

\[
c \dot{\theta} = D^P_{\text{mech}} + D^\nu - \mathcal{H} - J \text{div}(q) + R.
\]

(2.107)
2.3.4 Application: A model example

Free energy function

The preceding general formulations developed for both formulations can now be specialized to obtain a thermo-viscoelastic-plastic model at finite deformations. Of interest for this study is consideration of rubber-like materials. To do this, for both equilibrium and non-equilibrium parts, we work with the class of compressible Ogden materials. Considering a volumetric and deviatoric split, \( \psi_0^{ep} \) and \( \psi_0^{ev} \) can be written

\[
\psi_0^{ep}(c_{ep}, \xi) = \psi_0^{ev}(b_{ev}, \xi) = \psi_0^{ev}(J_{ep}) + \psi_0^{ev}(\lambda_1^{ep}, \lambda_2^{ep}, \lambda_3^{ep}) + KC(\xi),
\]

(2.108a)

\[
\psi_0^{ev}(C_{ev}) = \psi_0^{ev}(b_{ev}) = \psi_0^{ev}(J_{ev}) + \psi_0^{ev}(\lambda_1^{ev}, \lambda_2^{ev}, \lambda_3^{ev}),
\]

(2.108b)

where \( J_{ep} = \det(F_{ep}) \) and \( J_{ev} = \det(F_{ev}) \), \( K(\xi) \) is a potential characterizing the plastic hardening of the material and \( \lambda_a^{ep} = J_{ep}^{1/3} \lambda_a^{ep} \) \& \( \lambda_a^{ev} = J_{ev}^{1/3} \lambda_a^{ev} \) \( \forall a = 1,2,3 \) in which \( \lambda_a^{ep} \) and \( \lambda_a^{ev} \) represent the square roots of the eigenvalues of the Finger tensors \( b_{ep} \) and \( b_{ev} \), respectively. For the volumetric and isochoric parts of the free energy in the above equations, let

\[
\psi_0^{ep}(J_{ep}) = \frac{\kappa_{ep}}{4} G(J_{ep}) \quad \text{with:} \quad G(J_{ep}) = (J_{ep}^2 - 2 \ln J_{ep} - 1),
\]

(2.109a)

\[
\psi_0^{ev}(J_{ev}) = \frac{\kappa_{ev}}{4} G(J_{ev}) \quad \text{with:} \quad G(J_{ev}) = (J_{ev}^2 - 2 \ln J_{ev} - 1),
\]

(2.109b)

\[
\psi_{0iso}^{ep}(\lambda_1^{ep}, \lambda_2^{ep}, \lambda_3^{ep}) = \sum_{k=1}^{N} \sum_{a=1}^{3} \frac{\mu_k^{ep}}{\alpha_k^{ep}} \left[ \left( \frac{\lambda_a^{ep}}{\lambda_a^{ep}} \right)^{\alpha_k^{ep}} - 1 \right],
\]

(2.109c)

\[
\psi_{0iso}^{ev}(\lambda_1^{ev}, \lambda_2^{ev}, \lambda_3^{ev}) = \sum_{k=1}^{N} \sum_{a=1}^{3} \frac{\mu_k^{ev}}{\alpha_k^{ev}} \left[ \left( \frac{\lambda_a^{ev}}{\lambda_a^{ev}} \right)^{\alpha_k^{ev}} - 1 \right],
\]

(2.109d)

where \( \kappa_{ep} \) and \( \kappa_{ev} \) denote the bulk modulus for the plastoelastic and viscoelastic parts, respectively; \( N \) represents the integer number which determines the number of terms in the isochoric part of the strain-energy functions; \( \mu_k^{ep} \) and \( \mu_k^{ev} \) are the constant shear modulus; and \( \alpha_k^{ep} \) and \( \alpha_k^{ev} \) are dimensionless constants with the linearization consistency condition \( 2 \mu_p = \sum_{k=1}^{N} \mu_k^{ep} \alpha_k^{ep} \) \& \( 2 \mu_v = \sum_{k=1}^{N} \mu_k^{ev} \alpha_k^{ev} \) in which \( \mu_p \) and \( \mu_v \) denote the shear modulus for the plastoelastic and viscoelastic parts, respectively. For the equilibrium and non-equilibrium parts of the internal energy at the reference temperature \( \theta_R \), let (Chadwick, 1973; and Chadwick and Creasy, 1984)

\[
\epsilon_0^{ep} = 3 \kappa_{ep} \alpha_0^{ep} \theta_R \ln J_{ep},
\]

(2.110a)
\[ e_{0}^{ev} = 3 \kappa_{ev} \alpha_{0}^{ev} \theta_{R} \ln J_{ev}, \]  

(2.110b)

where \( \alpha_{0}^{ep}, \alpha_{0}^{ev} \) are the volumetric thermal expansion coefficients of the plastoelastic and viscoelastic parts, respectively.

Considering the thermal effects, Eqs. (2.108)-(2.110) can now be employed to present the following final form of the free energy function for the thermo-viscoelastic-plastic response of class of the compressible Ogden materials

\[
\psi(b_{ep}, b_{ev}, \xi, \theta) = \frac{\theta}{\theta_{R}} \left[ \psi_{0}^{ep}(b_{ep}, \xi) + \psi_{0}^{ev}(b_{ev}) \right] + \left( 1 - \frac{\theta}{\theta_{R}} \right) (e_{0}^{ep} + e_{0}^{ev}) + T(\theta)
\]

\[
= \left\{ \frac{\kappa_{ep}(\theta)}{4} \bar{g}(J_{ep}) + \sum_{k=1}^{N} \sum_{a=1}^{3} \frac{\lambda_{a}^{ep}(\theta)}{\alpha_{k}^{ep}} \left[ \left( \lambda_{a}^{ep} \right)^{a_{k}^{ep}} - 1 \right] - 3 \kappa_{ep} \alpha_{0}^{ep} \ln J_{ep} + \frac{\theta}{\theta_{R}} \kappa(\xi) + T(\theta) \right\}
\]

\[
+ \left\{ \frac{\kappa_{ev}(\theta)}{4} \bar{g}(J_{ev}) + \sum_{k=1}^{N} \sum_{a=1}^{3} \frac{\lambda_{a}^{ev}(\theta)}{\alpha_{k}^{ev}} \left[ \left( \lambda_{a}^{ev} \right)^{a_{k}^{ev}} - 1 \right] - 3 \kappa_{ev} \alpha_{0}^{ev} \ln J_{ev} \right\},
\]

(2.111)

where

\[
\dot{\kappa}_{ep}(\theta) = \frac{\theta}{\theta_{R}} \kappa_{ep}, \quad \dot{\kappa}_{ev}(\theta) = \frac{\theta}{\theta_{R}} \kappa_{ev},
\]

\[
\dot{\mu}_{k}^{ep}(\theta) = \frac{\theta}{\theta_{R}} \mu_{k}^{ep}, \quad \dot{\mu}_{k}^{ev}(\theta) = \frac{\theta}{\theta_{R}} \mu_{k}^{ev}, \quad \mathbb{S} = \theta - \theta_{R}.
\]

Here it is seen that despite the complete coupling between the thermal effects and plastoelastic and viscoelastic deformations, there exits the coupling between the thermal deformation and plastic hardening mechanism. As a consequence of restriction to isotropy, the principal directions of the equilibrated Kirchhoff stress tensor \( \tau_{p}^{eq} \) and the elastic Finger tensor \( b_{ep} \) coincide and similarly this holds for non-equilibrium stress tensor \( \tau_{v}^{neq} \) and the elastic Finger tensor \( b_{ev} \) as follows

\[
b_{ep} = \sum_{a=1}^{3} (\lambda_{a}^{ep})^{2} n_{a}^{ep} \otimes n_{a}^{ep} \quad \& \quad \tau_{p}^{eq} = \sum_{a=1}^{3} \tau_{a}^{eq} n_{a}^{ep} \otimes n_{a}^{ep},
\]

(2.112a)

\[
b_{ev} = \sum_{a=1}^{3} (\lambda_{a}^{ev})^{2} n_{a}^{ev} \otimes n_{a}^{ev} \quad \& \quad \tau_{v}^{neq} = \sum_{a=1}^{3} \tau_{a}^{ev} n_{a}^{ev} \otimes n_{a}^{ev},
\]

(2.112b)

where \( n_{a}^{ep} \) (\( \forall a = 1,2,3 \)) are the spatial directions of \( b_{ep} \) and \( \tau_{p}^{eq} \), and \( n_{a}^{ev} \) (\( \forall a = 1,2,3 \)) are the spatial directions of \( b_{ev} \) and \( \tau_{v}^{neq} \). For the subsequent developments, the following definitions are introduced
\[
\begin{align*}
\tau^{ep} &= \begin{cases} 
\tau_1^{ep} \\
\tau_2^{ep} \\
\tau_3^{ep}
\end{cases}, \\
\tau^{ev} &= \begin{cases} 
\tau_1^{ev} \\
\tau_2^{ev} \\
\tau_3^{ev}
\end{cases}, \\
\varepsilon^{ep} &= \begin{cases} 
\ln \lambda_1^{ep} \\
\ln \lambda_2^{ep} \\
\ln \lambda_3^{ep}
\end{cases}, \\
\varepsilon^{ev} &= \begin{cases} 
\ln \lambda_1^{ev} \\
\ln \lambda_2^{ev} \\
\ln \lambda_3^{ev}
\end{cases}, \\
1 &= \begin{cases} 
1 \\
1 \\
1
\end{cases}.
\end{align*}
\]

(2.113)

Yield and creep functions

So far we have presented the strain-energy function in Eq. (2.111); from which the constitutive Eqs. (2.62a, b) for the first formulation and the constitutive Eqs. (2.96a, b) for the second formulation can be obtained. To complete this thermo-viscoelastic-plastic model of compressible rubber-like materials all that remains to do is specializing the yield criterion \( \hat{\varphi} \) and the creep-like potential \( \varphi_v \) (as presented in Eqs. (2.66) and (2.69) for the first formulation and likewise in Eqs. (2.99) and (2.101) for the second formulation) from which the evolution equations for the internal variables can be provided.

- **Thermo-plasticity: The first formulation**

For the thermoplastic part, the thermomechanical version of the \( J_2 \)-flow theory is assumed in which the yield function \( \hat{\varphi} \) in Eq. (2.66) is given by the von Mises yield criterion

\[
\hat{\varphi}(\tau_p^{eq}, \beta, \theta) = \|\text{dev}[\tau_p^{eq}]\| - \sqrt{\frac{2}{3}[\sigma_y(\theta) - \beta]} \leq 0,
\]

(2.114)

where \( \sigma_y(\theta) > 0 \) is initial flow stress.

- **Thermo-plasticity: The second formulation**

Considering the thermoelastic domain (2.99), let the following functional form for the yield function \( \hat{\varphi} \) by

\[
\hat{\varphi}(\tau_p^{eq}, \tau_v^{eq}, \beta, \theta) = \|\text{dev}[\tau_p^{eq}] - \text{dev}[\tau_v^{eq}]\| - \sqrt{\frac{2}{3}[\sigma_y(\theta) - \beta]}
\]

\[
\leq 0.
\]

(2.115)

- **Thermo-viscoelasticity**
2.3. THERMO-VISCOPLASTICITY AT FINITE STRAINS

For the thermo-viscoelastic part it is assumed that

\[ \varphi_v(\tau_v^{neq}) = \frac{1}{2} (\tau_v^{neq} : \mathbf{X}^{-1} : \tau_v^{neq}), \quad (2.116) \]

where \( \mathbf{X}^{-1} \) is an isotropic rank four tensor given by (Fung, 1994)

\[ \mathbf{X}^{-1} = \frac{1}{2\zeta_D} (\mathbb{I} - \frac{1}{3} \mathbf{I} \otimes \mathbf{I}) + \frac{1}{9\zeta_V} \mathbf{I} \otimes \mathbf{I}, \quad (2.117) \]

where \( \mathbb{I} \) and \( \mathbf{I} \) denote the fourth and second order identity tensors, \( \zeta_D \) and \( \zeta_V \) are deviatoric and volumetric shear viscosities. Using Eq. (2.117), Eq. (2.116) takes the form

\[ \varphi_v = \frac{1}{4\zeta_D} (\tau_v^{neq} : \tau_v^{neq} - \frac{1}{3} [\tau_v^{neq} : \mathbf{I}]^2) + \frac{1}{18\zeta_V} [\tau_v^{neq} : \mathbf{I}]^2. \quad (2.118) \]

Remark on the endochronic plasticity

The \( J_2 \)-flow theory has been assumed throughout the work but some major differences with endochronic plasticity are addressed in what follows. For endochronic plasticity the yield function does not exist anymore and therefore, the plastic consistency parameter \( \gamma \) does not evolve. Also, for the assumed thermo-plasticity theory the plastic entropy does not evolve since \( \eta^p \) designed as a result of temperature dependency of the yield function. Therefore, the total entropy should be considered as elastic entropy for the case of endochronic plasticity and the term \( \theta \dot{\eta}^p \) should be excluded in the above dissipation functions.

Endochronic plasticity: first formulation

Now, if endochronic theory is of interest, the plastic flow rules should be revised and given by

Linear theory: \[ \dot{\epsilon}^p = \frac{\dot{z}}{\omega_p} \frac{\partial \hat{\phi}}{\partial \sigma_p^eq}, \quad (2.119) \]

Finite deformations: \[ \mathbf{L}_p \mathbf{b}_{ep} = -2 \frac{\dot{z}}{\omega_p} \frac{\partial \hat{\phi}}{\partial \tau_p^eq} \mathbf{b}_{ep}, \quad (2.120) \]

where \( \omega_p \) can be termed plastic shear viscosity and \( \dot{z} \) presents the time rate of arclength as \( \dot{z} = \|\dot{\epsilon}\| \) for the geometrically linear theory and \( \dot{z} = \|\dot{C}\| \) in the finite deformations. Finally, the yield criterions can be assumed

Linear theory: \[ \hat{\phi}(\sigma_p^{eq}) = \frac{1}{2} \sigma_p^{eq} : \sigma_p^{eq}, \quad (2.121a) \]
Finite deformations: \[ \dot{\phi}(\tau^e_p) = \frac{1}{2} \tau^e_p : \tau^e_p. \] (2.121b)

\[ \boxdot \] Endochronic plasticity: second formulation

Now the linearized plastic flow rule and yield criterions can be assumed of the form

Linear theory: \[ \dot{\epsilon}^p = \frac{z}{\omega_p} \frac{\partial \hat{\phi}}{\partial \sigma} \quad , \quad \hat{\phi}(\sigma^e_p, \sigma_n^e) = \frac{1}{2} \sigma : \sigma, \] (2.122)

Finite deformations: \[ \mathcal{L}_v b_{ep} = -2 \frac{z}{\omega_p} \frac{\partial \hat{\phi}}{\partial \tau^e_p} b_{ep} \cdot \hat{\phi}(\tau^e_p, \tau^n_v) \]
\[ = \frac{1}{2} \tau : \tau. \] (2.123)

This completes the required material modeling formulations for the class of compressible Ogden materials. In the next subsection, the algorithmic treatment of the above constitutive formulations is discussed. From mathematical point of view, the \( J_2 \)-flow theory needs more consideration rather than endochronic plasticity and also from algorithmic point of view thermo-viscoelastic behavior of rubber-like materials can be recovered if \( \sigma_v \) is artificially a very large number. Therefore, the endochronic plasticity is not considered in what follows. A summary of the main results of the subsections 2.3.1-2.3.4 is given in table 2.1.

Table 2.1: A summary of the subsections 2.3.1-2.3.4.

<table>
<thead>
<tr>
<th>I.</th>
<th>Strain-energy function:</th>
</tr>
</thead>
<tbody>
<tr>
<td>[ \psi(b_{ep}, b_{ev}, \xi, \theta) = \psi^{ep}(b_{ep}, \xi, \theta) + \psi^{ev}(b_{ev}, \theta) ]</td>
<td></td>
</tr>
<tr>
<td>with</td>
<td></td>
</tr>
<tr>
<td>[ \psi^{ep}(b_{ep}, \xi, \theta) = \psi^{ep}<em>{vol}(J</em>{ep}, \theta) + \psi^{ep}<em>{iso}(\lambda_1, \lambda_2, \lambda_3, \theta) + \frac{\theta}{\theta_0} \kappa_r(e</em>{ep}) + \frac{\theta}{\theta_0} \varepsilon_0 + T(\theta), ]</td>
<td></td>
</tr>
<tr>
<td>[ \psi^{ev}(b_{ev}, \theta) = \psi^{ev}<em>{vol}(J</em>{ev}, \theta) + \psi^{ev}_{iso}(\lambda_1, \lambda_2, \lambda_3, \theta) + \frac{\theta}{\theta_0} \varepsilon_0 + T(\theta), ]</td>
<td></td>
</tr>
<tr>
<td>where</td>
<td></td>
</tr>
<tr>
<td>[ \psi^{ep}<em>{vol}(J</em>{ep}, \theta) = \frac{k_{ep}(\theta)}{4} G(J_{ep}) \quad &amp; \quad \psi^{ep}<em>{iso}(\lambda_1, \lambda_2, \lambda_3, \theta) = \frac{\theta}{\theta_0} \psi^{ep}</em>{iso}(\lambda_1, \lambda_2, \lambda_3), ]</td>
<td></td>
</tr>
<tr>
<td>[ \psi^{ev}<em>{vol}(J</em>{ev}, \theta) = \frac{k_{ev}(\theta)}{4} G(J_{ev}) \quad &amp; \quad \psi^{ev}<em>{iso}(\lambda_1, \lambda_2, \lambda_3, \theta) = \frac{\theta}{\theta_0} \psi^{ev}</em>{iso}(\lambda_1, \lambda_2, \lambda_3). ]</td>
<td></td>
</tr>
<tr>
<td>II.</td>
<td>Constitutive equations (( b_{ep} = F_{ep} F_{ep}^T ); ( b_{ev} = F_{ev} F_{ev}^T ); ( b_{ep} = j_{ep}^{2/3} b_{ep} ); ( b_{ev} = j_{ev}^{2/3} b_{ev} )).</td>
</tr>
</tbody>
</table>
2.3. THERMO-VISCOPLASTICITY AT FINITE STRAINS

a. \[ \mathbf{t} = \mathbf{t}_p^{eq} + \mathbf{t}_v^{neq} = 2\frac{\partial \psi_f}{\partial \mathbf{b}_p} \mathbf{b}_p + 2\frac{\partial \psi_f}{\partial \mathbf{b}_v} \mathbf{b}_v \]

with

\[ \mathbf{t}_p^{eq} = J_{ep} \mathbf{P}_p \mathbf{I} + \mathbf{t}_{p_{iso}}^{eq} \quad \& \quad \mathbf{t}_v^{eq} = J_{ev} \mathbf{P}_v \mathbf{I} + \mathbf{t}_{v_{iso}}^{eq} \]

where

\[ \mathbf{P}_p = \left( \kappa_{ep}(\theta)/4 \right) \partial J_{ep} G(J_{ep}) - \left( \varepsilon / \theta \right) \partial J_{ep} e_0^{ep} = \left( \kappa_{ep}(\theta)/2 \right) (J_{ep} - J_{ep}^{-1}) - (3 \kappa_{ep} a_{0}^{ep} \zeta) J_{ep}^{-1}, \]
\[ \mathbf{P}_v = \left( \kappa_{ev}(\theta)/4 \right) \partial J_{ev} G(J_{ev}) - \left( \varepsilon / \theta \right) \partial J_{ev} e_0^{ev} = \left( \kappa_{ev}(\theta)/2 \right) (J_{ev} - J_{ev}^{-1}) - (3 \kappa_{ev} a_{0}^{ev} \zeta) J_{ev}^{-1}. \]

\[ \mathbf{t}_{p_{iso}}^{eq} = \text{dev} \mathbf{t}_p^{eq} = \text{dev} \left( 2 \frac{\partial \psi_f}{\partial \mathbf{b}_p} \mathbf{b}_p \right) = \sum_{a=1}^{3} \left( \frac{\partial \psi_f}{\partial \mathbf{b}_p} \right)_a \mathbf{n}_a \otimes \mathbf{n}_a, \]
\[ \mathbf{t}_{v_{iso}}^{eq} = \text{dev} \mathbf{t}_v^{eq} = \text{dev} \left( 2 \frac{\partial \psi_f}{\partial \mathbf{b}_v} \mathbf{b}_v \right) = \sum_{a=1}^{3} \left( \frac{\partial \psi_f}{\partial \mathbf{b}_v} \right)_a \mathbf{n}_a \otimes \mathbf{n}_a, \]

in which

\[ \left( \frac{\partial \psi_f}{\partial \mathbf{b}_p} \right)_a = \text{dev} \left( \lambda_a \frac{\partial \psi_f}{\partial \lambda_a} \right) = \lambda_a \frac{\partial \psi_f}{\partial \lambda_a} - \frac{1}{3} \sum_{c=1}^{3} \lambda_c \frac{\partial \psi_f}{\partial \lambda_c} = \sum_{k=1}^{N} \mu_k^{ep}(\theta) \left[ \left( \frac{\partial \psi_f}{\partial \lambda_a} \right)^{a}\mu_k^{ep} - \frac{1}{3} \sum_{c=1}^{3} \lambda_c \left( \frac{\partial \psi_f}{\partial \lambda_c} \right)^{a}\mu_k^{ep} \right], \]
\[ \left( \frac{\partial \psi_f}{\partial \mathbf{b}_v} \right)_a = \text{dev} \left( \lambda_a \frac{\partial \psi_f}{\partial \lambda_a} \right) = \lambda_a \frac{\partial \psi_f}{\partial \lambda_a} - \frac{1}{3} \sum_{c=1}^{3} \lambda_c \frac{\partial \psi_f}{\partial \lambda_c} = \sum_{k=1}^{N} \mu_k^{ev}(\theta) \left[ \left( \frac{\partial \psi_f}{\partial \lambda_a} \right)^{a}\mu_k^{ev} - \frac{1}{3} \sum_{c=1}^{3} \lambda_c \left( \frac{\partial \psi_f}{\partial \lambda_c} \right)^{a}\mu_k^{ev} \right]. \]

b. \[ \eta = \eta^{\text{vol}} + \eta^{\text{iso}} + \eta^{\text{hard}} + \eta^{\text{ener}} \]

with

\[ -\eta^{\text{vol}} = \eta^{\text{vol}} + \eta^{\text{iso}} + \eta^{\text{hard}} + \eta^{\text{ener}} \]
\[ -\eta^{\text{ev}} = \eta^{\text{vol}} + \eta^{\text{iso}} + \eta^{\text{ener}}, \]

where

\[ \eta^{\text{vol}} = \frac{K_{ep}}{4 \theta_R} G(J_{ep}), \quad \eta^{\text{iso}} = \frac{1}{\theta_R} \psi_{0_{iso}} \left( \lambda_1^{\text{vol}}, \lambda_2^{\text{vol}}, \lambda_3^{\text{vol}} \right), \quad \eta^{\text{hard}} = \frac{1}{\theta_R} \psi_{\text{hard}}(\xi) \quad \eta^{\text{ener}} = \frac{-1}{\theta_R} e_0^{\text{vol}} \quad \eta^{\text{therm}} = \partial \theta T(\theta), \]
\[ \eta^{\text{vol}} = \frac{K_{ev}}{4 \theta_R} G(J_{ev}), \quad \eta^{\text{iso}} = \frac{1}{\theta_R} \psi_{0_{iso}} \left( \lambda_1^{\text{vol}}, \lambda_2^{\text{vol}}, \lambda_3^{\text{vol}} \right), \quad \eta^{\text{ener}} = \frac{-1}{\theta_R} e_0^{\text{ev}}. \]

III. Evolution equations:

A. First formulation:

a. Thermo-plastoelastic part:

i. J2-flow theory \( \gamma \geq 0, \quad \phi(\mathbf{t}_p^{eq}, \beta, \theta) \leq 0, \quad \gamma \phi(\mathbf{t}_p^{eq}, \beta, \theta) = 0; \)
CHAPTER 2. MATERIAL MODELING

\[ \phi(\tau^e, \beta, \theta) = \| \text{dev} [\tau^e] \| - \frac{2}{3} |\sigma_y(\theta) - \beta| \leq 0, \]

\[ L_v b_{ep} = -2\gamma \frac{\partial \phi}{\partial \tau^e} b_{ep} = -2\gamma \| \text{dev} [\tau^e] / \| \text{dev} [\tau^e] \| \| b_{ep} \|
\]

\[ \xi = \gamma \frac{\partial \phi}{\partial \beta} = \frac{2}{\sqrt{3} \gamma}, \]

\[ \eta^p = \gamma \frac{\partial \phi}{\partial \theta} = -\frac{2}{\sqrt{3} \gamma} \left( \partial_\theta \sigma_y(\theta) \right). \]

\[ \phi(\tau^e, \beta, \theta) = \frac{1}{2} \tau^e : \tau^e, \]

\[ L_v b_{ep} = -2 \frac{\partial \phi}{\partial \tau^e} b_{ep} = -2 \frac{\partial}{\partial \tau^e} \tau^e b_{ep} \]

b. Thermo-viscoelastic part:

\[ l_v = \frac{L_v b_{ep} b_{ep}^{-1} \frac{\partial \phi}{\partial \tau^e} (\tau^e, \beta, \theta) = \frac{\partial}{\partial \tau^e} (\tau^e, \beta, \theta) = \frac{\partial}{\partial \tau^e} (\tau^e, \beta, \theta) \]

\[ \text{with: } \tau^e = \frac{1}{2\zeta_p} \left( \frac{1}{3} \mathbb{I} \otimes \mathbb{I} \right) + \frac{1}{9\zeta_V} \mathbb{I} \otimes \mathbb{I} \]

\[ l_v = \frac{1}{2\zeta_p} \text{dev} (\tau^e) + \frac{1}{9\zeta_V} (\tau^e : \mathbb{I}) \mathbb{I}. \]

B. Second formulation:

a. Thermo-plastoelastic part:

i. 1st flow theory \[ \gamma \geq 0, \phi(\tau^e, \tau^neq, \beta, \theta) \leq 0, \gamma \phi(\tau^e, \tau^neq, \beta, \theta) = 0]  

\[ \phi(\tau^e, \tau^neq, \beta, \theta) = \| \text{dev} [\tau^e - \tau^neq] \| - \frac{2}{3} |\sigma_y(\theta) - \beta| \leq 0, \]

\[ L_v b_{ep} = -2\gamma \frac{\partial \phi}{\partial \tau^e} b_{ep} = -2\gamma \| \text{dev} [\tau^e - \tau^neq] / \| \text{dev} [\tau^e - \tau^neq] \| \| b_{ep} \|
\]

\[ \xi = \gamma \frac{\partial \phi}{\partial \beta} = \frac{2}{\sqrt{3} \gamma}, \]

\[ \eta^p = \gamma \frac{\partial \phi}{\partial \theta} = -\frac{2}{\sqrt{3} \gamma} \left( \partial_\theta \sigma_y(\theta) \right). \]

ii. Endochronic plasticity:

\[ \phi(\tau^e, \tau^neq) = \frac{1}{2} \tau^e : \tau^e, \]

\[ L_v b_{ep} = -2 \frac{\partial \phi}{\partial \tau^e} b_{ep} = -2 \frac{\partial}{\partial \tau^e} \tau^e b_{ep} \]

b. Thermo-viscoelastic part:

\[ l_i = \frac{L_v b_{ep} b_{ep}^{-1} \frac{\partial \phi}{\partial \tau^e} (\tau^e, \beta, \theta) = \frac{\partial}{\partial \tau^e} (\tau^e, \beta, \theta) = \frac{\partial}{\partial \tau^e} (\tau^e, \beta, \theta) \]

IV. Heat fluxes and dissipation functions:
\[ q = -k \text{grad}(\theta), \]
\[ Q = -k/ C^{-1} \text{Grad}(\theta). \]

A. First formulation:
   a. Thermo-plastoelastic part:
      i. \( J_2 \)-flow theory:
         \[ \mathcal{D}^P_{\text{mech}} = \tau_p^e : - \frac{L_b b_{ep} b_{ep}^{-1}}{2} \beta \xi = \gamma [\text{dev} \tau_p^e / \|\text{dev} \tau_p^e\|] \cdot \tau_p^e + \frac{2}{\sqrt{3}} \gamma \beta = \frac{2}{\sqrt{3}} \sigma_y(\theta), \]
         \[ \mathcal{D}^P_{\text{ther}} = - \frac{2}{\sqrt{3}} \gamma \theta \left( \frac{\partial \sigma_y(\theta)}{\partial \theta} \right). \]
      ii. Endochronic plasticity:
         \[ \mathcal{D}^P_p = \tau_p^e : - \frac{L_b b_{ep} b_{ep}^{-1}}{2} \beta \xi = \frac{2}{\xi_p} \tau_p^e : \tau_p^e. \]
   b. Thermo-viscoelastic part:
      The same as the first formulation.

B. Second formulation:
   a. Thermo-plastoelastic part:
      i. \( J_2 \)-flow theory:
      ii. Endochronic plasticity:
         \[ \mathcal{D}^P_p = \tau_p^e : - \frac{L_b b_{ep} b_{ep}^{-1}}{2} \beta \xi = \frac{2}{\sqrt{3}} \gamma \sigma_y(\theta) + \gamma \text{dev}(\tau_v^{\text{neq}}): \frac{\text{dev}[\tau_p^e - \tau_v^{\text{neq}}]}{\|\text{dev}[\tau_p^e - \tau_v^{\text{neq}}]\|}, \]
      \[ \mathcal{D}^P_{\text{ther}} = - \frac{2}{\sqrt{3}} \gamma \theta \left( \frac{\partial \sigma_y(\theta)}{\partial \theta} \right). \]
   b. Thermo-viscoelastic part: The same as the first formulation.

2.3.5 Integration of evolution equations

Since both formulations have the same structures, it is mainly focused on the first formulation in this subsection and therefore the algorithmic treatment of the second formulation can be followed in a straightforward manner. Let’s start with time discretization of the problem where a typical time sub-interval \([t_n, t_{n+1}]\) is considered to govern the subsequent equations. In an initial boundary value problem (BVP) it is typically assumed that the solution is known at time \(t_n\) and the goal is to determine the solution at time \(t_{n+1}\). For this reason it is assumed that the deformation \(\varphi\) and the temperature \(\theta\) with their gradients \((F\) and \(\text{grad}(\theta)\), respectively), and the primary internal variables \(\{C_p^{-1}, C_v^{-1}, \xi, \eta^p\}\) are known at the time \(t_n\). Now, the goal is updating
the set \( \{ \varphi, \theta, C_{p_n}^{-1}, C_{v_n}^{-1}, \xi_n, \eta_n^p \} \rightarrow \{ \varphi_{n+1}, \theta_{n+1}, C_{p_{n+1}}^{-1}, C_{v_{n+1}}^{-1}, \xi_{n+1}, \eta_{n+1}^p \} \) for a given incremental temperature \( \Delta \theta_t \) and incremental displacement \( \mathbf{u}_t(x_n) \) with its relative deformation gradient \( f_t(x_n) = I + \nabla \mathbf{u}_t(x_n) \). Note that by introducing the relative deformation gradient, the total deformation gradient will be \( F_t(X) = f_t(x_n)F_n(X) \) and, hence, the set \( \{ F_{n+1}, \theta_{n+1} \} \) is known. In what follows the monolithic scheme is used to solve the governing equations.

For thermo-viscoelastic-plastic response of the material, the viscous and plastic flows; and the local deformation at point \( X \in B_0 \) and at time \( t \in [t_n, t_{n+1}] \) are governed by the following first-order constrained equations using Eqs. (2.33), (2.68) and (2.69)

\[
\begin{align*}
\dot{f}_t &= l_t \dot{f}_t \quad \text{with:} \quad l_t &= \dot{f}_t f_t^{-1} = \dot{F}_t F_t^{-1}, \\
\dot{b}_{ev_t} &= (l_t b_{ev_t} + b_{ev_t} l_t^T) - 2 \frac{\partial \varphi_v(t_{neq}^{eq})}{\partial \tau_v^{eq}} \dot{b}_{ev_t}, \\
\dot{b}_{ep_t} &= (l_t b_{ep_t} + b_{ep_t} l_t^T) - 2 \gamma_t \frac{\partial \hat{\varphi}(\tau_{eq}^{eq}, \beta_t, \theta_t)}{\partial \tau_p^{eq}} \dot{b}_{ep_t}, \\
\dot{\xi}_t &= \gamma_t \frac{\partial \hat{\varphi}(\tau_{eq}^{eq}, \beta_t, \theta_t)}{\partial \theta}, \\
\dot{\eta}_t^p &= \gamma_t \frac{\partial \hat{\varphi}(\tau_{eq}^{eq}, \beta_t, \theta_t)}{\partial \theta},
\end{align*}
\]

where the set \( \{ \tau_{eq}^{eq}, \tau_{neq}^{eq}, \beta_t \} \) are dependent variables obtained by the constitutive equations

\[
\begin{align*}
\tau_{eq}^{eq} &= 2 \frac{\partial \psi_{ep}}{\partial b_{ep}} b_{ep_t}, \\
\tau_{neq}^{eq} &= 2 \frac{\partial \psi_{ev}}{\partial b_{ev}} b_{ev_t}, \\
\beta_t &= - \frac{\partial \psi_{ep}}{\partial \xi}.
\end{align*}
\]

\[
\{ f_t, b_{ep_t}, b_{ev_t}, \xi_t, \eta_t^p \} = \{ I, b_{ep_t}, b_{ev_t}, \xi_t, \eta_t^p \}
\]

where \( \hat{\varphi} \) and \( \varphi_v \) explicitly given in Eqs. (2.114) and (2.116) written here implicitly and in subsequent equations for convenience.

**Operator split**

To solve the above governing equations using the product formula algorithm (Simo, 1992), the structure of equations suggests the following operator splits as

Problem 1. Trial thermoelastic state
\[ \dot{f}_t = l_t f_t, \quad (2.127a) \]
\[ \dot{b}_{ev_t} = (l_t b_{ev_t} + b_{ev_t} l_t^T), \quad (2.127b) \]
\[ \dot{b}_{ep_t} = (l_t b_{ep_t} + b_{ep_t} l_t^T), \quad (2.127c) \]
\[ \xi_t = 0, \quad (2.127d) \]
\[ \eta^p_t = 0, \quad (2.127e) \]

Constraints: None

Problem 2. Thermo-viscoelastic corrector step

\[ \dot{f}_t = 0, \quad (2.128a) \]
\[ \dot{b}_{ev_t} = -2 \frac{\partial \varphi_v(t^{neq}_v)}{\partial t^{neq}_v} b_{ev_t}, \quad (2.128b) \]
\[ \dot{b}_{ep_t} = 0, \quad (2.128c) \]
\[ \xi_t = 0, \quad (2.128d) \]
\[ \eta^p_t = 0, \quad (2.128e) \]

Constraints: None

Problem 3. Thermoplastic return mapping

\[ \dot{f}_t = 0, \quad (2.129a) \]
\[ \dot{b}_{ev_t} = 0, \quad (2.129b) \]
\[ \dot{b}_{ep_t} = -2 \gamma_t \frac{\partial \tilde{\varphi}(t^q_p, \beta, \theta)}{\partial t^q_p} b_{ep_t}, \quad (2.129c) \]
\[ \xi_t = \gamma_t \frac{\partial \varphi(t^q_p, \beta, \theta)}{\partial \beta}, \quad (2.129d) \]
\[ \eta^p_t = \gamma_t \frac{\partial \tilde{\varphi}(t^q_p, \beta, \theta)}{\partial \beta}, \quad (2.129e) \]

Constraints: \[ \gamma_t \geq 0, \quad \hat{\varphi}(t^q_p, \beta, \theta) \leq 0, \quad \gamma_t \hat{\varphi}(t^q_p, \beta, \theta) = 0. \]
Product formula algorithm

Problem 1 physically means that the viscoelastic and plastic flows are frozen at the time $t_n$. The solution to this problem is exact and given by the closed form formula

$$f_{tr}^n = f_t, \quad \xi_{tr}^n = \xi_n, \quad \eta_{tr}^n = \eta_n^p,$$  \hspace{1cm} (2.130a)

$$b_{ep t}^{tr} = f_t b_{ep} f_t^n F_{t}^{-1} C_p, \quad b_{ev t}^{tr} = f_t b_{ev} f_t^n F_{t}^{-1} C_p.$$  \hspace{1cm} (2.130b)

\[
\begin{align*}
(\tau_p^{eq})_{tr}^n & = 2 \frac{\partial \psi_{ep} \left( \frac{b_{ep}^{tr} \xi_{tr}, \theta_t}{\partial b_{ep}} \right)}{\partial b_{ep}} b_{ep t}^{tr}, \\
(\tau_v^{eq})_{tr}^n & = 2 \frac{\partial \psi_{ev} \left( \frac{b_{ev}^{tr} \xi_{tr}, \theta_t}{\partial b_{ev}} \right)}{\partial b_{ev}} b_{ev t}^{tr}, \\
\beta_{tr}^n & = - \frac{\partial \psi_{ep} \left( \frac{b_{ep}^{tr} \xi_{tr}, \theta_t}{\partial \xi} \right)}{\partial \beta}.
\end{align*}
\]  \hspace{1cm} (2.131a)

From a physical point of view the problems 2 and 3 are obtained by freezing the current configuration via $\dot{f}_t = 0$. The solution to these equations are relied on the so called exponential mapping algorithms (Weber and Anand, 1990; Cuitino and Ortiz, 1992; and Simo, 1992 among others). So, based on the exponential approximations and employing the implicit Euler backward method, the general solutions of the problem are

- **Thermo-viscoelastic part:**

$$b_{ev t} = \exp \left[ -2\Delta t \frac{\partial \varphi_v \left( \tau_v^{eq} \right)}{\partial \tau_v^{eq}} \right] b_{ev t}^{tr}.$$  \hspace{1cm} (2.132a)

- **Thermo-plastoelastic part:**

$$b_{ep t} = \exp \left[ -2\Delta \gamma_t \frac{\partial \hat{\varphi} \left( \tau_p^{eq}, \beta_t, \theta_t \right)}{\partial \tau_p^{eq}} \right] b_{ep t}^{tr},$$  \hspace{1cm} (2.132b)

$$\xi_t = \xi_n + \Delta \gamma_t \frac{\partial \hat{\varphi} \left( \tau_p^{eq}, \beta_t, \theta_t \right)}{\partial \beta},$$  \hspace{1cm} (2.132c)

$$\eta_t^p = \eta_n^p + \Delta \gamma_t \frac{\partial \hat{\varphi} \left( \tau_p^{eq}, \beta_t, \theta_t \right)}{\partial \theta},$$  \hspace{1cm} (2.132d)

$$\Delta \gamma_t \geq 0, \quad \hat{\varphi} \left( \tau_p^{eq}, \beta_t, \theta_t \right) \leq 0, \quad \Delta \gamma_t \hat{\varphi} \left( \tau_p^{eq}, \beta_t, \theta_t \right) = 0.$$
where $\Delta t = t - t_n$ denotes the time increment and $\Delta \gamma_t = \Delta t \gamma_t$ is Lagrangian multiplier presented algorithmically in table 2.3. Note that as a consequence of employing the Euler backward scheme the set \( \{ \tau_{eq}^t, \tau_{neq}^{t}, \beta_t \} \) should be evaluated at \( \{ b_{ep}, b_{ev}, \xi_t, \theta_t \} \).

Table 2.2: Local Newton scheme to solve thermo-viscoelastic part.

<table>
<thead>
<tr>
<th>I. Nonlinear equation:</th>
<th>$r = -\varepsilon_t^{eq} + \varepsilon_t^{eq,v} - \Delta t \partial \varphi_t(\tau_t^{eq})$.</th>
</tr>
</thead>
<tbody>
<tr>
<td>II. Initialize $k = 0$, $\varepsilon_t^{eq,v} = c t e$, $\Delta \theta_t = 0$, and linearize around $\tau_t^{eq} = \tau_t^{eq,(k)}$, $\tau_t^{eq,(k)} = \partial \varepsilon_t^{eq,v}(\varepsilon_t^{eq,(k)}, \theta_t)$:</td>
<td>$r^{(k+1)} = 0$, $r^{(k)} = -\varepsilon_t^{eq,(k)} + \varepsilon_t^{eq,v} - \Delta t \partial \varphi_t(\tau_t^{eq,(k)})$.</td>
</tr>
<tr>
<td>III. Compute the algorithmic tangent moduli and stress increment:</td>
<td>$A^{(k)} = \left[ \frac{\partial^2 \varphi_t^{eq,(k)}}{\partial \varepsilon_t^{eq,v} \partial \varepsilon_t^{eq,v}} \right]^{-1} + \Delta t \left[ \frac{\partial^2 \varphi_t^{eq,(k)}}{\partial \varphi_t^{eq,v} \partial \tau_t^{eq,v}} \right]^{-1}$, $\Delta r^{(k)} = -(A^{(k)})^{-1}\Delta \tau_t^{eq,(k)}$, $\Delta \tau_t^{eq,(k)} = A^{(k)}r^{(k)}$.</td>
</tr>
<tr>
<td>IV. Update the logarithmic non-equilibrated elastic stretch vectors:</td>
<td>$\Delta \varepsilon_t^{eq,(k)} = \left[ \frac{\partial^2 \varphi_t^{eq,(k)}}{\partial \varepsilon_t^{eq,v} \partial \varepsilon_t^{eq,v}} \right]^{-1} \Delta \tau_t^{eq,(k)}$, $\varepsilon_t^{eq,(k+1)} = \varepsilon_t^{eq,(k)} + \Delta \varepsilon_t^{eq,(k)}$.</td>
</tr>
<tr>
<td>V. Repeat until $| r^{(k)} | &lt; \text{tol}$.</td>
<td></td>
</tr>
</tbody>
</table>

**Spectral decompositions: Reduction to principal directions**

Since the isotropy was assumed from the outset and by presenting the yield criterion and creep potential in their classical format, it was seen that they are isotropic functions and, therefore, they can be written in terms of their principal stretches. This leads to an efficient implementation of the product formula algorithm described above. To do this, in this subsection, the yield function and creep potential; and the trial elastic tensors are written in terms of their principal directions. Note that the spectral decompositions of elastic tensors and the stresses were given in Eqs. (2.112). Setting

\[
\hat{\phi}\left( \tau_{ep}^t, \beta_t, \theta_t \right) = \hat{\phi}\left( \tau_{1e}^t, \tau_{2e}^t, \tau_{3e}^t, \beta_t, \theta_t \right), \quad \text{(2.133a)}
\]

\[
\varphi_v\left( \tau_{neq}^t \right) = \varphi_v\left( \tau_{1e}^t, \tau_{2e}^t, \tau_{3e}^t \right), \quad \text{(2.133b)}
\]
the trial elastic Finger tensors in (2.132a, b) take the form

\[
\begin{align*}
\mathbf{b}_{ev_t}^{tr} &= \sum_{a=1}^{3} \left( \lambda_{a}^{ev} \right)^{2} \left( \exp[2\Delta t \partial_{\tau_{a}^{ev}} \varphi_{v}] \right) \mathbf{n}_{a}^{ev} \otimes \mathbf{n}_{a}^{ev}_{t}, \\
\mathbf{b}_{ep_t}^{tr} &= \sum_{a=1}^{3} \left( \lambda_{a}^{ep} \right)^{2} \left( \exp[2\Delta \gamma_{t} \partial_{\tau_{a}^{ep}} \phi] \right) \mathbf{n}_{a}^{ep} \otimes \mathbf{n}_{a}^{ep}_{t},
\end{align*}
\]

(2.134a, 2.134b)

since \( \mathbf{b}_{ev_t} \), \( \tau_{p_t}^{eq} \) and \( \partial_{\tau_{a}^{eq}} \phi \) commute with each other and the similar results hold for \( \mathbf{b}_{ev_t} \), \( \tau_{p_t}^{ev} \) and \( \partial_{\tau_{a}^{ev}} \varphi_{v} \). On the other hand, the spectral decompositions of the elastic trial Finger tensors \( \mathbf{b}_{ev_t}^{tr} \) and \( \mathbf{b}_{ep_t}^{tr} \) can be written

\[
\begin{align*}
\mathbf{b}_{ev_t}^{tr} &= \sum_{a=1}^{3} \left( \lambda_{a}^{evtr} \right)^{2} \left( \mathbf{n}_{a}^{ev}_{t} \right)^{tr} \otimes \left( \mathbf{n}_{a}^{ev}_{t} \right)^{tr}, \\
\mathbf{b}_{ep_t}^{tr} &= \sum_{a=1}^{3} \left( \lambda_{a}^{eplot} \right)^{2} \left( \mathbf{n}_{a}^{ep}_{t} \right)^{tr} \otimes \left( \mathbf{n}_{a}^{ep}_{t} \right)^{tr}.
\end{align*}
\]

(2.135a, 2.135b)

Comparing Eqs. (2.134) and (2.135), and noting the uniqueness of the spectral decomposition leads to

\[
\begin{align*}
\left( \lambda_{a}^{evtr} \right)^{2} &= \left( \lambda_{a}^{ev} \right)^{2} \exp[2\Delta t \partial_{\tau_{a}^{ev}} \varphi_{v}] \quad \& \quad \left( \mathbf{n}_{a}^{ev}_{t} \right)^{tr} = \mathbf{n}_{a}^{ev}_{t}, \\
\left( \lambda_{a}^{eplot} \right)^{2} &= \left( \lambda_{a}^{ep} \right)^{2} \exp[2\Delta \gamma_{t} \partial_{\tau_{a}^{ep}} \phi] \quad \& \quad \left( \mathbf{n}_{a}^{ep}_{t} \right)^{tr} = \mathbf{n}_{a}^{ep}_{t}.
\end{align*}
\]

(2.136a, 2.136b)

Taking the logarithm on both sides of Eq. (2.136), and using vector notation leads to equivalently reformulating the algorithmic flows in Eqs. (2.132) in principal directions

\[
\begin{align*}
\epsilon_{t}^{ev} &= \epsilon_{t}^{evtr} - \Delta t \partial_{\tau_{t}^{ev}} \varphi_{v}(\tau_{t}^{ev}), \\
\epsilon_{t}^{ep} &= \epsilon_{t}^{eplot} - \Delta \gamma_{t} \partial_{\tau_{t}^{ep}} \phi(\tau_{t}^{ep}, \beta_{t}, \theta_{t}), \\
\xi_{t} &= \xi_{n} + \Delta \gamma_{t} \frac{\partial \phi(\tau_{t}^{ep}, \beta_{t}, \theta_{t})}{\partial \beta}, \\
\eta_{t}^{p} &= \eta_{n} + \Delta \gamma_{t} \frac{\partial \phi(\tau_{t}^{ep}, \beta_{t}, \theta_{t})}{\partial \theta},
\end{align*}
\]

(2.137a, 2.137b, 2.137c, 2.137d)

\[\Delta \gamma_{t} \geq 0, \quad \phi(\tau_{t}^{ep}, \beta_{t}, \theta_{t}) \leq 0, \quad \Delta \gamma_{t} \phi(\tau_{t}^{ep}, \beta_{t}, \theta_{t}) = 0.\]

The update formula (2.137a) presents a nonlinear algebraic equation expressed in terms of the primary variable \( \epsilon_{t}^{ev} \) in the fixed principal direction \( \left( \mathbf{n}_{a}^{ev}_{t} \right)^{tr} \) defined by the trial elastic Finger tensor \( \mathbf{b}_{ev_t}^{tr} \) - the thermo-viscoelastic part. On the other hand, the update formula (2.137b-d) defines a set of nonlinear algebraic equations expressed in terms of
the primary variables \((\varepsilon_t^{ep}, \xi_t, \eta_t^p)\) in the fixed principal direction \( (n_{\alpha}^{ep})_{t}^{tr} \) defined by the trial elastic tensor \( b_{\alpha}^{ttr} \) - the plastoelastic part. Eq. (2.137a) is solved by means of a Newton iterative scheme in table 2.2. This standard Newton scheme is called global method in a way that it converges to a solution from almost any starting point. Due to the highly nonlinear nature of Eqs. (2.137b-c), the global method fails to converge -as tested by the authors for some thermo-viscoplasticity process paths- when a starting point is not sufficiently close to the solution. Thus, the standard global setting in table 2.3 is accompanied with line searches and backtracking (Press et al., 1997). Since these equations should be satisfied at the Gauss point level, these iterative schemes can be termed local Newton iterations. It should be noted that during the local iterative schemes the elastic trial stretches and the temperature are held fixed.

Table 2.3: General return mapping in principal axes for perfect thermo-plasticity \( \bar{\psi}^{tr} > 0 \).

<table>
<thead>
<tr>
<th>Step</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>I. Initialize</td>
<td>( k = 0, \quad \varepsilon_t^{ep(0)} = \varepsilon_t^{ep tr}, \quad \xi_t^{(0)} = \xi_n, \quad \eta_t^{p(0)} = \eta_n, \quad \Delta Y_t^{(0)} = 0, \quad \Delta \theta_t = 0 )</td>
</tr>
</tbody>
</table>
| II. Set the nonlinear equations: | \[
\begin{align*}
\psi^{ep(k)} &= \psi^{ep} \left( \varepsilon_t^{ep(k)}, \xi_t^{(k)}, \theta_t \right), \\
\tau_t^{ep(k)} &= \nabla \varepsilon_t^{ep} \left( \psi^{ep(k)} \right), \\
d^{(k)} &= \nabla \varepsilon_t^{ep} \left( \tau_t^{ep(k)} \right), \\
\beta_t^{(k)} &= -\partial_{\varepsilon_t} \left( \psi^{ep(k)} \right), \\
d_{\varepsilon_t} \left( \tau_t^{ep(k)} \right) &= 0, \\
\nabla \varepsilon_t^{ep} \left( \beta_t^{(k)} \right) &= 0,
\end{align*}
\]
| \( \bar{\psi}^{tr} = \left\{ \begin{array}{c} r_1^{(k)} \\ r_2^{(k)} \\ r_3^{(k)} \end{array} \right\} \) in which | \( \begin{align*}
\bar{r}_1^{(k)} &= -\varepsilon_{t}^{ep(k)} + \varepsilon_{t}^{ep tr} - \Delta Y_t^{(k)} \partial_{\varepsilon_t} \left( \bar{\psi}^{(k)} \right), \\
\bar{r}_2^{(k)} &= -\xi_{t}^{(k)} + \xi_{n} + \Delta Y_t^{(k)} \partial_{\xi_t} \left( \bar{\psi}^{(k)} \right), \\
\bar{r}_3^{(k)} &= -\eta_{t}^{p(k)} + \eta_{n} + \Delta Y_t^{(k)} \partial_{\eta_t} \left( \bar{\psi}^{(k)} \right).
\end{align*} \) |
| IF \( \| \bar{r}_2^{(k)} \| > tol \) or \( \bar{\psi}^{(k)} > 0 \) | go to Step III |
| Else | set \( \varepsilon_t^{ep} = \varepsilon_t^{ep(k)}, \quad \xi_t = \xi_t^{(k)}, \quad \eta_t^p = \eta_t^{p(k)} \) |
| END IF | |
| III. Compute the algorithmic tangent moduli: | \( \begin{align*}
\bar{U}^{(k)} &= \left( \bar{d}^{(k)} \right)^{-1} + \Delta Y_t^{(k)} \partial_{\varepsilon_t}^2 \left( \bar{\psi}^{(k)} \right), \\
U^{(k)} &= \left( D^{(k)} \right)^{-1} + \Delta Y_t^{(k)} \partial_{\beta_t}^2 \left( \bar{\psi}^{(k)} \right),
\end{align*} \) |
IV. Compute increments of consistency parameter, logarithmic stretch, equivalent plastic strain and plastic entropy:

\[
\Delta \chi_2 = \frac{\hat{\varphi}^{(k)} - \left[ \begin{array}{c} \partial_{\chi} \varphi^{(k)} \\ \partial_{\gamma} \varphi^{(k)} \end{array} \right] \psi_1^{(k)} R_1^{(k)} - \partial_{\chi} \varphi^{(k)} \right]}{\psi_1^{(k)} R_1^{(k)} - \partial_{\chi} \varphi^{(k)}}.
\]

\[
\left\{ \begin{array}{c}
\Delta \chi_1 \\
\Delta \chi_2 \\
\Delta \chi_{\eta}^{(k)}
\end{array} \right\} = \left[ \begin{array}{ccc}
(d^{(k)})^{-1} & 0_{3 \times 1} & 0_{3 \times 1} \\
0_{1 \times 3} & -(D^{(k)})^{-1} & 0_{1 \times 3} \\
0_{1 \times 3} & 0 & -1
\end{array} \right] \left\{ \begin{array}{c}
\psi_1^{(k)} \\
\psi_2^{(k)} \\
R_2^{(k)} - \Delta \chi_2
\end{array} \right\}.
\]

V. Update the consistency parameter, logarithmic stretch, equivalent plastic strain and plastic entropy:

\[
\chi_2^{(k+1)} = \chi_2^{(k)} + \Delta \chi_2^{(k)}
\]

\[
\varepsilon_t^{ep,(k+1)} = \varepsilon_t^{ep,(k)} + \Delta \varepsilon_t^{ep,(k)}
\]

\[
\xi_t^{(k+1)} = \xi_t^{(k)} + \Delta \xi_t^{(k)}
\]

\[
\eta_t^{p,(k+1)} = \eta_t^{p,(k)} + \Delta \eta_t^{p,(k)}
\]

Set \( k + 1 \leftarrow k \) ans return to Step II.

### 2.3.6 Variational formulations and consistent linearization

The outline of this subsection is as follows: first, the weak formulations of the Cauchy's first equation of motion and the energy balance equation are presented and then their corresponding consistent linearization is carried out which leads to the definition of the elasticity tensors. At the end, the elasticity tensors in the current configuration suitable for finite element implementation are derived for both thermo-plastoelastic and thermo-viscoelastic parts.

**Weak forms**

The linear momentum balance (2.102) and the energy Eq. (2.107) have been written in the strong form which are not suitable for the finite element implementation. Hence, by considering the arbitrary variations (\( \delta \mathbf{u}, \delta \theta \)) their weak forms may be written by
\[
\int_{B_0} \delta \mathbf{e} : \mathbf{t} \, dV + \int_{B_0} \delta \mathbf{u} \cdot (\rho_0 \mathbf{\dot{v}} - \rho_0 \mathbf{f}_b) \, dV - \int_{\partial B_0^p} \delta \mathbf{u} \cdot \overline{\mathbf{p}} \, dA = 0, \tag{2.138a}
\]

\[
\int_{B_0} j_q \, \nabla \delta \theta \, dV + \int_{B_0} \left( D_{\text{mech}}^p + D^v - \mathcal{H} - c \dot{\theta} + \mathcal{R} \right) \delta \theta \, dV - \int_{\partial B_0^Q} \mathbf{Q} \cdot \mathbf{N} \, dA = 0, \tag{2.138b}
\]

where \( \delta \) represents the variational symbol; \( \mathbf{N} \) denotes the unit outward normal to the element surface \( dA \); \( \overline{\mathbf{p}} = \overline{\mathbf{P}} \mathbf{N} \) is the traction vector and again \( B_0 \) is the reference volume with \( \partial B_0 = \partial B_0^u \cup \partial B_0^p = \partial B_0^\theta \cup \partial B_0^Q \) in which \( \partial B_0^u \cap \partial B_0^p = \partial B_0^\theta \cap \partial B_0^Q = 0 \). Note that displacements, tractions, temperatures and heat fluxes should be prescribed on \( \partial B_0^u, \partial B_0^p, \partial B_0^\theta \) and \( \partial B_0^Q \), respectively. Also, \( \delta \mathbf{e} \) denotes the variation of the Almansi strain tensor given by

\[
\delta \mathbf{e} = \text{sym} ( \nabla \delta \mathbf{u} ) = \frac{1}{2} \mathbf{F}^{-T} \delta \mathbf{C} \mathbf{F}^{-1}, \quad \delta \mathbf{C} = \text{sym}( \mathbf{F}^T \nabla \delta \mathbf{u} ). \tag{2.139}
\]

The above weak formulations may be written in short hand notation as

\[
\mathcal{W}_M = \int_{B_0} \frac{1}{2} \delta \mathbf{C} : ( \mathbf{S}_p^{eq} + \mathbf{S}_v^{neq} ) \, dV + \mathcal{W}_M^L, \tag{2.140a}
\]

\[
\mathcal{W}_\theta = \int_{B_0} j_q \, \nabla \delta \theta \, dV + \int_{B_0} \left( D_{\text{mech}}^p + D^v - \mathcal{H} - c \dot{\theta} + \mathcal{R} \right) \delta \theta \, dV + \mathcal{W}_\theta^b \tag{2.140b}
\]

where \( \mathcal{W}_M^L \) and \( \mathcal{W}_M^b \) are defined through the comparison to Eqs. (2.138).

### Consistent linearization

Next, the linearization of the above nonlinear variational functionals (2.140) is considered suitable for a numerical iterative scheme such as Newton method.

#### Linear momentum equation

Let’s start with the linearization of Eq. (2.140a) about a known state \( \mathcal{W}_M^p \).
\[ W_M \approx W_M^p + \Delta W_M = \]
\[ W_M^p + \int_{\mathcal{B}_0} \frac{1}{2} \delta \mathcal{C} : (\mathcal{S}_p^{eq} + \mathcal{S}_v^{neq}) dV \]
\[ + \int_{\mathcal{B}_0} \frac{1}{2} \delta \mathcal{C} : 2 \left( \frac{\partial \mathcal{S}_p^{eq}}{\partial \mathcal{C}} + \frac{\partial \mathcal{S}_v^{neq}}{\partial \mathcal{C}} \right) : \frac{1}{2} \Delta \mathcal{C} dV + \int_{\mathcal{B}_0} \delta \mathcal{e} : \left( \frac{\partial \mathcal{r}}{\partial \mathcal{\theta}} \right) \Delta \mathcal{\theta} dV, \]

(2.141)

where the first term requires \( \Delta \mathcal{C} = \text{sym}[(\text{Grad}^T \mathcal{\Delta} \mathcal{u}) \text{Grad} \delta \mathcal{u}] \) but the second term desires more consideration. Note that this term has some alternative forms

\[ \frac{1}{2} \delta \mathcal{C} : 2 \left( \frac{\partial \mathcal{S}_p^{eq}}{\partial \mathcal{C}} \right) : \frac{1}{2} \Delta \mathcal{C} = \frac{1}{2} \delta \mathcal{C}_{ep} : 2 \left( \frac{\partial \mathcal{S}_p^{eq}}{\partial \mathcal{C}_{ep}} \right) : \frac{1}{2} \Delta \mathcal{C}_{ep} \]
\[ = \frac{1}{2} \delta \mathcal{C}_{tr}^{ep} : 2 \left( \frac{\partial \mathcal{S}_p^{eq}}{\partial \mathcal{C}_{tr}^{ep}} \right) : \frac{1}{2} \Delta \mathcal{C}_{tr}^{ep}, \]

(2.142a)

and

\[ \frac{1}{2} \delta \mathcal{C} : 2 \left( \frac{\partial \mathcal{S}_v^{neq}}{\partial \mathcal{C}} \right) : \frac{1}{2} \Delta \mathcal{C} = \frac{1}{2} \delta \mathcal{C}_{ev} : 2 \left( \frac{\partial \mathcal{S}_v^{neq}}{\partial \mathcal{C}_{ev}} \right) : \frac{1}{2} \Delta \mathcal{C}_{ev} \]
\[ = \frac{1}{2} \delta \mathcal{C}_{tr}^{ev} : 2 \left( \frac{\partial \mathcal{S}_v^{neq}}{\partial \mathcal{C}_{tr}^{ev}} \right) : \frac{1}{2} \Delta \mathcal{C}_{tr}^{ev}, \]

(2.142b)

where \( \mathcal{S}_p^{eq} \) presents the second Piola-Kirchhoff stress tensor defined in the fixed intermediate plastic configuration and \( \mathcal{S}_v^{neq} \) is the second Piola-Kirchhoff stress tensor defined in the fixed intermediate viscous configuration; given by

\[ \mathcal{S}_p^{eq} = (\mathcal{F}_p)_n \mathcal{S}_p^{eq} (\mathcal{F}_p^T)_n = (\mathcal{F}_{tr}^{ep})_{n+1}^{-1} \mathcal{r}_p (\mathcal{F}_{tr}^{ep})_{n+1}^{-T}, \]

(2.143a)

\[ \mathcal{S}_v^{neq} = (\mathcal{F}_v)_n \mathcal{S}_v^{neq} (\mathcal{F}_v^T)_n = (\mathcal{F}_{tr}^{ev})_{n+1}^{-1} \mathcal{r}_v (\mathcal{F}_{tr}^{ev})_{n+1}^{-T}, \]

(2.143b)

and also \( \mathcal{S}_p^{eq} = 2 \delta \mathcal{S}_p^{eq} / \partial \mathcal{C}_{tr}^{ep} \) and \( \mathcal{S}_v^{neq} = 2 \delta \mathcal{S}_v^{neq} / \partial \mathcal{C}_{tr}^{ev} \) denote the elasticity tensors in the respective intermediate configurations. Among the alternative choices in Eqs. (2.142), here the last terms are chosen. The advantage is that since they are defined in the fixed intermediate configurations, \( (\mathcal{F}_p)_n \) and \( (\mathcal{F}_v)_n \) can be regarded as constants during the global Newton iterations and hence

\[ \Delta \mathcal{F} = \Delta \mathcal{F}_{tr}^{ep} (\mathcal{F}_p)_n = \Delta \mathcal{F}_{tr}^{ev} (\mathcal{F}_v)_n, \]

(2.144a)

\[ \delta \mathcal{F} = \delta \mathcal{F}_{tr}^{ep} (\mathcal{F}_p)_n = \delta \mathcal{F}_{tr}^{ev} (\mathcal{F}_v)_n, \]

\[ \Delta \mathcal{C}_{tr}^{ep} = (\mathcal{F}_p^T)_n \Delta \mathcal{C} (\mathcal{F}_p^{-1})_n = (\mathcal{F}_{tr}^{ep})_{n+1}^{-T} (2 \Delta \mathcal{e}) (\mathcal{F}_{tr}^{ep})_{n+1}^{-1}, \]

(2.144b)

\[ \Delta \mathcal{C}_{tr}^{ev} = (\mathcal{F}_v^T)_n \Delta \mathcal{C} (\mathcal{F}_v^{-1})_n = (\mathcal{F}_{tr}^{ev})_{n+1}^{-T} (2 \Delta \mathcal{e}) (\mathcal{F}_{tr}^{ev})_{n+1}^{-1}, \]
\[ \delta C_{eq}^{tr} = (F_p^{-T})_n \delta C (F_p^{-1})_n = (F_{eq}^{tr})^{-T}_{n+1} (2\delta e)(F_{eq}^{tr})^{-1}_{n+1}, \]
\[ \delta C_{ev}^{tr} = (F_v^{-T})_n \delta C (F_v^{-1})_n = (F_{ev}^{tr})^{-T}_{n+1} (2\delta e)(F_{ev}^{tr})^{-1}_{n+1}. \]

All that remains to do is computation of the elasticity tensors \( \hat{e}_{eq} \) and \( \hat{e}_{ev} \) and making push-forward to the current configuration (Marsden and Hughes, 1983). Following the same procedure as in Simo, 1998 and Wriggers, 2008, leads to

\[ \hat{e}_{eq} = \sum_{a=1}^{3} \sum_{b=1}^{3} \frac{C_{ab}^{eq} - 2(\tau_{ta}/\tau_{tb})\delta_{ab}}{(\lambda_{ab}^{eq})^2} (M_{ab}^{eq})^{tr}_t \otimes (M_{ab}^{eq})^{tr}_t \]
\[ \hat{e}_{ev} = \sum_{a=1}^{3} \sum_{b=1}^{3} \frac{C_{ab}^{ev} - 2(\tau_{ta}/\tau_{tb})\delta_{ab}}{(\lambda_{ab}^{ev})^2} (M_{ab}^{ev})^{tr}_t \otimes (M_{ab}^{ev})^{tr}_t \]

where

\[ (M_{ab}^{eq})^{tr}_t = (N_{a}^{eq})^{tr}_t \otimes (N_{b}^{eq})^{tr}_t \]
\[ (M_{ab}^{ev})^{tr}_t = (N_{a}^{ev})^{tr}_t \otimes (N_{b}^{ev})^{tr}_t \]

with \( (N_{a}^{eq})^{tr}_t \) and \( (N_{a}^{ev})^{tr}_t \) being the principal directions in the fixed plastic and viscous intermediate configurations; and also \( C_{ab}^{eq} = \partial \tau_{ta}/\partial \epsilon_{eq}^{tr} \) presents a thermo-plastoelastic \( 3 \times 3 \) algorithmic tensor obtained by linearization of the algorithmic flows (2.137b)-(2.137d) and \( C_{ab}^{ev} = \partial \tau_{ta}/\partial \epsilon_{ev}^{tr} \) denotes a thermo-viscoelastic \( 3 \times 3 \) algorithmic tensor obtained by linearization of the algorithmic flow (2.137a). They have been presented in Appendix A. Applying a push-forward to the last terms in Eqs. (2.142), one can obtain (Simou and Marsden, 1984; Sansour, 1993)

\[ \frac{1}{2} \delta C: \hat{e}_{eq} = 2 \frac{\partial S_{eq}^{eq}}{\partial C} : \frac{1}{2} \delta C = \frac{1}{2} \delta C_{eq}^{tr} : \hat{e}_{eq} : \frac{1}{2} \Delta C_{eq}^{tr} = \delta e: \hat{e}_{eq} : \Delta e, \]
\[ \frac{1}{2} \delta C: \hat{e}_{ev} = 2 \frac{\partial S_{ev}^{neq}}{\partial C} : \frac{1}{2} \delta C = \frac{1}{2} \delta C_{ev}^{tr} : \hat{e}_{ev} : \frac{1}{2} \Delta C_{ev}^{tr} = \delta e: \hat{e}_{ev} : \Delta e, \]

where \( \hat{e}_{eq} \) and \( \hat{e}_{ev} \) are the elasticity tensors in the current configuration given by
\[
\varepsilon_p^{eq} = \sum_{a=1}^{3} \sum_{b=1}^{3} \left( C_{ab}^{ep} - 2 \tau_a^{ep} \delta_{ab} \right) (m_{ab}^{ep})_t^{tr} \otimes (m_{ba}^{ep})_t^{tr} \\
+ \sum_{a=1}^{3} \sum_{b=1}^{3} \left( \lambda_{ab}^{eptr} \tau_{ta}^{ep} - \lambda_{ba}^{eptr} \tau_{tb}^{ep} \right) \left( m_{ab}^{ep} \right)_t^{tr} \otimes \left( m_{ab}^{ep} \right)_t^{tr} + \left( m_{ab}^{ep} \right)_t^{tr} \otimes \left( m_{ba}^{ep} \right)_t^{tr},
\]

where

\[
\begin{align*}
\left( m_{ab}^{ep} \right)_t^{tr} &= \left( n_a^{ep} \right)_t^{tr} \otimes \left( n_b^{ep} \right)_t^{tr} \\
\left( m_{ab}^{ev} \right)_t^{tr} &= \left( n_a^{ev} \right)_t^{tr} \otimes \left( n_b^{ev} \right)_t^{tr}
\end{align*}
\]

The linearization of the last term in Eq. (2.141) requires the computation of \( \partial \tau / \partial \theta \)

\[
\frac{\partial \tau}{\partial \theta} = \sum_{a=1}^{3} \left( \xi_1^{ep} \right)_a (n_a^{ep})_t^{tr} \otimes (n_a^{ep})_t^{tr} \\
+ \sum_{a=1}^{3} \left( \xi_1^{ev} \right)_a (n_a^{ev})_t^{tr} \otimes (n_a^{ev})_t^{tr},
\]

where the algorithmic thermo-plastoelastic (thermo-viscoelastic) vector \( \xi_1^{ep} (\xi_1^{ev}) \) has been given in Appendix A. This completes the linearization of the weak form of the momentum balance equation.

### Energy balance equation

In what follows, the linearization of the energy balance equation is pursued. Let a constant heat source and heat capacity. Taking into account the time discretization of the term \( c \dot{\theta} \) and based on the backward Euler method, one can write

\[
\Delta W_\theta = \int_{\mathcal{V}_0} \frac{\partial (q \cdot \text{grad}(\delta \theta))}{\partial \theta} \Delta \theta + \frac{\partial (q \cdot \text{grad}(\delta \theta))}{\partial C} : \Delta C \ dV + \int_{\mathcal{V}_0} \delta \theta \frac{\partial D_{\text{mech}}^p}{\partial \theta} \Delta \theta \ dV \\
+ \int_{\mathcal{V}_0} \delta \theta \frac{\partial D_{\text{mech}}^v}{\partial C_{\text{ep}}} : \Delta C_{\text{ep}}^{tr} \ dV + \int_{\mathcal{V}_0} \delta \theta \frac{\partial D_{\text{ev}}}{\partial \theta} \Delta \theta \ dV + \int_{\mathcal{V}_0} \delta \theta \frac{\partial D_{\text{ev}}}{\partial C_{\text{ev}}} : \Delta C_{\text{ev}}^{tr} \ dV \\
- \int_{\mathcal{V}_0} \Delta H \delta \theta - \delta \theta \left( \frac{\dot{C}}{\Delta t} \right) \Delta \theta \ dV.
\]
Upon the Fourier assumption for the Cauchy heat flux, \( q = -k \text{grad}(\theta) \), with \( k \) being the thermal conductivity, the linearization of the first two terms in the above equation takes the form

\[
- \int_{B_0} \Delta (J q \cdot \text{grad}(\delta \theta)) \, dV = \int_{B_0} k J [\text{grad}(\delta \theta) \cdot \text{grad}(\theta)] (I : \Delta e) dV
\]

\[
+ \int_{B_0} k J [\text{grad}(\delta \theta) \cdot \text{grad}(\Delta \theta)] dV - \int_{B_0} k J [\text{grad}(\delta \theta) \cdot 2 \Delta e \cdot \text{grad}(\theta)] dV.
\]

The linearization of the dissipation functions and STVPH desires more consideration which has been stated in Appendixes B and C, respectively.
Chapter 3

Asymptotic expansion approach

Many homogenization methods have been proposed so far. The simplest one is loading a material sample in tension and compression tests and presenting the average constitutive response experimentally. Although this approach provides the fundamental idea of relating the averages but it is clear that mathematically/theoretically cannot present any basis for further challenging homogenization problems. Another simple way to obtain homogenized moduli of an inhomogeneous material is based on the rule of mixtures. Since this approach is based on the volume ratio of heterogeneities only, one microstructural characteristic of the material can be taken into account and therefore effects of the other aspects might be ignored. A more rigorous method is the equivalent inclusion method using Eshelby tensor (Eshelby, 1957). This method further extended which is well known in the literature by the so-called self-consistent approach. See e.g., Budiansky (1965), Mori and Tanaka (1973), Hill (1965), and Christensen and Lo (1979) among others. In these methods typically the inclusions of one material/phase with the specified geometry are distributed in an infinite matrix of another material for the former method (in an effective material with unknown material properties for the latter case) and equivalent material properties are derived analytically (semi-analytically). Accurate prediction of the overall behavior of the clustered structure is major shortcoming of this method. Hashin and Shtrikman (1963) and Hashin (1983) further extended the self-consistent approach to the so-called variational bounding methods to provide upper and lower bounds for the overall material properties of heterogeneous materials. A more mathematically sophisticated method is asymptotic homogenization theory proposed in 1970s and early 1980s, for instance, by Babuska (1976), Sanchez-Palencia (1980) and Bakhvalov and Panasenko (1989). The asymptotic expansion analysis naturally enforces a separation of scales thereby presenting first- or higher-order homogenization frameworks which gained much attention from computational point of view. The overall material properties can be accurately predicted by this method but it is confined to the problems with simple microscopic geometries. The so-called unit cell method proposed in the early 1990s is suitable for the heterogeneous materials with complex nature in the linearized settings. In this method typically a unit cell at the
microlevel is loaded along the certain specific path and the resulted averaged stress-strain curve is fitted to the known phenomenological constitutive equations at macrolevel to provide the effective material properties. Considering the finite deformations of heterogeneous mediums or the materials with (materially) nonlinear behavior would be out of the scope of this method since it is really difficult to present a priori a macroscopic constitutive equation. For more details on this method see the works of Tvergaard (1990), Brockenbrough et al. (1991) and McHugh et al. (1993). Multiscale computational homogenization is a powerful method of treating inhomogeneous materials in a way that it has the ability of treating the above mentioned shortcomings. We will further speak about this approach in the next chapter. Here, the AE method is applied to the derived governing equations in chapter 2 to build up the multiscale procedure. The AE approach is considered to be a basic theory of homogenization which makes a clear starting point for further homogenization methods. Especially in the case of multiphysics problems where additional weak forms and governing equations appear, AE analysis provides the fundamental information about the homogenization process and the consistent governing equations which should be solved in the both micro- and macrolevel. In what follows, some pioneering works on mechanical/thermal (or thermomechanical) behavior of a heterogeneous solid using the AE homogenization method are addressed. Takano et al. (2000) were first to apply the AE homogenization method to consider the purely mechanical behavior of composite materials with periodic microstructure in finite deformation regime while an AE treatment in the infinitesimal deformation regime is well-known (Sanchez-Palencia, 1980). Based on assumptions of microstructure periodicity and uniformity of macroscopic fields within a unit cell domain, Laschet (2002) applied AE approach to nonlinear thermal conduction equation in a quasi-static setting for homogenization of the thermal properties of transpiration cooled multi-layer plates while the treatment of the linearized setting is again well-known (Sanchez-Palencia, 1980). The first treatment of the coupled transient thermoelastic problem in a linearized setting was presented in Francfort (1983). The coupled quasistatic problem was further investigated by Alzina et al. (2007) while the transient case with viscous dissipation effects was considered in Francfort (1986) and Yu and Fish (2002). Extension of the above mechanical and thermal coupling to the finite deformation regime motivated Temizer (2012) to consider the AE treatment of two-scale finite TE. He presented the (macro) thermal equations in a fully transient setting and showed deformation-induced thermal anisotropy due to the presence of heterogeneities in the material. His procedure is mainly followed here and its extension to the case that inelastic effects evolve is the main goal of this chapter.

3.1 Two-scale setting for a heterogeneous solid

The AE theory of homogenization is based on the assumption that the microheterogeneous material at a fine scale is assembled by a periodic repetition of unit cells. Within this framework two distinct scales are taken to explain the physically behavior of the body. One is a macroscale position vector \( X \) (usually referred to as fast
variable) and the other is its microscale counterpart \( Y \) (slow variable) which defines the heterogeneities. These two scales are related to each other by \( X = Y/\varepsilon \) where \( \varepsilon = l_{\text{micro}}/l_{\text{macro}} \) denotes the aspect ratio between representative length scales of the microstructural features and the macro-structural problem. In what follows, the conventional AE method is applied to a most general case of thermoinelastic problem (the previously derived mechanical and thermal governing equations is taken as a basis in which with slightly changes, they are extended to the most general case of thermoinelastic material) to present the corresponding microscopic and macroscopic governing equations. To do this, all physically highly-oscillatory primal variables \( \{u_\varepsilon, \theta_\varepsilon\} \) and subsequently dual variables \( \{P_\varepsilon, Q_\varepsilon\} \) are asymptotically expanded with respect to the characteristic size of the unit cell and the results are inserted into the original governing equations. Finally, a separation of scales (i.e., \( \varepsilon \to 0 \)) is enforced to separate the consistent governing equations in two-scales. Let a position vector \( X_\varepsilon \) (the subscript \( \varepsilon \) is attached to the following variables to emphasize that they depend on the microstructure in the original heterogeneous body) has the asymptotic expansion of the form

\[
X_\varepsilon = X + \varepsilon Y. \tag{3.1}
\]

Thus, the differential operators can be derived as

\[
\text{Grad}_\varepsilon(*) = \nabla_{X_\varepsilon}(*) = \frac{\partial(*)}{\partial X} \cdot \frac{\partial X}{\partial X_\varepsilon} + \frac{\partial(*)}{\partial Y} \cdot \frac{\partial Y}{\partial X_\varepsilon} = \text{Grad}_X(*) + \frac{1}{\varepsilon} \text{Grad}_Y(*), \tag{3.2a}
\]

\[
\text{Div}_\varepsilon(*) = \nabla_{X_\varepsilon}.(*) = \text{Grad}_X.(*) + \frac{1}{\varepsilon} \text{Div}_Y.(*) = \text{Div}_X.(*) + \frac{1}{\varepsilon} \text{Div}_Y.(*) \tag{3.2b}
\]

### 3.1.1 Asymptotic expansion of primal variables

Let the physically primal variables \( u_\varepsilon \) and \( \theta_\varepsilon \) have the following AEs

\[
u_\varepsilon(X) = u(X, Y) = u_0(X, Y) + \varepsilon u_1(X, Y) + \varepsilon^2 u_2(X, Y) + O(\varepsilon^3), \tag{3.3a}
\]

where the symbol \( O \) is the Landau’s symbol which describes the asymptotically behavior of the displacement function in a way that here the third-order term with respect to \( \varepsilon \) is an asymptotic upper bound of the all remaining higher-order terms when \( \varepsilon \) tends to zero and

\[
\theta_\varepsilon(X) = \theta(X, Y) = \theta_0(X, Y) + \varepsilon \theta_1(X, Y) + \varepsilon^2 \theta_2(X, Y) + O(\varepsilon^3). \tag{3.3b}
\]

For the subsequent developments, the gradients of the above primal variables are given by
\[ F_\varepsilon(X) = I + \frac{\partial u_\varepsilon}{\partial X_\varepsilon} = \varepsilon^{-1}F - 1 + \varepsilon^0F_0 + \varepsilon^1F_1 + O(\varepsilon^2), \]  
\[ G_\varepsilon(X) = \frac{\partial \theta_\varepsilon}{\partial X_\varepsilon} = \varepsilon^{-1}G - 1 + \varepsilon^0G_0 + \varepsilon^1G_1 + O(\varepsilon^2), \]

where

\[
\begin{align*}
F - 1 &= \frac{\partial u_0}{\partial Y} , & F_0 &= I + \left(\frac{\partial u_0}{\partial X} + \frac{\partial u_1}{\partial Y}\right) , & F_1 &= \frac{\partial u_1}{\partial X} + \frac{\partial u_2}{\partial Y}, \\
G - 1 &= \frac{\partial \theta_0}{\partial Y} , & G_0 &= \frac{\partial \theta_0}{\partial X} + \frac{\partial \theta_1}{\partial Y} , & G_1 &= \frac{\partial \theta_1}{\partial X} + \frac{\partial \theta_2}{\partial Y}.
\end{align*}
\]

Upon enforcing the separation of scales, it is concluded that \( u_0 \) and \( \theta_0 \) are independent of the slow variable \( Y \) and also one can obtain

\[
F_\varepsilon(X) = F_0 , \quad G_\varepsilon(X) = G_0.
\]

Using the cell average operator \( \langle * \rangle \)

\[
\langle * \rangle = \frac{1}{y} \int_y (*) dy,
\]

and making use of the divergence theorem together with \( y \)-periodicity of the fluctuation fields \( u_1 \) and \( \theta_1 \), mean and fluctuation parts of the above deformation and temperature gradients can be written

\[
\begin{align*}
\overline{F}_\varepsilon &= \langle F_0 \rangle = I + \frac{\partial u_0}{\partial X} , & \overline{F}_\varepsilon &= \overline{F}_0 = \frac{\partial u_1}{\partial Y}, \\
\overline{G}_\varepsilon &= \langle G_0 \rangle = \frac{\partial \theta_0}{\partial X} , & \overline{G}_\varepsilon &= \overline{G}_0 = \frac{\partial \theta_1}{\partial Y}.
\end{align*}
\]

Within the framework of the AE approach, it is further assumed that all of the microstructural field variables have a \( y \)-periodic structure.

### 3.1.2 Asymptotic expansion of dual variables

In order to derive AEs of the dual variables and subsequently the governing equations, first the microstructural sensitivities of the dual variables with respect to the set \( \{\theta_\varepsilon, G_\varepsilon, F_\varepsilon, \zeta_\varepsilon\} \) are introduced via

**Mechanical sensitivities:**

\[
M_\varepsilon = \frac{\partial P_\varepsilon}{\partial \theta_\varepsilon} , \quad K_\varepsilon = \frac{\partial P_\varepsilon}{\partial F_\varepsilon} , \quad Z_\varepsilon = \frac{\partial P_\varepsilon}{\partial \zeta_\varepsilon},
\]  
(3.9a)
Thus, using Eqs. (3.2b), (3.10a), (3.11a) and (3.12)

\[
\mathbf{m}_\varepsilon = -\frac{\partial \mathbf{Q}_\varepsilon}{\partial \theta_\varepsilon}, \quad K_\varepsilon = -\frac{\partial \mathbf{Q}_\varepsilon}{\partial \mathbf{G}_\varepsilon}, \quad \mathbf{Q}_\varepsilon = -\frac{\partial \mathbf{Q}_\varepsilon}{\partial \mathbf{F}_\varepsilon}, \quad \mathbf{Z}_\varepsilon^0 = -\frac{\partial \mathbf{Q}_\varepsilon}{\partial \zeta_\varepsilon},
\] (3.9a)

where the vector \(\zeta_\varepsilon\) represents all internal variables due to the evolution of inelastic effects. Thus, one can write AEs of the first Piola-Kirchhoff stress tensor \(P_\varepsilon\) and the Piola-Kirchhoff heat flux \(Q_\varepsilon\)

\[
P_\varepsilon(\theta_\varepsilon, \mathbf{F}_\varepsilon, \zeta_\varepsilon) = P_0(\theta_0, \mathbf{F}_0, \zeta_0) + \varepsilon P_1(\theta_0, \theta_1, \mathbf{F}_0, \mathbf{F}_1, \zeta_0, \zeta_1) + O(\varepsilon^2), \quad (3.10a)
\]

\[
Q_\varepsilon(\theta_\varepsilon, \mathbf{G}_\varepsilon, \mathbf{F}_\varepsilon, \zeta_\varepsilon) = Q_0(\theta_0, \mathbf{G}_0, \mathbf{F}_0, \zeta_0) + \varepsilon Q_1(\theta_0, \theta_1, \mathbf{G}_0, \mathbf{G}_1, \mathbf{F}_0, \mathbf{F}_1, \zeta_0, \zeta_1) + O(\varepsilon^2), \quad (3.10b)
\]

where

\[
\begin{align*}
P_0(\theta_0, \mathbf{F}_0, \zeta_0) &= \lim_{\varepsilon \to 0} P_\varepsilon(\theta_\varepsilon, \mathbf{F}_\varepsilon, \zeta_\varepsilon), \\
P_1(\theta_0, \theta_1, \mathbf{F}_0, \mathbf{F}_1, \zeta_0, \zeta_1) &= \lim_{\varepsilon \to 0} \frac{dP_\varepsilon}{d\varepsilon} = M_0 \theta_1 + \mathbb{K}_0 : \mathbf{F}_1 + \mathbf{Z}_0^P \cdot \zeta_1, \\
Q_0(\theta_0, \mathbf{G}_0, \mathbf{F}_0, \zeta_0) &= \lim_{\varepsilon \to 0} Q_\varepsilon(\theta_\varepsilon, \mathbf{G}_\varepsilon, \mathbf{F}_\varepsilon, \zeta_\varepsilon), \\
Q_1(\theta_0, \theta_1, \mathbf{G}_0, \mathbf{G}_1, \mathbf{F}_0, \mathbf{F}_1, \zeta_0, \zeta_1) &= \lim_{\varepsilon \to 0} \frac{dQ_\varepsilon}{d\varepsilon} \\
&= -m_0 \theta_1 - K_0 \mathbf{G}_1 - Q_0 : \mathbf{F}_1 - \mathbf{Z}_0^Q \zeta_1,
\end{align*}
\] (3.11a)

(3.11b)

and \(\zeta_0\) and \(\zeta_1\) are the terms obtained by AE of \(\zeta_\varepsilon\). Since \(\zeta_\varepsilon\) is not considered as an fundamental primal variable, its relevant AE has not been presented in Eq. (3.3) for convenience.

### 3.2 Two-scale governing equations

#### 3.2.1 Linear momentum equation

In order to present the AE of the linear momentum balance (2.102), first one should have AEs of the body force and the inertia term (it is assumed that referential density does not have any AE with respect to the field variables)

\[
f^b_\varepsilon(X) = f^b_0 + \varepsilon f^b_1 + O(\varepsilon^2), \quad (3.12a)
\]

\[
\rho_0 \ddot{u}_\varepsilon(X) = \rho_0 [\ddot{u}_0(X, Y) + \varepsilon \ddot{u}_1(X, Y) + O(\varepsilon^2)]. \quad (3.12b)
\]

Thus, using Eqs. (3.2b), (3.10a), (3.11a) and (3.12), Eq. (2.102) can be expanded
\[
\text{Div}_X(P_\varepsilon) + \frac{1}{\varepsilon} \text{Div}_Y(P_\varepsilon) + f_0^b + O(\varepsilon) = \rho_0 \ddot{u}_0 + O(\varepsilon) \quad \Rightarrow \\
\text{Div}_X(P_0) + \frac{1}{\varepsilon} \text{Div}_Y(P_0) + \text{Div}_Y\left(M_0 \theta_1 + \mathbb{K}_0 : F_1 + \mathbf{Z}_0^p : \mathbf{c}_1\right) + f_0^b + O(\varepsilon) \\
= \rho_0 \ddot{u}_0 + O(\varepsilon).
\]

(3.13)

Note that Eq. (3.13) has been expanded up to the order of \( \varepsilon^0 \) since it can represent the consistent micro and macro governing equations to provide the set \( \{u_0, u_1, \theta_0, \theta_1\} \) which is the main goal of the first-order homogenization approach. Upon enforcing the separation of scales one can obtain

\[
\text{Div}_Y(P_0(\theta_0, F_0, \mathbf{c}_0)) = 0, 
\]

(3.14a)

\[
\text{Div}_X(P_0) + \text{Div}_Y\left(M_0 \theta_1 + \mathbb{K}_0 : F_1 + \mathbf{Z}_0^p : \mathbf{c}_1\right) + f_0^b = \rho_0 \ddot{u}_0. 
\]

(3.14b)

Eq. (3.14a) represents the micro purely mechanical governing equation in \( y \) (Temizer, 2012). It is seen that \( \theta_0 \) enters this cell problem as a constant which describes the fact that the temperature distribution within the cell does not influence the stress distribution in \( y \) while the scale separation has been enforced. This cell problem is solved iteratively for \( u_1 \) at an elevated/reduced temperature \( \theta_0 \) which is uniform within the cell. Considering the \( y \)-periodicity of the field variables \( \{u_1, u_2, \theta_1, \mathbf{c}_1\} \) and the sensitivities \( \{M_0, \mathbb{K}_0, \mathbf{Z}_0^p\} \), divergence theorem and using the fact that the cell average \( \langle \ast \rangle \) is interchangebale with \( \text{Div}_X(\ast) \), the cell average of Eq. (3.14b) presents the macroscopic linear momentum balance

\[
\text{Div}_X(P) + \bar{f}^b = \bar{\rho}_0 \ddot{u}_0, 
\]

(3.15)

where \( P = \langle P_0 \rangle \) denotes the macroscopic stress, \( \bar{f}^b = \langle f_0^b \rangle \) represents the macroscopic body force, and \( \bar{\rho}_0 = \langle \rho_0 \rangle = \rho_0 \) is the macroscopic density.

**Remark 3.1:**

Eqs. (3.14a) and (3.15) have been derived without specifying any particular constitutive choices and they have been identically reported by Temizer (2012). This shows the fundamental nature of balance of linear momentum that should be satisfied for equilibrium in both micro- and macrolevel. Clearly solutions of these fundamental governing equations differ if the internal variables evolve.

### 3.2.2 Energy equation

The energy balance (2.107) is only applicable to thermo-viscoelastic-plastic materials. Here, this restriction is excluded and, therefore, a general thermoinelastic medium is assumed in order to keep generality of the following AE approach. Thus, the energy balance (2.107), with slightly change, can be assumed of the following form
3.2. TWO-SCALE GOVERNING EQUATIONS

\[ c \dot{\theta} = \mathcal{D} - \mathcal{H} - \text{Div}(\mathcal{Q}) + \mathcal{R} \]

where \( \mathcal{D} \) denotes the total dissipation induced by a general internal variable vector \( \zeta \) as introduced before. Before expanding the general energy balance (3.16), AEs of the heat capacity, heat source, total dissipation function, and structural thermoinelastic heating (or cooling) are given by (up to the \( \varepsilon^0 \) order)

\[
\begin{align*}
    c_\varepsilon(X) &= c_0 + O(\varepsilon), \quad \mathcal{R}_\varepsilon(X) = \mathcal{R}_0 + O(\varepsilon), \quad (3.17a) \\
    \mathcal{D}_\varepsilon(X) &= \mathcal{D}_0 + O(\varepsilon), \quad \mathcal{H}_\varepsilon(X) = \mathcal{H}_0 + O(\varepsilon), \quad (3.17b)
\end{align*}
\]

where

\[
\begin{align*}
    c_0 &= \lim_{\varepsilon \to 0} \left( -\theta_\varepsilon \frac{\partial^2 \psi_\varepsilon}{\partial \theta^2} \right) = -\theta_0 \frac{\partial^2 \psi_0}{\partial \theta^2}, \\
    \mathcal{R}_0 &= \lim_{\varepsilon \to 0} (\mathcal{R}_\varepsilon) = \mathcal{R}_0, \\
    \mathcal{D}_0 &= \lim_{\varepsilon \to 0} [\mathcal{D}_\varepsilon(\theta_\varepsilon, \mathcal{F}_\varepsilon, \zeta_\varepsilon)] = \mathcal{D}_0(\theta_0, \mathcal{F}_0, \zeta_0), \quad (3.18a) \\
    \mathcal{H}_0 &= \lim_{\varepsilon \to 0} (\mathcal{H}_\varepsilon) = -\theta_0 \frac{\partial \mathcal{P}_0}{\partial \theta_0} : \mathcal{F}_0 - \theta_0 \frac{\partial^2 \psi_0}{\partial \theta_0 \partial \zeta_0} \zeta_0 \\
    &= -\theta_0 \mathcal{M}_0 : \mathcal{F}_0 + \theta_0 \frac{\partial \mathcal{D}_0}{\partial \theta_0} \quad (3.18b) \\
\end{align*}
\]

Now, using Eqs. (3.2b), (3.3b), (3.10b), (3.11b) and (3.17), the AE of Eq. (3.16) can be obtained

\[
\begin{align*}
    c_0 \dot{\theta}_0 + O(\varepsilon) &= \mathcal{D}_0 + \theta_0 \mathcal{M}_0 : \mathcal{F}_0 - \theta_0 \frac{\partial \mathcal{D}_0}{\partial \theta_0} - \left[ \text{Div}_\chi(\mathcal{Q}_0) + \frac{1}{\varepsilon} \text{Div}_\gamma(\mathcal{Q}_0) \right] \\
    - \text{Div}_\gamma(-\mathbf{m}_0 \theta_1 - \mathbf{K}_0 \mathbf{G}_1 - \mathbf{Q}_0 : \mathbf{F}_1 - \mathbf{E}_0^Q \zeta_1) + \mathcal{R}_0 + O(\varepsilon).
\end{align*}
\]

By enforcing the separation of scales, one can write

\[
\begin{align*}
    \text{Div}_\gamma[\mathcal{Q}_0] &= \text{Div}_\gamma[\mathcal{Q}_0(\theta_0, \mathbf{G}_0, \mathbf{F}_0, \zeta_0)] = 0, \quad (3.20a) \\
    c_0 \dot{\theta}_0 &= \mathcal{D}_0 + \theta_0 \mathcal{M}_0 : \mathcal{F}_0 \\
    - \theta_0 \frac{\partial \mathcal{D}_0}{\partial \theta_0} - \text{Div}_\chi(\mathcal{Q}_0) - \text{Div}_\gamma(-\mathbf{m}_0 \theta_1 - \mathbf{K}_0 \mathbf{G}_1 - \mathbf{Q}_0 : \mathbf{F}_1 - \mathbf{E}_0^Q \zeta_1) + \mathcal{R}_0. \quad (3.20b)
\end{align*}
\]

Eq. (3.20a) presents the same result as in Temizer (2012) (except the evolution of the internal variables). This microscopic purely thermal governing equation within the cell provides two results. First, \( \theta_0 \) appears as a constant in this thermal cell problem. This shows that the temperature-dependent thermal material properties should be evaluated at this elevated/reduced temperature and therefore they are independent of the temperature distribution throughout the cell. Second, the appearance of \( \mathbf{F}_0 \) which
presents the equilibrium configuration of the body in the mechanical phase, reveals the fact that Eq. (3.20a) must be solved at the deformed configuration of the solid which is already known by solving the purely mechanical cell problem (3.14a). By following the same procedure that led to Eq. (3.15), one can obtain from Eq. (3.20b) the following general macroscopic energy balance equation

\[
\langle c_0 \dot{\theta}_0 \rangle = \langle D_0 \rangle + \theta_0 \langle M_0 : \dot{F}_0 \rangle - \dot{\theta}_0 \langle \partial D_0 / \partial \theta_0 \rangle - \text{Div}_X(\langle Q_0 \rangle) + \langle R_0 \rangle - \langle \mathcal{H}_0 \rangle - \text{Div}_X(\langle Q \rangle) + \langle R \rangle.
\]  

(3.21)

Here \( \langle D_0 \rangle \) denotes the macroscopic dissipation function, \( \langle Q_0 \rangle \) is the macroscopic referential heat flux and \( \langle R_0 \rangle \) represents the macroscopic heat source. Considering Eq. (3.16), one may want to present the above equation in the following convenient form

\[
\bar{c} \dot{\theta}_0 = \bar{D} + \theta_0 \frac{\partial \bar{P}}{\partial \theta_0} : \dot{\bar{F}} - \theta_0 \frac{\partial \bar{D}}{\partial \theta_0} - \text{Div}_X(\bar{Q}) + \bar{R}
\]

(3.22)

In what follows, it is verified that Eq. (3.21) can be rewritten in the convenient form (3.22). Let

\[
\langle D_0 \rangle = \bar{D} \quad , \quad \langle Q_0 \rangle = \bar{Q} \quad , \quad \langle R_0 \rangle = \bar{R},
\]

(3.23a)

this verification can be completed by proving the following equality

\[
\langle c_0 \dot{\theta}_0 + \mathcal{H}_0 \rangle = \bar{c} \dot{\theta}_0 + \bar{H}.
\]

(3.23b)

One can proceed by postulating the following formulation

\[
\bar{\eta} = \langle \eta_0 \rangle \rightarrow \tilde{\eta} = - \frac{\partial \bar{\psi}}{\partial \theta_0}
\]

\[
= - \frac{\partial}{\partial \theta_0} \langle \psi_0 \rangle = - \langle \psi_0 \rangle \frac{\partial}{\partial \theta_0} - \langle \psi_0 \circ \partial F_0 : \partial \theta_0 \rangle = \langle \eta_0 \rangle - \bar{P} \frac{\partial \bar{F}}{\partial \theta_0},
\]

(3.24)

which indicates that the volume average of the partial sensitivity of the microscopic inelastic free energy function with respect to the enforced macroscopic temperature equals to the its total sensitivity counterpart. This result is only guaranteed when the macroscopic deformation gradient and internal variables are held fixed which can identically be seen in the thermoelastic problems \cite{Temizer and Wriggers, 2011}. In the next chapter, we also show this consistency for thermo-viscoelastic-plastic problems as \( \bar{\eta}^e = \langle \eta^e_0 \rangle \) (due to the additively decomposition of the total entropy to the elastic and plastic entropies, the internal energy is a function of elastic entropy in the both micro- and macrolevel). Its consistency in the general framework of thermonelastic materials can be verified in a straightforward manner. Since the equality (3.23b) is just the material time derivative of the equality (3.24), therefore Eqs. (3.21) and (3.22) are equivalent.
The above procedure does not provide any information regarding the relation between macroscopic and microscopic specific heat or structural thermoinelastic heating (or cooling). Following the consistent representation of the mentioned macroscopic thermodynamic variables, the equivalence of Eqs. (3.21) and (3.22) is shown in an alternative way. From the right hand side of Eq. (3.23b), it follows

\[
\bar{c}\dot{\theta}_0 + \bar{H} = -\theta_0 \frac{\partial^2 \langle \psi_0 \rangle}{\partial \theta_0^2} \dot{\theta}_0 - \theta_0 \frac{\partial \bar{P}}{\partial \theta_0} : \dot{\bar{F}} - \theta_0 \frac{\partial^2 \bar{\psi}}{\partial \theta_0 \partial \bar{\xi}} : \ddot{\bar{\xi}}
\]

\[
= -\theta_0 \frac{\partial}{\partial \theta_0} \left( \frac{\partial \psi_0}{\partial \theta_0} + \frac{\partial \psi_0}{\partial F_0} \right) \dot{\theta}_0 - \theta_0 \frac{\partial \langle P_0 \rangle}{\partial \theta_0} : \dot{F}_0 - \theta_0 \frac{\partial \bar{P}}{\partial \theta_0} \left( \frac{\partial \bar{\psi}}{\partial \bar{\xi}} \right) \dot{\bar{\xi}}
\]

\[
= -\theta_0 \left( \frac{\partial^2 \psi_0}{\partial \theta_0^2} + \left( \frac{\partial^2 \psi_0}{\partial \theta_0 \partial F_0} \right) \right) \dot{\theta}_0 - \theta_0 \langle P_0 : \dot{\bar{F}}_0 + \ddot{\bar{F}}_0 \rangle \frac{\partial F_0}{\partial \theta_0} \frac{\partial P_0}{\partial \theta_0} \frac{\partial F_0}{\partial \theta_0}
\]

\[
- \theta_0 \langle \frac{\partial P_0}{\partial \theta_0} : \dot{F}_0 - \frac{\partial F_0}{\partial \bar{\xi}} \frac{\partial P_0}{\partial \theta_0} - \frac{\partial F_0}{\partial \bar{\xi}} \frac{\partial P_0}{\partial \theta_0} \rangle F_{0 \theta_0 \bar{\xi}}
\]

\[
= (c_0 \dot{\theta}_0 - \theta_0 \langle \frac{\partial P_0}{\partial \theta_0} : \dot{F}_0 \rangle)
\]

\[
- \left( \langle \frac{\partial F_0}{\partial \theta_0} : \left( \frac{\partial P_0}{\partial \theta_0} \frac{\partial \bar{\xi}}{\partial \theta_0} - \frac{\partial P_0}{\partial \bar{\xi}} \frac{\partial \bar{\xi}}{\partial \theta_0} \right) \right) F_{0 \bar{\xi} \bar{\xi}}
\]

\[
= (c_0 \dot{\theta}_0 + H_{0}), \quad (3.25)
\]

which clearly underlines that the energy balance (3.22) can be consistently employed at macrolevel. Note that in Eq. (3.25), \( \bar{D} = -\left( \frac{\partial \bar{\psi}}{\partial \bar{\xi}} \right) \dot{\bar{\xi}} \) has been used where its consistency can be straightforwardly verified in view of the consistency conditions discussed in the chapter 4. The above results are in the most general case without any specific constitutive assumption and inelastic theory. These results can be easily specialized to the case of thermo-viscoelastic-plastic problems (in order to keep their consistency with the material modeling developed in the previous chapter) by assuming microscopic free energy function of the form

\[
\psi_0 = \psi_0 \left( \theta_0, F_0, C_{0}^{-1}, \bar{\xi}_0, C_{0v}^{-1} \right), \quad (3.26)
\]
which represents the canonical form of the previously defined free energy function in a way that its consistency with the above developed AE methodology has been preserved via \( b_{ep0} = F_0 C_0^{-1} F_0^T \) and \( b_{ev0} = F_0 C_{0v}^{-1} F_0^T \). Thus, replacing the general internal variable vector \( \zeta_0 \) by the set \( \{ C_0^{-1}, \xi_0, C_{0v}^{-1} \} \) which induces replacing \( (D_0) \) with \( (D_{mech0}^P + D^v_0) \) in the above formulations can make the homogenized form of the energy balance (2.107) consistently employable at the macroscale.
Chapter 4
Classical multiscale homogenization approach

Multiscale computational homogenization or the so-called global-local analysis has gained much attention in recent years due to some advantages such as; it circumvents the need to construct an explicit constitutive equation at macrolevel; small and finite deformations can be accurately addressed by this method; it is general in a way that existing numerical techniques such as FEM, BEM, DQM can be applied to solve the governing equations on the microscale. See e.g. the pioneering works of Suquet (1985), Guedes and Kikuchi (1990), Ghosh et al. (1995) among others. Increased computational cost is a major concern of researchers to apply this method. Although this concern can be overcome by parallel computation (Feyel and Chaboche, 2000) still it is an open issue for research. For a multiscale material with 3 (possibly N) scales of interest such as the macroscale, the microscale and the nanoscale, a general multi-resolution framework can be used (Hao et al., 2004; McVeigh et al., 2006). The classical/practical (first-order) computational homogenization method cannot monitor the localization effects since this method provides satisfactory results when the macroscopic deformation gradient is considered as a constant over the length scale of the microstructural features which is not a consistent assumption for the localization problems (for a discussion of the local homogenized solution quality see e.g., Fish and Belsky, 1995; and Temizer and Wriggers, 2011) in addition to the sufficiently smallness assumption of the aspect ratio between representative length scales of the microstructural features and the macro-structural problem to make the separation of scales reliable as discussed in the previous chapter. The latter condition holds when the microstructural features embedded in \( u_0 \) can statistically represent the real microstructural constituents of \( \mathcal{B} \) and therefore the test sample \( u_0 \) can be termed representative volume element (RVE).
4.1 Macroscopic governing equations

A numerical RVE has been assumed throughout the developments and therefore all homogenized (macroscopic) variables are distinguished from their microscopic counterparts by sign on a generally microscopic tensorial variable. For the thermo-viscoelastic-plastic problems, the following homogenized linear momentum and energy balance equations are assumed from the outset

\[
\text{Div}(\mathbf{P}) + \mathbf{f} = \tilde{\rho}_0 \mathbf{\ddot{u}}, \quad \tilde{c} \dot{\theta} = \mathcal{D}^{p}_{\text{ mech}} + \mathcal{D}^v - \tilde{\mathbf{H}} - \text{Div}(\mathbf{Q}) + \mathcal{R},
\]

(4.1)

where \( \tilde{\mathbf{H}} \) is the macroscopic STVPH defined

\[
\tilde{\mathbf{H}} = -\theta \frac{\partial \mathbf{P}}{\partial \theta} : \mathbf{F} + \theta \frac{\partial \mathcal{D}^{p}_{\text{ mech}}}{\partial \theta} + \theta \frac{\partial \mathcal{D}^v}{\partial \theta}.
\]

(4.2)

In order to determine

\[
\mathbf{P} = \mathbf{P}(\tilde{\theta}, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v), \quad \tilde{c} = \tilde{c}(\tilde{\theta}, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v),
\]

(4.3a)

\[
\mathcal{D}^{p}_{\text{ mech}} = \mathcal{D}^{p}_{\text{ mech}}(\tilde{\theta}, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v), \quad \mathcal{D}^v
\]

(4.3b)

one needs to have a knowledge of

\[
\tilde{e} = \tilde{e}(\tilde{\theta}, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v), \quad \tilde{\eta}^e = \tilde{\eta}^e(\tilde{\theta}, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v),
\]

(4.4)

\[
\mathbf{Q} = \mathbf{Q}(\tilde{\theta}, \mathbf{F}, \mathbf{G}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v).
\]

where \( \tilde{\xi}_p \) represents a vector of all macroscopic internal variables which comes from the microscopic internal variables \( C_p^{-1}, \tilde{\xi}_h \) denotes homogenized internal variable due to the hardening effects on the macroscopic, and \( \tilde{\xi}_v \) is macroscopic viscous internal variable associated with the microscopic internal variable \( C_v^{-1} \). Eqs. (4.4) and (2.38) motivates macroscopic Legendre transformation of the following form

\[
\tilde{e} = \tilde{\psi} + \tilde{\eta}^e \tilde{\theta},
\]

(4.5)

where \( \tilde{\psi} = \tilde{\psi}(\tilde{\theta}, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v) \) & \( \tilde{e} = \tilde{e}(\tilde{\eta}^e, \mathbf{F}, \tilde{\xi}_p, \tilde{\xi}_h, \tilde{\xi}_v) \) and the reason for the contribution of the homogenized elastic entropy \( \tilde{\eta}^e \) in Eq. (4.5) becomes clear through the developments. Note that in view of the theory and assumptions of the chapter 2, the microscopic heat flux \( \mathbf{Q} \) does not explicitly depend on the microscopic internal variables, but the macroscopic one in (4.4) should have this dependency since \( \mathbf{Q} \) is sensitive to the microstructural changes (see figure 5.20). Introduction of the macroscopic elastic entropy \( \tilde{\eta}^e \) motivates the assumption of the homogenized total and plastic entropies

\[
\tilde{\eta} = \tilde{\eta}^e + \tilde{\eta}^p.
\]

(4.6)

The homogenized Clausius-Plank form of the second law can be written
4.1. MACROSCOPIC GOVERNING EQUATIONS

\[
\bar{D}^{\text{tot}}_{\text{int}} = \bar{P} : \dot{\bar{F}} - \dot{\bar{e}} + \bar{\theta} \ddot{\bar{\eta}} = \bar{P} : \dot{\bar{F}} - \dot{\bar{\psi}} - \bar{\eta}^e \dot{\bar{\theta}} + \bar{\theta} \ddot{\bar{\eta}}^p = \\
\bar{P} : \dot{\bar{F}} - \frac{\partial \bar{\psi}}{\partial \bar{F}} : \dot{\bar{F}} - \frac{\partial \bar{\psi}}{\partial \bar{\theta}} \dot{\bar{\theta}} - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_p} \dot{\bar{\xi}}_p - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_h} \dot{\bar{\xi}}_h - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_v} \dot{\bar{\xi}}_v + \bar{\theta} \ddot{\bar{\eta}}^e + \bar{\theta} \ddot{\bar{\eta}}^p = \\
\bar{P} : \dot{\bar{F}} - \frac{\partial \bar{\psi}}{\partial \bar{F}} : \dot{\bar{F}} - \frac{\partial \bar{\psi}}{\partial \bar{\theta}} \dot{\bar{\theta}} - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_p} \dot{\bar{\xi}}_p - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_h} \dot{\bar{\xi}}_h - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_v} \dot{\bar{\xi}}_v - \bar{\eta}^e \ddot{\bar{\theta}} + \bar{\theta} \ddot{\bar{\eta}}^p \geq 0.
\]

(4.7)

The above inequality must hold for the all admissible thermodynamic processes on the macroscale and, therefore, applying the Coleman-Noll procedure leads to the following constitutive equations

\[
\bar{P} = \frac{\partial \bar{\psi}}{\partial \bar{F}} \quad \text{or} \quad \bar{P} = \frac{\partial \bar{\psi}}{\partial \bar{\theta}},
\]

(4.8)

and macroscopic dissipation functions take the form

\[
\bar{D}^{\text{tot}}_{\text{int}} = \bar{D}^p + \bar{D}^\nu = \bar{D}_M + \bar{D}_{\text{ther}} \geq 0,
\]

(4.9)

where

\[
\bar{D}^p = \bar{\beta}_p \dot{\bar{\xi}}_p + \bar{\beta}_h \dot{\bar{\xi}}_h + \bar{\theta} \ddot{\bar{\eta}}^p \geq 0 \quad \text{or} \quad \bar{D}^\nu = \bar{\beta}_v \dot{\bar{\xi}}_v \geq 0,
\]

(4.10)

in which

\[
\bar{\beta}_p = - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_p}, \quad \bar{\beta}_h = - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_h}, \quad \bar{\beta}_v = - \frac{\partial \bar{\psi}}{\partial \bar{\xi}_v}.
\]

(4.11)

As discussed above, one does not need to explicitly construct the macroscopic free energy function \( \bar{\psi} \) which it is extremely difficult in this nonlinear setting. To solve the nonlinear coupled BVPs (4.1) using the multiscale homogenization approach (the so-called FE\(^2\)) one does need to attach to a typical spatial point at the macrolevel an accompanying test sample and solve its associated BVPs to obtain the desired macroscopic variables mostly defined above through the volume averaging. Then, applying these averaged variables in the solution of the above macroscopic BVPs completes the homogenization framework. One does need to perform this volume averaging in a consistent way in which the macroscopic Eqs. (4.5)-(4.9) do not violate. Thus, using the above equations, one can define the following thermodynamic consistency conditions as a criterion that should hold for all thermo-viscoplastic deformation processes in the macroscale to guarantee the consistent macroscopic constitutive response via

\[
\bar{\theta} = - \frac{\partial \bar{\psi}}{\partial \bar{\eta}^e} \quad \text{or} \quad \bar{\eta}^e = - \frac{\partial \bar{\psi}}{\partial \bar{\theta}}, \quad \bar{P} = \frac{\partial \bar{\psi}}{\partial \bar{F}} \quad \text{or} \quad \bar{P} = \frac{\partial \bar{\psi}}{\partial \bar{\theta}}.
\]

(4.12a)
\[
\mathcal{D}_{ther}^p = \mathcal{D}_{int}^{tot} - \mathcal{D}_M = \theta \hat{\eta}^p \geq 0, \quad \bar{c} = -\frac{\partial^2 \psi}{\partial \bar{\theta}^2} = \frac{\partial \bar{\varepsilon}}{\partial \bar{\theta}}. \quad (4.12b)
\]

The desire for presenting alternative forms of the thermodynamic potentials based on characterizing the elastic/inelastic behavior of the material at the reference temperature (and motivated by the defined microscopic thermodynamic potentials), leads to the following most general form for the internal energy, elastic entropy and free energy functions at the macrolevel

\[
\bar{\varepsilon}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) = \bar{\varepsilon}_o(\bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) + \int_{\bar{\theta}_R}^{\bar{\theta}} \bar{c}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) d\bar{\theta}, \quad (4.13a)
\]

\[
\bar{\eta}^e(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) = \bar{\eta}_o^e(\bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) + \int_{\bar{\theta}_R}^{\bar{\theta}} \frac{1}{\bar{\theta}} \bar{c}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) d\bar{\theta}, \quad (4.13b)
\]

\[
\bar{\psi}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) = \bar{\theta} \bar{\psi}_o(\bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) + (1 - \frac{\bar{\theta}}{\bar{\theta}_R}) \bar{c}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) d\bar{\theta}. \quad (4.13c)
\]

### 4.2 Scale transitions

Computational homogenization methods are truly based on the solution of two nested BVPs on the macro and microlevel. The solutions to the both macroscopic and microscopic BVPs are coupled to each other through scale transitions. Thus, in a standard homogenization framework where an accompanying test sample is simultaneously analyzed with the macrostructure at the all associated spatial points, the solution scheme to the BVPs (4.1) consists of the two following main steps:

i. **Macro-to-micro transition**: The governing macroscopic quantities \( \{\bar{F}, \bar{\theta}, \bar{G}\} \) are transferred to the microscale analysis in order to solve the BVPs on the numerical RVE which induces solution field \( \{x, \theta\} \) in \( \nu_0 \).

ii. **Micro-to-macro-transition**: The resulted solution field \( \{x, \theta\} \) with the constitutive formulations should be employed to present the all desired macroscopic quantities which are necessary for the solution of the homogenized BVPs through volume averaging.

These desired macroscopic variables are extracted from their microscopic counterparts based on the identifications of some fundamental thermodynamic quantities (Maugin, 1992; Temizer and Wriggers, 2011) as
\[ \bar{\rho}_0 = \langle \rho_0 \rangle, \quad \bar{\varepsilon} = \langle \varepsilon \rangle, \quad \bar{\eta}^e = \langle \eta^e \rangle, \quad \bar{D}_{\text{int}}^{\text{Tot}} = \langle D_{\text{int}}^{\text{Tot}} \rangle, \]  

(4.14)

which guarantees that the total mass, internal energy, elastic entropy and the total dissipation are preserved in the micro-to-macro transition where the original heterogeneous material \( B \) is replaced by the homogenized medium \( \bar{B} \). It can be shown that the identification of all other relevant macroscopic variables can be followed from the above fundamental ones. Note that from Eq. (4.14), one cannot obtain \( \bar{\rho} = \langle \rho \rangle \) unless the micro-macro mass criterion \( \bar{f} = \langle f \rangle \) is satisfied. It has been shown that this criterion is not satisfied for all of the standard boundary conditions when the test sample does not qualify as a RVE (Temizer and Wriggers, 2008a). Hence, to identify the alternative form of density in the current configuration the evolution as induced by the macroscale kinematics should be employed. Using Eqs. (4.13) and (4.14), one can obtain

\[ \bar{e}_o(\bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) + \int_{\bar{\theta}_R}^{\bar{\theta}} \overline{c}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) d\bar{\theta} = 
\]

(4.15a)

\[ \langle e_o(F, C_p^{-1}, \xi, C_v^{-1}) \rangle + \int_{\bar{\theta}_R}^{\bar{\theta}} \overline{c}(\bar{\theta}, F, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) d\bar{\theta} = 
\]

(4.15b)

\[ \bar{\eta}^e_o(\bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) + \int_{\bar{\theta}_R}^{\bar{\theta}} \frac{1}{\bar{\theta}} \overline{c}(\bar{\theta}, \bar{F}, \bar{\xi}_p, \bar{\xi}_h, \bar{\xi}_v) d\bar{\theta} = 
\]

(4.15c)

\[ \langle \eta^e_o(F, C_p^{-1}, \xi, C_v^{-1}) \rangle + \int_{\bar{\theta}_R}^{\bar{\theta}} \frac{1}{\bar{\theta}} c(\bar{\theta}, F, C_p^{-1}, \xi, C_v^{-1}) d\bar{\theta} \]

Since \( b_{ep} = FC_p^{-1}F^T \), the above microscopic thermodynamic potentials \( e_o \) and \( \psi_o \), and therefore \( \eta^e_o \) and \( c \) have been canonically written as a function of \( F \) and \( C_p^{-1} \) (and also the thermo-viscoelastic part) to be more consistent with their relevant macroscopic counterparts. Note that \( e_o \) and \( c \) have been written in most general form although in the material modeling developed in chapter 2 it was assumed that \( e_o \) can vary independent of the hardening variable \( \xi \). The readers should note that we have explicitly employed the macroscopic temperature \( \bar{\theta} \) in the above formulations based on the AE analysis of the previous chapter. Besides the AE analysis, if this enforcement is not applied two major inconsistencies may appear. First, let a purely thermal medium which is additionally
homogeneous with a constant specific heat on the microscale. Based on these assumptions, Eqs. (4.15a) and (4.15b) are reduced to
\begin{align}
\tilde{e}_o + \tilde{c}(\bar{\theta} - \theta_R) &= e_o + c(\langle \theta \rangle - \theta_R), \\
\tilde{n}_o^\varepsilon + \tilde{c}(\ln \bar{\theta} - \ln \theta_R) &= n_o^\varepsilon + c(\langle \ln \theta \rangle - \ln \theta_R),
\end{align}
(4.16)
which is clearly impossible to satisfy \( \bar{\theta} = \langle \theta \rangle \) and \( \ln \bar{\theta} = \langle \ln \theta \rangle \) simultaneously. Second, since one does have a distribution of temperature at the microlevel, therefore \( e \) will be affected by changes of temperature which leads to the changes of \( \tilde{e} \). Now, by changing \( \bar{G} \) while \( \bar{\theta} \) is fixed, the distribution of the microscopic temperature will change which may change \( \tilde{e} \). Therefore, there is no guarantee to have a constant homogenized internal energy while macroscopic temperature gradient changes. See Temizer and Wriggers (2011) for more discussions on these inconsistencies.

### 4.3 Micromechanical analysis

Here, we apply the results of AE analysis as a fundamental basis to build up the micromechanical analysis. Thus, a split of the micromechanical testing procedure into the mechanical and thermal phases is pursued. It is also assumed that the microscopic deformation and temperature fields \( \{x, \theta\} \) have no jumps throughout \( \nu_0 \) in a standard setting.

#### 4.3.1 Mechanical phase

Of interest for intrinsic response of the heterogeneous material on the microscale is excluding the body forces and dynamic effects from the linear momentum balance equation which reads via
\[ \text{Div}[P(\bar{\theta}, F, C_p^{-1}, C_v^{-1})] = 0, \]
(4.17)
which was previously derived in the chapter 3 for the thermoinelastic problems. This BVP is solved by imposing the macroscale deformation gradient \( \bar{F} \) on \( \nu_0 \) while the macroscopic temperature \( \bar{\theta} \) is held fixed -which induces the deformed microstructural configuration \( \nu \)- in order to characterize the all desired macroscopic variables that are necessary for the solution scheme of the macroscopic BVPs. Then, it is highlighted that macroscale gradient \( \bar{F} \) enters the BVP (4.17) through the boundary conditions imposed on the test sample. In this work, the standard boundary conditions LN, PR and UF are taken where in a standard setting they satisfy the Hill-Mandel condition (Hill, 1963; Hill, 1984)
\[ \bar{P}:\bar{F} = \langle P:F \rangle, \]
(4.18)
which states that macroscopic volume average of the rate of the work performed on the
test sample should match the local rate of the work on the macroscale in such a way that

\[
\bar{F} \xrightarrow{\text{enforced}} \langle F \rangle \quad \& \quad \bar{P} \xleftarrow{\text{measured}} \langle P \rangle.
\] (4.19)

Thus, one then obtains

\[
\bar{P} : \dot{\bar{F}} = \langle P \rangle : \dot{\langle F \rangle}.
\] (4.20)

See Temizer and Wriggers (2008b) and Lillbacka et al. (2006) for the case \( \bar{P} \) \xrightarrow{\text{enforced}} \langle P \rangle \& \bar{F} \xleftarrow{\text{measured}} \langle F \rangle.

### 4.3.2 Thermal phase

Derivation of the Eq. (3.20a) clearly showed that the STVPH, dissipation function, heat
supply term, and the term with the evolution of temperature on the microscale have not
any influence on the intrinsic response of the heterogeneous material which should be
excluded from the energy balance Eq. (2.107). Thus, the microscopic BVP that should be
considered is given by (it is rewritten here for convenience)

\[
\text{Div}[\bar{Q}(\bar{\theta}, \bar{G}, \bar{F})] = 0.
\] (4.21)

This BVP is solved by imposing the macroscale temperature gradient \( \bar{G} \) on \( v_0 \) while the
microscopic deformation gradient \( \bar{F} \) -transferred from the mechanical testing
procedure- is held fixed in order to determine the macroscopic heat flux vector \( \bar{Q} \) and its
relevant sensitivities which should be applied in the solution scheme of the macroscopic
energy balance Eq. (4.1b). The same procedure as in the mechanical phase is pursued in
a way that the macroscale gradient \( \bar{G} \) enters the BVP (4.21) through the boundary
conditions imposed on the test sample which are assumed as LN, PR and UF (Appendix
E). The micro-macro work criterion in the mechanical phase can now be -loosely
speaking- restated as:

The macroscopic volume average of the thermal energy dissipated on the test sample
should match the local thermal dissipation on the macroscale as

\[
\bar{D}_0^\theta = -\bar{Q} : \bar{G} = \langle D_0^\theta \rangle = \langle -\frac{\bar{Q} : \bar{G}}{\bar{\theta}} \rangle,
\] (4.22)

where \( \bar{D}_0^\theta \) \( (D_0^\theta) \) denotes the macroscopic (microscopic) thermal dissipation in the
referential coordinates. Eq. (4.22) can be satisfied by applying the above BCs and

\[
\bar{G} \xrightarrow{\text{enforced}} \langle G \rangle \quad \& \quad \bar{Q} \xleftarrow{\text{measured}} \langle Q \rangle.
\] (4.23)

Finally, one can conclude
\[ \bar{Q} \cdot \bar{G} = \langle Q \rangle \cdot \langle G \rangle. \quad (4.24) \]

The micro-macro thermal dissipation criterion (4.22) can be alternatively defined in the current configuration via \( \bar{q} \cdot \bar{g} = \langle q \rangle \cdot \langle g \rangle \). But it cannot be satisfied for all of the above BCs when the test sample does not qualify as a RVE. To consider this, Temizer and Wriggers (2011) defined a supplementary dissipation criterion

\[ \langle g \rangle_v = \bar{F}^{-T} \langle G \rangle_v \quad \text{and} \quad \langle q \rangle_v = \bar{f}^{-1} \bar{F} \langle Q \rangle_v, \quad (4.25) \]

and showed that if this criterion holds, the micro-macro thermal criterion can be alternatively satisfied in the both referential and current configurations. This has been thoroughly investigated in Appendix F. Based on applying the above different boundary conditions on the solution of the microscopic BVPs, one can have three possibilities for the macroscopic dual variable \( \bar{P} \) (since the mechanical phase should be solved first) and then there are nine different possibilities for the homogenized dual variable \( \bar{Q} \).

**Remark 4.1:**

Note that we did not present the thermal dissipation in the both macro and microscale energy balance equations since we have assumed from the outset that the microscopic one is automatically satisfied using the Fourier assumption for the Cauchy heat flux. This is a typical assumption in thermomechanical analysis of the homogeneous solids which based on Eqs. (4.22) and (4.24), one can conclude that the thermal dissipations preserved in micro-to-macro transition and \( \bar{D}_\theta^p \geq 0 \) while the separation of scales is enforced. Since Eq. (4.22) defined on the reference configuration can lead to its current counterpart under the appropriate BCs upon using Eq. (4.23), here we consider it as -loosely speaking- micro-macro energy criterion that should be satisfied.

### 4.3.3 Consistency conditions

Here, the results of the previous chapter and equations derived in the subsection 4.1 are used to prove the consistency conditions defined in (4.12). Assuming a single time scale for the present setting and based on the identification Eq. (4.14), one can conclude that the material time derivative of the two sides along a prescribed macroscopic process path imposed on an equilibrium state of the microstructural test sample should match

\[ \dot{e} = \frac{\partial \bar{e}}{\partial \bar{F}} : \dot{F} + \frac{\partial \bar{e}}{\partial \eta^e} \dot{\eta}^e - \bar{D}_M = \langle \dot{e} \rangle = \langle P : \dot{F} + \frac{\partial \bar{e}}{\partial \eta^e} \dot{\eta}^e - D_{mech}^p - D^v \rangle = \langle P : \dot{F} + \bar{g} \dot{\eta}^e - \langle D_{mech}^p \rangle - \langle D^v \rangle, \quad (4.26) \]

where in view of the AE analysis of the previous section, one can have

\[ \bar{D}_M = \langle D_{mech}^p + D^v \rangle, \quad (4.27a) \]
and then one can ideally conclude
\[
\frac{\partial \bar{\epsilon}}{\partial \bar{F}} : \dot{\bar{F}} = \langle P : \dot{\bar{F}} \rangle, \quad \frac{\partial \bar{\epsilon}}{\partial \bar{\eta}^e} \dot{\bar{\eta}}^e = \bar{\theta} \langle \eta^e \rangle, \tag{4.27b}
\]
in a way that they have the same structure as in the thermoelastic problems.

i. Since the rates of the two sides of Eq. (4.14), equal and \( \bar{\epsilon} \) is independent of \( \bar{\eta}^e \), one can obtain the first consistency equation defined in Eqs. (4.12)
\[
\bar{\theta} = \frac{\partial \bar{\epsilon}}{\partial \bar{\eta}^e} \quad \text{Legendre transformation} \quad \bar{\eta}^e = - \frac{\partial \bar{\psi}}{\partial \bar{\theta}}. \tag{4.28}
\]
Note that although we defined the \( \bar{\eta}^e = \langle \eta^e \rangle \), but eventually it was not necessary since from (4.27b) this result could be obtained.

Remember that the homogenized internal energy assumed as a function of the elastic entropy at the beginning of this chapter. This is due to the evolution of \( \langle \eta^e \rangle \) in (4.27b) which stems from the fact that the microscopic internal energy is plastic entropy independent and therefore this result motivates the additively decomposition of total entropy to the elastic and plastic entropies in the macrolevel.

ii. By applying the micro-macro criterion (4.20), the second consistency equation can be obtained
\[
\langle P \rangle = \frac{\partial \bar{\epsilon}}{\partial \bar{F}} \quad \text{Legendre transformation} \quad \langle P \rangle = \frac{\partial \bar{\psi}}{\partial \bar{F}}. \tag{4.29}
\]

iii. To obtain the third consistency condition, one should consider the definitions of the dissipation functions in Eq. (4.14)
\[
\mathcal{D}^\text{Tot}_{\text{int}} = \mathcal{D}^\text{M} + \mathcal{D}^\text{p}_{\text{ther}} = \langle \mathcal{D}^\text{Tot}_{\text{int}} \rangle = \langle \mathcal{D}^\text{p}_{\text{mech}} \rangle + \langle \mathcal{D}^\text{p} \rangle + \langle \mathcal{D}^\text{p}_{\text{ther}} \rangle. \tag{4.30}
\]
Using Eqs. (4.27a) and (4.30), one can finally obtain the third consistency equation
\[
\mathcal{D}^\text{p}_{\text{ther}} = \bar{\theta} \langle \eta^p \rangle \quad \rightarrow \quad \bar{\eta}^p = \langle \eta^p \rangle. \tag{4.31}
\]
Note that one could alternatively define the last equation in (4.14) as \( \bar{\eta}^p = \langle \eta^p \rangle \) and finally check the consistency of \( \mathcal{D}^\text{Tot}_{\text{int}} = \langle \mathcal{D}^\text{Tot}_{\text{int}} \rangle \). With Eqs. (4.14), and (4.31) at hand, one can conclude that the total entropy preserved in the micro-to-macro scale transition.

Remark 4.2:

Through the developments in this chapter, we have neglected the possible interactions between the microscopic internal variables through the scale transitions. Therefore, since we had four sources for dissipation on the microscale, i.e., the plastic part of
deformation gradient, the hardening parameter, the viscous part of deformation gradient and the plastic entropy; we identically assumed four sources for dissipation in macrolevel in a way that they are exactly representing their microscopic counterparts. Even with this simple ideal assumption it is extremely difficult to explicitly construct a free energy function to model these internal variables on the macroscale in a way that the macroscopic volume average of the dissipation functions can be preserved during the micro-to-macro transition which renders the multiscale homogenization approach as a powerful method to consider the behavior of the heterogeneous materials. Among these internal variables, the plastic entropy has different nature. First, it does not appear in the microscopic and macroscopic free energy functions. Then, although the result of Eq. (4.31) shows that the plastic entropy preserves through the micro-to-macro scale transition, its importance relies on the fact that it explicitly represents the relation between a microscopic internal variable with its associated macroscopic counterpart. This explicit relation is really hard to achieve for the other internal variables employed in this work.

The micro-macro work condition (4.20) had an important role to guarantee Eq. (4.28) since by vanishing \( \bar{F} \) the term presenting the volume average of the work performed on the microscale vanishes. By neglecting any inelastic effects, Eqs. (4.26) and (4.28) reduce to their thermoelastic counterparts that previously reported by Temizer and Wriggers (2011).

iv. Although the macroscopic specific heat was investigated in the previous chapter for the general thermoinelastic materials, its thermodynamic consistency is further considered on the basis of the specific constitutive formulation employed through the developments (Chadwick, 1973).

From Eqs. (4.14) and (4.15c), one can write

\[
\bar{c} = -\bar{\theta} \frac{\partial}{\partial \bar{\theta}} \langle \frac{\partial \bar{\psi}}{\partial \bar{\theta}} \rangle = -\frac{\partial}{\partial \bar{\theta}} \langle \psi_o - e_o \rangle + c + \int_{\bar{\theta}_R}^{\bar{\theta}} \left( \frac{\partial c}{\partial \bar{F} : \frac{\partial \bar{F}}{\partial \bar{\theta}}} \right) d\bar{\theta} = \left( \frac{\partial e_o}{\partial \bar{F} : \frac{\partial \bar{F}}{\partial \bar{\theta}}} \right) + \left( \frac{d}{d\bar{\theta}} \int_{\bar{\theta}_R}^{\bar{\theta}} c(\bar{\theta}, F, C_p^{-1}, \xi, C_v^{-1}) d\bar{\theta} \right) = \frac{d\bar{e}}{d\bar{\theta}} = \frac{\partial \bar{e}}{\partial \bar{\theta}},
\]

(4.32)

where \( \partial F / \partial \bar{\theta} \) represents the sensitivity of the microscopic deformation gradient with respect to the macroscopic temperature at a fixed macroscopic deformation and internal variables states. The evolution of this term relies on the definition of the specific heat; the amount of energy to generate unit increase in the temperature of a unit volume of the heterogeneous material keeping the (macroscopic) deformation and the internal variables fixed. Therefore, since the microscopic deformation is allowed this sensitivity evolves as a result of microstructural changes in the medium (see Yu and Tang, 2007; and Temizer and Wriggers, 2011 for the thermoeelastic problems in the linearized and finite deformations settings). And this clearly shows that \( \bar{c} \) is a function of \( \bar{F} \) and \( \bar{\theta} \) with the
associated internal variables even if $c$ is a constant. This completes the verification of the consistency equations defined in Eqs. (4.12).

### 4.4 Macroscale solution

To solve the linear momentum balance Eqs. (4.1) using FEM, one does need to have their relevant weak forms as

$$\mathcal{W}_M = \int_{\Omega} \delta \mathbf{F} : \mathbf{p} \, dV + \int_{\Omega} \delta \mathbf{u} \cdot (\bar{\rho}_0 \ddot{\mathbf{u}} - \ddot{\mathbf{f}}) dV - \int_{\partial \Omega} \delta \mathbf{u} \cdot \mathbf{p} \, dA = 0, \quad (4.33a)$$

$$\mathcal{W}_\theta = \int_{\Omega} \delta \mathbf{G} : \mathbf{Q} \, dV + \int_{\Omega} (\mathbf{B}_m - \mathbf{R} - \dot{c} \dot{\mathbf{\theta}} + \mathbf{\bar{R}}) \delta \mathbf{\theta} \, dV - \int_{\partial \Omega} \mathbf{Q} \cdot \delta \mathbf{\theta} \, dA = 0, \quad (4.33b)$$

together with their consistent linearization (in the monolithic manner)

$$\Delta \mathcal{W}_M = \int_{\Omega} \delta \mathbf{F} \left( \frac{\partial \mathbf{P}}{\partial \mathbf{\theta}} \equiv \mathbf{M} \right) \Delta \mathbf{\theta} \, dV + \int_{\Omega} \delta \mathbf{F} \left( \frac{\partial \mathbf{P}}{\partial \mathbf{\bar{F}}} \equiv \mathbf{K} \right) : \Delta \mathbf{\bar{F}} \, dV, \quad (4.34a)$$

$$\Delta \mathcal{W}_\theta = - \int_{\Omega} \delta \mathbf{G} \left( - \frac{\partial \mathbf{\bar{Q}}}{\partial \mathbf{\bar{\theta}}} \equiv \mathbf{\bar{K}} \right) \Delta \mathbf{\bar{\theta}} \, dV - \int_{\Omega} \delta \mathbf{G} \left( - \frac{\partial \mathbf{\bar{Q}}}{\partial \mathbf{\bar{F}}} \equiv \mathbf{\bar{Q}} \right) : \Delta \mathbf{\bar{F}} \, dV$$

$$\quad + \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{M}}}{\partial \mathbf{\bar{\theta}}} \right) : \Delta \mathbf{\bar{F}} \, dV + \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{M}}}{\partial \mathbf{\bar{\theta}}} \right) \Delta \mathbf{\bar{\theta}} \, dV$$

$$\quad - \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{F}}}{\partial \mathbf{\bar{\theta}}} \right) : \Delta \mathbf{\bar{F}} \, dV - \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{F}}}{\partial \mathbf{\bar{\theta}}} \right) \Delta \mathbf{\bar{\theta}} \, dV$$

$$\quad - \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{c}}}{\partial \mathbf{\bar{F}}} \right) : \Delta \mathbf{\bar{F}} \Delta \mathbf{\bar{\theta}} \, dV - \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{c}}}{\partial \mathbf{\bar{\theta}}} \right) \Delta \mathbf{\bar{\theta}} \, dV - \int_{\Omega} \delta \mathbf{\bar{G}} \left( \frac{\partial \mathbf{\bar{c}}}{\partial \mathbf{\bar{\theta}}} \right) \Delta \mathbf{\bar{\theta}} \, dV,$$

where the sensitivities are defined in view of Eqs. (3.9). Based on the multilevel implementation within FEM, each Gauss point of the BVPs (4.33) is accompanied by an attached microstructural test sample where by solving the cell problems (4.17) and (4.21) and applying the appropriate macroscopic data—such that the consistency Eqs. (4.12) are satisfied—in (4.33) and (4.34), the developed homogenization procedure is completed. So far, the appropriate data in BVPs (4.33) has been presented, and in what follows the sensitivity analysis is performed to provide required data for applying (4.34a) and (4.34b). The tangents computation necessitates the knowledge of $\partial \mathbf{F}/\partial \mathbf{\theta}$ and/or $\partial \mathbf{F}/\partial \mathbf{\bar{F}}$ where they are obtained in a straightforward manner in what follows. These terms already exist in $\bar{c}$ (Eq. (4.32)) and $\bar{H}$ (this is clarified in what follows) and therefore their linearization individually requires the higher-order terms $\partial^2 \mathbf{F}/\partial \mathbf{\theta}^2, \partial^2 \mathbf{F}/\partial \mathbf{\theta} \partial \mathbf{\bar{F}}$ and $\partial (\partial \mathbf{F}/\partial \mathbf{\bar{F}})/\partial \mathbf{\bar{F}}$ which does not seem to be feasible. Hence, a parameter update scheme to evaluate $\bar{c}$ and
makes sense. In another way, one can apply staggering methods to linearize the weak forms (4.33) and calculate the terms $\bar{c}$ and $\bar{H}$ at the end of the latest time step in the mechanical phase. In this way, one can consider them as a heat source in the thermal part. Note that by applying the staggering methods the terms consist of $\frac{\partial(\ast)}{\partial \bar{\theta}}$ in (4.34a) and $\frac{\partial(\ast)}{\partial \bar{F}}$ in (4.34b) vanish. Also, isothermal and isentropic operator split algorithms can be applied in this case. See e.g., Simo and Miehe (1992) for both monolithic and isothermal operator split algorithms and Holzapfel and Simo (1996b) for the isentropic one. But, it can be shown that the linearization of the both terms together as $(\bar{H} + \bar{c}\dot{\bar{\theta}})$ exclude the knowledge of the above higher-order terms since eventually this term is a volume average of its microscopic counterpart.

### 4.4.1 Mechanical tangent computations

To apply the linearized mechanical weak form (4.34a), the sensitivities of the homogenized first Piola-Kirchhoff stress tensor $\bar{P}$ with respect to the set $\{\bar{\theta}, \bar{F}\}$ should be obtained

$$\bar{M} = \left\langle \frac{dP}{d\bar{\theta}} \right\rangle = \left\langle \mathbb{K} \frac{\partial F}{\partial \bar{\theta}} + M \right\rangle, \quad \bar{\mathbb{K}} = \left\langle \frac{dP}{dF} \right\rangle = \left\langle \mathbb{K} \frac{\partial F}{\partial F} \right\rangle, \tag{4.35}$$

which clearly requires the evaluation of sensitivities of the microscopic deformation gradient with respect to the set $\{\bar{\theta}, \bar{F}\}$ under the BCs employed during the mechanical phase. To do this, since $P$ is divergence-free in Eq. (4.17), its relevant changes should remain divergence-free under arbitrary changes to the set $\{\bar{\theta}, \bar{F}\}$ for any micromechanical testing procedure

$$\text{Div} \left[ \mathbb{K} \frac{\partial F}{\partial \bar{\theta}} + M \right] = \text{Div} \left[ \mathbb{K} : A_M^\theta + M \right] = 0, \tag{4.36a}$$

$$\text{Div} \left[ A_M^\theta \frac{\partial F}{\partial F_{JB}} \right] = \text{Div} \left[ \mathbb{K} : \left( A_M^F \right)^{JB} \right] = 0, \quad \forall j, B = 1,2,3 \tag{4.36b}$$

where

$$A_M^\theta = \frac{\partial a_M^\theta}{\partial X} \quad \& \quad \left( A_M^F \right)^{JB} = \frac{\partial (a_M^F)^{JB}}{\partial X} \quad \text{in which}$$

$$a_M^\theta = \frac{\partial x}{\partial \bar{\theta}} \quad \& \quad (a_M^F)^{JB} = \frac{\partial x}{\partial F_{JB}}. \tag{4.37}$$

Eqs. (4.36a) and (4.36b) are linear BVPs for $A_M^\theta$ and $(a_M^F)^{jB}$ respectively, and they are constructed at the converged solution states of the mechanical phase which should be complemented by appropriate BCs for a unique solution. The set $\{a_M^\theta, (a_M^F)^{jB}\}$ is eventually a perturbation to $x$ and therefore it is free of jump in $u_0$ and subject to the
the linearization of the second with respect to the intermediate configurations)

\[
\begin{align*}
\{\partial \bar{F} / \partial \bar{\theta} = 0, & \quad \partial \bar{F}_{iA} / \partial F_{jB} = \delta_{ij}\delta_{AB} \} \\
\{ (A^g_M) = 0, & \quad (A^g_M)_{ia} = \delta_{ij}\delta_{AB} \}.
\end{align*}
\] (4.38)

To solve the BVPs (4.36), one should clearly have \( \mathbb{K} \) and \( \mathbb{M} \). Since the developed numerical algorithm on the microscale is based on the Kirchhoff stress tensor with its associated consistent linearization, therefore \( \mathbb{K} \) and \( \mathbb{M} \) should be derived in a consistent manner as follows. Let right Cauchy-Green strain tensor \( C^{tr}_{ep} \), stress \( \mathring{S}^e_{p} \), and elasticity tensor \( \mathring{e}_{p}^{eq} \) all defined in the fixed plastic intermediate configuration (\( C^{tr}_{ev}, \mathring{S}^e_{v}, \mathring{e}_{v}^{eq} \) for the non-equilibrium part), since

\[
P_{iA} = F_{iB}(S^e_{p})_{AB} + F_{iB}(S^{neq}_{v})_{AB} = \\
(F^{tr}_{ep})_{i \varphi}(S^e_{p})_{\varphi \eta}(F^{-1}_{p})_{\eta \eta} + (F^{tr}_{ev})_{i \varphi}(\mathring{S}^e_{v})_{\varphi \eta}(F^{-1}_{v})_{\eta \eta},
\] (4.39)

one can obtain (the Greek letters were used to emphasize that the variables are defined with respect to the intermediate configurations)

\[
\Delta P_{iA} = \Delta F_{iB} \left[ (S^e_{p})_{AB} + (S^{neq}_{v})_{AB} \right] \\
+ (F^{tr}_{ep})_{i \varphi} \Delta (\mathring{S}^e_{p})_{\varphi \eta}(F^{-1}_{p})_{\eta \eta} + (F^{tr}_{ev})_{i \varphi} \Delta (\mathring{S}^{neq}_{v})_{\varphi \eta}(F^{-1}_{v})_{\eta \eta}.
\] (4.40)

The linearization of the second Piola-Kirchhoff stress tensors defined with respect to the fixed intermediate configurations is given by

\[
\Delta(\mathring{S}^e_{p})_{\varphi \eta} = (\mathring{e}_{p}^{eq})_{\varphi \eta \alpha \epsilon} \frac{\Delta(C^{tr}_{ep})_{\alpha \epsilon}}{2} = \\
\left[(a^{eq}_{p})_{abj}(F^{tr}_{ep})_{\varphi a}(F^{tr}_{ep})_{\eta b}(F_{Bd})^{-1}\right] \Delta F_{jB} + \sum_{a=1}^{3} \left( \lambda_{a}^{tr} \right)^{-2} \partial (a^{eq}_{p})_{\varphi \alpha \epsilon} / \partial \bar{\theta} \left( N_{a}^{tr} \right)_{\varphi}(N_{a}^{tr})_{\eta} \Delta \bar{\theta},
\] (4.41a)

\[
\Delta(\mathring{S}^{neq}_{v})_{\varphi \eta} = (\mathring{e}_{v}^{eq})_{\varphi \eta \alpha \epsilon} \frac{\Delta(C^{tr}_{ev})_{\alpha \epsilon}}{2} = \\
\left[(a^{neq}_{v})_{abj}(F^{tr}_{ev})_{\varphi a}(F^{tr}_{ev})_{\eta b}(F_{Bd})^{-1}\right] \Delta F_{jB} + \sum_{a=1}^{3} \left( \lambda_{a}^{tr} \right)^{-2} \partial (a^{eq}_{v})_{\varphi \alpha \epsilon} / \partial \bar{\theta} \left( N_{a}^{tr} \right)_{\varphi}(N_{a}^{tr})_{\eta} \Delta \bar{\theta}.
\] (4.41b)

Now, Eq. (4.40) takes the form
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\[ \Delta P_{IA} = \left\{ \left( S^p_{eq} \right)_{AB} + \left( S^v_{neq} \right)_{AB} \right\} \delta_{ij} + \left\{ \left( e^p_{eq} \right)_{ibdj} + \left( e^v_{neq} \right)_{ibdj} \right\} F_{Ab}^{-1} F_{Bd}^{-1} \Delta F_{jB} \]

\[ + \sum_{a=1}^{3} \frac{\partial \tau^{ep}_{a}}{\partial \tilde{\theta}} \left( n^e_{a} \right)_{i} \left( n^e_{a} \right)_{j} \Delta \tilde{\theta} + \sum_{a=1}^{3} \frac{\partial \tau^{ev}_{a}}{\partial \tilde{\theta}} \left( n^{ev}_{a} \right)_{i} \left( n^{ev}_{a} \right)_{j} \Delta \tilde{\theta}, \]

and therefore one can finally obtain \( \mathbb{K} \) and \( M \)

\[ \mathbb{K}_{IAjB} = \left\{ \left( S^p_{eq} \right)_{AB} + \left( S^v_{neq} \right)_{AB} \right\} \delta_{ij} + \left\{ \left( e^p_{eq} \right)_{ibdj} + \left( e^v_{neq} \right)_{ibdj} \right\} F_{Ab}^{-1} F_{Bd}^{-1}, \]

\[ M = \sum_{a=1}^{3} \frac{\partial \tau^{ep}_{a}}{\partial \tilde{\theta}} \left( n^e_{a} \right)_{i} \left( n^e_{a} \right)_{j} \Delta \tilde{\theta} + \sum_{a=1}^{3} \frac{\partial \tau^{ev}_{a}}{\partial \tilde{\theta}} \left( n^{ev}_{a} \right)_{i} \left( n^{ev}_{a} \right)_{j} \Delta \tilde{\theta}, \]

where \( \frac{\partial \tau^{ep}_{a}}{\partial \tilde{\theta}} \) and \( \frac{\partial \tau^{ev}_{a}}{\partial \tilde{\theta}} \) have been given in Eqs. (A.8) and (A.11), respectively. Note that in Eqs. (4.35) and (4.36), the sensitivity of \( P \) with respect to the internal variables has not been encountered since the flow rules of the theory have been already applied and therefore the internal variables implicitly contribute to \( P \) in a way that one can assume \( P = P(\tilde{\theta}, F) \) which is an obvious result as it can be seen in Eq. (4.42). Please also note that Eqs. (4.39)-(4.43) are consistent with the thermo-viscoplasticity, i.e. \( \dot{\phi} \geq 0 \) but for the thermo-viscoelastic processes \( (\dot{\phi} \leq 0) \) the equilibrium parts of the above derived equations should be consistently revised (Temizer and Wriggers, 2011).

4.4.2 Thermal tangent computations and sensitivities

For the thermal phase, one should obtain the sensitivities of the referential Piola-Kirchhoff heat flux \( \mathbf{Q} \) with respect to the set \( \{ \tilde{\theta}, \overline{G}, \overline{F} \} \) and the sensitivities of the macroscopic dissipation functions with respect to the set \( \{ \tilde{\theta}, \overline{F} \} \) together with the linearization of the STVPH and specific heat to have the appropriate data for applying the linearized thermal weak form (4.34b). The same procedure as in the mechanical phase is pursued and therefore one can write

- The homogenized referential heat flux sensitivities

\[ \mathbf{\bar{m}} = \left\{ \frac{d \mathbf{Q}}{d \tilde{\theta}} \right\} = \left\{ \mathbf{Q} : \frac{\partial \mathbf{F}}{\partial \tilde{\theta}} + \mathbf{K} : \frac{\partial \overline{G}}{\partial \tilde{\theta}} + \mathbf{m} \right\}, \]

\[ \mathbf{\bar{K}} = \left\{ \frac{d \mathbf{Q}}{d \overline{G}} \right\} = \left\{ \mathbf{K} : \frac{\partial \overline{G}}{\partial \overline{G}} \right\}, \]

\[ \mathbf{\bar{Q}} = \left\{ \frac{d \mathbf{Q}}{d \overline{F}} \right\} = \left\{ \mathbf{Q} : \frac{\partial \mathbf{F}}{\partial \overline{F}} + \mathbf{K} : \frac{\partial \overline{G}}{\partial \overline{F}} \right\}, \]

where \( \frac{\partial \mathbf{F}}{\partial \tilde{\theta}} \) and \( \frac{\partial \mathbf{F}}{\partial \overline{F}} \) have already been evaluated in the mechanical phase and, therefore, the set \( \{ \partial \overline{G} / \partial \tilde{\theta}, \partial \overline{G} / \partial \overline{G}, \partial \overline{G} / \partial \overline{F} \} \) are the unknowns of Eqs. (4.44). Since the
microscale field \( \mathbf{Q} \) remains divergence-free under the arbitrary changes in \( \bar{\theta}, \mathbf{G}, \) and \( \mathbf{F}, \) the associated thermal ATPs take the form

\[
\text{Div}\left[ \mathbf{K}(\mathbf{A}_{M}^{\bar{\theta}}) + \mathbf{Q} : \mathbf{A}_{M}^{\bar{\theta}} + \mathbf{m} \right] = 0, \\
\text{Div}\left[ \mathbf{K} : \mathbf{A}_{M}^{\bar{\theta}} \right] = 0, \\
\text{Div}\left[ \mathbf{K} \cdot (\mathbf{A}_{M}^{F})^{jB} + \mathbf{Q} : (\mathbf{A}_{M}^{F})^{jB} \right] = 0, \quad \forall \ j, B = 1, 2, 3, 
\]

where

\[
\begin{cases}
\mathbf{A}_{T}^{\bar{\theta}} = \frac{\partial \mathbf{a}_{T}^{\bar{\theta}}}{\partial \mathbf{X}}, \\ (\mathbf{A}_{T}^{G})^{B} = \frac{\partial (\mathbf{a}_{T}^{G})^{B}}{\partial \mathbf{X}}, \\ (\mathbf{A}_{T}^{F})^{jB} = \frac{\partial (\mathbf{a}_{T}^{F})^{jB}}{\partial \mathbf{X}}
\end{cases}
\]

in which

\[
\begin{cases}
\mathbf{a}_{T}^{\bar{\theta}} = \frac{\partial \theta}{\partial \bar{\theta}}, \\ (\mathbf{a}_{T}^{G})^{B} = \frac{\partial \theta}{\partial \mathbf{G}^{B}}, \\ (\mathbf{a}_{T}^{F})^{jB} = \frac{\partial \theta}{\partial \mathbf{F}^{jB}}
\end{cases}
\]

Note that the thermal set \( \{ \mathbf{A}_{T}^{\bar{\theta}}, (\mathbf{A}_{T}^{G})^{B}, (\mathbf{A}_{T}^{F})^{jB} \} \) is a first-order tensor whereas the mechanical set \( \{ \mathbf{A}_{M}^{\bar{\theta}}, (\mathbf{A}_{M}^{G})^{B}, (\mathbf{A}_{M}^{F})^{jB} \} \) is a second-order tensor. As in the mechanical phase, these ATPs are constructed at the equilibrium solution states of the thermal phase in which the set \( \{ \mathbf{a}_{T}^{\bar{\theta}}, (\mathbf{a}_{T}^{G})^{B}, (\mathbf{a}_{T}^{F})^{jB} \} \) is a perturbation to \( \bar{\theta} \) and therefore it is free of jump in \( \nu_{0} \) and subject to the same class of BCs imposed on \( \bar{\theta} \) to provide a unique solution. The thermal counterparts of the constraints (4.38) now take the following form

\[
\begin{cases}
\left( \frac{\partial \mathbf{G}}{\partial \bar{\theta}} \right) = \mathbf{0}, \\ \frac{\partial \mathbf{G}}{\partial \mathbf{G}} = \mathbf{I}, \\ \frac{\partial \mathbf{G}}{\partial \mathbf{F}^{jB}} = \mathbf{0}
\end{cases}
\]

\[
\{ (\mathbf{A}_{T}^{\bar{\theta}})^{B} = \mathbf{0}, \quad \langle (\mathbf{A}_{T}^{G})^{B} \rangle_{\mathbf{A}} = \delta_{AB}, \quad \langle (\mathbf{A}_{T}^{F})^{jB} \rangle = \mathbf{0} \}.
\]

This completes the tangent computations for the mechanical and thermal phases.

\[\bullet\] The macroscopic dissipation functions sensitivities

After applying the flow rules and based on the algorithmic procedure for the solution of the problem, one can clearly assume \( \mathcal{D}^{p}_{\text{mech}} = \mathcal{D}^{p}_{\text{mech}}(\mathbf{F}, \bar{\theta}) \) and \( \mathcal{D}^{v} = \mathcal{D}^{v}(\mathbf{F}, \bar{\theta}) \) -which leads to their associated macroscopic counterpart as \( \mathcal{D}^{p}_{\text{mech}} = \mathcal{D}^{p}_{\text{mech}}(\mathbf{F}, \bar{\theta}) \) and \( \mathcal{D}^{v} = \mathcal{D}^{v}(\mathbf{F}, \bar{\theta}) \) - and write
\[
\Delta \mathcal{D}_{\text{mech}}^p = \frac{\partial \mathcal{D}_{\text{mech}}^p}{\partial \mathbf{F}} : \Delta \mathbf{F} + \frac{\partial \mathcal{D}_{\text{mech}}^p}{\partial \bar{\theta}} \Delta \bar{\theta} = \frac{\partial \langle \mathcal{D}_{\text{mech}}^p \rangle}{\partial \mathbf{F}} : \Delta \mathbf{F} + \frac{\partial \langle \mathcal{D}_{\text{mech}}^p \rangle}{\partial \bar{\theta}} \Delta \bar{\theta}, \\
\]
\[
\Delta \mathcal{V} = \frac{\partial \mathcal{V}}{\partial \mathbf{F}} : \Delta \mathbf{F} + \frac{\partial \mathcal{V}}{\partial \bar{\theta}} \Delta \bar{\theta} = \frac{\partial \langle \mathcal{V} \rangle}{\partial \mathbf{F}} : \Delta \mathbf{F} + \frac{\partial \langle \mathcal{V} \rangle}{\partial \bar{\theta}} \Delta \bar{\theta},
\]

where considering \( \partial \mathbf{F} / \partial \bar{\theta} \) and \( \partial \mathbf{F} / \partial \bar{\theta} \) as known data and in view of the above discussions, the sensitivity of the set \( \{ \mathcal{D}_{\text{mech}}^p, \mathcal{V} \} \) with respect to \( \{ \mathbf{F}, \bar{\theta} \} \) is derived as follows. On the basis of equations derived in the Appendixes A, B and D, they are given by

\[
\frac{\partial \mathcal{D}_{\text{mech}}^p}{\partial \mathbf{F}} = \sqrt{\frac{2}{3\Delta t^2}} \sum_{a=1}^{3} \sigma_y \frac{\partial (\Delta y)}{\partial \varepsilon_a^{\text{eptr}}} (\mathbf{n}_a^{\text{ep}})^{tr} \otimes \mathbf{F}^{-1} (\mathbf{n}_a^{\text{ep}})^{tr},
\]
\[
\frac{\partial \mathcal{D}_{\text{mech}}^p}{\partial \bar{\theta}} = \sqrt{\frac{2}{3\Delta t^2}} \left( \sigma_y \frac{\partial (\Delta y)}{\partial \bar{\theta}} + \Delta y \sigma_y \right),
\]
\[
\frac{\partial \mathcal{V}}{\partial \mathbf{F}} = \sum_{a=1}^{3} \frac{\partial \mathcal{V}}{\partial \varepsilon_a^{\text{evtr}}} (\mathbf{n}_a^{\text{ev}})^{tr} \otimes \mathbf{F}^{-1} (\mathbf{n}_a^{\text{ev}})^{tr}, \quad \frac{\partial \mathcal{V}}{\partial \bar{\theta}} = \frac{\partial \mathcal{V}}{\partial \bar{\theta}} \bigg|_{\varepsilon_a^{\text{evtr}}=\text{cte}},
\]

where \( \partial (\Delta y) / \partial \varepsilon_a^{\text{eptr}} \) and \( \partial (\Delta y) / \partial \bar{\theta} \) have been presented in Eqs. (A.6) of Appendix A; and \( \partial \mathcal{V} / \partial \varepsilon_a^{\text{evtr}} \) and \( \partial \mathcal{V} / \partial \bar{\theta} \) are computable in view of Eqs. (B.5)-(B.7) of Appendix B. Now, introduction of Eqs. (4.49) in (4.48) completes the evaluation of the sensitivities of the macroscopic dissipation functions.

**The homogenized STVPH**

The macroscopic STVPH was consistently given in Eq. (4.2) and it can be computable whenever \( \partial \mathcal{H} / \partial \bar{\theta} \) and the set \( \mathcal{D}_{\text{sen}}^\bar{\theta} = \{ \partial \mathcal{D}_{\text{mech}}^p / \partial \bar{\theta}, \partial \mathcal{V} / \partial \bar{\theta} \} \) is known. Note that the term \( \partial \mathcal{H} / \partial \bar{\theta} \) given in Eq. (4.43b) and the set \( \mathcal{D}_{\text{sen}}^\bar{\theta} \) in (4.48) are not applicable here. Since based on the definition, the macroscopic set \( \mathcal{D}_{\text{sen}}^\bar{\theta} \) here is obtained by taking the internal variables constant (this also holds for the microscopic set \( \mathcal{D}_{\text{sen}}^\bar{\theta} \)) but the appropriate changes with \( \bar{\theta} \) induced by changes of the relevant internal variables have been taken into account in the evaluation of Eqs. (4.48). Here, \( \mathcal{H} \) is obtained in an alternative way as
Thus, using Eqs. (4.32), (C.3) of Appendix C, and (4.50), \( \hat{\mathcal{H}} \) can be consistently computed. The importance of the above equation relies on the fact that its left hand side explicitly contributes to the homogenized thermal weak form (4.33b) and therefore its linearization simply takes the form

\[
\Delta \left( \hat{\mathcal{H}} + c\dot{\theta} \right) = \langle \Delta \mathcal{H} \rangle + \langle \Delta c \rangle \dot{\theta} + \left( \frac{c}{\Delta t} \right) \Delta \theta, 
\]

which can be applied in the linearized macroscopic thermal weak form (4.34b) once \( \Delta \mathcal{H} \) and \( \Delta c \) are known. Since the linearization of the terms \( \mathcal{H} \) and \( c \) requires the knowledge of utmost the first partial derivative of the microscopic deformation gradient with respect to its macroscopic counterpart and \( \dot{\theta} \), one does not need to have any knowledge of the higher-order terms \( \partial^2 F / \partial \dot{\theta}^2 \), \( \partial^2 F / \partial \theta \partial \dot{\theta} \), and \( \partial (\partial F / \partial \theta) / \partial \dot{\theta} \). Hence, the macroscopic solution scheme can be completed in the monolithic way. By assuming the constant specific heat at the microlevel, \( \Delta c \) vanishes and the linearization of (4.51) in view of equations derived in the Appendixes C and D takes the following form

\[
\langle \Delta \mathcal{H} + \frac{c}{\Delta t} \Delta \theta \rangle = \langle \left( \frac{\mathcal{H}}{\dot{\theta}} + \hat{\mathcal{H}}_\theta \right) + \left( \frac{c}{\Delta t} \right) \Delta \theta \rangle
\]

\[
+ \left( \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ep} \rangle_a \left( n_a^{ep} \otimes F^{-1} n_a^{ep} \right) + \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ev} \rangle_a \left( n_a^{ev} \otimes F^{-1} n_a^{ev} \right) \right] : \left[ \frac{\partial F}{\partial \theta} \right] \Delta \theta
\]

\[
+ \left( \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ep} \rangle_a \left( n_a^{ep} \otimes F^{-1} n_a^{ep} \right) + \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ev} \rangle_a \left( n_a^{ev} \otimes F^{-1} n_a^{ev} \right) \right] : \left[ \frac{\partial F}{\partial F} \right] \dot{\theta} \dot{F}.
\]

Using Eqs. (4.51) and (4.52), one can finally obtain

\[
\frac{\partial}{\partial \theta} \left( \hat{\mathcal{H}} + c\dot{\theta} \right) = \langle \left( \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ep} \rangle_a \left( n_a^{ep} \otimes F^{-1} n_a^{ep} \right) + \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ev} \rangle_a \left( n_a^{ev} \otimes F^{-1} n_a^{ev} \right) \right] : \left[ \frac{\partial F}{\partial \theta} \right] \rangle,
\]

\[
\frac{\partial}{\partial F} \left( \frac{\mathcal{H}}{\dot{\theta}} + \hat{\mathcal{H}}_\theta \right) = \langle \left( \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ep} \rangle_a \left( n_a^{ep} \otimes F^{-1} n_a^{ep} \right) + \sum_{a=1}^{3} \langle \hat{\mathcal{H}}_{ev} \rangle_a \left( n_a^{ev} \otimes F^{-1} n_a^{ev} \right) \right] : \left[ \frac{\partial F}{\partial \theta} \right] + \frac{c}{\Delta t} \rangle.
\]

This complete the derivation of the all appropriate data required for the functionals (4.33) and (4.34).
Chapter 5

Representative numerical examples

Numerical investigations of the developed constitutive theories and the homogenization framework are demonstrated here. To do this, for the material modeling a homogenized specimen and for the global-local analysis a model microstructure with a matrix and an inclusion phases is considered. This numerical simulation is based on a global Newton iterative solution procedure with a linear line search algorithm for the thermoplastic part. For the material modeling nearly incompressible responses are sought but for the microstructural testing procedure a (numerically) compressible material is assumed to avoid any numerical (volumetric) locking problems. Material data for the Ogden’s model together with non-linear hardening law and temperature dependent yield stress employed in this thesis are summarized in table 5.1. Based on the standard Galerkin finite element method, all examples in this thesis have been implemented in a numerical user programmed code in the software Fortran.

In homogenization examples, digital microstructures (figure 5.1) have been generated using a random field model (Torquato, 2002) at a fixed intrinsic length scale with a referential volume fraction of $VF_{2D} = 0.3$ for 2D and $VF_{3D} = 0.25$ for 3D examples. The inclusion phase consists of dispersed metallic particles to enrich its properties. Thus, the inclusion phase also admits thermo-viscoelastic-plastic response. This enrichment is modeled by mismatch ratio $m$ which presents the ratio of the inclusion phase to that of the matrix. In this work, the mismatch ratio $m$ has been applied to the set $\{\kappa_{ep}, \kappa_{ev}, \mu_{p}, \mu_{v}, k\}$ and a constant specific heat was taken on the microscale. For this reason, deviation of the macroscopic specific heat from its constant microscopic counterpart has been plotted in all figures. A 2D square plate and a cube both with a fixed length $L = 1$ mm have been considered for all examples although based on AE of chapter 3, the RVE size has no significance for the present classical homogenization theory. All tests are controlled through $\bar{H}_{IA} = \bar{F}_{IA} - \delta_{IA} = \bar{H}$ in the mechanical phase and for the thermal phase through $\bar{G}_{A} = \bar{G}$. In all examples except figure 5.15, the same BCs for the both mechanical and thermal phases have been taken. Examples of this chapter are based
on the finite thermo-elasticity (TE), thermo-viscoelasticity (TVE), the developed first formulation of thermo-viscoplasticity (TVP1) and the second formulation of thermo-viscoplasticity (TVP2).

The first example is related to material modeling. It depicts the effect of heating in the specimen induced by viscosity and plasticity of the rubber-like materials. To do this, we consider a homogenized square plate and a cube with $10^{sd}$ quadrilateral elements (also used for the homogenization examples where $sd$ denotes the space dimension), edge length $L = 1$ m, and 100 time steps (schematically shown in figure 5.2). The test sample is sinusoidally loaded by controlling the displacement of the top edge (surface) of the specimen via $F = I + 0.5(e_{sd} \otimes e_{sd}) \sin(2\pi ft)$ whereas temperature of the bottom edge (surface) is held fixed at $\theta = 314.15$ K. Results of this analysis based on TVP1 and TVP2 are depicted in figures 5.2-5.3. It is seen that with increasing loading, the temperature increase becomes more significant when the internal variables highly evolve. Moreover, the frequency of loading significantly affects the rate of heating.

In what follows, some examples are presented to provide macroscopic results by conducting the micromechanical testing analysis. The study is mainly focused on the derived set \{\overline{P}, \overline{c}, \overline{D}_M, \overline{Q}\} based on the driving set \{\overline{F}, \overline{\theta}, \overline{G}\}. To investigate the effects of BCs on the test sample, the value of the referential heat flux vector and the first Piola-Kirchhoff stress tensor contours are represented in figures 5.4-5.9 for TVE, TVP1 and TVP2 in 3D and 2D. Note that (results of) TVE can be obtained from TVP1 by artificially selecting a very high value for the yield stress to prevent plasticity. As one expects, the stress and heat flux decrease in transitions from LN- to PR- to UF-BCs. It is also seen that the stress predicted by TVP1 is less than its TVE counterpart due to the fact that the plasticity imposes a limitation on the elastic part of TVE. But this difference is not substantial since viscosity is more dominant than the plasticity in rubber-like materials and this can be seen in figure 5.14. Moreover, it can be concluded that the TVP2 is very close to the TVE and therefore this model is more appropriate for stiffer rubber-like materials in a way that while the viscous effects are more substantial, plastic internal variables do not highly evolve as in TVP1.
Temperature dependencies of some macroscopic thermodynamic quantities are depicted in figures 5.10-5.13 for TVE, TVP1 and TVP2 in 3D and 2D. It is seen that by increasing the macroscopic temperature, homogenized specific heat and mechanical dissipation decrease due to the softening occurring in the sample. Figures 5.14-5.15 present deformation dependencies and comparison of the macroscopic quantities on the basis of TE, TVE and TVP1. Note that TE can be obtained from TVP1 by neglecting the non-equilibrium quantities (free energy, stress and so on) and assuming a very high value for the yield stress. By neglecting this amount of energy, decrease in the stress and specific heat is evident. The mechanical dissipation graph in figure 5.14a shows that up to the moderate deformation, $\bar{D}_M$ is almost the same for TVE and TVP1 which presents the fact that viscosity in the rubber-like materials is more predominant than plasticity. For large deformations where internal variables considerably evolve still viscosity is central but the high evolution of plastic internal variables leads to a slightly decrease in the rate of increase of viscoelastic internal variables due to the microstructural changes in the material such as hardening. In this condition, the material needs a higher amount of energy to let the unit increase in the temperature of its unit reference volume, i.e., $\bar{c}_{ep} + \bar{c}_{ev} > \bar{c}_e + \bar{c}_{ev}$. Figure 5.16 presents the thermal version of figure 5.14 which reveals the same result: by increasing the gradient of macroscopic temperature (displacement), heat flux (stress) in the sample increases. To show the discrepancy between the results of investigating a real 3D problem and its simplified 2D counterpart, the 3D and 2D results have also been compared in this figure. For a standard purely thermomechanical problem (in the absence of the other forms of energy such as electric, magnetic, chemical and nuclear), it is just amount of deformation and/or temperature that may cause plasticity in a homogenized material. These effects may be avoided or even accelerated in the presence of inhomogeneities in heterogeneous materials. This is mathematically mainly modeled by the mismatch ratio (in addition to shape, size and volume fraction of the constituents) which is an important parameter design for the engineers. For this reason, effects of the mismatch ratio on the macroscopic thermodynamic variables are considered in figure 5.17 for TVE, TVP1 and TVP2 in 3D and 2D. As one expects, by increasing $m$, more amount of energy is required to deform and/or heat up the material. Another important parameter is relaxation time which is a required time for a system to return to equilibrium in response to a sudden disturbance. Reese and Govindjee (1998b) presented a temperature dependent relaxation time for thermo-viscoelastic problems and considered the effects of this dependency on the response of the material. Although this was assumed as a constant in this work but still it considerably affects the homogenized material response. For this reason, variation of some macroscopic quantities with this time constant is considered in figure 5.18. It is understood that the

---

2 This predominance only happens for the thermo-viscoplastic processes which are close to the equilibrium states, otherwise it is clear that by increasing time for larger processes away from equilibrium states, the dashpot effects diminish.
materials with higher relaxation time bear higher stress since they experience more nonequilibrium states and this leads to more evolution of the internal variables for the developed constitutive theories. It is also seen that by increasing \( \hat{\tau} \), heat capacity decreases since relaxation time is eventually a measurement of difference from equilibrium states. Figure 5.19 depicts variation of some macroscopic variables against \( \omega \) through a sinusoidal loading \( \vec{F} = I + \bar{H} \sin \left[ \frac{2\pi}{T} \omega t \right] \) for TVE and TVP1 in 2D. It is seen that after a certain frequency, a macroscopic equilibrium state is reached. Moreover, it is concluded that with increasing the frequency stress in the sample decreases while heat capacity increases. From figure 5.1 remember that with increasing the frequency, material heats up which clearly shows that more amount of energy has been consumed to heat up the specimen. This result is in accordance with the results of figure 5.19 for inhomogenous materials.

Table 5.1: Material parameters employed are summarized.

<table>
<thead>
<tr>
<th></th>
<th>( \mu_p = 1.0 )</th>
<th>( \mu_v = 1.0 )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Bulk Modulus</strong> (N/mm(^2))</td>
<td></td>
<td></td>
</tr>
<tr>
<td>For homogenized problem,</td>
<td>( \kappa_{ep} = 100 )</td>
<td>( \kappa_{ev} = \kappa_{ep} )</td>
</tr>
<tr>
<td>For microstructural testing procedure,</td>
<td>( \kappa_{ep} = 4 )</td>
<td>( \kappa_{ev} = \kappa_{ep} )</td>
</tr>
<tr>
<td><strong>Shear Modulus</strong> (N/mm(^2))</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Ogden Material parameters:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>((N = 2 \rightarrow 2\mu_p = \sum_{k=1}^{N} \mu_k^p \alpha_k^{ep})) for equilibrium part,</td>
<td>( \mu_1^p = 9.92 \times 10^3; \mu_2^p = 8.68 \times 10^{-5} ),</td>
<td></td>
</tr>
<tr>
<td>((N = 1 \rightarrow 2\mu_v = \sum_{k=1}^{N} \mu_k^v \alpha_k^{ev})) for nonequilibrium part,</td>
<td>( \alpha_1^{ep} = 2.01 \times 10^{-4}; \alpha_2^{ep} = 1.40 \times 10^1 )</td>
<td></td>
</tr>
<tr>
<td>Volumetric thermal expansion coefficient (K(^{-1}))</td>
<td>( \kappa_0^{ep} = \kappa_0^{ev} = 22.333 \times 10^{-5} )</td>
<td></td>
</tr>
<tr>
<td><strong>Thermal conductivity</strong> (N/sK)</td>
<td>( k = 0.15 )</td>
<td></td>
</tr>
<tr>
<td><strong>Specific heat</strong> (N/mm(^2)K)</td>
<td>( c = 1.7385 )</td>
<td></td>
</tr>
<tr>
<td><strong>Reference temperature</strong> (K), and macro temperature rate (K/s)</td>
<td>( \theta_R = 293.15, \quad \dot{\theta} = 1 )</td>
<td></td>
</tr>
<tr>
<td><strong>Mismatch ratio</strong></td>
<td>( m = 10 )</td>
<td></td>
</tr>
<tr>
<td><strong>Relaxation time</strong> ( \hat{\tau} ), and maximum time ( T )</td>
<td>( \hat{\tau} = 5s, \quad 0 \leq t \leq T = 20s )</td>
<td></td>
</tr>
<tr>
<td><strong>Temperature dependent yield stress:</strong></td>
<td>( \sigma_y(\theta) = y_0(\theta_R)(1 - w_0(\theta - \theta_R)), \quad y_0(\theta_R) = 0.15 \text{ N/mm}^2, \quad w_0 = 3.0 \times 10^{-4} \text{ K}^{-1} )</td>
<td></td>
</tr>
<tr>
<td><strong>Hardening Law:</strong></td>
<td>( \psi(\xi) = (\sigma_y^\infty - \sigma_y^o)(1 - e^{-\delta t}) + h\xi, \quad \sigma_y^\infty = 0.2 \text{ N/mm}^2; \quad \sigma_y^o = 0.15 \text{ N/mm}^2, \quad \delta = 8.75; \quad h = 0.1 \text{ N/mm}^2. )</td>
<td></td>
</tr>
</tbody>
</table>
Figure 5.20 aims to depict macroscopic internal variables dependencies of homogenized stress and heat flux for the simplest case of TVE. To do this, the enforced displacement gradient is linearly increased to a certain value and then it is fixed (the macroscopic temperature gradient has been kept constant). It is clearly seen that the macroscopic variables change while the loading is constant which illustrates the microstructural changes. Moreover, this figure shows the macroscopic relaxation for different BCs and relaxation times, and this has been done by numerically increasing time to a large number in order to diminish the dashpot effects. The last example is dealt with sample size effects to examine the convergence of the macroscopic results. To monitor the decrease in macroscopic response scatter, voxel dimension $V_D$ which depicts the number of voxels per spatial dimension should be sequentially increased. Figure 5.21 schematically shows this sample size effect for TVP1 under PR-BCs. To ensure the above mentioned convergence, volume fraction of the constituents is also successively increased with $V_D$. As one expects, the effect of $V_F$ on the homogenized response is similar to $m$ ($m > 1$) in a way that by increasing the volume fraction, stress and heat flux in the material increase.
Figure 5.2: TVP1 Temperature, mechanical dissipation and structural thermoinelastic heating versus time for a homogenized (2D square) plate and cube. Here a sinusoidal loading has been applied with 100 time steps per cycle.
Figure 5.3: TVP2 Temperature, mechanical dissipation and structural thermoinelastic heating versus time for a homogenized (2D square) plate and cube. Here a sinusoidal loading has been applied with 100 time steps per cycle.
Figure 5.4: Macroscopic TVE Piola-Kirchhoff heat flux $\|\vec{Q}\|$ on the current configuration of the 3D microstructure for combinations of BCs on the mechanical and thermal phases with $\{\bar{H}, \bar{G}, \bar{\theta} - \bar{\theta}_0, V\} = \{0.1, 10^3, 10, 50\}$. 
Figure 5.5: Macroscopic TVP1 Piola-Kirchhoff heat flux $||\bar{\mathbf{Q}}||$ on the current configuration of the 3D microstructure for combinations of BCs on the mechanical and thermal phases with $\{\bar{H}, \bar{G}, \bar{\theta} - \bar{\theta}_0, V\} = \{0.1, 10^3, 10, 50\}$.
Figure 5.6: Macroscopic TVP2 Piola-Kirchhoff heat flux $\|\overrightarrow{Q}\|$ on the current configuration of the 3D microstructure for combinations of BCs on the mechanical and thermal phases with $\{\overline{H}, \overline{G}, \overline{\theta} - \overline{\theta}_0, V\} = \{0.1, 10^3, 10, 50\}$. 
Figure 5.7: Macroscopic TVE, TVP1 and TVP2 first Piola-Kirchhoff stress $\|\vec{P}\|$ on the current configuration of the 3D microstructure for different BCs on the mechanical phase with 
\[
\{H, G, \bar{\theta} - \bar{\theta}_0, V\} = \{0.1, 10^3, 10, 50\}.
\]
Figure 5.8: Macroscopic TVE and TVP1 norms $\|\mathbf{Q}\|$ and $\|\mathbf{P}\|$ on the current configuration of the 2D microstructure for different BCs with $\{\bar{H}, \bar{G}, \bar{\theta} - \bar{\theta}_0, V\} = \{0.1, 10^3, 10, 50\}$. 
Figure 5.9: Macroscopic TVP2 norms $\|\overline{Q}\|$ and $\|\overline{P}\|$ on the current configuration of the 2D microstructure for different BCs with $\{\overline{H}, \overline{G}, \overline{\theta} - \overline{\theta}_0, V\} = \{0.25, 10^3, 10, 50\}$. 
Figure 5.10a: Temperature dependencies of the macroscopic TVE thermodynamic quantities for combinations of BCs on the mechanical and thermal phases. Here \( \{\bar{H}, \bar{G}, \bar{V}\} = \{0.05, 10^3, 50\} \).
CHAPTER 5. REPRESENTATIVE NUMERICAL EXAMPLES

Figure 5.10b: Temperature dependencies of the sensitivities of the macroscopic TVE stress, heat flux and the rate of entropy for combinations of BCs on the mechanical and thermal phases. Here \( \{H, \tilde{G}, V\} = \{0.05, 10^3, 50\} \).
Figure 5.11: Temperature dependencies of the macroscopic TVP1 thermodynamic quantities for combinations of BCs on the mechanical and thermal phases. Here \( \{\overline{H}, \overline{G}, V\} = \{0.05, 10^3, 50\} \).
Figure 5.12: Temperature dependencies of the macroscopic TVP2 thermodynamic quantities for combinations of BCs on the mechanical and thermal phases. Here \( \{H, \tilde{G}, V\} = \{0.1, 10^3, 50\} \).
Figure 5.13: Comparison of the macroscopic TVE, TVP1 and TVP2 thermodynamic quantities with respect to the temperature for PR- and LN-BCs on the mechanical and thermal phases in 2D. Here \( \{\bar{H}, \bar{G}, V\} = \{0.1, 10^3, 50\} \).
Fig. 5.14a: Deformation dependencies of the macroscopic TE, TVE and TVP1 thermodynamic quantities for PR-BCs. Here $\{\bar{G}, \bar{\theta} - \tilde{\theta}_0, V \} = \{10^3, 10, 50\}$. 
Fig. 5.14b: Deformation dependencies of the sensitivities of the macroscopic TE, TVE and TVP1 stress, heat flux and mechanical dissipation. Here \( \{ \bar{\sigma}, \bar{\theta} - \bar{\theta}_0, V \} = \{ 10^3, 10, 50 \} \).
Figure 5.15: Comparison of the macroscopic TVE, TVP1 and TVP2 thermodynamic quantities for combinations of BCs on the mechanical and thermal phases in 2D. Here \( \{ G, \tilde{\theta} - \theta_0, V \} = \{ 10^3, 10, 50 \} \).
Figure 5.16: Variation of the macroscopic TVE, TVP1 and TVP2 thermodynamic quantities with the macroscopic temperature gradient for combinations of BCs on the mechanical and thermal phases in 3D and 2D. Here \( \{ \bar{H}, \bar{\theta} - \bar{\theta}_0, V \} = \{ 0.1, 10, 50 \} \).
Figure 5.17: Variation of the macroscopic TVE, TVP1 and TVP2 specific heat ($\bar{H} = 0.1$) and structural thermoinelastic heating ($\bar{H} = 0.25$) with the mismatch ratio for different BCs on the mechanical and thermal phases. Here $\{\bar{G}, \bar{\theta} - \bar{\theta}_0, V\} = \{10^3, 10, 50\}$. 
Figure 5.18: Variation of the TVE, TVP1 and TVP2 macroscopic stress, specific heat and mechanical dissipation with the relaxation time for combinations of BCs on the mechanical and thermal phases. Here \( \{ \bar{H}, \bar{\theta} - \theta_0, V, VF_{3D}, VF_{2D} \} = \{ 0.25, 10, 50, 0.25, 0.3 \} \).
Figure 5.19: Variation of TVE and TVP1 macroscopic stress, specific heat, mechanical dissipation and referential heat flux with $\omega$ for a sinusoidal loading $F = I + \bar{H} \sin \left( \frac{2\pi}{T} \omega t \right)$ with $0 \leq t \leq T$ for PR- and LN-BCs on the mechanical and thermal phases. Here $\{\bar{H}, \bar{\theta} - \bar{\theta}_0, V\} = \{0.25, 10, 50\}$. 
Figure 5.20: Macroscopic internal variable dependencies of the TVE homogenized heat flux and stress for different BCs and relaxation times. Here $\vec{H} = \begin{cases} 0.005t & 0 \leq t \leq 20 \\ 0.1 & 20 < t \leq T^* \end{cases}$ and $\{\bar{G}, \bar{\theta} - \bar{\theta}_0, T^*\} = \{10^3, 15, 150\}$. 
Figure 5.21: TVP1 macroscopic referential heat flux $||\vec{Q}||$ at the end of the thermal phase for combinations of voxel dimension and volume fraction. Here PR-BCs have been applied and $\{H, \bar{G}, \bar{\theta} - \bar{\theta}_0\} = \{0.2, 10^3, 10\}$. 
Chapter 6

Conclusions

Rubber-like materials exhibit highly nonlinear behavior with complex physics of inelastic deformation. Their high deformability property dictates a finite deformation analysis. In this thesis, a two-scale thermo-viscoplasticity analysis framework has been presented for heterogeneous compressible rubber-like materials at finite strains in a fully transient setting and a thermodynamically consistent framework based on a homogenization approach which consists of three main parts: material modeling, asymptotic expansion approach and classical homogenization method.

On the material modeling side and in order to account for inelastic effects of different nature such as viscoelasticity and plasticity combined with thermal effects, multiple decompositions of deformation gradient have been assumed based on the generalization of two developed thermo-mechanical devises (rheological models). The underlying kinematical assumption of multiplicative decompositions of the deformation gradient leads to the associated thermo-viscoelastic and thermo-plastoelastic formulations decoupled from each other in the first formulation whereas interacting between viscous and plastic intermediate configurations in the second formulation is unavoidable. An accompanying decomposition involving thermal expansion is not pursued since the form of the free energy function is based on the modified entropic theory of elasticity.

Subsequently, an asymptotic expansion approach has been applied to consistently build up the homogenization analysis for a general thermoelastic problem wherein two microscopically decoupled mechanical and thermal cell problems have been obtained as in the thermoelastic case. Consequently, the stress distribution in the mechanical phase, temperature-dependent material properties in the mechanical/thermal phases, as well as all microscale functionals are responsive only to the macroscopic temperature.

Finally, computational homogenization approach was followed by imposing the macroscopic deformation gradient and temperature and measuring the stress on the mechanical phase, and imposing the macroscopic temperature gradient on the deformed
microstructural configuration (characterized by an obtained current deformation at a converged equilibrium state of the mechanical phase) and measuring the macroscopic heat flux. The microstructural computations was completed by consistently applying the volume average of the stress and heat flux with their relevant sensitivities, dissipations functions, specific heat and structural thermo-viscoelastic-plastic heating (or cooling) together with their associated sensitivities, in the both macroscopic variational formulations and their associated consistently linearized weak forms in the monolithic manner which did not necessitate any knowledge of higher-order sensitivity terms. The above mentioned macroscopic variables obtained through micro-to-macro transition based on the proper identification of the macroscopic density, internal energy, elastic entropy and total dissipation function and their thermodynamical consistency has been thoroughly considered.

It was seen that as a result of additively decomposition of the microscopic total entropy as elastic and plastic entropies, the microscopic internal energy was a function of elastic entropy which was lead to the elastic entropy dependency of the internal energy at the macroscale. Moreover, the thermal dissipation evolved on the macroscale as a result of total dissipation function identification which was lead to the conclusion that the plastic entropy is preserved through the scale transitions.

Although TVP1 is computationally efficient to address the thermo-viscoplastic behavior of the rubber-like materials, its results are very close to TVE for inelastic processes which are relatively close to the equilibrium states. It was shown that the evolution of plastic internal variables did not have any substantial effects on the prime macroscopic variables such as stress and heat flux. This motivated the development of TVP2 besides the physics of the problem which excludes investigation of the inelastic material behaviors separately and decoupled from each other. Thus, TVP2 takes advantage of less evolution of plastic internal variables in comparison with TVP1.

In summary, some novel aspects of this thesis are highlighted as follows.

- Two finite thermo-viscoplasticity models have been developed to provide a constitutive basis.
- Multiscale finite thermo-inelasticity has been investigated through asymptotic expansion.
- The novel homogenization framework guaranteed two-scale thermodynamic consistency.
- A unique identification of the macroscopic entropy production rate has been provided.
- Feasibility of an implicit-monolithic macroscopic solution scheme has been established.

The present framework also constitutes a basis for the two-scale homogenization and thermodynamic analysis of soft micro-heterogeneous materials which are responsive not only to mechanical and thermal but also to chemical and electrical fields.
Appendix A

In this appendix, the algorithmic equilibrium and non-equilibrium tensors $C^{ep} = \partial \tau^{ep}_t / \partial \epsilon^{ep}_{t\text{tr}}$ and $C^{ev}_a = \partial \tau^{ev}_t / \partial \epsilon^{ev}_{t\text{tr}}$ are derived. It is assumed that 

$$\partial^2 \epsilon_{\xi_t}^{ep} \psi^{ep} = \partial^2 \epsilon_{\xi_t}^{ep} \psi^{ep} = 0,$$  \hspace{1em} (A.1) 

$$\partial^2 \epsilon_{\beta_t}^{ep} \phi = \partial^2 \epsilon_{\beta_t}^{ep} \phi = \partial^2 \epsilon_{\theta_t}^{ep} \phi = \partial^2 \epsilon_{\theta_t}^{ep} \phi = \partial^2 \epsilon_{\beta_t}^{ep} \phi = 0.$$  \hspace{1em} (A.2)

A.1 Thermo-plastoelastic part

Differential forms of Eqs. (2.137b) and (2.137c) are assumed in what follows. Considering the following equations

$$\tau^{ep}_t = \frac{\partial \psi^{ep}}{\partial \epsilon^{ep}_t} \Rightarrow d \tau^{ep}_t = \frac{\partial^2 \psi^{ep}}{\partial \epsilon^{ep}_t \partial \epsilon^{ep}_t} d \epsilon^{ep}_t + \frac{\partial^2 \psi^{ep}}{\partial \epsilon^{ep}_t \partial \theta_t} d \theta_t,$$

$$\beta_t = - \frac{\partial \psi^{ep}}{\partial \xi_t} \Rightarrow d \beta_t = - \frac{\partial^2 \psi^{ep}}{\partial \xi_t \partial \xi_t} d \xi_t - \frac{\partial^2 \psi^{ep}}{\partial \xi_t \partial \theta_t} d \theta_t,$$  \hspace{1em} (A.3)

and using (differential forms of) Eqs. (2.137b) and (2.137c), the above equations can be written

$$d \tau^{ep}_t = \mathbb{U}^* d \epsilon^{ep}_{t\text{tr}} - \mathbb{U}^* \frac{\partial \phi}{\partial \tau^{ep}_t} d(\Delta \gamma_t) + \mathbb{U}^* d \theta_t,$$

$$d \beta_t = - \mathbb{U}^* \frac{\partial \phi}{\partial \beta_t} d(\Delta \gamma_t) - \mathbb{U}^* d \theta_t,$$  \hspace{1em} (A.4)

where
\[
\begin{align*}
\mathbb{U}^* &= \left[ \left( \frac{\partial^2 \psi_{ep}}{\partial \varepsilon_{ep} \partial \varepsilon_{ep}} \right)^{-1} + \Delta \gamma_t \left( \frac{\partial^2 \phi}{\partial t_{ep} \partial t_{ep}} \right) \right]^{-1} , \\
\mathbb{U}^\ast &= \mathbb{U}^* \left( \frac{\partial^2 \psi_{ep}}{\partial \varepsilon_{ep} \partial \varepsilon_{ep}} \right)^{-1} \frac{\partial^2 \psi_{ep}}{\partial t_{ep} \partial \theta_t}, \\
\mathbb{U}^* &= \left[ \left( \frac{\partial^2 \psi_{ep}}{\partial \xi_t \partial \xi_t} \right)^{-1} + \Delta \gamma_t \frac{\partial \phi}{\partial \beta_t} \right]^{-1} , \\
\mathbb{U}^\ast &= \mathbb{U}^* \left( \frac{\partial^2 \psi_{ep}}{\partial \xi_t \partial \xi_t} \right)^{-1} \frac{\partial^2 \psi_{ep}}{\partial \xi_t \partial \theta_t} .
\end{align*}
\]  

Since for plastic loading \( \Delta \gamma_t > 0 \), the Kuhn-Tucker conditions imply \( \hat{\phi} = 0 \) and therefore \( d \hat{\phi} = 0 \). Using this equation and Eq. (A.4), one can obtain

\[
d(\Delta \gamma_t) = \frac{1}{\mathcal{M}} \left( \frac{\partial \phi}{\partial t_{ep}} \mathbb{U}^* \right) d \varepsilon_{ep}^{tr} + \frac{1}{\mathcal{M}} \left( \frac{\partial \phi}{\partial t_{ep}} \mathbb{U}^* - \frac{\partial \phi}{\partial \beta_t} \mathbb{U}^* + \frac{\partial \phi}{\partial \theta_t} \right) d \theta_t ,
\]

where

\[
\mathcal{M} = \frac{\partial \phi}{\partial t_{ep}} \mathbb{U}^* + \frac{\partial \phi}{\partial \beta_t} U^* \frac{\partial \phi}{\partial \beta_t}.
\]

Finally, from Eqs. (A.4) and (A.6), one can write \( d t_{ep} = \left( \frac{\partial t_{ep}}{\partial \varepsilon_{ep}^{tr}} \right) d \varepsilon_{ep}^{tr} + \left( \frac{\partial t_{ep}}{\partial \theta_t} \right) d \theta_t \) in which

\[
\begin{align*}
\mathcal{C}_1^{ep} &= \frac{\partial t_{ep}}{\partial \varepsilon_{ep}^{tr}} = \left( I - \frac{1}{\mathcal{M}} \mathbb{U}^* \mathcal{N} \right) \mathbb{U}^*, \\
\mathcal{C}_1^{ep} &= \frac{\partial t_{ep}}{\partial \theta_t} = \left( I - \frac{1}{\mathcal{M}} \mathbb{U}^* \mathcal{N} \right) \mathbb{U}^* + \frac{1}{\mathcal{M}} \left( \frac{\partial \phi}{\partial \beta_t} \mathbb{U}^* - \frac{\partial \phi}{\partial \theta_t} \right) \left( \mathbb{U}^* \frac{\partial \phi}{\partial t_{ep}} \right),
\end{align*}
\]

where

\[
\mathcal{N} = \frac{\partial \phi}{\partial t_{ep} \partial \varepsilon_{ep}^{tr}} \frac{\partial \phi}{\partial t_{ep}}.
\]

**A.2 Thermo-viscoelastic part**

To compute the algorithmic tensor \( \mathcal{C}^{ev} \), the same procedure as in the thermo-plastoelastic part is pursued. From the incremental form of \( t_{ep}^{ev} \) and Eq. (2.137a), one can obtain
\[
\begin{aligned}
&\begin{cases}
\tau_t^{ev} = \frac{\partial^2 \psi^{ev}}{\partial \varepsilon_t^{ev} \partial \varepsilon_t^{ev}} d\varepsilon_t^{ev} + \frac{\partial^2 \psi^{ev}}{\partial \varepsilon_t^{ev} \partial \theta_t} d\theta_t, \\
\varepsilon_t^{ev} = \varepsilon_t^{ev, tr} - \Delta t \frac{\partial^2 \varphi_v}{\partial \tau_t^{ev} \partial \tau_t^{ev}} d\tau_t^{ev}
\end{cases} \Rightarrow \\
\tau_t^{ev} = \frac{\partial \varepsilon_t^{ev}}{\partial \varepsilon_t^{ev, tr}} d\varepsilon_t^{ev, tr} + \frac{\partial \tau_t^{ev}}{\partial \theta_t} d\theta_t,
\end{aligned}
\]  

(A.10)

where

\[
\begin{aligned}
C_1^{ev} = \left( \frac{\partial^2 \psi^{ev}}{\partial \varepsilon_t^{ev} \partial \varepsilon_t^{ev}} \right)^{-1} + \Delta t \left( \frac{\partial^2 \varphi_v}{\partial \tau_t^{ev} \partial \tau_t^{ev}} \right)^{-1}, \\
\tilde{C}_1^{ev} = C_t^{ev} \left( \frac{\partial^2 \psi^{ev}}{\partial \varepsilon_t^{ev} \partial \varepsilon_t^{ev}} \right)^{-1} \frac{\partial^2 \psi^{ev}}{\partial \varepsilon_t^{ev} \partial \theta_t}.
\end{aligned}
\]  

(A.11)
Appendix B

In this appendix, linearization of the plastic and viscous dissipation functions $D^p_{mech}$ and $D^v$ is carried out. Recall that these functions are (table 2.1)

$$D^p_{mech} = \sqrt{\frac{2}{3}} \gamma \sigma_y(\theta).$$  \hfill (B.1)

$$D^v = \tau^v_{neq} \cdot \frac{\partial \varphi_v(\tau^v_{neq})}{\partial \tau^v_{neq}} = \tau^v_{neq} \left[ \frac{1}{2 \zeta_D} d e v (\tau^v_{neq}) + \frac{1}{\partial \zeta_v} (\tau^v_{neq} \cdot I) I \right].$$

Applying time discretization to Eq. (B.1) and using Eq. (2.137a), the above equations can be written

$$D^p_{mech,t} = \sqrt{\frac{2}{3}} \Delta t \sigma_{yt}^{\gamma t}, \quad D^v_t = -\frac{1}{\Delta t} \tau^v_t \cdot (e^v_t - e^{eptr}_t).$$  \hfill (B.2)

Now, the linearization of the first equation in (B.2) is given by

$$\Delta D^p_{mech,t} = \sqrt{\frac{2}{3}} \Delta t \sigma_{yt}^{\gamma t} \left\{ \sigma_{yt} \frac{\partial (\Delta \gamma_t)}{\partial e^{eptr}_t} \Delta e^{eptr}_t + \left( \sigma_{yt} \frac{\partial (\Delta \gamma_t)}{\partial \theta_t} + \Delta \gamma_t \sigma_{yt}^{\gamma t} \right) \Delta \theta_t \right\},$$  \hfill (B.3)

where $\frac{\partial (\Delta \gamma_t)}{\partial e^{eptr}_t}$ and $\frac{\partial (\Delta \gamma_t)}{\partial \theta_t}$ are given in Eq. (A.6) of Appendix A. Then, the increment of the second equation in (B.2) becomes

$$\Delta D^v_t = \frac{\partial D^v_t}{\partial e^{eptr}_t} \Delta e^{eptr}_t + \frac{\partial D^v_t}{\partial \theta_t} \Delta \theta_t.$$  \hfill (B.4)
All that remains to do is computation of partial derivatives of the viscous dissipation \( \mathcal{D}_t^v \) with respect to the principal trial elastic logarithmic stretch \( \varepsilon_{t}^{evtr} \) and temperature \( \theta_t \). They are given by

\[
\frac{\partial \mathcal{D}_t^v}{\partial \varepsilon_{t}^{evtr}} = -\frac{1}{\Delta t} \left\{ (\varepsilon_{t}^{ev} - \varepsilon_{t}^{evtr}) C_1^{ev} + \tau_t^{ev} \left( \frac{\partial \varepsilon_{t}^{ev}}{\partial \varepsilon_{t}^{evtr}} - I \right) \right\},
\]

\[
\frac{\partial \mathcal{D}_t^v}{\partial \theta_t} = -\frac{1}{\Delta t} \left\{ \tilde{C}_1^{ev} \cdot (\varepsilon_{t}^{ev} - \varepsilon_{t}^{evtr}) + \tau_t^{ev} \cdot \left( \frac{\partial \varepsilon_{t}^{ev}}{\partial \theta_t} \right) \right\},
\]

where \( C_1^{ev} \) and \( \tilde{C}_1^{ev} \) have been obtained in Eqs. (A.11) of Appendix A. To compute the partial derivatives of \( \varepsilon_{t}^{ev} \) with respect to \( \varepsilon_{t}^{evtr} \) and \( \theta_t \), again take Eqs. (A.10)

\[
\begin{align*}
\frac{d \tau_t^{ev}}{d \varepsilon_t^{ev}} &= \frac{\partial^2 \psi_t^{ev}}{\partial \varepsilon_t^{ev} \partial \varepsilon_t^{ev}} d \varepsilon_t^{ev} + \frac{\partial^2 \psi_t^{ev}}{\partial \varepsilon_t^{ev} \partial \theta_t} d \theta_t \\
\frac{d \tau_t^{ev}}{d \theta_t} &= \left( \frac{\partial^2 \varphi_t}{\partial \tau_t^{ev} \partial \tau_t^{ev}} \right)^{-1} \left( \frac{-d \varepsilon_t^{ev} + d \varepsilon_t^{evtr}}{\Delta t} \right) \\
\frac{d \theta_t}{d \varepsilon_t^{evtr}} &= \mathcal{K}_1 d \varepsilon_t^{evtr} + \tilde{\mathcal{K}}_1 d \theta_t,
\end{align*}
\]

where

\[
\mathcal{K}_1 = \frac{\partial \varepsilon_t^{ev}}{\partial \varepsilon_t^{evtr}} = \left( I + \Delta t \frac{\partial^2 \varphi_t}{\partial \tau_t^{ev} \partial \tau_t^{ev}} \frac{\partial^2 \psi_t^{ev}}{\partial \varepsilon_t^{ev} \partial \varepsilon_t^{ev}} \right)^{-1},
\]

\[
\tilde{\mathcal{K}}_1 = \frac{\partial \varepsilon_t^{ev}}{\partial \theta_t} = -\Delta t \mathcal{K}_1 \frac{\partial^2 \varphi_t}{\partial \tau_t^{ev} \partial \tau_t^{ev}} \frac{\partial^2 \psi_t^{ev}}{\partial \varepsilon_t^{ev} \partial \theta_t}.
\]
Appendix C

In this appendix, linearization of STVPH is performed. Recall from Eq. (2.106) that

$$\mathcal{H} = -\theta \frac{\partial}{\partial \theta} [\mathbf{r} : \mathbf{d} - \mathcal{D}^p_{mech} - \mathcal{D}^v].$$  (C.1)

The above equation can be easily rewritten

$$\mathcal{H} = -\theta \frac{\partial \dot{\psi}}{\partial \theta} + \theta \frac{\partial^2 \psi}{\partial \theta \partial \theta} \dot{\theta} = -\theta \frac{\partial^2 \psi^e_p}{\partial \theta \partial \mathbf{b}^e_p} : \dot{\mathbf{b}}^e_p - \theta \frac{\partial^2 \psi^e_v}{\partial \theta \partial \mathbf{b}^e_v} : \dot{\mathbf{b}}^e_v. \quad (C.2)
$$

Finally, taking advantage of isotropy, performing time discretization using Euler method and using Eq. (2.111), the above equation can be written

$$\mathcal{H} = -\frac{\theta_t}{\theta_R} \left\{ \left( \frac{\partial \psi^e_o}{\partial \xi^e_t} - \frac{\partial \epsilon^e_n}{\partial \xi^e_t} \right) \cdot \left( \frac{\epsilon^e_t - \epsilon^e_n}{\Delta t} \right) \right\} \frac{\partial \mathcal{K}}{\partial \xi_t} \left( \frac{\xi_t - \xi_n}{\Delta t} \right) + \left( \frac{\partial \psi^e_o}{\partial \epsilon^e_t} - \frac{\partial \epsilon^e_n}{\partial \epsilon^e_t} \right) \cdot \left( \frac{\epsilon^e_t - \epsilon^e_n}{\Delta t} \right). \quad (C.3)
$$

The above form of STVPH is more suitable for linearization than the alternative form of Eq. (C.1) from implementation point of view. Thus, its linearization is given by

$$\Delta \mathcal{H} = \frac{\mathcal{H}}{\theta_t} \Delta \theta_t - \frac{\theta_t}{\Delta t \theta_R} \left\{ \frac{\partial^2 \mathcal{K}}{\partial \xi_t^2} \left( \frac{\xi_t - \xi_n}{\Delta t} \right) + \frac{\partial \mathcal{K}}{\partial \xi_t} \right\} \Delta \xi_t$$

$$- \frac{\theta_t}{\Delta t \theta_R} \left\{ \left( \frac{\partial \psi^e_o}{\partial \epsilon^e_t} - \frac{\partial \epsilon^e_n}{\partial \epsilon^e_t} \right) + \left( \epsilon^e_t - \epsilon^e_n \right) \left( \frac{\partial^2 \psi^e_o}{\partial \epsilon^e_t^2} \frac{\partial \epsilon^e_t}{\partial \epsilon^e_t} \right) \right\} \Delta \epsilon^e_t$$

$$- \frac{\theta_t}{\Delta t \theta_R} \left\{ \left( \frac{\partial \psi^e_o}{\partial \epsilon^e_t} - \frac{\partial \epsilon^e_n}{\partial \epsilon^e_t} \right) + \left( \epsilon^e_t - \epsilon^e_n \right) \left( \frac{\partial^2 \psi^e_o}{\partial \epsilon^e_t^2} \frac{\partial \epsilon^e_t}{\partial \epsilon^e_t} \right) \right\} \Delta \epsilon^e_t. \quad (C.4)$$
\[
- \frac{\theta_t}{\Delta t \theta_R} \left( (\epsilon_t^{ep} - \epsilon_n^{ep}) \cdot \left( \frac{\partial^2 \psi_o^{ep}}{\partial \epsilon_t^{ep} \partial \theta} \right) + (\epsilon_t^{ev} - \epsilon_n^{ev}) \cdot \left( \frac{\partial^2 \psi_o^{ev}}{\partial \epsilon_t^{ev} \partial \theta} \right) \right) \Delta \theta_t.
\]

One does only need to have the strain-like increment $\Delta \xi_t$ and also elastic-plastic and elastic-viscous logarithmic stretch increments $\Delta \epsilon_t^{ep}$ and $\Delta \epsilon_t^{ev}$ in Eq. (C.4). Using Eqs. (2.137c), (2.114), (A.3), (A.4) and (A.6), they are given by

\[
\{ \Delta \epsilon_t^{ep} \} = \left[ T_{3 \times 3} \quad T_{3 \times 1} \right] \left\{ \Delta \epsilon_t^{epr} \right\},
\]

where

\[
T = \left( \frac{\partial^2 \psi}{\partial \epsilon_t^{ep} \partial \epsilon_t^{ep}} \right)^{-1} \left[ I - \frac{1}{M} U^* \bar{N} \right] U^*,
\]

\[
\bar{T} = \left( \frac{\partial^2 \psi}{\partial \epsilon_t^{ep} \partial \epsilon_t^{ep}} \right)^{-1} \left[ -\frac{\partial^2 \psi}{\partial \epsilon_t^{ep} \partial \theta_t} \right]
\]

\[
\left. + \left( I - \frac{1}{M} U^* \bar{N} \right) U^* + \frac{1}{M} \left( \frac{\partial \dot{\phi}}{\partial \beta_t} \bar{U} + \frac{\partial \phi}{\partial \beta_t} \right) \left( U^* \frac{\partial \phi}{\partial \epsilon_t^{ep}} \right) \right].
\]

Now, upon substitution for $\Delta \epsilon_t^{ep}$ and $\Delta \xi_t$ from Eq. (C.5) and also Eq. (B.6), for $\Delta \epsilon_t^{ev}$, the increment of STVPH takes the following final form

\[
\Delta \mathcal{H} = \left( \frac{\mathcal{H}}{\dot{\theta}_t} + \bar{H}_t \right) \Delta \theta_t + \bar{H}_{ep} \cdot \Delta \epsilon_t^{epr} + \bar{H}_{ev} \cdot \Delta \epsilon_t^{evr},
\]

where

\[
\bar{H}_{ep} = -\dot{\theta}_t (\bar{\epsilon}_t^{ep} T + \xi_t^{*} T^T),
\]

\[
\bar{H}_{ev} = -\dot{\theta}_t (\bar{\epsilon}_t^{ev} \bar{K}_1),
\]

\[
\bar{H}_\theta = -\dot{\theta}_t (\bar{\epsilon}_t^{ep} \bar{T} + \xi_t^{*} \bar{F} + \bar{\epsilon}_t^{ev} \bar{K}_1 + \omega),
\]

in which

\[
\bar{\epsilon}_t^{ep} = \left( \frac{\partial^2 \psi}{\partial \epsilon_t^{ep} \partial \epsilon_t^{ep}} \right) (\epsilon_t^{ep} - \epsilon_n^{ep}) + \left( \frac{\partial \psi}{\partial \epsilon_t^{ep}} - \frac{\partial \psi_o}{\partial \epsilon_t^{ep}} \right),
\]

\[
\bar{\epsilon}_t^{ev} = \left( \frac{\partial^2 \psi}{\partial \epsilon_t^{ev} \partial \epsilon_t^{ev}} \right) (\epsilon_t^{ev} - \epsilon_n^{ev}) + \left( \frac{\partial \psi}{\partial \epsilon_t^{ev}} - \frac{\partial \psi_o}{\partial \epsilon_t^{ev}} \right).
\]
\[
\bar{\xi}_t = \frac{\partial^2 \mathcal{K}}{\partial \xi_t^2} (\xi_t - \xi_n) + \frac{\partial \mathcal{K}}{\partial \xi_t},
\]

\[
\omega = (\varepsilon_{te}^{ep} - \varepsilon_{ne}^{ep}) \left( \frac{\partial^2 \psi_{o}^{ep}}{\partial \varepsilon_{te}^{ep} \partial \theta} \right) + (\varepsilon_{te}^{ev} - \varepsilon_{ne}^{ev}) \left( \frac{\partial^2 \psi_{o}^{ev}}{\partial \varepsilon_{te}^{ev} \partial \theta} \right), \quad \bar{\theta}_t = \frac{\theta_t}{\Delta t \theta_R}. \quad \text{(C.9b)}
\]
Appendix D

In this appendix, it is algorithmically shown that $\varepsilon^{ep}$, $\varepsilon^{ev}$, and $\xi$ are functions of $\{\theta, F\}$. Since the thermo-plastoelastic and thermo-viscoelastic parts have the same structure for the developed models, it is mainly focused on $\varepsilon^{ep}$ and the results can be consistently applied to the viscoelastic part. First, one should have the trial stretches as a function of the deformation gradient. To do this, remember that

$$C_{ep}^{tr} = \sum_{a=1}^{3} (\lambda_{a}^{ep tr})^2 N_{a}^{ep} \otimes N_{a}^{ep}, \quad \varepsilon_{a}^{ep tr} = \ln(\lambda_{a}^{ep tr}). \quad (D.1)$$

From the above equation, one can easily obtain

$$\frac{\partial \lambda_{a}^{ep tr}}{\partial C_{ep}^{tr}} = \frac{1}{2\lambda_{a}^{ep tr}} N_{a}^{ep} \otimes N_{a}^{ep} = \frac{e^{-\varepsilon_{a}^{ep tr}}}{2} N_{a}^{ep} \otimes N_{a}^{ep}. \quad (D.2)$$

The increment of the elastic-plastic trial stretch $\lambda_{a}^{ep tr}$ delivers

$$\Delta \lambda_{a}^{ep tr} = \lambda_{a}^{ep tr} \Delta \varepsilon_{a}^{ep tr} = \frac{1}{2\lambda_{a}^{ep tr}} N_{a}^{ep} \otimes N_{a}^{ep} : \Delta C_{ep}^{tr} \Rightarrow$$

$$\Delta \varepsilon_{a}^{ep tr} = \frac{1}{2\lambda_{a}^{ep tr}} N_{a}^{ep} \otimes N_{a}^{ep} : \Delta C_{ep}^{tr}. \quad (D.3)$$

Applying the increment of the Euler-Almansi strain tensor $\Delta e = F_{ep}^{tr - T}(\Delta C_{ep}^{tr}/2) F_{ep}^{tr - 1}$ in the result of the above equation gives

$$\Delta \varepsilon_{a}^{ep tr} = \frac{1}{(\lambda_{a}^{ep tr})^2} N_{a}^{ep} \otimes N_{a}^{ep} : F_{ep}^{tr - T} \Delta e F_{ep}^{tr}$$

$$= n_{a}^{ep} \otimes n_{a}^{ep} : \Delta e = n_{a}^{ep} \otimes n_{a}^{ep} : \Delta FF^{-1} = n_{a}^{ep} \otimes F^{-1} n_{a}^{ep} : \Delta F. \quad (D.4)$$

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In the similar way, one can obtain the increment of the logarithmic elastic-viscous stretch $\Delta \varepsilon_{a}^{\text{evtr}}$

\[
\Delta \varepsilon_{a}^{\text{evtr}} = \frac{\partial \varepsilon_{a}^{\text{evtr}}}{\partial F} : \Delta F = n_{a}^{\text{ev}} \otimes F^{-1} n_{a}^{\text{ev}} : \Delta F. \tag{D.5}
\]

In what follows, Eq. (D.5) is derived in an alternative way for the interested readers. This time, $\varepsilon_{a}^{\text{eptr}}$ is a function of $b_{ep}^{tr}$ and

\[
\Delta \varepsilon_{a}^{\text{eptr}} = \frac{\partial \varepsilon_{a}^{\text{eptr}}}{\partial b_{ep}^{tr}} : \frac{\partial b_{ep}^{tr}}{\partial F} : \Delta F \quad \text{where}
\]

\[
\frac{\partial \varepsilon_{a}^{\text{eptr}}}{\partial b_{ep}^{tr}} = \frac{\partial \varepsilon_{a}^{\text{eptr}}}{\partial \left(\lambda_{a}^{\text{eptr}}\right)^2} \frac{\partial \lambda_{a}^{\text{eptr}}}{\partial b_{ep}^{tr}} = \frac{1}{2 \left(\lambda_{a}^{\text{eptr}}\right)^2} \left(n_{a}^{\text{ep}} \otimes n_{a}^{\text{ep}}\right). \tag{D.6}
\]

To derive $\frac{\partial b_{ep}^{tr}}{\partial F}$, one can consider $b_{ep}^{tr} = F(C_{p}^{-1})_{n} F^{T}$ and write

\[
\frac{\partial b_{ep}^{tr}}{\partial F} = \frac{\partial \left(F(C_{p}^{-1})_{n} F^{T}\right)}{\partial F} \bigg|_{C_{p}} \Rightarrow
\]

\[
\frac{\partial b_{ep}^{tr}}{\partial F} = \frac{\partial \left(F(C_{p}^{-1})_{n} F^{T}\right)}{\partial F} \bigg|_{C_{p}} = \frac{\partial \left(F_{iB}[C_{p}^{-1}]_{BC} F_{jC}\right)}{\partial F_{kA}} = 
\]

\[
\delta_{ik} \delta_{AB} [C_{p}^{-1}]_{BC} F_{jC} + F_{iB}[C_{p}^{-1}]_{BC} \delta_{jk} \delta_{AC} = \delta_{ik} [C_{p}^{-1}]_{AC} F_{jC} + F_{iB}[C_{p}^{-1}]_{BA} \delta_{jk}.
\]

Now, the contraction between the first two terms on the right hand side of the first equation in (D.6) can be performed

\[
\left(\frac{\partial \varepsilon_{a}^{\text{eptr}}}{\partial b_{ep}^{tr}}\right)_{ij} \left(\frac{\partial b_{ep}^{tr}}{\partial F}\right)_{ijkA} = 
\]

\[
\frac{1}{2 \left(\lambda_{a}^{\text{eptr}}\right)^2} \left\{ \left(n_{a}^{\text{ep}}\right)_{i} \left(n_{a}^{\text{ep}}\right)_{j} \left[ \delta_{ik} [C_{p}^{-1}]_{AC} F_{jC} + F_{iB}[C_{p}^{-1}]_{BA} \delta_{jk} \right] \right\} = \tag{D.8}
\]

\[
\frac{1}{2 \left(\lambda_{a}^{\text{eptr}}\right)^2} \left\{ \left(n_{a}^{\text{ep}}\right)_{k} \left(n_{a}^{\text{ep}}\right)_{j} F_{jC}[C_{p}^{-1}]_{CA} + \left(n_{a}^{\text{ep}}\right)_{i} F_{iB}[C_{p}^{-1}]_{BA} \right\}.
\]

The above equation can be written

\[
\frac{\partial \varepsilon_{a}^{\text{eptr}}}{\partial b_{ep}^{tr}} : \frac{\partial b_{ep}^{tr}}{\partial F} = \frac{1}{\left(\lambda_{a}^{\text{eptr}}\right)^2} n_{a}^{\text{ep}} \otimes C_{p}^{-1} F^{T} n_{a}^{\text{ep}}. \tag{D.9}
\]

Note that
\[
\begin{aligned}
\left\{ \begin{array}{l}
C_p^{-1} F^T = F^{-1} b_{ep}^{tr} \\
(b_{ep}^{tr} n_{\alpha}^{ep} = (\lambda_{ev}^{tr})^2 n_{\alpha}^{ep} \Rightarrow \quad C_p^{-1} F^T n_{\alpha}^{ep} = (\lambda_{ev}^{tr})^2 F^{-1} n_{\alpha}^{ep}.
\end{array} \right.
\end{aligned}
\] (D.10)

Applying the result of Eq. (D.10) in Eq. (D.9), and the introduction of the resulted equation in equation (D.6) presents the $\varepsilon^{ep tr}$ as a function of the deformation gradient as derived in Eq. (D.4). Finally, using Eqs. (C.5), (B.6), (D.4) and (D.5), one can obtain

\[
\begin{aligned}
\Delta \varepsilon_i^{ep} &= \frac{\partial \varepsilon_i^{ep}}{\partial F} \Delta F + \frac{\partial \varepsilon_i^{ep}}{\partial \theta} \Delta \theta, \\
\Delta \xi &= \frac{\partial \xi}{\partial F} \Delta F + \frac{\partial \xi}{\partial \theta} \Delta \theta, \\
\Delta \varepsilon_i^{ev} &= \frac{\partial \varepsilon_i^{ev}}{\partial F} \Delta F + \frac{\partial \varepsilon_i^{ev}}{\partial \theta} \Delta \theta,
\end{aligned}
\] (D.11)

where

\[
\begin{aligned}
\frac{\partial \varepsilon_i^{ep}}{\partial F} &= \sum_{a=1}^{3} (\mathcal{J})_{ia} n_{a}^{ep} \otimes F^{-1} n_{a}^{ep}, \quad \frac{\partial \varepsilon_i^{ep}}{\partial \theta} = (\mathcal{J})_{i}, \\
\frac{\partial \xi}{\partial F} &= \sum_{a=1}^{3} (\mathcal{J}^*)_{a} n_{a}^{ep} \otimes F^{-1} n_{a}^{ep}, \quad \frac{\partial \xi}{\partial \theta} = (\mathcal{J}^*), \\
\frac{\partial \varepsilon_i^{ev}}{\partial F} &= \sum_{a=1}^{3} (\mathcal{K}_1)_{ia} n_{a}^{ev} \otimes F^{-1} n_{a}^{ev}, \quad \frac{\partial \varepsilon_i^{ev}}{\partial \theta} = (\mathcal{K}_1)_{i}.
\end{aligned}
\]
Appendix E

Assume a domain $\mathcal{B}_0$ with position vector $X$, the element surface $dA$ and outward unit vector $N$. The following equations hold for mechanical and thermal parts,

### E.1 Mechanical part

\[
\langle F \rangle_{v_0} = \frac{1}{|v_0|} \int_{v_0} \left( F = \frac{\partial x}{\partial X} \right) dV = \frac{1}{|v_0|} \int_{v_0} x \otimes N \; dA, \quad (E.1a)
\]

\[
\frac{1}{|v_0|} \int_{\partial v_0} p \otimes X \; dA = \frac{1}{|v_0|} \int_{\partial v_0} PN \otimes X \; dA = \frac{1}{|v_0|} \int_{v_0} \text{Div}(P) \otimes X \; dV, \quad (E.1b)
\]

\[
\frac{1}{|v_0|} \int_{\partial v_0} p.\dot{x} \; dA = \frac{1}{|v_0|} \int_{\partial v_0} PN.\dot{x} \; dA = \frac{1}{|v_0|} \int_{v_0} \frac{\partial (P^T \dot{x})}{\partial X} \; dV = \frac{1}{|v_0|} \int_{v_0} P.\dot{F} \; dV + \frac{1}{|v_0|} \int_{v_0} \text{Div}(P).\dot{x} \; dV. \quad (E.1c)
\]
E.2 Thermal part

\[
\langle G \rangle_{v_0} = \frac{1}{|v_0|} \int_{v_0} \left( G = \frac{\partial \theta}{\partial \mathbf{X}} \right) dV = \frac{1}{|v_0|} \int_{\partial v_0} \theta \mathbf{N} dA, \quad \text{(E.2a)}
\]
\[
\frac{1}{|v_0|} \int_{\partial v_0} (-\mathbf{Q} \cdot \mathbf{N} \equiv \mathbf{q}) \mathbf{X} dA = -\frac{1}{|v_0|} \int_{v_0} \text{Div}(\mathbf{Q}) \mathbf{X} dV - \frac{1}{|v_0|} \int_{v_0} \mathbf{Q} dV, \quad \text{(E.2b)}
\]
\[
\frac{1}{|v_0|} \int_{\partial v_0} (-\mathbf{Q} \cdot \mathbf{N} \equiv \mathbf{q}) \theta dA
\]
\[
= -\frac{1}{|v_0|} \int_{v_0} \mathbf{Q} \cdot \mathbf{G} dV - \frac{1}{|v_0|} \int_{v_0} \text{Div}(\mathbf{Q}) \theta dV. \quad \text{(E.2c)}
\]

Thus,

\[
\langle P \rangle_{v_0} = \frac{1}{|v_0|} \int_{\partial v_0} \mathbf{p} \otimes \mathbf{X} dA, \quad \text{(E.3a)}
\]
\[
\langle P : \dot{\mathbf{F}} \rangle_{v_0} = \frac{1}{|v_0|} \int_{\partial v_0} \mathbf{p} \cdot \dot{\mathbf{x}} dA, \quad \text{(E.3b)}
\]
\[
\langle Q \rangle_{v_0} = -\frac{1}{|v_0|} \int_{\partial v_0} \mathbf{q} \mathbf{X} dA, \quad \text{(E.3c)}
\]
\[
\langle Q : \mathbf{G} \rangle_{v_0} = -\frac{1}{|v_0|} \int_{\partial v_0} \mathbf{q} \theta dA. \quad \text{(E.3d)}
\]

In order to satisfy the micro-macro energy criterion for the mechanical and thermal parts, one should have (based on Eqs. (E.3))

\[
\langle P : \dot{\mathbf{F}} \rangle_{v_0} = \langle P \rangle_{v_0} : \langle \dot{\mathbf{F}} \rangle_{v_0}, \quad \text{(E.4a)}
\]
\[
\langle Q : \mathbf{G} \rangle_{v_0} = \langle Q \rangle_{v_0} : \langle \mathbf{G} \rangle_{v_0}. \quad \text{(E.4b)}
\]

This can be done by considering the following three types of BCs for the given set \{\mathbf{F}, \mathbf{G}, \mathbf{P}, \mathbf{Q}\} in the standard way

1. Linear (LN): \( x = \mathbf{F} \mathbf{X} \), \( \theta = (\mathbf{G} \cdot \mathbf{X}) \).
2. Periodic (PR): For a periodic \( x, \theta \) and an anti-periodic \( p, \varphi \):

\[
x^+ - x^- = \bar{F}(X^+ - X^-), \quad \theta^+ - \theta^- = \bar{G}.(X^+ - X^-),
\]

\[
p^+ = \bar{P}N^+ = -\bar{P}N^- = -p^- , \quad q^+ = -\bar{Q}.N^+ = \bar{Q}.N^- = -q^-.
\]

3. Uniform (UF): \( p = \bar{P}N \), \( q = -\bar{Q}.N \).

In this work, the framework is driven via \( \bar{F} \) and \( \bar{G} \) such that \( \langle F \rangle \leftarrow \bar{F} \) \& \( \langle G \rangle_{\nu_0} \leftarrow \bar{G} \) is enforced and \( \bar{P} \leftarrow \langle P \rangle_{\nu_0} \) \& \( \bar{Q} \leftarrow \langle Q \rangle_{\nu_0} \) is measured. Please note that to ensure the uniqueness of the results, current position and temperature should be prescribed at a single point on the boundary (periodic and uniform boundary conditions).
Appendix F

Here, the consistent BCs under whom the criterion (4.25) holds are examined. To do this, one should investigate that the macroscopic current configuration quantities \( \bar{g} = \bar{F}^{-T} \bar{G} \) \& \( \bar{q} = \bar{j}^{-1} \bar{F} \bar{Q} \) equal the volume average of their microscopic counterparts

\[
\bar{g} = \langle g \rangle \quad \& \quad \bar{q} = \langle q \rangle,
\]  

(F.1)

where \( g \) and \( q \) are induced by the thermal phase on the \( v_0 \). Defining \( \bar{g}^* = \langle g \rangle_v \) \& \( \bar{q}^* = \langle q \rangle_v \) one should show \( \bar{g} = \bar{g}^* \) \& \( \bar{q} = \bar{q}^* \) as follows.

F.1 Temperature gradient

Based on the standard BCs employed during the mechanical phase, the analysis is resolved into the three parts:

1. LN-BCs: In this case \( \bar{\rho}_0 = \bar{\rho} \bar{f} \) \& \( |B| = |v| = \bar{j}|v_0| \) and \( x = \bar{F}X \) is independent of the internal microstructure. Based on the Nanson’s formula, one can have

\[
\bar{g}^* = \frac{1}{|B|} \int_{\partial v} \theta n \, da = \frac{1}{|v_0|} \int_{\partial v_0} \theta \bar{f} \bar{F}^{-T} \bar{N} \, dA = \frac{\bar{F}^{-T}}{|v_0|} \int_{\partial v_0} \theta \bar{N} \, dA
\]

(F.2)

Thus, one can conclude \( \bar{g} = \bar{g}^* \) independent of the BCs employed during the thermal phase.

2. PR-BCs: In this case again \( \bar{\rho}_0 = \bar{\rho} \bar{f} \) \& \( |v| = \bar{j}|v_0| \) holds. Assuming \( \theta \) satisfies periodicity on \( B_0 \), one can obtain
\( \bar{g}^* = \frac{1}{|v|} \int_\partial v \theta n \, da = \frac{1}{|v|} \int_{\partial v^+} \theta^+ n^+ \, da + \frac{1}{|v|} \int_{\partial v^-} \theta^- n^- \, da \)

\[ = \frac{1}{|v|} \int_{\partial v^+} (\theta^+ - \theta^-) n^+ \, da = \frac{1}{|v|} \int_{\partial v^+} \bar{G} \cdot (X^+ - X^-) n^+ \, da \]

\[ = \frac{1}{|v|} \int_{\partial v^+} \bar{G} \bar{F}^{-1} (x^+ - x^-) n^+ \, da = \frac{\bar{F}^{-T} \bar{G}}{|v|} \int_{\partial v^+} (x^+ - x^-) \otimes n^+ \, da \]

\[ = \frac{\bar{F}^{-T} \bar{G}}{|v|} \int \nabla(x) \, dv = \bar{F}^{-T} \bar{G}. \]

Thus, LN- or PR-BCs should be applied during the thermal phase to ensure \( \bar{g} = \bar{g}^* \).

3. **UF-BCs:** In this case \( \bar{\rho}_0 \neq \bar{\rho} \bar{f} \) since \( \bar{f} \neq \langle f \rangle \), and therefore \( \bar{g} = \bar{g}^* \) is not guaranteed.

### F.2 Heat flux

Again the procedure is decomposed into three parts based on the mechanical phase BCs:

1. **LN-BCs:** In view of the above assumptions to obtain \( \bar{g}^* \), one can have

\[ hda = -(q). (nda) = -(q). (\bar{f} F^{-T} N \, dA) = -(\bar{f} F^{-1} q). (N \, dA) = -(Q). (N \, dA) = h_0 dA \]

Consequently,

\[ \bar{q}^* = \frac{-1}{|v|} \int_{\partial v} h x \, da = \frac{-1}{|\mathcal{B}_0|} \int_{\partial v_0} h_0 \bar{F}X \, dA = \frac{-\bar{F}}{|\mathcal{B}_0|} \int_{\partial v_0} h_0 X \, dA \]

\[ = \bar{f}^{-1} \bar{F}(Q)_{v_0}. \]

Therefore, one can conclude \( \bar{q} = \bar{q}^* \) independent of the BCs employed during the thermal phase as in the temperature gradient case.

2. **PR-BCs:** Taking into account \( \bar{\rho}_0 = \bar{\rho} \bar{f} \) & \( |v| = \bar{f}|v_0| \) and assuming \( h \) satisfies anti-periodicity on \( \mathcal{B}_0 \), one can write
\[ \bar{q}^* = -\frac{1}{|\mathcal{U}|} \int h_x \, da = -\frac{1}{|\mathcal{B}|} \int h^+ x^+ \, da - \frac{1}{|\mathcal{B}|} \int h^- x^- \, da \]

\[ = -\frac{1}{|\mathcal{B}|} \int h^+(x^+ - x^-) \, da = -\frac{1}{|\mathcal{B}|} \int h^+ \bar{F}(X^+ - X^-) \, da \quad (F.6) \]

\[ = - \frac{\bar{F}}{\mathcal{J}|\mathcal{B}_0|} \int h_0^+(X^+ - X^-) \, dA = \frac{-(\bar{J}^{-1} \bar{F})}{|\mathcal{U}_0|} \int h_0 X \, dA = \bar{J}^{-1} \bar{F}(\mathcal{Q})_{\mathcal{B}_0}. \]

Thus, PR- or UF-BCs should be applied during the thermal phase to guarantee \( \bar{q} = \bar{q}^* \).

3. **UF-BCs**: As before since \( \bar{J} \neq \langle J \rangle \), in general \( \bar{g} = \bar{g}^* \) cannot be guaranteed. So, it is understood that one cannot always revert to a definition \( \bar{g}^* = \langle g \rangle_{\mathcal{B}} \) while \( \langle G \rangle \leftarrow \bar{G} \) is enforced unless its value equals to the evolution of \( \bar{g} \) induced by the macroscale problem. In other words, the supplementary dissipation criterion (4.25) must hold which guarantees that from \( \bar{D}_{\mathcal{B}_0} = \langle D_{\mathcal{B}_0} \rangle_{\mathcal{U}_0} \) one can always revert to \( \bar{D} = \langle D \rangle_{\mathcal{U}} \)

\[ \bar{D}_{\mathcal{B}_0} = - \frac{\bar{Q} \cdot \bar{G}}{\bar{\theta}} = \langle - \frac{Q \cdot G}{\theta} \rangle_{\mathcal{U}_0} = - \frac{1}{\bar{\theta}} \langle Q \rangle_{\mathcal{U}_0} \cdot \langle G \rangle_{\mathcal{U}_0} = \langle D_{\mathcal{B}_0} \rangle_{\mathcal{U}_0} = - \frac{1}{\bar{\theta}|\mathcal{U}_0|} \int Q \cdot G \, dV \]

\[ = - \frac{\bar{J}}{\theta|\mathcal{U}|} \int q \cdot g \, dv = \bar{J} \langle - \frac{q \cdot g}{\theta} \rangle_{\mathcal{U}} = - \frac{\bar{J}}{\bar{\theta}} \langle q \rangle_{\mathcal{U}} \cdot \langle g \rangle_{\mathcal{U}} = \bar{J} \langle D \rangle_{\mathcal{U}}. \quad (F.7) \]
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