A VARIATIONAL FORMULATION FOR A SET OF HYPERELASTIC-VISCOPLASTIC MATERIAL MODELS IN A FULLY COUPLED THERMO-MECHANICAL PROBLEM

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Abstract. Many different contexts in solid mechanics demand the consideration of thermal effects during deformation. Be it intrinsic material properties (e.g. glass transition temperatures of rubber-like polymers) or specific deformation regimes (large strain and strain rates), there is plenty of motivation for the study of thermo-mechanical coupling. In this paper, an adiabatic problem is considered. A fully coupled thermo-mechanical problem is formulated. Isotropic hyperelastic-viscoplastic materials are considered in a variational structure. The classical multiplicative decomposition of deformation in elastic and inelastic (plastic) parts is used in the construction of the incremental pseudo-potential, together with the hypothesis of isochoric inelastic deformation. This leads to the use of separate potentials associated with volumetric, isochoric elastic and plastic deformations, purely thermal accumulation and dissipated energy. The use of different potentials commonly found in literature is explored. Temperature dependence for all the potentials, the essence of the fully coupled thermo-mechanical problem, is briefly discussed. It is important to note that assuming no local heat generation or heat flux allows for temperature to be considered as an additional internal variable. A radial-return mapping scheme and elastic predictor states are used in the solution of the resulting non-linear problem with respect to temperature and cumulated plastic strain. Temperature increase, heat dissipation and entropy change are examples of what can be predicted by the model. Applications to selected materials are presented.

Keywords: Thermo-mechanical coupling, Variational formulation, Constitutive updates

1. INTRODUCTION

The application of variational principles for dissipative mechanical systems has been the theme of many recent papers. Ortiz and Stainier (1999) developed variational constitutive updates for a rather general range of material models, including irreversible, dissipative and rate-dependent behaviors. The works of Fancello et al. (2006), with application to nonlinear finite viscoelasticity problems, and Fancello et al. (2008), extending the approach of the previous paper to finite isotropic viscoplasticity, base the construction of constitutive updates on the use of spectral quantities of independent variables. This allowed for the adoption of a wider variety of potentials within the same formalism.

Owing to the need to consider thermal effects in many contexts, the study of thermo-mechanically coupled formulations has also been of recent interest. Yang et al. (2006) and Stainier and Ortiz (2008) list a number of fields of application where the assumption of mechanical behavior independent of thermal effects proves to be insufficient. In such diverse applications such as metal forming and ballistic penetration, common characteristics such as high strain rates and heat dissipation due to plastification indicate the conditions that motivate the construction of coupled thermo-mechanical models for dissipative materials.

The aim of the present paper is to extend the formulation used by Fancello et al. (2008) to an adiabatic fully-coupled thermo-viscoplastic model. Potentials based on spectral quantities are used in order to allow for more versatility. By considering the problem to be adiabatic (a reasonable hypothesis when the time range under consideration is short, according to Stainier and Ortiz (2008)), thermal effects can be treated locally, and temperature becomes an internal variable.

2. INCREMENTAL FORMULATIONS FOR PURELY MECHANICAL PROBLEMS

In searching for variational formulations for general inelastic problems, the existence of a pseudo-potential function $\psi$, dependent on strains and internal variables describing the dissipative behavior of the material, is assumed. It is referred to as a pseudo-potential because, despite not being able to describe the state of stress for any strain state (i.e. despite not being hyperelastic in strict sense), it holds hyperelastic-like properties within the load increment:
\[
P_{n+1} = \frac{\partial \Psi(F_{n+1}; \epsilon_n)}{\partial F_{n+1}} = 2F_{n+1} \frac{\partial \Psi(C_{n+1}; \epsilon_n)}{\partial C_{n+1}} \tag{1}
\]

Where: \(P_{n+1}\) is the first Piola-Kirchhoff stress tensor at load step \(n+1\); \(F\) is the deformation gradient; \(C\) is the right Cauchy-Green tensor; and \(\epsilon_n\) is a set of internal variables, defined accordingly to the considered problem.

Such a formulation, based on the construction of an incremental pseudo-potential for every load step, is elsewhere explored in detail, e.g. in the works of Ortiz and Stainier (1999), Radovitzky and Ortiz (1999), Fancello et al. (2006) and Fancello et al. (2008). When no thermal effects are considered, the pseudo-potential used to describe a wide variety of inelastic problems takes on the following form:

\[
\Psi(F_{n+1}, \epsilon_n) = \min_{\epsilon_{n+1}} \left\{ W(\epsilon_{n+1}) - W(\epsilon_n) + \Delta t \Psi(\dot{\epsilon}_{n+1}; \epsilon_n) \right\}
\tag{2}
\]

Where \(W\) denotes a Helmholtz free energy density; \(\psi\) denotes a dissipation potential; \(\epsilon\) includes external variable \(F\) (deformation gradient) and internal variables \(F^\text{P}\) (inelastic part of deformation gradient) and \(Q\) (describing remaining internal processes); and \(\dot{\epsilon}\) denotes the rate equations for the set of variables \(\epsilon\).

Since we wish to extend the previous formulation to a thermo-mechanical context, it is necessary to define an appropriate set of internal variables, to redefine the Helmholtz free energy density and to explore the laws of thermodynamics in order to build an incrementally consistent pseudo-potential.

### 3. EXTENSION OF THE VARIATIONAL FORMULATION TO THERMO-MECHANICAL VISCOPLASTIC PROBLEMS

#### 3.1. Definitions and hypotheses

Before we delve into the thermodynamical aspects of the present model, some basic hypotheses are presented.

The classical multiplicative decomposition of the deformation gradient in elastic (\(F^\text{E}\)) and plastic (\(F^\text{P}\)) parts is also used here:

\[
F = F^\text{E}F^\text{P} \tag{3}
\]

It is assumed that all plastic deformations are isochoric. Therefore, we may consider the following multiplicative decomposition of the deformation gradient, in volumetric (\(F^\text{vol}\)) and isochoric (\(F\)) parts, and the consequent useful definitions of an isochoric elastic right Cauchy-Green tensor (\(\hat{C}^\text{e}\)), and the related natural strain (\(\epsilon^\text{e}\)), both decomposed in their respective spectral quantities:

\[
F = F^\text{vol}F \tag{4}
\]

\[
J = \det F \quad \hat{F} = \frac{1}{J^{1/3}} F \tag{5}
\]

\[
\hat{F} = \hat{F}^\text{P}\hat{F}^\text{E} \quad \det F^\text{P} = 1 \tag{6}
\]

\[
\hat{C}^\text{e} = \hat{F}^\text{E}^T\hat{F}^\text{E} = \sum_{i=1}^{3} c_i^\text{e}E_i^\text{e} \quad \epsilon^\text{e} = \frac{1}{2} \ln \hat{C}^\text{e} = \sum_{i=1}^{3} \epsilon_i^\text{e}E_i^\text{e} \quad \epsilon_i^\text{e} = \frac{1}{2} \ln c_i^\text{e} \tag{7}
\]

Considering a von Mises type flow rule for the plastic part, the rate of plastic deformation (\(D^\text{P}\)) may be decomposed in terms of amplitude (\(\dot{q}\)) and direction (\(M\)). Ortiz and Stainier (1999) show that combining this decomposition with logarithmic strains and quadratic hyperelastic (Hencky) potentials yields a complete separation of kinematic aspects (direction \(M\)) and constitutive aspects (\(\dot{q}\)). Thus, expressions similar to those of infinitesimal plasticity can be obtained.

\[
D^\text{P} = \text{sym}(L^\text{P}) = \hat{F}^\text{P}\hat{F}^\text{P}^{-1} \tag{8}
\]

\[
D^\text{P} = \dot{q}M \quad \dot{q} \in \mathbb{R}^+ \quad M \in K_M = \left\{ N \in \text{Sym}: N \cdot N = \frac{3}{2}; N \cdot I = 0 \right\} \tag{9}
\]

If a spectral decomposition of \(D^\text{P}\) is used, it is possible to extend the separation of kinematic and constitutive aspects to more general potentials:
\[ D^\circ = \dot{\mathbf{q}} \sum_{i=1}^{3} q_i \mathbf{M}_i \]  

(10)

\[ \dot{\mathbf{q}} \in \mathbb{R}^+ \quad q_i \in K_Q = \left\{ p_i \in \mathbb{R}^3 : \sum_{i=1}^{3} p_i = 0 ; \sum_{i=1}^{3} p_i^2 = \frac{3}{2} \right\} \]

(11)

\[ \mathbf{M}_i \in K_M = \left\{ N_1 \in \text{Sym}: N_1 \cdot N_1 = 1; N_1 \cdot N_j = 0, i \neq j \right\} \]

(12)

The set \( K_Q \) enforces the traceless properties of \( \mathbf{M} \), necessary since the plastic flow has to be incompressible and is considered irrotational (hypothesis of zero plastic spin), while the set \( K_M \) enforces properties of eigenprojections. The relations above allow for a complete representation of the plastic deformation gradient in terms of \( \dot{\mathbf{q}}, q_i \), and \( \mathbf{M}_i \).

### 3.2. Thermodynamic aspects

The inclusion of thermomechanical coupling within the present variational formalism was firstly stated in Yang et al. (2006). In this paper we combine that approach with spectral decomposition (Eqs. 10-12) in order to allow the use of general isotropic hyperelastic laws suitable e.g. to polymeric materials.

We begin by postulating the existence a Helmholtz free energy density \( W \), dependent on a set of external (an imposed \( \mathbf{F} \)) and internal variables (cumulated plastic strain on the load step \( \Delta \mathbf{q} = \dot{\mathbf{q}} \Delta t \), plastification directions \( q_i \), eigenprojections \( \mathbf{M}_i \), and temperature \( T \)). Derivatives of the Helmholtz free energy density with respect to independent variables give thermodynamic forces associated to them. The entropy density per unit of undeformed volume \( \eta \) is the thermodynamic force associated to the temperature \( T \), just as the first Piola-Kirchhoff stress tensor \( \mathbf{P} \) is the thermodynamic force associated to the total strain.

By means of a Legendre-Fenchel transform of the equation above, we define the specific internal energy (per unit of undeformed volume) as:

\[
U(\mathbf{F}, q, q_i, \mathbf{M}_i, \eta) = \sup_T [\rho_0 \eta T + W(\mathbf{F}, q, q_i, \mathbf{M}_i, T)]
\]

(13)

We may now introduce the first law of thermodynamics in local form, as deducted by Holzapfel (2000), with \( \mathbf{H} \) denoting the heat flux vector, \( Q \) denoting local heat generation per unit undeformed volume and the term \( \mathbf{P} : \dot{\mathbf{F}} \) representing the stress power:

\[
\dot{U} = \mathbf{P} : \dot{\mathbf{F}} - \text{Div} \mathbf{H} + Q
\]

(14)

The second law of thermodynamics is then introduced, in a local form of the Clausius-Duhem inequality, where \( \dot{\eta} \) indicates the local production of entropy:

\[
\mathbf{P} : \dot{\mathbf{F}} - \dot{U} + T\dot{\eta} - \frac{\mathbf{H}}{T} \text{Grad} T \geq 0
\]

(15)

The last term on the left-hand side indicates the production of entropy due to heat conduction. Heat flux occurs from warmer to colder regions of a body, which means that this term must be non-negative. Thus, a stronger form of the second law of thermodynamics, known as the Clausius-Planck inequality, introducing the concept of internal dissipation \( (D_{\text{int}}) \):

\[
D_{\text{int}} = \mathbf{P} : \dot{\mathbf{F}} - \dot{U} + T\dot{\eta} \geq 0
\]

(16)

Combining the Clausius-Planck inequality with the local form of the first law of thermodynamics presented above, we arrive at the energy balance in entropy form, which will later serve as the equation for entropy evolution along the load step of the incremental problem:

\[
T\dot{\eta} = D_{\text{int}} - \text{Div} \mathbf{H} + Q
\]

(17)

In this paper, we consider an adiabatic case. No heat flux or heat generation are considered, so that the last two terms of the equation above are equal to zero. In other words, we consider thermal effects to be local, and temperature behaves as a local variable of similar nature to cumulated plastic strain \( \Delta \mathbf{q} \). All entropy production is due to internal
dissipation during deformation, and is strictly associated to a dissipation potential that is a part of the incremental pseudo-potential, as shown below.

3.3. Incremental pseudo-potential

An additive decomposition of the free energy density is commonly used, representing the independence of elastic processes from internal processes, a very reasonable assumption for a wide range of materials. Furthermore, in the present work, we consider independent potentials for all different aspects of material behavior: \( \phi^{\text{vol}}(J,T) \) is responsible for the elastic volumetric response (associated to the material’s bulk modulus and volumetric dilation coefficient); \( \phi^e(\mathbf{C}^e,T) \) represents the isochoric elastic response; \( \phi^p(q,T) \) represents the plastic response of the material, including yield conditions and hardening (the form used in Vassoler (2007) was chosen for its versatility in describing various modes of hardening); and \( \phi^h(T) \) is responsible for the accumulation of energy in the form of heat (associated to the specific heat capacity).

\[
W(F,q,q_i,M,T) = \phi^{\text{vol}}(J,T) + \phi^e(\mathbf{C}^e,T) + \phi^p(q,T) + \phi^h(T) \tag{18}
\]

It is important to observe that all the individual potentials are considered to be dependent of temperature. In other words, thermal effects affect potentials describing mechanical behavior, and are affected by them.

We focus on the form of the isochoric elastic response adopted in the present model. It is an extension of the model proposed in Fancello (2006), based on spectral quantities (where values \( c^e_i \) are considered to be the eigenvalues of the elastic deformation \( \mathbf{C}^e \), related to the eigenvalues \( \mathbf{e}^s_i \) of the natural strain \( \mathbf{e}^s \)), so that a variety of isotropic hyperelastic materials may be represented.

\[
\phi^e(\mathbf{C}^e,T) = \phi^e(c^e_1,c^e_2,c^e_3,T) \tag{19}
\]

\[
e^e = \frac{1}{2} \ln \mathbf{C}^e \quad e^e_i = \frac{1}{2} \ln c^e_i \tag{20}
\]

\[
\phi^e(e^e,T) = \phi^e(e^e_1,e^e_2,e^e_3,T) \tag{21}
\]

Dissipative behaviors after yield are described in the dissipative potential \( \psi^h \). They are associated with the rate of internal variables. For a viscoplastic models the dissipation potential depends on the rate of plastic deformation \( \dot{q} \), usually represented by the rate of the cumulated plastic strain in the load step (\( \Delta \dot{q} \)). Since the temperature is now an internal variable of the model, we would also need to include dependence on the rate of temperature change. We represent both rates together, following the work of Stainier (2006), by assuming that temperature and cumulated plastic strain appear together on all rate expressions.

We report the reader interested in the specific forms used for all the potentials, as well as in a further discussion of the forms in which the thermo-mechanical coupling appears in them, to Selke et al (2009).

We are now well equipped to assemble the incremental potential, consistently representing the material behavior within a load step. The total deformation gradient at the end of the load step \( \mathbf{F}_{n+1} \) is imposed as an external variable.

\[
\Psi(F_{n+1}, e_n) = \inf_{M_i, q_i, \Delta q} \sup_{T_{n+1}} \left\{ \Delta W(F,e) + \rho_0 \eta_n (T_{n+1} - T_n) + \Delta t \psi \left( \frac{T_{n+1} \Delta q}{T_n}, T_n \right) \right\} \tag{22}
\]

Where:

\[
\Delta W(F,e) = W(F_{n+1}, e_{n+1}) - W(F_n, e_n) \tag{23}
\]

Subjected to the following constraints:

\[
q_i \in Q = \left\{ p_i \in \mathbb{R}; \sum_{i=1}^3 p_i = 0; \sum_{i=1}^3 p_i^2 = \frac{3}{2} \right\} \tag{24}
\]

\[
M_i \in \mathcal{K}_M = \left\{ \mathbf{N}_i \in \text{Sym}; \mathbf{N}_i \cdot \mathbf{N}_i = 1; \mathbf{N}_i \cdot \mathbf{N}_j = 0, i \neq j \right\} \tag{25}
\]
Details of the extremization of the incremental pseudo-potential are omitted due to space constraints. In Selke et al. (2009), the Lagrangian function associated to the problem and its primary optimality conditions are presented in detail. The minimization with respect to directions $M_i$ can be performed analytically, as demonstrated in Fancello et al. (2008).

### 3.4. Incremental updates

In an incremental context, it is necessary to determine evolution equations in terms of involved variables. We thus complete the brief overview of our model with the presentation of the incremental updates for plastic strain variables, and indicate how the stress can be updated in a hyperelastic manner.

An exponential mapping of the plastic part of the deformation gradient ($F^P$) is considered:

$$F^P_{n+1} = \exp \left[ \Delta q \sum_{i=1}^{3} q_i M_i \right] F^P_n$$  \hspace{1cm} (27)

The cumulated plastic strain for a certain point is considered to be the sum of the cumulated plastic strains of all previous steps:

$$q_{n+1} = q_n + \Delta t \dot{q} = q_n + \Delta q$$  \hspace{1cm} (28)

This allowed us to substitute $\dot{q}$ for $\Delta q$ in the list of independent variables.

Considering the separation between volumetric and isochoric parts, the expressions for the updated Piola-Kirchhoff ($P_{n+1}$) and Cauchy ($\sigma_{n+1}$) stresses are as follows:

$$P_{n+1} = 2F^P_{n+1} \frac{\partial \psi(F^p_{n+1}, \epsilon)}{\partial C_{n+1}} = F^P_{n+1} \left[ J_{n+1}^{-1/3} \text{DEV} \left( 2 \frac{\partial \psi^e}{\partial C_{n+1}} + \frac{\partial \psi^{vol}}{\partial J_{n+1}} J_{n+1}^{-1} C_{n+1}^{-1} \right) \right]$$  \hspace{1cm} (29)

$$\sigma_{n+1} = \frac{1}{J_{n+1}} P_{n+1} F_{n+1}^T$$  \hspace{1cm} (30)

### 4. APPLICATION TO SELECT MATERIALS

In order to show the versatility of our model, we present simulation results for two very different kinds of materials. We first take advantage of the complete thermo-mechanical characterization of rate dependent $\alpha$-titanium alloy presented in the work of Stainier and Ortiz (2008), and then present a fictitious material with an Ogden type of isochoric elastic potential. We basically seek to evidence thermo-mechanical coupling through stress-strain and temperature increase curves of numerically simulated uniaxial traction tests.
Figure 2 - Influence of initial temperature on stress-strain behavior and on temperature increase for a material with an Ogden type of isochoric elastic response ($\varepsilon = 0.001/s$).

5. CONCLUSIONS

In this paper, we have shown the application of a variational formulation to a fully-coupled thermo-mechanical problem. The general nature of the variational structure, with potentials dependent of spectral quantities, gives it great versatility in describing different sets of materials and material behaviors. The construction of an incrementally consistent pseudo-potential, together with the definition of constitutive updates for other variables, allows for the complete determination of the state of the material at any point in time.

Limitations of the present model are associated to its simplifying hypotheses. As is, there is restriction to isotropic materials. No viscoelastic effects are considered, which may somehow limit its applications to some polymeric materials, though the extension to include such effects should pose no serious obstacles. It also important to highlight that this paper presented a model restricted to adiabatic thermo-viscoplasticity. Although the inclusion of heat conduction and heat generation is theoretically straightforward, their implementation is the subject of future works.

6. REFERENCES

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