6th European Conference on Computational Mechanics (ECCM 6)
7th European Conference on Computational Fluid Dynamics (ECFD 7)
1115 June 2018, Glasgow, UK

VARIATIONAL FORMULATIONS FOR LARGE STRAIN THERMO-ELASTODYNAMICS BASED ON THE GENERIC FORMALISM

Peter Betsch, Mark Schiebl

Institute of Mechanics, Karlsruhe Institute of Technology, Germany,
{peter.betsch,mark.schiebl}@kit.edu, http://www.ifm.kit.edu/english/index.php

Key words: Thermomechanical Problems, Thermoelasticity, Structure-Preserving Numerical Methods

Abstract. We newly propose a GENERIC-based variational formulation for initial boundary value problems of finite strain thermoelasticity. The transformation properties of the underlying GENERIC formalism make possible the free choice of the thermodynamic state variable. Moreover, due to the structure properties of GENERIC the proposed variational formulation provides a solid foundation for the structure-preserving discretization in space and time.

1 INTRODUCTION

GENERIC (General Equation for the Non-Equilibrium Reversible-Irreversible Coupling) is a double-generator formalism for the thermodynamically consistent formulation of problems from continuum mechanics. The GENERIC-based formulation relies on an additive decomposition of the evolution equations into a reversible part and a dissipative part. While the reversible part is generated by the total energy of the system, the irreversible part is generated by the total entropy. Originally, GENERIC has been developed in the context of complex fluids. We refer to the book by Öttinger [1] for a comprehensive account of the GENERIC formalism up to the year 2005.

More recently, the GENERIC framework has been extended to solid mechanics (see [2]-[4]). Romero [5, 6] recognized at an early stage the great potential of the GENERIC framework for the design of structure-preserving numerical schemes and coined the notion of a thermodynamically consistent (TC) method (see also [7]-[11]). If a TC scheme is also capable of conserving momentum maps associated to symmetries of the underlying mechanical system, it may be termed Energy-Momentum-

Entropy (EME) scheme. EME schemes can be viewed as extension to dissipative systems of earlier developed Energy-Momentum (EM) schemes for conservative systems with symmetry such as large strain elastodynamics and flexible multibody dynamics (see [12] for a comprehensive overview of previous developments in this direction).

Previously developed GENERIC-based TC methods for thermomechanically coupled solids are typically subject to serious limitations such as (i) the use of the entropy density as thermodynamical variable, and (ii) the restriction to isolated (or closed) systems in which the boundaries are neglected. We newly propose a generalized GENERIC-based formulation that (i) allows for the free choice of the thermodynamical variable among either the temperature, internal energy density or entropy density, and (ii) takes into account the boundaries of the system. Full details of the proposed approach can be found in our recent work [13]. The new formulation lays the ground for the design of structure-preserving methods for the solution of initial boundary value problems for thermomechanically coupled solids. In the present work we focus on the dynamics of thermoelastic solids with heat conduction.

2 GENERIC FOR CLOSED SYSTEMS

The GENERIC formalism was originally developed in the context of closed (or isolated) systems. That is, boundaries of the domain under consideration are typically disregarded. The GENERIC framework relies on an additive decomposition of the evolution equations into reversible and irreversible parts. Correspondingly, the time-evolution of an arbitrary functional $\mathcal{A}$ can be written in the form

$$\frac{\mathrm{d}\mathcal{A}}{\mathrm{d}t} = \big\{\mathcal{A},\mathcal{E}\big\} + \big[\mathcal{A},\mathcal{S}\big] \tag{1}$$

This equation represents a 2-generator formalism in which the reversible part is generated by the total energy $\mathcal{E}$ of the system via the Poisson bracket $\{\cdot,\cdot\}$, while the irreversible part is generated by the total entropy $\mathcal{S}$ of the system via the dissipative bracket $[\cdot,\cdot]$.

Consider a continuum body with material points $\mathbf{X} = X_i\mathbf{e}_i$ in the reference configuration $\mathcal{B} \subset \mathbb{R}^3$ (Fig. 1). Here and in the sequel the summation convention applies to repeated indices. Moreover, $\mathbf{e}_i$ denote the canonical base vectors in $\mathbb{R}^3$. Within the Lagrangian description of continuum mechanics the deformed configuration of the body at time t is characterized by the deformation map $\boldsymbol{\varphi}_t : \mathcal{B} \mapsto \mathbb{R}^3$. The velocity of the material point $\mathbf{X} \in \mathcal{B}$ located at $\mathbf{x} = \boldsymbol{\varphi}_t(\mathbf{X})$ is given by $\mathbf{v}_t = \partial\boldsymbol{\varphi}_t/\partial t$. Alternatively we will often write $\mathbf{v}_t = \dot{\boldsymbol{\varphi}}_t$. The conjugate momentum density is defined by $\mathbf{p}_t = \rho\mathbf{v}_t$.

The deformation gradient corresponds to the Jacobian of the deformation map, $\mathbf{F}_t = \partial\boldsymbol{\varphi}_t/\partial\mathbf{X}$. In what follows the partial derivative with respect to the material

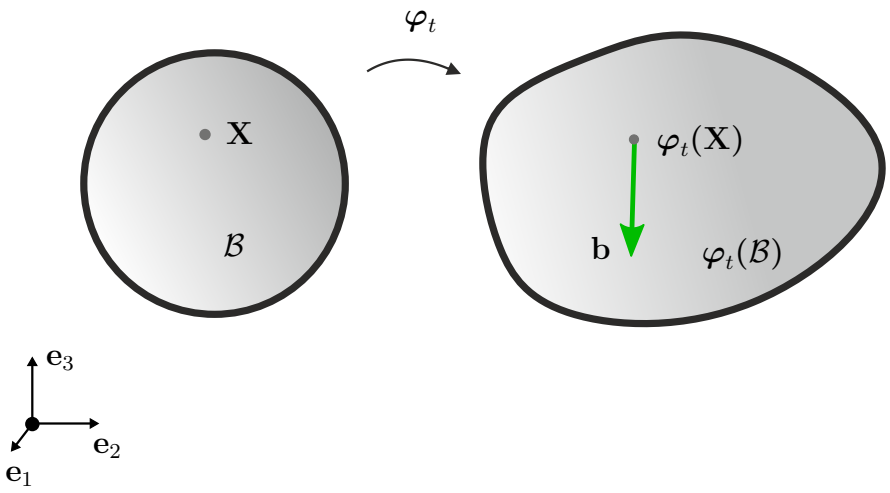

Figure 1: Reference configuration $\mathcal{B}$ and deformed configuration $\varphi_t(\mathcal{B})$ at time t.

coordinates will be denoted by the nabla operator. Accordingly, the deformation gradient assumes the form

$$\mathbf{F}_t = \nabla \varphi_t \tag{2}$$

A natural choice for the thermodynamic state variable is the absolute temperature $\theta_t : \mathcal{B} \mapsto \mathbb{R}_+$. Alternatively, the entropy density $\eta_t : \mathcal{B} \mapsto \mathbb{R}$ or the internal energy density $u_t : \mathcal{B} \mapsto \mathbb{R}$ could be chosen.

The generalized GENERIC formulation developed in [13] makes possible the free choice of the thermodynamic state variable $\tau_t \in \{\theta_t, \eta_t, u_t\}$. An arbitrary functional $\mathcal{A}$ can now be written in the form

$$\mathcal{A} = \mathcal{A}'(\varphi_t, \mathbf{p}_t, \tau_t) = \int_{\mathcal{B}} a'(\varphi_t, \nabla\varphi_t, \mathbf{p}_t, \tau_t)\, \mathrm{d}V \tag{3}$$

with the corresponding density function $a'(\varphi_t, \nabla\varphi_t, \mathbf{p}_t, \tau_t)$. Now the Poisson bracket required in the GENERIC evolution equation (1) can be written as

$$\begin{aligned} \{\mathcal{A}', \mathcal{B}'\} = &\int_{\mathcal{B}} \left(\delta_{\varphi} a' \cdot \delta_{\mathbf{p}} b' - \delta_{\mathbf{p}} a' \cdot \delta_{\varphi} b'\right) \mathrm{d}V \\ &+ \int_{\mathcal{B}} \left(\mathrm{Div}\left(\frac{\delta_\tau a'}{\partial_\tau \eta'} \partial_{\nabla\varphi} \eta'\right) \cdot \delta_{\mathbf{p}} b' - \delta_{\mathbf{p}} a' \cdot \mathrm{Div}\left(\frac{\delta_\tau b'}{\partial_\tau \eta'} \partial_{\nabla\varphi} \eta'\right)\right) \mathrm{d}V \end{aligned} \tag{4}$$

In addition to that, the dissipative bracket featuring in the GENERIC evolution equation (1) assumes the form

$$[\mathcal{A}', \mathcal{B}'] = \int_{\mathcal{B}} \nabla\left(\frac{\delta_\tau a'}{\partial_\tau u'}\right) \cdot (\theta')^2 \mathbf{K}_t \nabla\left(\frac{\delta_\tau b'}{\partial_\tau u'}\right) \mathrm{d}V \tag{5}$$

In the last equation, the absolute temparature can be calculated via the formula

$$\theta'(\nabla\boldsymbol{\varphi}_t,\tau_t)=\frac{\partial_\tau u'(\nabla\boldsymbol{\varphi}_t,\tau_t)}{\partial_\tau \eta'(\nabla\boldsymbol{\varphi}_t,\tau_t)} \tag{6}$$

which is valid for any $\tau_t\in\{\theta_t,\eta_t,u_t\}$ (see [3] and also [1]). Moreover, in (5), the material conductivity tensor is given by $\mathbf{K}_t=\mathbf{K}'(\nabla\boldsymbol{\varphi}_t,\tau_t)$. We further note that the functional derivatives in the brackets (4) and (5) are given by

$$\begin{aligned}\delta_{\boldsymbol{\varphi}}a'&=\partial_{\boldsymbol{\varphi}}a'-\mathrm{Div}(\partial_{\nabla\boldsymbol{\varphi}}a')\\ \delta_{\mathbf{p}}a'&=\partial_{\mathbf{p}}a'\\ \delta_\tau a'&=\partial_\tau a'\end{aligned} \tag{7}$$

The GENERIC evolution equation (1) can now be considered in more detail by using the previously derived Poisson bracket (4) along with the dissipative bracket (5). Accordingly, we obtain

$$\frac{\mathrm{d}\mathcal{A}'}{\mathrm{d}t}=\{\mathcal{A}',\mathcal{E}'\}+[\mathcal{A}',\mathcal{S}'] \tag{8}$$

We note that the evolution equation (8) represents a uniform description of thermo-elastodynamics in which the thermodynamic variable $\tau_t\in\{\theta_t,\eta_t,u_t\}$ can be freely chosen. In (8), the total energy of the system is given by the functional

$$\mathcal{E}'(\boldsymbol{\varphi}_t,\mathbf{p}_t,\tau_t)=\int_{\mathcal{B}}e'(\boldsymbol{\varphi}_t,\nabla\boldsymbol{\varphi}_t,\mathbf{p}_t,\tau_t)\,\mathrm{d}V \tag{9}$$

with associated density function

$$e'(\boldsymbol{\varphi}_t,\nabla\boldsymbol{\varphi}_t,\mathbf{p}_t,\tau_t)=\frac{1}{2}\rho^{-1}\mathbf{p}_t\cdot\mathbf{p}_t+u'(\nabla\boldsymbol{\varphi}_t,\tau_t)-\mathbf{b}\cdot\boldsymbol{\varphi}_t \tag{10}$$

In the last equation $\mathbf{b}:\mathcal{B}\mapsto\mathbb{R}^3$ represents prescribed body forces which are assumed to be dead loads. In addition to the total energy, the total entropy of the system acts as second generator in the GENERIC evolution equation (8) and is given by the functional

$$\mathcal{S}'(\boldsymbol{\varphi}_t,\tau_t)=\int_{\mathcal{B}}\eta'(\nabla\boldsymbol{\varphi}_t,\tau_t)\,\mathrm{d}V \tag{11}$$

3 GENERIC FOR OPEN SYSTEMS

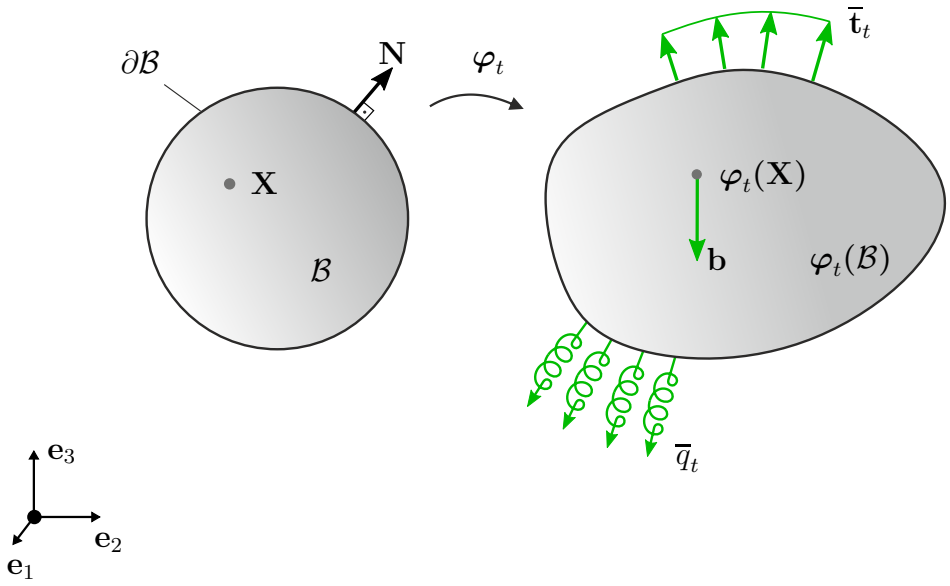

Figure 2: Reference configuration $\mathcal{B}$ with boundary $\partial\mathcal{B}$ and current configuration $\varphi_t(\mathcal{B})$ at time t. External tractions $\overline{\mathbf{t}}_t = \mathbf{P}_t\mathbf{N}$ act on the boundary of the current configuration. In addition to that, the heat flux accross the current boundary is denoted by $\overline{q}_t = \mathbf{Q}_t \cdot \mathbf{N}$.

The GENERIC formulation for closed systems outlined in the last section can be extended to open systems (Fig. 2) by means of a straightforward procedure (see [14] and [13]). Accordingly, the Poisson bracket (4) and the dissipative bracket (5) are now viewed as full brackets that can be decomposed according to

$$\begin{aligned} \{\mathcal{A}', \mathcal{B}'\} &= \{\mathcal{A}', \mathcal{B}'\}_{\text{bulk}} + \{\mathcal{A}', \mathcal{B}'\}_{\text{boun}} \\ [\mathcal{A}', \mathcal{B}'] &= [\mathcal{A}', \mathcal{B}']_{\text{bulk}} + [\mathcal{A}', \mathcal{B}']_{\text{boun}} \end{aligned} \tag{12}$$

That is, the full brackets are split additively into bulk and boundary parts, respectively. This split can be accomplished by applying integration by parts to the full brackets. Following [14], the proper interpretation of the GENERIC evolution equation (8) is now given by

$$\frac{\mathrm{d}\mathcal{A}'}{\mathrm{d}t} = \{\mathcal{A}', \mathcal{E}'\}_{\text{bulk}} + [\mathcal{A}', \mathcal{S}']_{\text{bulk}} \tag{13}$$

Invoking the symmetry properties of the full brackets, i.e. $\{\mathcal{A}', \mathcal{B}'\} = -\{\mathcal{B}', \mathcal{A}'\}$ and $[\mathcal{A}', \mathcal{B}'] = [\mathcal{B}', \mathcal{A}']$, (12) leads to

$$\begin{aligned} \big\{\mathcal{A}', \mathcal{B}'\big\}_{\text{bulk}} &= -\big\{\mathcal{B}', \mathcal{A}'\big\}_{\text{bulk}} - \Big(\big\{\mathcal{A}', \mathcal{B}'\big\}_{\text{boun}} + \big\{\mathcal{B}', \mathcal{A}'\big\}_{\text{boun}}\Big) \\ \big[\mathcal{A}', \mathcal{B}'\big]_{\text{bulk}} &= \quad \big[\mathcal{B}', \mathcal{A}'\big]_{\text{bulk}} - \Big(\big[\mathcal{A}', \mathcal{B}'\big]_{\text{boun}} - \big[\mathcal{B}', \mathcal{A}'\big]_{\text{boun}}\Big) \end{aligned} \tag{14}$$

Substitution from (14) into (13) yields the GENERIC evolution equation for open systems

$$\frac{\mathrm{d}\mathcal{A}'}{\mathrm{d}t} = -\big\{\mathcal{E}', \mathcal{A}'\big\}_{\text{bulk}} + \big[\mathcal{S}', \mathcal{A}'\big]_{\text{bulk}} - \Big(\big\{\mathcal{A}', \mathcal{E}'\big\}_{\text{boun}} + \big\{\mathcal{E}', \mathcal{A}'\big\}_{\text{boun}} + \big[\mathcal{A}', \mathcal{S}'\big]_{\text{boun}} - \big[\mathcal{S}', \mathcal{A}'\big]_{\text{boun}}\Big) \tag{15}$$

In the sequel, we use the above equation to derive the variational formulation for large strain thermo-elastodynamics.

3.1 Specific brackets

Next, we provide the specific brackets featering in the GENERIC evolution equation (15) pertaining to thermoelastic solids. Proceeding along the lines of [14], we start from the full brackets derived above and apply integration by parts. In this connection, the goal is to get the derivatives $(\delta_{\boldsymbol{\varphi}} a', \delta_{\mathbf{p}} a', \delta_\tau a')$ free of any spatial derivatives. To this end, we rewrite the full Poisson bracket (4) as

$$\begin{aligned} \big\{\mathcal{A}', \mathcal{B}'\big\} = &\int_{\mathcal{B}} \left(\partial_{\boldsymbol{\varphi}} a' \cdot \partial_{\mathbf{p}} b' - \partial_{\mathbf{p}} a' \cdot \left(\partial_{\boldsymbol{\varphi}} b' - \operatorname{Div}\left(\partial_{\nabla\boldsymbol{\varphi}} b' - \frac{\partial_\tau b'}{\partial_\tau \eta'} \partial_{\nabla\boldsymbol{\varphi}} \eta'\right)\right)\right) \mathrm{d}V \\ &- \int_{\mathcal{B}} \operatorname{Div}\left(\partial_{\nabla\boldsymbol{\varphi}} a' - \frac{\partial_\tau a'}{\partial_\tau \eta'} \partial_{\nabla\boldsymbol{\varphi}} \eta'\right) \cdot \partial_{\mathbf{p}} b' \, \mathrm{d}V \end{aligned} \tag{16}$$

Applying integration by parts to the second integral on the right-hand side of (16), and taking into account the additive decomposition $(12)_1$, we obtain

$$\begin{aligned} \big\{\mathcal{A}', \mathcal{B}'\big\}_{\text{bulk}} = &\int_{\mathcal{B}} \left(\partial_{\boldsymbol{\varphi}} a' \cdot \partial_{\mathbf{p}} b' - \partial_{\mathbf{p}} a' \cdot \left(\partial_{\boldsymbol{\varphi}} b' - \operatorname{Div}\left(\partial_{\nabla\boldsymbol{\varphi}} b' - \frac{\partial_\tau b'}{\partial_\tau \eta'} \partial_{\nabla\boldsymbol{\varphi}} \eta'\right)\right)\right) \mathrm{d}V \\ &+ \int_{\mathcal{B}} \left(\partial_{\nabla\boldsymbol{\varphi}} a' - \frac{\partial_\tau a'}{\partial_\tau \eta'} \partial_{\nabla\boldsymbol{\varphi}} \eta'\right) : \nabla \partial_{\mathbf{p}} b' \, \mathrm{d}V \end{aligned} \tag{17}$$

and

$$\big\{\mathcal{A}', \mathcal{B}'\big\}_{\text{boun}} = -\int_{\partial\mathcal{B}} \partial_{\mathbf{p}} b' \cdot \left(\partial_{\nabla\boldsymbol{\varphi}} a' - \frac{\partial_\tau a'}{\partial_\tau \eta'} \partial_{\nabla\boldsymbol{\varphi}} \eta'\right) \mathbf{N} \, \mathrm{d}A \tag{18}$$

Here, the vector $\mathbf{N}$ denotes the unit outward normal field on the boundary $\partial\mathcal{B}$ of the reference configuration (Fig. 2). Similarly, applying integration by parts to the full

dissipative bracket (5), yields the corresponding bulk bracket

$$\big[\mathcal{A}',\mathcal{B}'\big]_{\text{bulk}} = -\int_{\mathcal{B}} \frac{\partial_\tau a'}{\partial_\tau u'} \text{Div}\left((\theta')^2 \mathbf{K}_t \nabla\left(\frac{\partial_\tau b'}{\partial_\tau u'}\right)\right) \text{d}V \tag{19}$$

along with the boundary bracket

$$\big[\mathcal{A}',\mathcal{B}'\big]_{\text{boun}} = \int_{\partial\mathcal{B}} \frac{\partial_\tau a'}{\partial_\tau u'} \mathbf{N}\cdot(\theta')^2 \mathbf{K}_t \nabla\left(\frac{\partial_\tau b'}{\partial_\tau u'}\right) \text{d}A \tag{20}$$

Table 1 contains a summary of the specific brackets appearing in the GENERIC evolution equations (15) for open systems. In Table 1, the material heat flux vector and the first Piola-Kirchhoff stress tensor are given by

$$\begin{aligned} \mathbf{Q}' &= (\theta')^2 \mathbf{K}_t \nabla\left(\frac{\partial_\tau \eta'}{\partial_\tau u'}\right) \\ \mathbf{P}' &= \partial_\nabla \boldsymbol{\varphi} u' - \frac{\partial_\tau u'}{\partial_\tau \eta'} \partial_\nabla \boldsymbol{\varphi} \eta' \end{aligned} \tag{21}$$

Table 1: Summary of the brackets featuring in the GENERIC evolution equations (15) for open systems.

$$\begin{aligned}
\big\{\mathcal{E}',\mathcal{A}'\big\}_{\text{bulk}} &= -\int_{\mathcal{B}} \left(\mathbf{b}\cdot\partial_{\mathbf{p}} a' + \rho^{-1}\mathbf{p}_t \cdot \left(\partial_{\boldsymbol{\varphi}} a' - \text{Div}\left(\partial_\nabla \boldsymbol{\varphi} a' - \frac{\partial_\tau a'}{\partial_\tau \eta'} \partial_\nabla \boldsymbol{\varphi} \eta'\right)\right)\right) \text{d}V \\
&\quad + \int_{\mathcal{B}} \mathbf{P}' : \nabla \partial_{\mathbf{p}} a' \, \text{d}V \\
\big[\mathcal{S}',\mathcal{A}'\big]_{\text{bulk}} &= -\int_{\mathcal{B}} \frac{1}{\theta'} \text{Div}\left((\theta')^2 \mathbf{K}_t \nabla\left(\frac{\partial_\tau a'}{\partial_\tau u'}\right)\right) \text{d}V \\
\big\{\mathcal{A}',\mathcal{E}'\big\}_{\text{boun}} &= -\int_{\partial\mathcal{B}} \rho^{-1}\mathbf{p}_t \cdot \left(\partial_\nabla \boldsymbol{\varphi} a' - \frac{\partial_\tau a'}{\partial_\tau \eta'} \partial_\nabla \boldsymbol{\varphi} \eta'\right) \mathbf{N} \, \text{d}A \\
\big\{\mathcal{E}',\mathcal{A}'\big\}_{\text{boun}} &= -\int_{\partial\mathcal{B}} \partial_{\mathbf{p}} a' \cdot \mathbf{P}' \mathbf{N} \, \text{d}A \\
\big[\mathcal{A}',\mathcal{S}'\big]_{\text{boun}} &= \int_{\partial\mathcal{B}} \frac{\partial_\tau a'}{\partial_\tau u'} \mathbf{N}\cdot\mathbf{Q}' \, \text{d}A \\
\big[\mathcal{S}',\mathcal{A}'\big]_{\text{boun}} &= \int_{\partial\mathcal{B}} \frac{1}{\theta'} \mathbf{N}\cdot(\theta')^2 \mathbf{K}_t \nabla\left(\frac{\partial_\tau a'}{\partial_\tau u'}\right) \text{d}A
\end{aligned}$$

3.2 Initial boundary value problem

We next deal with the initial boundary value problem (IBVP) pertaining to large-strain thermoelastodynamics. To this end we decompose the boundary $\partial\mathcal{B}$ of the continuum body (Fig. 2) into a displacement boundary $\partial_\varphi\mathcal{B}$, on which $\boldsymbol{\varphi}_t = \overline{\boldsymbol{\varphi}}_t$, and a traction boundary $\partial_\sigma\mathcal{B}$, on which $\mathbf{P}_t\mathbf{N} = \overline{\mathbf{t}}_t$, where $\overline{\boldsymbol{\varphi}}_t$ and $\overline{\mathbf{t}}_t$ are prescribed functions for $t \geq 0$. Moreover, $\partial_\varphi\mathcal{B} \cup \partial_\sigma\mathcal{B} = \partial\mathcal{B}$ and $\partial_\varphi\mathcal{B} \cap \partial_\sigma\mathcal{B} = \varnothing$. Similarly, for the thermal part we consider the subsets $\partial_\tau\mathcal{B}$ and $\partial_q\mathcal{B}$, with the properties $\partial_\tau\mathcal{B} \cup \partial_q\mathcal{B} = \partial\mathcal{B}$ and $\partial_\tau\mathcal{B} \cap \partial_q\mathcal{B} = \varnothing$. Here, the thermodynamic variable is prescribed on $\partial_\tau\mathcal{B}$, i.e. $\tau_t = \overline{\tau}_t$, whereas the heat flux is prescribed on $\partial_q\mathcal{B}$, i.e. $\mathbf{Q}_t \cdot \mathbf{N} = \overline{q}_t$.

The goal is now to determine the motion $\boldsymbol{\varphi}_t : \mathcal{B} \mapsto \mathbb{R}^3$, the linear momentum density $\mathbf{p}_t : \mathcal{B} \mapsto \mathbb{R}^3$, and the thermodynamic variable $\tau_t : \mathcal{B} \mapsto \mathbb{R}$ for $t \in (0, T]$. The unknown fields are subject to initial conditions of the form $\boldsymbol{\varphi}_0 = \mathbf{X}$, $\mathbf{p}_0 = \rho\mathbf{V}_0$, and $\tau_0 = \tau^{\text{ini}}$ in $\mathcal{B}$. Here, $\mathbf{V}_0$ is a prescribed material velocity field and τ^{ini} is a prescribed field of the thermodynamic variable $\tau \in \{\theta, \eta, u\}$. The unknown fields are determined by the variational problem to be dealt with in the next section.

3.2.1 Variational formulation

To deduce the variational formulation of the present IBVP from the GENERIC evolution equation (15), we choose the specific density function $a' = w'$, where

$$w' = \mathbf{w}_\varphi \cdot \boldsymbol{\varphi}_t + \mathbf{w}_p \cdot \mathbf{p}_t + \mathrm{w}_\tau \tau_t \tag{22}$$

Here, $\mathbf{w}_\varphi, \mathbf{w}_p : \mathcal{B} \mapsto \mathbb{R}^3$ and $\mathrm{w}_\tau : \mathcal{B} \mapsto \mathbb{R}$ are test functions that have to satisfy the boundary conditions $\mathbf{w}_\varphi = \mathbf{0}$ and $\mathbf{w}_p = \mathbf{0}$ on $\partial_\varphi\mathcal{B}$, and $\mathrm{w}_\tau = 0$ on $\partial_\tau\mathcal{B}$. With the choice (22), the left-hand side of the GENERIC evolution equation (15) yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{W}' = \int_{\mathcal{B}} \left(\mathbf{w}_\varphi \cdot \dot{\boldsymbol{\varphi}}_t + \mathbf{w}_p \cdot \dot{\mathbf{p}}_t + \mathrm{w}_\tau \dot{\tau}_t\right) \mathrm{d}V \tag{23}$$

On the other hand, the specific brackets on the right-hand side of (15) assume the form (cf. Table 1)

$$\left\{\mathcal{E}', \mathcal{W}'\right\}_{\text{bulk}} = -\int_{\mathcal{B}} \left(\mathbf{b} \cdot \mathbf{w}_p + \rho^{-1}\mathbf{p}_t \cdot \left(\mathbf{w}_\varphi + \mathrm{Div}\left(\frac{\mathrm{w}_\tau}{\partial_\tau \eta'}\partial_\nabla \boldsymbol{\varphi}\eta'\right)\right) - \mathbf{P}' : \nabla\mathbf{w}_p\right) \mathrm{d}V$$

$$\left[\mathcal{S}', \mathcal{W}'\right]_{\text{bulk}} = -\int_{\mathcal{B}} \frac{1}{\theta'}\mathrm{Div}\left((\theta')^2 \mathbf{K}_t \nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)\right) \mathrm{d}V$$

and

$$\begin{aligned}
\big\{\mathcal{W}',\mathcal{E}'\big\}_{\text{boun}} &= -\int_{\partial\mathcal{B}} \rho^{-1}\mathbf{p}_t\cdot\left(-\frac{\mathrm{w}_\tau}{\partial_\tau\eta'}\partial_\nabla\boldsymbol{\varphi}\eta'\right)\mathbf{N}\,\mathrm{d}A\\
\big\{\mathcal{E}',\mathcal{W}'\big\}_{\text{boun}} &= -\int_{\partial\mathcal{B}} \mathbf{w}_p\cdot\mathbf{P}'\mathbf{N}\,\mathrm{d}A\\
\big[\mathcal{W}',\mathcal{S}'\big]_{\text{boun}} &= \int_{\partial\mathcal{B}} \frac{\mathrm{w}_\tau}{\partial_\tau u'}\mathbf{N}\cdot\mathbf{Q}'\,\mathrm{d}A\\
\big[\mathcal{S}',\mathcal{W}'\big]_{\text{boun}} &= \int_{\partial\mathcal{B}} \frac{1}{\theta'}\mathbf{N}\cdot(\theta')^2\mathbf{K}_t\nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)\mathrm{d}A
\end{aligned}$$

Accordingly, the GENERIC evolution equation (15) gives rise to the equations

$$\begin{aligned}
0 &= \int_{\mathcal{B}}\mathbf{w}_\varphi\cdot\left(\dot{\boldsymbol{\varphi}}_t-\rho^{-1}\mathbf{p}_t\right)\mathrm{d}V\\
0 &= \int_{\mathcal{B}}\left(\mathbf{w}_p\cdot(\dot{\mathbf{p}}_t-\mathbf{b})+\mathbf{P}':\nabla\mathbf{w}_p\right)\mathrm{d}V-\int_{\partial\mathcal{B}}\mathbf{w}_p\cdot\mathbf{P}'\mathbf{N}\,\mathrm{d}A
\end{aligned}\tag{24}$$

along with

$$\begin{aligned}
0 = \int_{\mathcal{B}}\Bigg(&\mathrm{w}_\tau\dot{\tau}_t-\mathrm{Div}\left(\frac{\mathrm{w}_\tau}{\partial_\tau\eta'}\partial_\nabla\boldsymbol{\varphi}\eta'\right)\cdot\rho^{-1}\mathbf{p}_t+\frac{1}{\theta'}\mathrm{Div}\left((\theta')^2\mathbf{K}_t\nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)\right)\Bigg)\,\mathrm{d}V\\
+\int_{\partial\mathcal{B}}\Bigg(&\rho^{-1}\mathbf{p}_t\cdot\left(\frac{\mathrm{w}_\tau}{\partial_\tau\eta'}\partial_\nabla\boldsymbol{\varphi}\eta'\right)\mathbf{N}-\frac{1}{\theta'}\mathbf{N}\cdot(\theta')^2\mathbf{K}_t\nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)+\frac{\mathrm{w}_\tau}{\partial_\tau u'}\mathbf{N}\cdot\mathbf{Q}'\Bigg)\,\mathrm{d}A
\end{aligned}$$

Integrating by parts twice, we arrive at an alternative representation of the last equation given by

$$\begin{aligned}
0 = \int_{\mathcal{B}}\Bigg(&\mathrm{w}_\tau\dot{\tau}_t+\nabla(\rho^{-1}\mathbf{p}_t):\left(\frac{\mathrm{w}_\tau}{\partial_\tau\eta'}\partial_\nabla\boldsymbol{\varphi}\eta'\right)-\nabla\left(\frac{1}{\theta'}\right)\cdot(\theta')^2\mathbf{K}_t\nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)\Bigg)\,\mathrm{d}V\\
+\int_{\partial\mathcal{B}}&\frac{\mathrm{w}_\tau}{\partial_\tau u'}\mathbf{N}\cdot\mathbf{Q}'\,\mathrm{d}A
\end{aligned}$$

Using expression $(21)_1$ for the material heat flux and the symmetry property $\mathbf{K}_t = \mathbf{K}_t^{\mathrm{T}}$, the above equation can be recast in the form

$$0 = \int_{\mathcal{B}}\left(\mathrm{w}_\tau\dot{\tau}_t+\nabla(\rho^{-1}\mathbf{p}_t):\left(\frac{\mathrm{w}_\tau}{\partial_\tau\eta'}\partial_\nabla\boldsymbol{\varphi}\eta'\right)-\nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)\cdot\mathbf{Q}'\right)\mathrm{d}V+\int_{\partial\mathcal{B}}\frac{\mathrm{w}_\tau}{\partial_\tau u'}\mathbf{N}\cdot\mathbf{Q}'\,\mathrm{d}A\tag{25}$$

Taking into account the above stated boundary conditions, (24) and (25) give rise to the following variational formulation of the present IBVP:

$$\begin{aligned}
0 &= \int_{\mathcal{B}}\mathbf{w}_\varphi\cdot\left(\dot{\boldsymbol{\varphi}}_t-\rho^{-1}\mathbf{p}_t\right)\mathrm{d}V\\
0 &= \int_{\mathcal{B}}\left(\mathbf{w}_p\cdot(\dot{\mathbf{p}}_t-\mathbf{b})+\mathbf{P}':\nabla\mathbf{w}_p\right)\mathrm{d}V-\int_{\partial_\sigma\mathcal{B}}\mathbf{w}_p\cdot\overline{\mathbf{t}}_t\,\mathrm{d}A\\
0 &= \int_{\mathcal{B}}\left(\mathrm{w}_\tau\dot{\tau}_t+\nabla(\rho^{-1}\mathbf{p}_t):\left(\frac{\mathrm{w}_\tau}{\partial_\tau\eta'}\partial_\nabla\boldsymbol{\varphi}\eta'\right)-\nabla\left(\frac{\mathrm{w}_\tau}{\partial_\tau u'}\right)\cdot\mathbf{Q}'\right)\mathrm{d}V+\int_{\partial_q\mathcal{B}}\frac{\mathrm{w}_\tau}{\partial_\tau u'}\overline{q}_t\,\mathrm{d}A
\end{aligned}\tag{26}$$

These equations have to hold for all times $t \geq 0$ and for arbitrary test functions subject to the above mentioned boundary conditions.

3.2.2 Balance laws

Important balance laws can be directly deduced from the GENERIC-based variational formulation (26). For that purpose we confine our attention in this section to the pure Neumann problem (i.e. $\partial_\sigma \mathcal{B} = \partial_q \mathcal{B} = \partial\mathcal{B}$).

First, we choose $\mathbf{w}_\varphi = \partial_{\boldsymbol{\varphi}} j'_\xi$ and $\mathbf{w}_p = \partial_{\mathbf{p}} j'_\xi$, where $j'_\xi = \boldsymbol{\xi} \cdot (\boldsymbol{\varphi}_t \times \mathbf{p}_t)$ is the density function corresponding to the total angular momentum $\mathbf{J}_t = \int_\mathcal{B} \boldsymbol{\varphi}_t \times \mathbf{p}_t \, \mathrm{d}V$ projected onto the straight line specified by the constant vector $\boldsymbol{\xi} \in \mathbb{R}^3$. Inserting $\mathbf{w}_\varphi = \mathbf{p}_t \times \boldsymbol{\xi}$ and $\mathbf{w}_p = \boldsymbol{\xi} \times \boldsymbol{\varphi}_t$ into $(26)_{1,2}$, and subsequently adding both equations, we obtain the balance of angular momentum in the form

$$\boldsymbol{\xi} \cdot \frac{\mathrm{d}\mathbf{J}_t}{\mathrm{d}t} = \boldsymbol{\xi} \cdot \left(\int_\mathcal{B} \boldsymbol{\varphi}_t \times \mathbf{b} \, \mathrm{d}V + \int_{\partial\mathcal{B}} \boldsymbol{\varphi}_t \times \mathbf{P}'\mathbf{N} \, \mathrm{d}A \right) \tag{27}$$

To verify the balance of energy we choose for the test functions in (26)

$$\begin{aligned} \mathbf{w}_\varphi &= \partial_{\boldsymbol{\varphi}} e' & & \mathbf{w}_\varphi = -\mathbf{b} \\ \mathbf{w}_p &= \partial_{\mathbf{p}} e' \quad & \text{or} \quad & \mathbf{w}_p = \rho^{-1}\mathbf{p}_t \\ \mathrm{w}_\tau &= \partial_\tau e' & & \mathrm{w}_\tau = \partial_\tau u' \end{aligned}$$

Substituting these quantities into (26) and subsequently adding the three resulting equations, a straightforward calculation taking into account the identity $\dot{\boldsymbol{\varphi}}_t = \rho^{-1}\mathbf{p}_t$ and formula $(21)_2$ for the first Piola-Kirchhoff stress tensor yields

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\mathcal{B} \left(\frac{1}{2} \rho^{-1} \mathbf{p}_t \cdot \mathbf{p}_t + u' \right) \mathrm{d}V = \int_\mathcal{B} \mathbf{b} \cdot \dot{\boldsymbol{\varphi}}_t \, \mathrm{d}V + \int_{\partial\mathcal{B}} \left(\dot{\boldsymbol{\varphi}}_t \cdot \mathbf{P}'\mathbf{N} - \mathbf{N} \cdot \mathbf{Q}' \right) \mathrm{d}A \tag{28}$$

This equation corresponds to the balance law for the energy. Concerning the balance of entropy, we insert $\mathrm{w}_\tau = \partial_\tau \eta'$ into $(26)_3$, to obtain

$$\begin{aligned} 0 &= \int_\mathcal{B} \left(\partial_\tau \eta' \dot{\tau}_t + \nabla(\rho^{-1}\mathbf{p}_t) : \left(\partial_{\nabla\boldsymbol{\varphi}} \eta' \right) - \nabla \left(\frac{\partial_\tau \eta'}{\partial_\tau u'} \right) \cdot \mathbf{Q}' \right) \mathrm{d}V + \int_{\partial\mathcal{B}} \frac{\partial_\tau \eta'}{\partial_\tau u'} \mathbf{Q}' \cdot \mathbf{N} \, \mathrm{d}A \\ &= \int_\mathcal{B} \left(\frac{\mathrm{d}\eta'}{\mathrm{d}t} - \nabla \left(\frac{1}{\theta'} \right) \cdot (\theta')^2 \mathbf{K}_t \nabla \left(\frac{1}{\theta'} \right) \right) \mathrm{d}V + \int_{\partial\mathcal{B}} \frac{1}{\theta'} \mathbf{Q}' \cdot \mathbf{N} \, \mathrm{d}A \end{aligned}$$

Here, use has been made of formula (6) for the temperature along with expression $(21)_1$ for the material heat flux vector. Moreover, the identity $\dot{\boldsymbol{\varphi}}_t = \rho^{-1}\mathbf{p}_t$ has again

been taken into account. The above equation can be rewritten as

$$\frac{\mathrm{d}\mathcal{S}'}{\mathrm{d}t} = \underbrace{\int_{\mathcal{B}} \nabla\left(\frac{1}{\theta'}\right)\cdot(\theta')^2\mathbf{K}_t\nabla\left(\frac{1}{\theta'}\right)\mathrm{d}V}_{\geq 0} - \int_{\partial\mathcal{B}}\frac{1}{\theta'}\mathbf{Q}'\cdot\mathbf{N}\,\mathrm{d}A \tag{29}$$

which complies with the second law of thermodynamics.

4 CONCLUSIONS

We have developed a new GENERIC-based variational formulation for large strain elastodynamics. Two salient features of the newly proposed weak formulation (26) are (i) the possibility to freely choose from among three options for the thermodynamic state variable (the absolute temperature, the internal energy density, or the entropy density), and (ii) the nonstandard form provided by the underlying GENERIC formalism. These features make possible the design of alternative thermodynamically consistent Energy-Momentum-Entropy schemes. This is shown in the companion contribution [15].

Acknowledgement

Support for this research was provided by the Deutsche Forschungsgemeinschaft (DFG) under Grant BE 2285/13-1. This support is gratefully acknowledged.

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