European Congress on Computational Methods
in Applied Sciences and Engineering (ECCOMAS 2012)
J. Eberhardsteiner et.al. (eds.)
Vienna, Austria, September 10-14, 2012

DYNAMIC FINITE DEFORMATION THERMO-VISCOELASTICITY USING ENERGY-CONSISTENT TIME-INTEGRATION

Melanie Krüger[1], Michael Groß[2] & Peter Betsch[1]

[1]University of Siegen
Paul-Bonatz-Straße 9-11, 57068 Siegen
e-mail: melanie.krueger@uni-siegen.de, peter.betsch@uni-siegen.de

[2] Chemnitz University of Technology
Straße der Nationen 62, 09111 Chemnitz
e-mail: michael.gross@mb.tu-chemnitz.de

Keywords: enhanced GENERIC, enhanced TC algorithm, partitioned discrete gradients

Abstract. *The main goal of the present work is the description of a dynamic finite deformation thermo-viscoelastic continuum in the enhanced GENERIC (General equations for non-equilibrium reversible irreversible coupling) format. Therefore the time integration is done with partitioned discrete derivatives for the thermodynamically consistent system. The system of partial differential equations is described in an enhancement of the so called GENERIC format. This GENERIC format was introduced for thermo-elastodynamic systems. The considered variables of the system are the Poissonian variables, which are the linear momentum, the configuration, the entropy and the internal variable.*

There are two constitutive equations for the thermo-viscoelastic continuum necessary. The thermal evolution equation is described with Fourier's law of isotropic heat conduction and the viscous part is given by the fourth order compliance tensor.

The enhanced numerical stability of the newly developed structure-preserving integrators in comparison to standard integrators is demonstrated by means of numerical examples.

1 INTRODUCTION

Structure preserving time integrators are meanwhile well-known as time integrators, which lead to enhanced robustness and longtime stability. An often used time approach is the discrete derivative of Gonzalez [1]. Furthermore, the Hamiltonian formulation leads for elastodynamics to an energy-momentum scheme (see Gonzalez [2]). Öttinger [9] introduced for thermodynamics a GENERIC (General Equations for Non-Equilibrium Reversible Irreversible Coupling) format which includes a dissipative term. The state variables are the Poissonian variables (configuration, linear momenta and entropy). This framework is given for closed systems. In Romero [11, 12, 13] the GENERIC format is applied with partitioned discrete gradients (see Gonzalez [1]) for a thermoelastic double pendulum and a thermoelastic continuum. This time integrator is called the TC (Thermodynamically Consistent) integrator and preserves the underlying structural properties. In Krüger et al.[5] a comparison of the TC integrator and two other structure preserving time integrators is presented.

In the present work, the GENERIC framework and the TC integrator will be enhanced to thermoviscoelastic systems. For a double pendulum, the enhanced GENERIC format and the enhanced TC algorithm is considered in Krüger et al.[6]

2 THERMOVISCOELASTIC CONTINUUM

The motion of a continuum $\mathcal{B}$ with a particle P and the boundary $\partial\mathcal{B}$ over a time t is described with two configurations (see Figure 1). Here, the reference configuration $\mathcal{B}_0$ is given

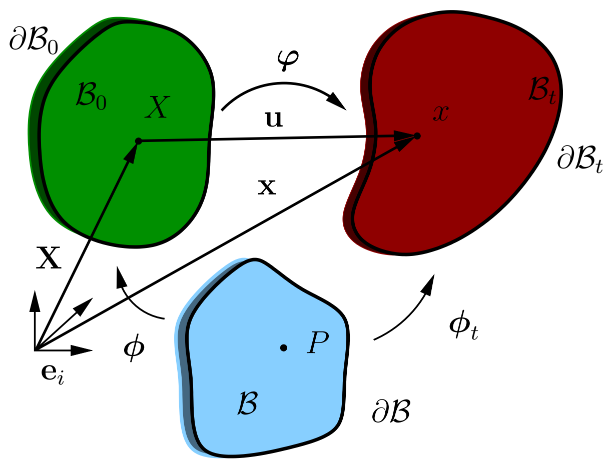

Figure 1: Configurations of a continuum

at time $t = 0$ and the current configuration $\mathcal{B}_t$ is defined at a time $t > 0$. $\partial\mathcal{B}_0$ and $\partial\mathcal{B}_t$ are the corresponding boundaries. The particle P is transformed with the nonlinear mappings ϕ and ϕ_t to the reference configuration $\mathcal{B}_0$ and the current configuration $\mathcal{B}_t$ (see Holzapfel [4]), respectively:

$$\mathbf{X} = \phi(P, t) \qquad\qquad \mathbf{x} = \phi_t(P, t) \tag{1}$$

$\mathbf{X}$ and $\mathbf{x}$ denote the position vectors of the points X and x, respectively. The nonlinear mapping φ maps the position vector $\mathbf{X}$ to the current configuration $\mathbf{x}$ by:

$$\mathbf{x} = \varphi(\mathbf{X}, t) \tag{2}$$

The displacement field $\mathbf{u}$ is defined by the difference of the position vectors:

$$\mathbf{u}(\mathbf{X},t) = \mathbf{x}(\mathbf{X},t) - \mathbf{X} \tag{3}$$

The velocity and acceleration field can be derived by the first and second partial time derivative of the mapping $\boldsymbol{\varphi}$:

$$\mathbf{v}(\mathbf{X},t) = \frac{\partial \boldsymbol{\varphi}(\mathbf{X},t)}{\partial t} =: \dot{\boldsymbol{\varphi}} \qquad\qquad \mathbf{a}(\mathbf{X},t) = \frac{\partial^2 \boldsymbol{\varphi}(\mathbf{X},t)}{\partial t^2} =: \ddot{\boldsymbol{\varphi}} \tag{4}$$

These derivatives can also be written $\mathbf{v} = \dot{\mathbf{x}}$ and $\mathbf{a} = \ddot{\mathbf{x}}$. Hence, a dot denotes a partial time derivative at a fixed position vector $\mathbf{X}$. The deformation of the continuum is given by the deformation gradient

$$\mathcal{F} = \frac{\partial \boldsymbol{\varphi}(\mathbf{X},t)}{\partial \mathbf{X}} = \mathrm{Grad}\,\boldsymbol{\varphi}(\mathbf{X},t) \tag{5}$$

With the definition of the Jacobian determinant $J = \det \mathcal{F} > 0$, the volume element of the reference configuration $\underset{\cdot}{\mathrm{V}}$ can be related to the current volume $\underset{\cdot}{\mathrm{v}} = J\,\underset{\cdot}{\mathrm{V}}$. The deformation gradient leads to the strain of continuum, which is denoted by the right Cauchy-Green strain tensor

$$\mathcal{C} = \mathcal{F}^{\mathrm{T}}\,\mathcal{F} \tag{6}$$

In order to describe thermal behavior, the entropy is chosen as state variable:

$$s = s(\mathbf{X},t) \tag{7}$$

This variable was also selected in the works of Romero [12, 13]. The underlying constitutive law of the internal energy e yields the temperature

$$\theta = \frac{\partial e}{\partial s} \tag{8}$$

The viscous (history dependend) material behavior is described by an isotropic internal variable (see Reese et al. [10] & Groß [3]):

$$\mathcal{C}_i = \mathcal{F}_i^{\mathrm{T}}\,\mathcal{F}_i \tag{9}$$

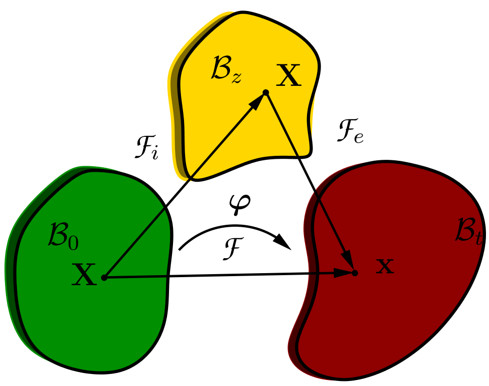

Figure 2: Intermediate configuration of the continuum

$\mathcal{F}_e$ describes the elastic deformation gradient. The internal variable $\mathcal{C}_i$ is symmetric and characterizes the internal structure of the continuum with irreversible (dissipative) effects. Note that the internal deformation gradient $\mathcal{F}_i$ is given on the intermediate configuration $\mathcal{B}_z$ (see Figure 2), which is a transformation of two inelastic states. In Noll [7, 8] the material isomorphism is introduced, which establishes a connection between two particles. The isotropic material behavior leads to the elastic strain measure

$$\mathcal{C}_e = \mathcal{C}\,\mathcal{C}_i^{-1} \tag{10}$$

3 PHYSICAL STRUCTURE

The total energy H of the continuum is given by the total kinetic energy T and the total internal energy E:

$$H = T\,(\mathbf{p}) + E\,(\mathcal{C}, s, \mathcal{C}_i) \tag{11}$$

The total kinetic energy T and the total internal energy E are the integrals over the domain of the kinetic energie $\mathcal{T}$ and the internal energy e:

$$T\,(\mathbf{p}) = \int\limits_{\mathcal{B}_0} \mathcal{T}\,(\mathbf{p}) \qquad\qquad E\,(\mathcal{C}, s, \mathcal{C}_i) = \int\limits_{\mathcal{B}_0} e\,(\mathcal{C}, s, \mathcal{C}_i) \tag{12}$$

Furthermore, the total kinetic energy T is given in terms of the linear momenta $\mathbf{p} = \rho_0\,\mathbf{v}$ and the constant density ρ_0 by:

$$T\,(\mathbf{p}) = \int\limits_{\mathcal{B}_0} \frac{1}{2\,\rho_0}\,\mathbf{p}\cdot\mathbf{p} \tag{13}$$

The total entropy of the system S is defined by the local entropy s functions:

$$S = \int\limits_{\mathcal{B}_0} s \tag{14}$$

As stability criterion, the Lyapunov function L is introduced:

$$L = H - \theta_\infty\,S \tag{15}$$

The temperatur θ_∞ is the reference temperature.

4 STRONG EVOLUTION EQUATIONS

The strong evolution equations are the two equations of motion, which are well known from elastodynamics, the thermal evolution equation and the viscous evolution equation:

$$\begin{aligned}
\dot{\boldsymbol{\varphi}} &= \frac{1}{\rho_0}\,\mathbf{p} \\
\dot{\mathbf{p}} &= \mathrm{Div}\,\mathcal{P} \\
\dot{s} &= -\frac{1}{\theta}\,\left[\mathrm{Div}\,\mathbf{Q} - D^{int}\right] \\
\dot{\mathcal{C}}_i &= 2\,\mathcal{C}_i\,\mathbb{V}^{-1} : \varSigma^{vis}
\end{aligned} \tag{16}$$

The first Piola-Kirchhoff stress tensor $\mathcal{P}$ depends on the second Piola-Kirchhoff stress tensor $\mathcal{S}$:

$$\mathcal{P} = \mathcal{F}\,\mathcal{S} \qquad\qquad \mathcal{S} = 2\,\frac{\partial e}{\partial \mathcal{C}} \tag{17}$$

As constitutive equation for the first Piola-Kirchhoff heat flux $\mathbf{Q}$ the Fouriers law of heat conduction is used with the assumption of isotropy:

$$\mathbf{Q} = -\mathcal{K}\ \mathrm{Grad}\,\theta \tag{18}$$

The isotropic heat conduction tensor $\mathcal{K}$ is defined by

$$\mathcal{K} = \kappa\, J\, \mathcal{C}^{-1} \tag{19}$$

where $\kappa > 0$ denotes the heat conduction parameter and the Jacobian determinant $J = \sqrt{\det \mathcal{C}}$ is evaluated with the right Cauchy-Green strain tensor $\mathcal{C}$. The viscous evolution equation leads to the viscous Mandel stress Σ^{vis}, which depends on the inelastic stress tensor Γ:

$$\Sigma^{vis} = 2\,\mathcal{C}_i\,\Gamma \qquad\qquad \Gamma = -\frac{\partial e}{\partial \mathcal{C}_i} \tag{20}$$

This inelastic stress Γ can be recovered in the internal dissipation

$$D^{int} = \Gamma : \dot{\mathcal{C}}_i \tag{21}$$

The fourth order compliance tensor $\mathbb{V}^{-1}$ is split into a deviatoric and volumetric part:

$$\mathbb{V}^{-1} = \frac{1}{2\,V^{dev}}\,\mathbb{I}^{dev^{\mathrm{T}}} + \frac{1}{V^{vol}\,n_{dim}}\,\mathbb{I}^{vol} \tag{22}$$

with

$$\begin{aligned} \mathbb{I}^{dev^{\mathrm{T}}} &= \mathbb{I}^{\mathrm{T}} - \mathbb{I}^{vol} \\ \mathbb{I}^{vol} &= \frac{1}{n_{dim}}\, I \otimes I \\ \mathbb{I}^{\mathrm{T}} &= I \underline{\otimes} I \end{aligned} \tag{23}$$

The deviatoric and volumetric parameter V^{dev} and V^{vol} as well as the dimension n_{dim} define this compliance tensor with the restrictions

$$V^{dev} > 0 \qquad\qquad V^{vol} > \frac{2\,V^{dev}}{n_{dim}} \tag{24}$$

5 ENHANCED GENERIC

The GENERIC format was introduced by Öttinger [9]. This format is given for thermal and mechanical isolated systems. For the thermoviscoelastic continuum, the GENERIC system will be enhanced. The initial value problem is stated by

$$\begin{aligned} \dot{\mathbf{z}} &= \left[\mathbf{L}(\mathbf{z}) + \mathbf{L}^{vis}(\mathbf{z})\right]\ \delta H(\mathbf{z}) + \left[\mathbf{M}(\mathbf{z}) + \mathbf{M}^{vis}(\mathbf{z})\right]\ \delta S(\mathbf{z}) \\ \mathbf{z}(t=0) &= \mathbf{z}^0 \end{aligned} \tag{25}$$

The state vector $\mathbf{z} \in \mathbb{R}^{13}$ is defined by the mapping $\boldsymbol{\varphi}$, the linear momenta $\mathbf{p}$, the entropy s and the internal variable in Voigt notation $\mathcal{C}_i$:

$$\mathbf{z} = \begin{bmatrix} \boldsymbol{\varphi} \\ \mathbf{p} \\ s \\ [\mathcal{C}_i]_{vn} \end{bmatrix} \tag{26}$$

The matrices $\mathbf{L}$ and $\mathbf{M}$ denote the skew-symmetric Poisson matrix and the symmetric positive-semidefinite friction matrix, respectively. The viscous evolution equation leads to the enhanced symmetric matrices $\mathbf{L}^{vis}$ and $\mathbf{M}^{vis}$. These matrices are as follows:

$$\mathbf{L} = \begin{bmatrix} \mathbf{0}^{3\times3} & \mathbf{I}^{3\times3} & \mathbf{0}^{3\times7} \\ -\mathbf{I}^{3\times3} & \mathbf{0}^{3\times3} & \mathbf{0}^{3\times7} \\ \mathbf{0}^{7\times3} & \mathbf{0}^{7\times3} & \mathbf{0}^{7\times7} \end{bmatrix} \qquad \mathbf{L}^{vis} = \begin{bmatrix} \mathbf{0}^{7\times7} & \mathbf{0}^{7\times6} \\ \mathbf{0}^{6\times7} & -4\,\left[V_1\,\mathcal{C}_i \underline{\otimes} \mathcal{C}_i + V_2\,\mathcal{C}_i \otimes \mathcal{C}_i\right]_{vn} \end{bmatrix}$$
$$\mathbf{M} = \begin{bmatrix} \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \\ \mathbf{0}^{1\times6} & -\dfrac{1}{\theta}\,\mathrm{Div}\,\mathbf{Q} & \mathbf{0}^{1\times6} \\ \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \end{bmatrix} \qquad \mathbf{M}^{vis} = \begin{bmatrix} \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \\ \mathbf{0}^{1\times6} & \dfrac{1}{\theta}\,D^{int} & \mathbf{0}^{1\times6} \\ \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \end{bmatrix} \tag{27}$$

Here, the parameter V_1 and V_2 are shorthand notations for the expressions

$$V_1 = \frac{1}{2\,V_{dev}} \qquad V_2 = \frac{1}{V_{vol}\,n_{dim}^2} - \frac{1}{2\,V_{dev}\,n_{dim}} \tag{28}$$

The functional derivatives of the total energy δH and total entropy δS with respect to the state vector $\mathbf{z}$ are

$$\delta H = \begin{bmatrix} -\,\mathrm{Div}\,\mathcal{P} \\ \dfrac{1}{\rho_0}\,\mathbf{p} \\ \theta \\ -\,[\varGamma]_{vn} \end{bmatrix} \qquad \delta S = \begin{bmatrix} \mathbf{0}^{(3\times1)} \\ \mathbf{0}^{(3\times1)} \\ 1 \\ \mathbf{0}^{(6\times1)} \end{bmatrix} = \text{const.} \tag{29}$$

The related degeneracy conditions for the enhanced GENERIC format are similar to the degeneracy conditions of the GENERIC format, which means:

$$\int\limits_{\mathcal{B}_0} \delta H \cdot \mathbf{M}\,\delta S = 0 \qquad \int\limits_{\mathcal{B}_0} \delta S \cdot \left[\mathbf{L} + \mathbf{L}^{vis}\right]\,\delta H = 0 \tag{30}$$

Furthermore, the following enhanced degeneracy condition is necessary:

$$\int\limits_{\mathcal{B}_0} \delta H \cdot \mathbf{M}^{vis}\,\delta S = -\int\limits_{\mathcal{B}_0} \delta H \cdot \mathbf{L}^{vis}\,\delta H \tag{31}$$

5.1 Structural properties

The enhanced GENERIC format is linked to certain structural properties, which are fullfilled neglegting external forces. The first special property is the total energy consistency:

$$\dot{H} = \int\limits_{\mathcal{B}_0} \delta H \cdot \dot{\mathbf{z}} \tag{32}$$

Including the skew-symmetry of $\mathbf{L}$ and the degeneracy condition of Eq. $(30)_1$, the rate of the total energy yields

$$\begin{aligned}\dot{H} &= \int_{\mathcal{B}_0} \delta H \cdot \mathbf{L}^{vis}\, \delta H + \delta H \cdot \mathbf{M}^{vis}\, \delta S \\ &= 0\end{aligned} \tag{33}$$

due to the enhanced degeneracy condition Eq. (31). Analogously, the rate of the total entropy $\dot{S}$ is given as follows:

$$\begin{aligned}\dot{S} &= \int_{\mathcal{B}_0} \delta S \cdot \dot{\mathbf{z}} \\ &= \int_{\mathcal{B}_0} \delta S \cdot \left[\mathbf{M} + \mathbf{M}^{vis}\right]\, \delta S\end{aligned} \tag{34}$$

Here, the degeneracy condition of Eq. $(30)_2$ is inserted. The evaluation of the Matrices $\mathbf{M}$ and $\mathbf{M}^{vis}$, as well as the vector δS leads to

$$\begin{aligned}\dot{S} &= \int_{\mathcal{B}_0} \frac{1}{\theta}\left[\kappa\, J\, \theta^3\ \mathrm{Grad}\,\frac{1}{\theta} \cdot \mathcal{C}^{-1}\ \mathrm{Grad}\,\frac{1}{\theta} + D^{int}\right] \geq 0 \\ &= \int_{\mathcal{B}_0} \frac{D^{tot}}{\theta}\end{aligned} \tag{35}$$

Generally, the rate of the Lyapunov function V implies a stable equilibrium state, iff

$$\dot{V} \leq 0 \tag{36}$$

Here, the rate of the Lyapunov function is once more given by:

$$\dot{V} = \dot{H} - \theta_\infty\, \dot{S} \tag{37}$$

Inserting the two properties of Eqs. $(33)_2$ and $(35)_2$, the stable equilibrium state is guaranteed by:

$$\dot{V} = -\theta_\infty \int_{\mathcal{B}_0} \frac{D^{tot}}{\theta} \leq 0 \tag{38}$$

5.2 Weak evolution equations

The weak evolution equations of the enhanced GENERIC format can be derived by the total energy balance of Eq. (32). The functional dervative of the total energy δH yields the test functions $\mathbf{w}_z$. The first and second entry will be replaced by the strong evolution equations:

$$\mathbf{w}_z = \begin{bmatrix} \mathbf{w}_\varphi \\ \mathbf{w}_p \\ w_s \\ [w_{C_i}]_{vn} \end{bmatrix} = \begin{bmatrix} -\dot{\mathbf{p}} \\ \dot{\boldsymbol{\varphi}} \\ \theta \\ -[\mathit{\Gamma}]_{vn} \end{bmatrix} \tag{39}$$

The four weak equations of the enhanced GENERIC are

$$\begin{aligned}\int\limits_{\mathcal{B}_0} \mathbf{w}_z \cdot \dot{\mathbf{z}} = \int\limits_{\mathcal{B}_0} \mathbf{w}_\varphi \cdot \frac{1}{\rho_0}\,\mathbf{p} + \int\limits_{\mathcal{B}_0} \mathbf{w}_p \cdot \mathrm{Div}\,\mathcal{P} - \int\limits_{\mathcal{B}_0} \frac{w_s}{\theta}\,\left[\mathrm{Div}\,\mathbf{Q} - D^{int}\right] \\ + \int\limits_{\mathcal{B}_0} w_{C_i} : 2\,\mathcal{C}_i\,\mathbb{V}^{-1} : \Gamma^{vis}\end{aligned} \tag{40}$$

6 DISCRETIZATION IN TIME

The weak evolution equations are now discretized in time with the enhanced TC (Thermodynamically consistent) integrator. The TC integrator for thermoelastic systems was introduced by Romero [11] for a thermoelastic double pendulum. This integrator is now enhanced for the thermoviscoelastic continuum.

The time interval $\mathcal{I} = [0,\,\mathrm{T}]$ is split into finite time elements of the number $n = [1, \ldots, n_{tp}]$ with the time intervals $\mathcal{I}_n = [t_n, t_{n+1}]$. The time step size is denoted by $h_n = t_{n+1} - t_n$. The enhanced TC integrator is based upon the G-equivariant functional derivative of Gonzalez [1]. The time discrete weak evolution equations are given by

$$\begin{aligned}\frac{H_{n+1} - H_n}{h_n} &= \int\limits_{\mathcal{B}_0} \mathtt{w}_z \cdot \frac{\mathbf{z}_{n+1} - \mathbf{z}_n}{h_n} \\ &= \int\limits_{\mathcal{B}_0} \mathtt{w}_z \cdot \left(\left[\mathtt{L} + \mathtt{L}^{vis}\right]\,\Delta^G H + \left[\mathtt{M} + \mathtt{M}^{vis}\right]\,\Delta^G S\right)\end{aligned} \tag{41}$$

where

$$\mathtt{L} = \begin{bmatrix} \mathbf{0}^{3\times3} & \mathbf{I}^{3\times3} & \mathbf{0}^{3\times7} \\ -\mathbf{I}^{3\times3} & \mathbf{0}^{3\times3} & \mathbf{0}^{3\times7} \\ \mathbf{0}^{7\times3} & \mathbf{0}^{7\times3} & \mathbf{0}^{7\times7} \end{bmatrix},\ \mathtt{L}^{vis} = \begin{bmatrix} \mathbf{0}^{7\times7} & \mathbf{0}^{7\times6} \\ \mathbf{0}^{6\times7} & -4\,\left[V_1\,\mathcal{C}_{i_{n+\frac12}} \underline{\otimes} \mathcal{C}_{i_{n+\frac12}} + V_2\,\mathcal{C}_{i_{n+\frac12}} \otimes \mathcal{C}_{i_{n+\frac12}}\right]_{vn} \end{bmatrix}$$

$$\mathtt{M} = \begin{bmatrix} \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \\ \mathbf{0}^{1\times6} & -\dfrac{1}{\theta_{\frac12}}\,\mathrm{Div}\,\mathbf{Q}_{\frac12} & \mathbf{0}^{1\times6} \\ \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \end{bmatrix},\ \mathtt{M}^{vis} = \begin{bmatrix} \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \\ \mathbf{0}^{1\times6} & \dfrac{1}{\theta}\,D^{int}_{\frac12} & \mathbf{0}^{1\times6} \\ \mathbf{0}^{6\times6} & \mathbf{0}^{6\times1} & \mathbf{0}^{6\times6} \end{bmatrix} \tag{42}$$

The specific evaluation of the internal variables $\mathcal{C}_{i_{n+\frac12}}$, the temperatures $\theta_{\frac12}$, the heat flux vector $\mathbf{Q}_{\frac12}$ and the internal Dissipation $D^{int}_{\frac12}$ is done in the following way:

$$\begin{aligned} (\cdot)_{n+\frac12} &= \frac12\,\left[(\cdot)_n + (\cdot)_{n+1}\right] & \qquad \mathbf{Q}_{\frac12} &= -\kappa\,\sqrt{\det \mathcal{C}_{n+\frac12}}\,\mathcal{C}^{-1}_{n+\frac12}\,\mathrm{Grad}\,\theta_{\frac12} \\ \theta_{\frac12} &= \mathtt{D}_s e & D^{int}_{\frac12} &= 2\,\mathcal{C}_{i_{n+\frac12}}\,\Gamma_{\frac12} : \mathbb{V}^{-1} : 2\,\mathcal{C}_{i_{n+\frac12}}\,\Gamma_{\frac12} \end{aligned} \tag{43}$$

Here, the partitioned discrete gradient operator $\mathtt{D}\,(\cdot)$ is used (see Gonzalez [1]) for the derivative of the internal energy e with respect to the entropy s. The G-equivariant functional derivatives of the total energy and entropy are given by

$$\Delta^G H = \begin{bmatrix} -\operatorname{Div}\left(\mathcal{F}_{n+\frac{1}{2}}\,\mathcal{S}_{\frac{1}{2}}\right) \\ \mathtt{D}_{||\mathbf{p}||^2}\mathcal{T}\,2\,\mathbf{p}_{n+\frac{1}{2}} \\ \theta_{\frac{1}{2}} \\ -\left[\Gamma_{\frac{1}{2}}\right]_{vn3} \end{bmatrix} \qquad \Delta^G S = \begin{bmatrix} \mathbf{0}^{(3\times 1)} \\ \mathbf{0}^{(3\times 1)} \\ \mathtt{D}_s s \\ \mathbf{0}^{(6\times 1)} \end{bmatrix} \tag{44}$$

The second Piola-Kirchhoff stress tensor $\mathcal{S}_{\frac{1}{2}}$ and the inelastic stress tensor $\Gamma_{\frac{1}{2}}$ are also evaluated with partitioned discrete gradients:

$$\mathcal{S}_{\frac{1}{2}} = 2\,\mathtt{D}_{\mathcal{C}} e \qquad \Gamma_{\frac{1}{2}} = -\mathtt{D}_{\mathcal{C}_i} e \tag{45}$$

7 DISCRETIZATION IN SPACE

The spatial discretization of the weak evolution equations is performed with the Finite-Element-Method. Therefore, the continuum body $\mathcal{B}$ is approximated with n_e elements of $\Omega_e \subset \mathcal{B}^h$:

$$\mathcal{B} \approx \mathcal{B}^h = \bigcup_{e=1}^{n_e} \Omega_e \tag{46}$$

The discrete boundary $\partial\mathcal{B}^h$ is analogously given by $\partial\mathcal{B}^h = \bigcup_{e=1}^{n_e} \partial\Omega_e$. The isoparametric concept leads to ansatz functions, which are used for the geometry as well as for the field variables. These ansatz functions $N^A(\boldsymbol{\xi})$ are defined on a reference element $\Omega_\square$ with normalized coordinates $\boldsymbol{\xi}$. This leads to the following approximated test and trial functions:

$$\begin{aligned} \mathbf{X}^e &= \sum_{A=1}^{n_{af}} N^A\,\mathbf{X}^{eA} & \mathbf{w}^e_\varphi &= \sum_{A=1}^{n_{af}} N^A\,\mathbf{w}^{eA}_\varphi \\ \mathbf{x}^e &= \sum_{A=1}^{n_{af}} N^A\,\mathbf{x}^{eA} & \mathbf{w}^e_p &= \sum_{A=1}^{n_{af}} N^A\,\mathbf{w}^{eA}_p \\ \mathbf{p}^e &= \sum_{A=1}^{n_{af}} N^A\,\mathbf{p}^{eA} & w^e_s &= \sum_{A=1}^{n_{af}} N^A\,w^{eA}_s \\ s^e &= \sum_{A=1}^{n_{af}} N^A\,s^{eA} \end{aligned} \tag{47}$$

The viscous test and trial functions are evaluated on the element level. Hence, it is not necessary to approximate these functions in space. We denote the test function by $w^e_{\mathcal{C}_i}$ and the internal variable by $\mathcal{C}^e_i$. The deformation gradient $\mathcal{F}^e$ is approximated as follows:

$$\mathcal{F}^e = j^e\,\jmath^{e^{-1}} \tag{48}$$

The gradients j^e and $\jmath^e$ are defined as

$$\jmath^e = \frac{\partial\mathbf{X}^e}{\partial\boldsymbol{\xi}} \qquad j^e = \frac{\partial\mathbf{x}^e}{\partial\boldsymbol{\xi}} \tag{49}$$

The ordinary finite element approximation of the testfunction w^e_s in Eq. (47) pose a problem. An admissible testfunction is the temperature θ^e, but this testfunction is not approximated in

Eq. (47) and is not consistent with Eq. (32). Therefore, a projection of the testfunction θ^{P^e} leading to stability (see Romero [12]) with the node vector $\theta^{p^{eA}} = w_s^{eA}$:

$$\theta^{p^e} = \sum_{A=1}^{n_{af}} N^A \, \theta^{p^{eA}} \tag{50}$$

based on an additional time discrete equation:

$$\int_{\mathcal{B}_0} \mathtt{w}_{\theta^p} \, \theta^p = \int_{\mathcal{B}_0} \mathtt{w}_{\theta^p} \, \theta_{\frac{1}{2}} \tag{51}$$

is necessary. The testfunction of this equation can be approximated like the other testfunctions and is given by:

$$\mathtt{w}_{\theta^p} = -\frac{s_{n+1} - s_n}{h_n} \tag{52}$$

8 DISCRETE EVOLUTION EQUATIONS

The discrete weak evolution equations are now given for the enhanced GENERIC system. The global system includes the equations of motion, the thermal evolution equation and the projection:

$$\begin{aligned}
\bigcup_{e=1}^{n_e} \sum_{A,B=1}^{n_{af}} \mathtt{w}_{\varphi}^{eA} \cdot H^{AB} \, \frac{\mathbf{x}_{n+1}^{eB} - \mathbf{x}_n^{eB}}{h_n} &= \bigcup_{e=1}^{n_e} \sum_{A,B=1}^{n_{af}} \mathtt{w}_{\varphi}^{eA} \cdot M_{\rho_0^{-1}}^{AB} \, \mathbf{p}_{n+\frac{1}{2}}^{eB} \\
\bigcup_{e=1}^{n_e} \sum_{A,B=1}^{n_{af}} \mathtt{w}_{p}^{eA} \cdot H^{AB} \, \frac{\mathbf{p}_{n+1}^{eB} - \mathbf{p}_n^{eB}}{h_n} &= \bigcup_{e=1}^{n_e} \sum_{A=1}^{n_{af}} \mathtt{w}_{p}^{eA} \cdot \left(\mathbf{F}_{\frac{1}{2}}^{ext^{eA}} - \mathbf{F}_{\frac{1}{2}}^{int^{eA}} \right) \\
\bigcup_{e=1}^{n_e} \sum_{A,B=1}^{n_{af}} \mathtt{w}_{s}^{eA} \, H^{AB} \, \frac{s_{n+1}^{eB} - s_n^{eB}}{h_n} &= \bigcup_{e=1}^{n_e} \sum_{A=1}^{n_{af}} \mathtt{w}_{s}^{eA} \, \left(T^{ext^{eA}} - T^{int^{eA}} \right) \\
\bigcup_{e=1}^{n_e} \sum_{A,B=1}^{n_{af}} \mathtt{w}_{\theta^p}^{eA} \, H^{AB} \, \theta^{p^{eB}} &= \bigcup_{e=1}^{n_e} \sum_{A=1}^{n_{af}} \mathtt{w}_{\theta^p}^{eA} \int_{\Omega_\square} N^A \, \theta_{\frac{1}{2}}^e \det \mathcal{J}^e
\end{aligned} \tag{53}$$

The local system is given by the viscous evolution equation:

$$\bigcup_{e=1}^{n_e} \int_{\Omega_\square} \mathtt{w}_{C_i}^e : \frac{\mathcal{C}_{i_{n+1}}^e - \mathcal{C}_{i_n}^e}{h_n} = \bigcup_{e=1}^{n_e} \int_{\Omega_\square} \mathtt{w}_{C_i}^e : 2\, \mathcal{C}_{i_{n+\frac{1}{2}}}^e \, \mathbb{V}^{-1^e} : 2\, \mathcal{C}_{i_{n+\frac{1}{2}}}^e \, \Gamma_{\frac{1}{2}}^e \tag{54}$$

The internal forces $\mathbf{F}_{\frac{1}{2}}^{int^{eA}}$ and external forces $\mathbf{F}_{\frac{1}{2}}^{ext^{eA}}$ are given below:

$$\mathbf{F}_{\frac{1}{2}}^{int^{eA}} = \int_{\Omega_\square} \mathcal{F}_{n+\frac{1}{2}}^e \otimes \operatorname{Grad} N^A : \mathcal{S}_{\frac{1}{2}}^e \det \mathcal{J}^e \qquad\qquad \mathbf{F}_{\frac{1}{2}}^{ext^{eA}} = \sum_{B=1}^{n_{af}} H_r^{AB} \, \mathbf{T}_{\frac{1}{2}}^{eB} \tag{55}$$

The vector $\mathbf{T}_{\frac{1}{2}}^{eB}$ is the node vector of the first Piola-Kirchhoff stress vector $\mathbf{T}_{\frac{1}{2}}^{e} = \sum_{A=1}^{n_{af}} N^A \, \mathbf{T}_{\frac{1}{2}}^{eA}$. Analogously, the thermal evolution equation exhibits internal and external parts with the external heat flux $Q^e_{\frac{1}{2}} = \sum_{A=1}^{n_{af}} N^A\, Q^{eA}_{\frac{1}{2}}$:

$$\begin{aligned} T^{int^{eA}} &= \int\limits_{\Omega_\square} \left[\left[\frac{\operatorname{Grad} N^A}{\theta^{p^e}} - \frac{N^A}{\theta^{p^{e2}}} \operatorname{Grad} \theta^{p^e} \right] \cdot \mathcal{K}^e_{\frac{1}{2}} \operatorname{Grad} \theta^{p^e} - \frac{N^A}{\theta^{p^e}} D^{int^e}_{\frac{1}{2}} \right] \det \mathcal{J}^e \\ T^{ext^{eA}} &= \sum_{B=1}^{n_{af}} \int\limits_{\partial\Omega_\square} \frac{1}{\theta^{p^e}} N^A\, N^B \det \mathcal{J}^e_r\, Q^{eB}_{\frac{1}{2}} \end{aligned} \tag{56}$$

The scalars H^{AB}, $M^{AB}_{\rho_0^{-1}}$ and H^{AB}_r denote the boundary and volume integrals over the ansatz functions with the determinant over the boundaries $\det \mathcal{J}^e_r = ||\mathbf{X}^e_{,\xi} \times \mathbf{X}^e_{,\eta}||$:

$$H^{AB} = \int\limits_{\Omega_\square} N^A\, N^B \det \mathcal{J}^e \qquad M^{AB}_{\rho_0^{-1}} = \frac{1}{\rho_0} H^{AB} \qquad H^{AB}_r = \int\limits_{\partial\Omega_\square} N^A\, N^B \det \mathcal{J}^e_r \tag{57}$$

9 NUMERICAL EXAMPLES

The internal energy e is of Simo-Pister type and can be split into a compressible, a viscous and a thermal part:

$$e(\mathcal{C},\, s,\, \mathcal{C}_i) = \psi^{com}(\mathcal{C}) + \psi^{vis}(\mathcal{C},\, \mathcal{C}_i) + e^{the}(\mathcal{C},\, s) \tag{58}$$

with

$$\begin{aligned} \psi^{com} &= \frac{\mu}{2} (\operatorname{tr} \mathcal{C} - n_{dim} - 2 \ln) + \psi^{vol}(J) \\ \psi^{vis} &= \frac{\mu_e}{2} (\operatorname{tr} \mathcal{C}_e - n_{dim} - 2 \ln J_e) + \psi^{vol}(J_e) \\ e^{the} &= k\, [\theta(\mathcal{C}, s) - \theta_\infty] + \theta_\infty\, n_{dim}\, \beta\, \frac{\partial \psi^{vol}(J)}{\partial J} \end{aligned} \tag{59}$$

μ and λ are the Lamé parameters, μ_e and λ_e are the viscous Lamé parameters, k is the heat coefficient and β is the coupling parameter. The volumetric free energy $\psi^{vol}(J_{(\cdot)})$ is given by:

$$\psi^{vol}(J_{(\cdot)}) = \frac{\lambda_{(\cdot)}}{2} [\ln^2 J_{(\cdot)} + (J_{(\cdot)} - 1)^2] \tag{60}$$

The parameters for the following examples are given below:

$$\begin{array}{llll} \lambda = 3000 & \mu = 750 & \rho_0 = 8.93 & \\ \lambda_e = 3000 & \mu_e = 750 & V_{dev} = 100 & V_{vol} = 500 \\ \kappa = 2 & k = 150 & \theta_\infty = 300 & \beta = 0.0001 \end{array} \tag{61}$$

The continuum body is a disk (see Figure 3). This disk has an inner radius $r_1 = 0.8$ and an outer radius $r_2 = 2.0$. The thickness of the disk is $t = 0.4$. The initial temperature is logarithmic distributed from the temperature at the outer ring of 380 K to a temperature at the inner ring of 310 K.

For the first example we prescribe mechanical Dirichlet boundaries for the inner ring, which means a fixed position, and an initial angular velocity $\omega^0_z = 60$ elsewhere (see Figure 4). In the second example we state mechanical Neumann-Boundaries given by the traction vector $\mathbf{T}^h_{n+\frac{1}{2}} = \sum_B^{n_{af}} N^B\, \mathbf{t}^B \sin\left(\frac{2\pi}{8}\, t_{n+\frac{1}{2}}\right)$ with $\mathbf{t}^B = \begin{bmatrix} 0 & 100 & 0 \end{bmatrix}^{\mathrm{T}}$, see Figure 5 and in the

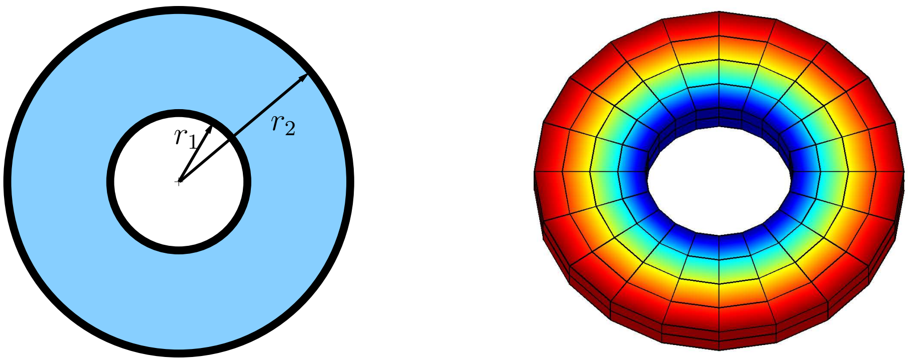

Figure 3: Continuum disk and the initial temperature contour

third example we prescribe thermal Neumann-boundaries with the boundary heat flux $Q^h_{n+\frac{1}{2}} = \sum_B^{n_{af}} N^B\, 1000 \sin\left(\frac{2\pi}{8}\, t_{n+\frac{1}{2}}\right)$, see Figure 6. These boundary conditions are applied for 8 s. After that the traction vector and the heat flux vanish and the system is totally closed. The time step size is $\Delta t = 0.02$ s.

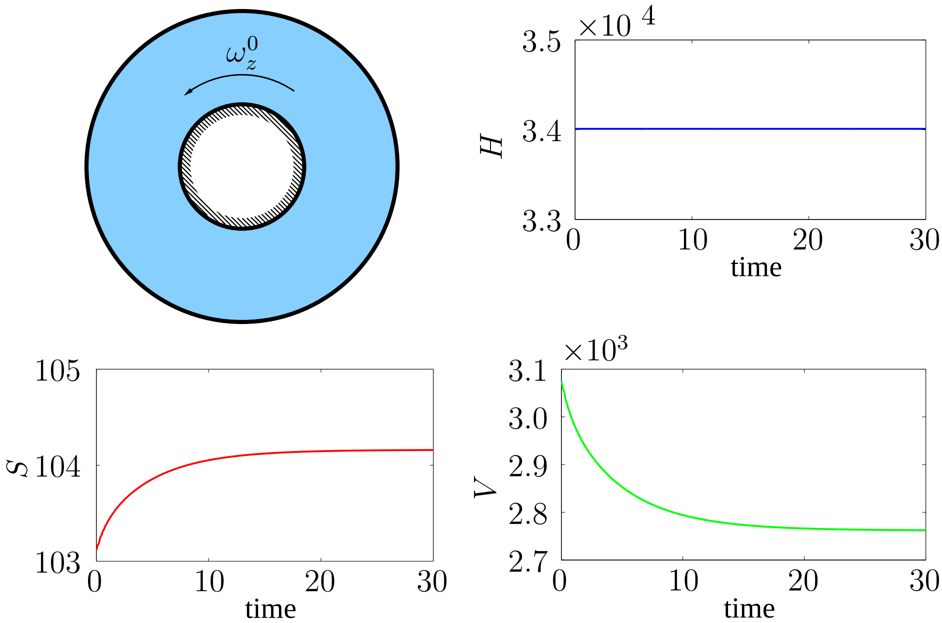

Figure 4: Example with Dirichlet boundaries and initial angular velocity, total energy H, total entropy S and Lyapunov function V

In Figure 4 the structural properties of the enhanced GENERIC system are shown for the first example. Here, external forces are neglected, this means that the disk is thermally and mechanically closed. The temperature balances to one temperature for the whole continuum. The total energy H is conserved for the total simulation time of 30 s. The total entropy S is increasing and the Lyapunov function V is decreasing, which indicates a stable system.

Figure 5 shows the result for the disk with Neumann boundaries related with the traction

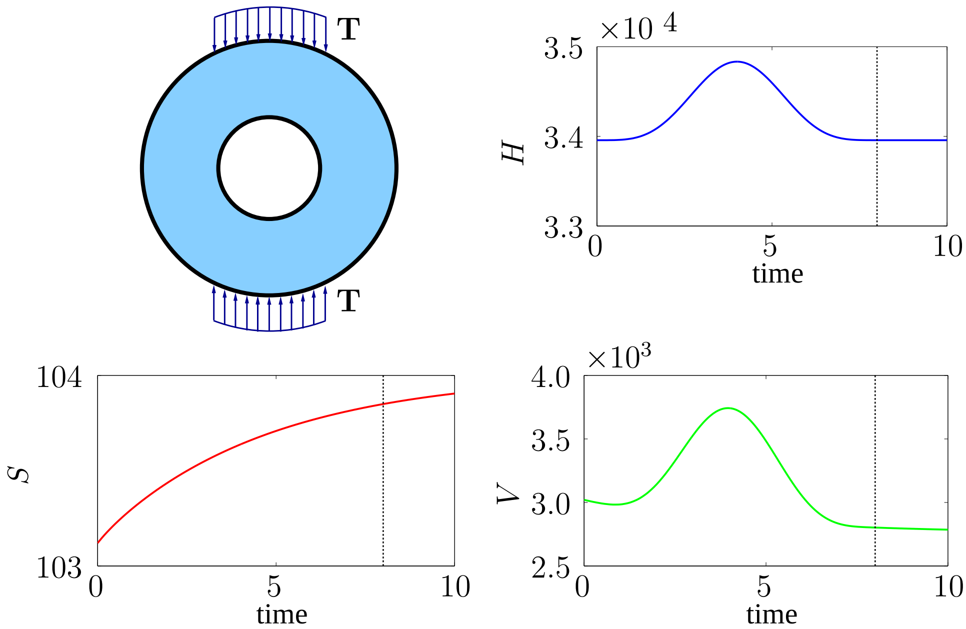

Figure 5: Example with Neumann boundaries for the traction vector, total energy H, total entropy S and Lyapunov function V

vector $\mathbf{T}^h_{n+\frac{1}{2}}$. This Neumann boundaries affect the total energy H, as well as the total entropy S and the Lyapunov function V. After 8 s the loads are removed and the structural properties of the enhanced GENERIC format are visible.

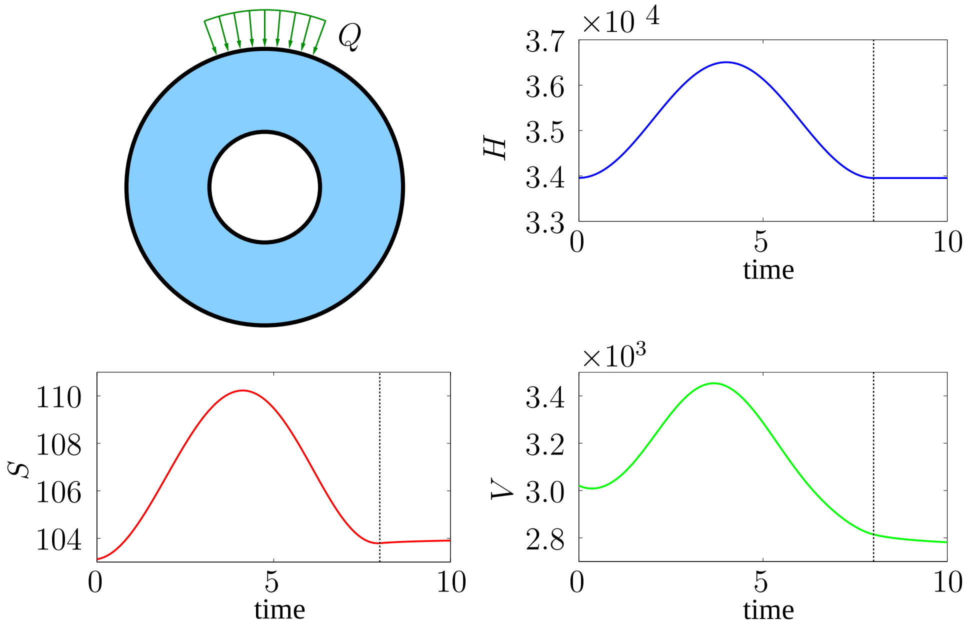

Figure 6: Example with Neumann boundaries for the heat flux, total energy H, total entropy S and Lyapunov function V

The third example is the disk with Neumann boundaries related to the boundary heat flux $Q^h_{n+\frac{1}{2}}$. The results are shown in Figure 6. Once again these boundaries affect the structural properties (H, S and V). After the 8 s of loads, the total energy H is conserved, the total entropy S increases and the Lyapunov function V decreases.

10 CONCLUSIONS

Structure preserving time integrators have become more and more important in the last decades. The preservation of the structural properties of the underlying system leads to long-time stability and computational robustness. In this work, we have newly proposed the enhanced GENERIC framework in connection with an enhanced TC integrator for thermoviscoelastic systems. This framework is based upon the Poissonian formulation of thermodynamics, which uses the configuration, the linear momenta, the entropy and the internal variables as state variables. The numerical examples show that the structural properties are preserved for closed systems. This means a constant total energy, an increasing total entropy and a decreasing Lyapunov function.

REFERENCES

[1] O. Gonzalez: Design and analysis of conserving integrators for nonlinear Hamiltonian systems with symmetry. Ph.D. Thesis, Department of Mechanical Engineering, Stanford University, March 1996.

[2] O. Gonzalez: Exact Energy and Momentum Conserving Algorithms for General Models in Nonlinear Elasticity. *Comput. Methods Appl. Mech. Engrg.*, 190 (2000), 1763–1783.

[3] M. Groß: Higher-order accurate and energy-momentum consistent discretisation of dynamic finite deformation thermo-viscoelasticity. Habilitationsschrift, urn:nbn:de:hbz:467-3890, Institut für Numerische Mechanik, Universität Siegen, Oktober 2008.

[4] G.A. Holzapfel: Nonlinear solid mechanics. A continuum approach for engineering. John Wiley & Sons Ltd., 2000.

[5] M. Krüger, M. Groß and P. Betsch: A comparison of structure-preserving integrators for discrete thermoelastic systems. *Comput. Mech.*, 47 (2011), 701–722.

[6] M. Krüger, M. Groß and P. Betsch: Energy-consistent time-integration for dynamic finite deformation thermo-viscoelasticity. *Proc. Appl. Math. Mech.*, 11 (2011), 239 – 240.

[7] W. Noll: A mathematical theory of the mechanical behavior of continuous media. *Arch. Rational Mech. Anal.*, 2 (1958), 197–226.

[8] W. Noll: A new mathematical theory of simple materials. *Arch. Rational Mech. Anal.*, 48 (1972), 1–50.

[9] H.C. Öttinger: Beyond equilibrium thermodynamics. John Wiley & Sons Inc., 2005.

[10] S. Reese and S. Govindjee: A theory of finite viscoelasticity and numerical aspects. *Int. J. Solids Structures*, 35 (1998), 3455–3482.

[11] I. Romero: Thermodynamically consistent time-stepping algorithms for non-linear thermomechanical systems. *Int. J. Numer. Meth. Engng*, 79 (2009), 706–732.

[12] I. Romero: Algorithms for coupled problems that preserve symmetries and the laws of thermodynamics. Part I: Monolithic integrators and their application to finite strain thermoelasticity. *Comput. Methods Appl. Mech. Engrg.*, (2010), 1841 – 1858.

[13] I. Romero: Algorithms for coupled problems that preserve symmetries and the laws of thermodynamics. Part II: Fractional step methods. *Comput. Methods Appl. Mech. Engrg.*, (2010), 2235 – 2248.