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Energy-Momentum-Entropy consistent time integration of dissipative thermomechanical systems in an extended framework of GENERIC

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Energy-Momentum-Entropy (EME) time-stepping schemes are distinguished by their numerical stable and robust behaviour, which stems from their ability to preserve the structure of the underlying system. In the context of closed dissipative thermomechanical systems, they are energy- and momentum-preserving as well as entropy-producing. In order to illustrate the qualification of the GENERIC framework for the design of EME integrators, a thermoviscoelastic double pendulum is chosen as discrete model problem to which the discrete gradient operator due to Gonzalez [1] is applied. The acronym GENERIC pertains to 'General Equation for Non-Equilibrium Reversible Irreversible Coupling' and provides by design a thermodynamic admissible mathematical framework for the evolution equations of dissipative thermomechanic systems. This contribution enlightens the incorporation of constraints in the GENERIC formalism and the necessity of a Lyapunov function as stability criterion.

1 Model problem

Despite its simplicity the model problem of a thermoviscoelastic double pendulum (Fig. 1) possesses essential structural properties of dissipative thermodynamic coupled systems. In this context, it facilitates the description of the GENERIC framework and therefore the design of thermodynamic consistent time-stepping schemes.

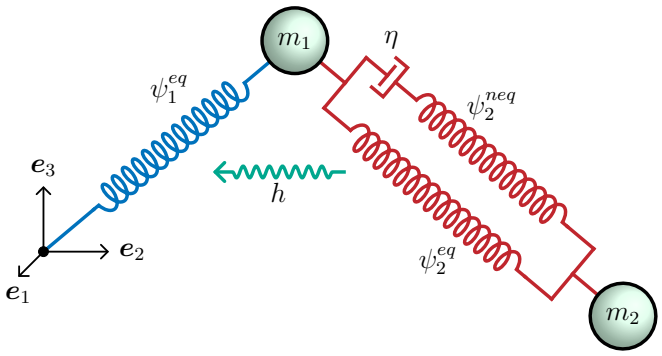

Fig. 1: The model problem of the thermoviscoelastic double pendulum.

The double pendulum's position in space is described through coordinates $\mathbf{q}_\alpha \in \mathbb{R}^3$, $(\alpha = 1, 2)$ that can be collected in the vector $\mathbf{q} = (\mathbf{q}_1, \mathbf{q}_2)$. They state the position of the mass points m_α, where $\mathbf{q}_2$ measures the distance from m_2 relative to m_1. Hence, the mass matrix has the form

$$\mathbf{m} = \begin{bmatrix} (m_1 + m_2)\mathbf{I} & m_2\mathbf{I} \\ m_2\mathbf{I} & m_2\mathbf{I} \end{bmatrix}, \tag{1}$$

with the identity matrix $\mathbf{I}$. The conjugate momenta are denoted $\mathbf{p} = (\mathbf{p}_1, \mathbf{p}_2)$ and calculated via $\mathbf{p} = \mathbf{m}\dot{\mathbf{q}}$, where the dot in the superscript denotes the temporal derivative. A thermoelastic spring connects the origin with m_1, while a thermoviscoelastic spring connects m_1 to m_2. Each spring's individual length is denoted by $l_\alpha = \sqrt{\mathbf{q}_\alpha \cdot \mathbf{q}_\alpha}$ and their unique temperature by θ_α. It is assumed that the thermoelastic behaviour of the first spring is governed by a free energy function $\psi_1(l_1, \theta_1)$. Similarly, the thermoviscoelastic behaviour is characterized by $\psi_2(l_2, \theta_2, \gamma)$, with γ being an internal variable that describes the inelastic strain in the damper. Both energy functions account for the Gough-Joule effect. According to Fourier's law, a heat flux takes place between the two springs.

An important advantage of GENERIC is the facilitation of the free choice of the thermodynamic variable τ_α among the entropy s_α, the temperature θ_α or the internal energy u_α due to its transformation properties (see [2]). The associated functions for the internal energy $U_1(l_1, \tau_1)$ and $U_2(l_2, \tau_2, \gamma)$ and the entropy $S_1(l_1, \tau_1)$ and $S_2(l_2, \tau_2, \gamma)$ can be determined from the two

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free energy functions by Legendre transformation. The temperature of the two springs can be calculated via

$$\Theta_\alpha = \frac{\partial_{\tau_\alpha} U_\alpha}{\partial_{\tau_\alpha} S_\alpha} \,. \tag{2}$$

Hence, the state vector, which completely describes the system follows as

$$\mathbf{z} = (\mathbf{q}, \mathbf{p}, \gamma, \tau) \,, \tag{3}$$

where $\tau = (\tau_1, \tau_2)$.

2 GENERIC-based formulation

The evolution equations within the GENERIC formalism according to Öttinger [3] follow as

$$\dot{\mathbf{z}} = \dot{\mathbf{z}}_{rev} + \dot{\mathbf{z}}_{irr} = \mathbf{L}(\mathbf{z}) \nabla E(\mathbf{z}) + \mathbf{K}(\mathbf{z}) \nabla S(\mathbf{z}) \,. \tag{4}$$

Herein, reversible processes are described through the gradient of the total energy E with the skew-symmetric Poisson matrix $\mathbf{L}$. In contrast, the irreversible evolution is generated through the gradient of the total entropy S with the symmetric and positive-semidefinite dissipative matrix $\mathbf{K}$. The framework is based on the thermodynamic consistency of the evolution equation (4), which is ensured through the degeneracy or non-interaction conditions

$$\begin{aligned} \mathbf{L} \nabla S &= \mathbf{0} \\ \mathbf{K} \nabla E &= \mathbf{0} \,. \end{aligned} \tag{5}$$

It is easily shown that GENERIC guarantees energy preservation ($\dot{E}(\mathbf{z}) = 0$) according to the first law of thermodynamics in a closed system as well as a non-decreasing entropy ($\dot{S}(\mathbf{z}) \geq 0$) as per second law of thermodynamics. Due to its thermodynamic admissibility, the GENERIC evolution equation (4) provides an ideal basis for the design of numerical time integration schemes for dissipative thermodynamic systems. If no external forces act on the point masses m_1 and m_2 and thermal interaction with the surrounding is prevented, the model problem constitutes a closed system. The total internal energy $U(\mathbf{z})$ and entropy $S(\mathbf{z})$ follow as the sum of the spring's internal energy and entropy. The total energy results in

$$E(\mathbf{z}) = \frac{1}{2} \mathbf{p} \cdot \mathbf{m}^{-1} \mathbf{p} + U(\mathbf{z}) \tag{6}$$

as the sum of the kinetic and internal energy, gravitation is considered by adding the corresponding potential.

The choice of the thermodynamic variable $\tau_\alpha \in \{\theta_\alpha, u_\alpha, s_\alpha\}$ influences the occupation of the structure-matrices $\mathbf{L}$ and $\mathbf{K}$ in the GENERIC formalism (4), which is illustrated in Fig. 2. Choosing the entropy ($\tau_\alpha = s_\alpha$) as thermodynamic variable does not lead to further contributions to the Poisson matrix $\mathbf{L}$, where only the entries due to the canonic Hamilton equations remain. In contrast, the choice of the temperature ($\tau_\alpha = \theta_\alpha$) leads to the maximum occupation.

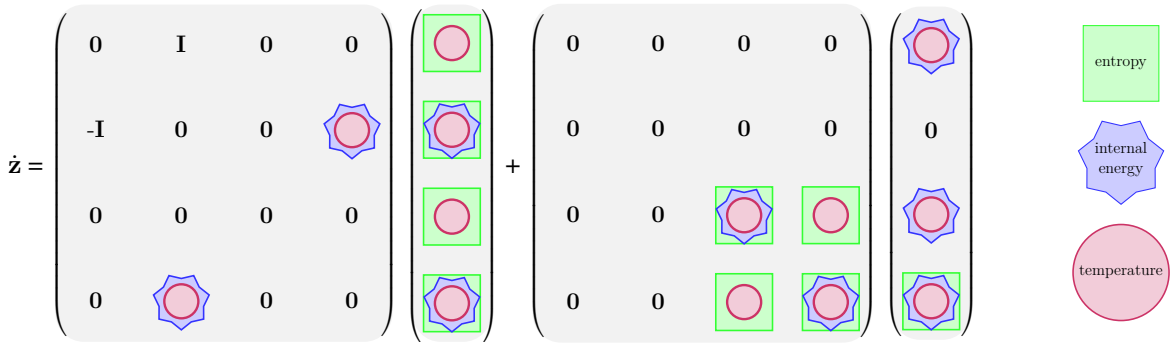

Fig. 2: Structure of the GENERIC evolution equation (4) dependent on the choice of the thermodynamic variable $\tau_\alpha \in \{\theta_\alpha, u_\alpha, s_\alpha\}$ for the model problem.

Mielke [2] proposed a special form of the GENERIC framework, which is based on a split of the Poisson matrix $\mathbf{L}$ and the dissipative matrix $\mathbf{K}$. Therefore, the matrices

$$\mathbf{M}_{\mathcal{H}}(\omega, \tau) = \begin{bmatrix} \mathbf{I} & \mathbf{0} \\ -\dfrac{1}{\nabla_\tau \mathcal{H}} \nabla_\omega \mathcal{H}^{\mathrm{T}} & \dfrac{1}{\nabla_\tau \mathcal{H}} \end{bmatrix} \quad \text{and} \quad \mathbf{M}^{\mathrm{T}}_{\mathcal{H}}(\omega, \tau) = \begin{bmatrix} \mathbf{I} & -\dfrac{1}{\nabla_\tau \mathcal{H}} \nabla_\omega \mathcal{H} \\ \mathbf{0} & \dfrac{1}{\nabla_\tau \mathcal{H}} \end{bmatrix} \tag{7}$$

are defined for a functional $\mathcal{H}$, where $\omega = (\mathbf{q}, \mathbf{p}, \gamma)$. The evolution equation in the specialized form follows as

$$\begin{bmatrix} \dot{\omega} \\ \dot{\tau} \end{bmatrix} = \mathbf{M}_S \mathbf{L}_0 \mathbf{M}_S^{\mathrm{T}} \nabla E + \mathbf{M}_E \mathbf{K}_0 \mathbf{M}_E^{\mathrm{T}} \nabla S = \mathbf{L} \nabla E + \mathbf{K} \nabla S \,, \tag{8}$$

where the mechanical matrices $\mathbf{M}_S$ and $\mathbf{M}_E$, as well as $\mathbf{M}_S^{\mathrm{T}}$ and $\mathbf{M}_E^{\mathrm{T}}$ correspond to the evaluation of (7) with respect to the functions of the total entropy and total energy. The matrices $\mathbf{L}_0$ and $\mathbf{K}_0$ possess a Poisson and dissipative structure, therefore the matrices $\mathbf{L} = \mathbf{M}_S \mathbf{L}_0 \mathbf{M}_S^{\mathrm{T}}$ and $\mathbf{K} = \mathbf{M}_E \mathbf{K}_0 \mathbf{M}_E^{\mathrm{T}}$ automatically define a Poisson and dissipative structure.

Multiplying the mechanical submatrices with the gradient of the total energy or total entropy gives

$$\mathbf{M}_E^{\mathrm{T}} \nabla E = \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \quad \text{and} \quad \mathbf{M}_S^{\mathrm{T}} \nabla S = \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \,, \tag{9}$$

which leads to the necessary condition

$$\mathbf{L}_0 \left(\omega, \tau\right) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \equiv 0 \equiv \mathbf{K}_0 \left(\omega, \tau\right) \begin{bmatrix} \mathbf{0} \\ \mathbf{1} \end{bmatrix} \tag{10}$$

for the fulfilment of the degeneracy conditions. The special form of GENERIC reveals the role of the reversible and irreversible driving forces as

$$\mathbf{M}_S^{\mathrm{T}} \nabla E = \begin{bmatrix} \nabla_\omega E - \theta \nabla_\omega S \\ \theta \end{bmatrix} \qquad \text{and} \qquad \mathbf{M}_E^{\mathrm{T}} \nabla S = \begin{bmatrix} \nabla_\omega S - \theta^{-1} \nabla_\omega E \\ \theta^{-1} \end{bmatrix} \,. \tag{11}$$

In contrast to the original GENERIC formulation due to Öttinger [3], the construction of the Poisson and dissipative matrices is very simple due to the split. The thermodynamic matrices $\mathbf{L}_0$ and $\mathbf{K}_0$ follow as

$$\mathbf{L}_0 = \begin{bmatrix} 0 & \mathbf{I} & 0 & 0 \\ -\mathbf{I} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \quad , \quad \mathbf{K}_0 = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \eta^{-1}\theta_2 & 0 \\ 0 & 0 & 0 & \mathbf{K}_{0,\tau\tau} \end{bmatrix} \quad \text{and} \quad \mathbf{K}_{0,\tau\tau} = \begin{bmatrix} \kappa\theta_2\theta_1 & -\kappa\theta_2\theta_1 \\ -\kappa\theta_2\theta_1 & \kappa\theta_2\theta_1 \end{bmatrix} \,. \tag{12}$$

Within the GENERIC framework constraints can be easily taken into account by adding an additional term, leading to

$$\dot{\mathbf{z}} = \dot{\mathbf{z}}_{rev} + \dot{\mathbf{z}}_{irr} = \mathbf{L}(\mathbf{z}) \nabla E(\mathbf{z}) + \mathbf{M}(\mathbf{z}) \nabla S(\mathbf{z}) + \mathbf{N}(\mathbf{z}) \lambda \tag{13}$$

as extension of the evolution equation (4). In this contribution two types of constraints will be addressed. Impeding the stretching of the first spring corresponds to the holonomic constraint $g_1(\mathbf{q}_1) = 0$ with $g_1 = \frac{1}{2}(l_1 - \bar{l}_1)$, where $\bar{l}_1$ denotes the prescribed distance of m_1 to the origin. The constraint force, which is necessary to that end, arises from the product of $\mathbf{N}(\mathbf{z})\lambda$. A variation of the first spring's temperature is prevented by $g_2(\mathbf{q_1}, \tau_1) = 0$, where $g_2 = \Theta_1 - \bar{\theta}_1$ with Θ_1 following (2) and $\bar{\theta}_1$ denoting the prescribed temperature. The corresponding entry in the matrix $\mathbf{N}$ with the entry in the vector λ governs the heat flux over the boundary of the system that is necessary to fulfil the temperature condition and which follows Fourier's law of heat conduction. In order to retain the GENERIC's thermodynamic consistency, the additional condition $\mathbf{N}^{\mathrm{T}} \nabla E = \mathbf{N}^{\mathrm{T}} \nabla S = \mathbf{0}$ has to hold for workless constraints. The condition on the temperature $g_2(\mathbf{q_1}, \tau_1) = 0$ leads to a heat flux over the system's boundary and therefore to a modification of the thermodynamic properties.

3 Energy-Momentum-Entropy consistent discretization

Structure-preserving time discretization methods are known for their numerical stable and robust behaviour (cf. [4, 5]). Previous work has shown that the midpoint rule as implicit integrator is only partially structure-preserving in dependence of the choice of the thermodynamic variable (compare [6–8]). The energy, which has proven to be a suitable numerical stability criterion for isothermal elastic systems is not adequate for the assessment of a dissipative thermomechanic system's stability. For this purpose

$$V(\mathbf{z}) = E(\mathbf{z}) - \theta_R S(\mathbf{z}) \tag{14}$$

has emerged as excellent indicator. Herein, θ_R denotes a constant reference temperature. It can be easily shown that V constitutes a Lyapunov function for the considered closed system. An integrator, which is able to correctly reproduce the first and second law of thermodynamics for arbitrary time step sizes, fulfils the stability criterion $V_{n+1} \leq V_n$ and is thermodynamically consistent. If the integrator additionally preserves the angular momentum, it is denoted as EME ('Energy-Momentum-Entropy') integrator. Dependent on the choice of the thermodynamic variable $\tau_\alpha \in \{\theta_\alpha, u_\alpha, s_\alpha\}$, three different time-stepping

schemes emerge ((EME)$_s$,(EME)$_\theta$,(EME)$_u$). The approximation of the differential-algebraic equations follows for initial values $\mathbf{z}_0$ of the state vector (3) at time $t = 0$ within the finite time interval $\mathcal{I}_n = (t_{n-1}, t_n]$ and time step size $\Delta t = t_{n+1} - t_n$ as

$$\begin{aligned} \Delta \mathbf{z} &= \frac{\mathbf{z}_{n+1} - \mathbf{z}_n}{\Delta t} = \mathrm{L}(\mathbf{z}_{n+1}, \mathbf{z}_n)\mathrm{DE}(\mathbf{z}_{n+1}, \mathbf{z}_n) + \mathrm{M}(\mathbf{z}_{n+1}, \mathbf{z}_n)\mathrm{DS}(\mathbf{z}_{n+1}, \mathbf{z}_n) + \mathrm{N}(\mathbf{z}_{n+1}, \mathbf{z}_n)\lambda_{n+1} \\ g_{n+1} &= 0 \,, \end{aligned} \tag{15}$$

where the functional values at time t_n are denoted by $(\bullet)_n$ and as $(\bullet)_{n+1}$ at time t_{n+1}. Herein, the derivatives are evaluated with the discrete derivative operator due to Gonzalez [1].

4 Numerical simulations

The free Helmholtz energy function that describes the thermoelastic and thermoviscoelastic behaviour of the two springs is chosen similarly to [9] as

$$\begin{aligned} \psi &= \psi_1^{eq}(\lambda_1, \theta_1) + \psi_2^{eq}(\lambda_2, \theta_2) + \psi_2^{neq}(\lambda_2, \theta_2, \gamma_2) \\ \psi_\alpha^{eq}(\lambda_\alpha, \theta_\alpha) &= \frac{\mu_\alpha^{eq}(\theta_\alpha)}{2} \ln^2\left(\frac{\lambda_\alpha}{\lambda_\alpha^0}\right) - \beta(\theta_\alpha - \theta_{ref}) \ln\left(\frac{\lambda_\alpha}{\lambda_\alpha^0}\right) + c_\alpha^0 \left(\theta_\alpha - \theta_{ref} - \theta_\alpha \ln\left(\frac{\theta_\alpha}{\theta_{ref}}\right)\right) \\ \psi_\alpha^{neq}(\lambda_\alpha, \theta_\alpha, \gamma_\alpha) &= \beta_\alpha^v \psi_\alpha^{eq}(\lambda_\alpha, \theta_\alpha) + \mu_\alpha^{neq}(\theta_\alpha)\gamma_\alpha^2 - \beta_\alpha^v \gamma_\alpha \frac{\partial \psi_\alpha^{eq}(\lambda_\alpha, \theta_\alpha)}{\partial \lambda_\alpha} \,. \end{aligned} \tag{16}$$

It is composed of the spring's free energy function ψ_α^{eq} and the Maxwell element's free energy function ψ_α^{neq}, where c_α^0, θ_{ref}, β and β^v denote the specific heat capacity, reference temperature and coupling parameters. The stiffness of the spring $\mu_\alpha^{eq}(\theta)$ and the Maxwell element $\mu_\alpha^{neq}(\theta)$ plus the viscosity parameter η are temperature-dependent and result from

$$\begin{aligned} &\mu_\alpha^{eq}(\theta) = \mu_{\alpha,cst}^{eq} - \mu_{\alpha,\theta}^{eq}(\theta - \theta_{ref}) \\ &\mu_\alpha^{eq}(\theta) = \mu_{\alpha,cst}^{neq} - \mu_{\alpha,\theta}^{neq}(\theta - \theta_{ref}) \\ &\eta = \eta_{cst} \exp\left[\eta_\theta \left(\frac{1}{\theta} - \frac{1}{\theta_{ref}}\right)\right] \end{aligned} \quad \text{with} \quad \begin{aligned} &\mu_{\alpha,cst}^{eq}, \mu_{\alpha,\theta}^{eq} > 0 \\ &\mu_{\alpha,cst}^{eq}, \mu_{\alpha,\theta}^{neq} > 0 \\ &\eta_{cst}, \eta_\theta > 0 \,. \end{aligned} \tag{17}$$

An overview of the chosen parameter values can be found in Table 1. The numeric data is produced within a time interval of $\mathcal{I} = [0, 20]$ s with a constant time step size of $\Delta t = 0.15$ s. The initial conditions are:

$$\theta_1^0 = 280 \text{ K}, \quad \theta_2^0 = 350 \text{ K}, \quad \mathbf{q}_1^0 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \text{m}, \quad \mathbf{q}_2^0 = \begin{bmatrix} 3 \\ 0 \\ 0 \end{bmatrix} \text{m}, \quad \mathbf{p}_1^0 = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \text{Ns}, \quad \mathbf{q}_2^0 = \begin{bmatrix} -1 \\ -1 \\ 0 \end{bmatrix} \text{Ns}, \quad \gamma_2^0 = 0 \text{ m}.$$

Table 1: Numerical data for the thermo-viscoelastic double pendulum.

Mass	m_1	1	m_2	1	kg
Natural length	λ_1^0	1.5	λ_2^0	2	m
Spring stiffness	$\mu_{1,cst}^{eq}$	200	$\mu_{2,cst}^{eq}$	200	J
	$\mu_{1,\theta}^{eq}$	0.5	$\mu_{2,\theta}^{eq}$	0.5	JK^{-1}
Maxwell element stiffness	-	-	$\mu_{2,cst}^{neq}$	5	Jm^{-2}
	-	-	$\mu_{2,\theta}^{neq}$	0.1	$\mathrm{J/m^2K}$
Specific heat capacity	c_1^0	10	c_2^0	10	JK^{-1}
Viscosity	-	-	η_{cst}	100	Nsm^{-1}
	-	-	η_θ	10	K
Thermal conductivity	k	1			$\mathrm{JK}^{-1}\mathrm{s}^{-1}$
Reference temperature	θ_{ref}	300			K
Coupling parameter	β	0.02			JK^{-1}
	β^v	0.5			m^{-2}
Gravitational vector	$\mathbf{g}$	$[0, 0, -9.81]^\mathrm{T}$			ms^{-2}
Newton tolerance		10e-8			-

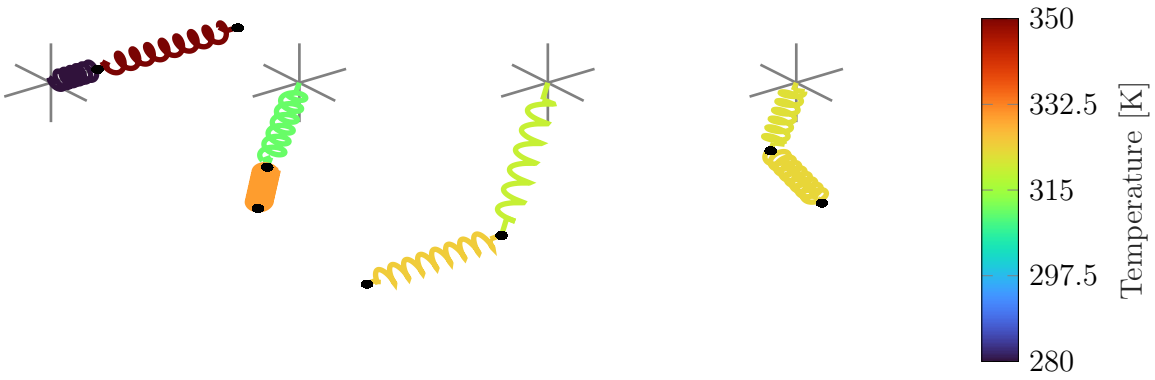

Fig. 3: Snapshots of the motion of the thermoviscoelastic double pendulum at time $t_n \in \{0, 8, 16, 24\}$.

Fig. 3 captures the motion of the double pendulum at discrete time steps and displays the approximation of the spring's temperatures due to the heat flux. Numeric results, that show the thermodynamic consistent behaviour of the EME integrators for all possible choices of the thermodynamic variable $\tau_\alpha \in (\theta_\alpha, u_\alpha, s_\alpha)$ are displayed in Fig. 4. Energy is preserved up to numeric errors, the entropy is an increasing function as per second law of thermodynamics due to heat flux and inelastic

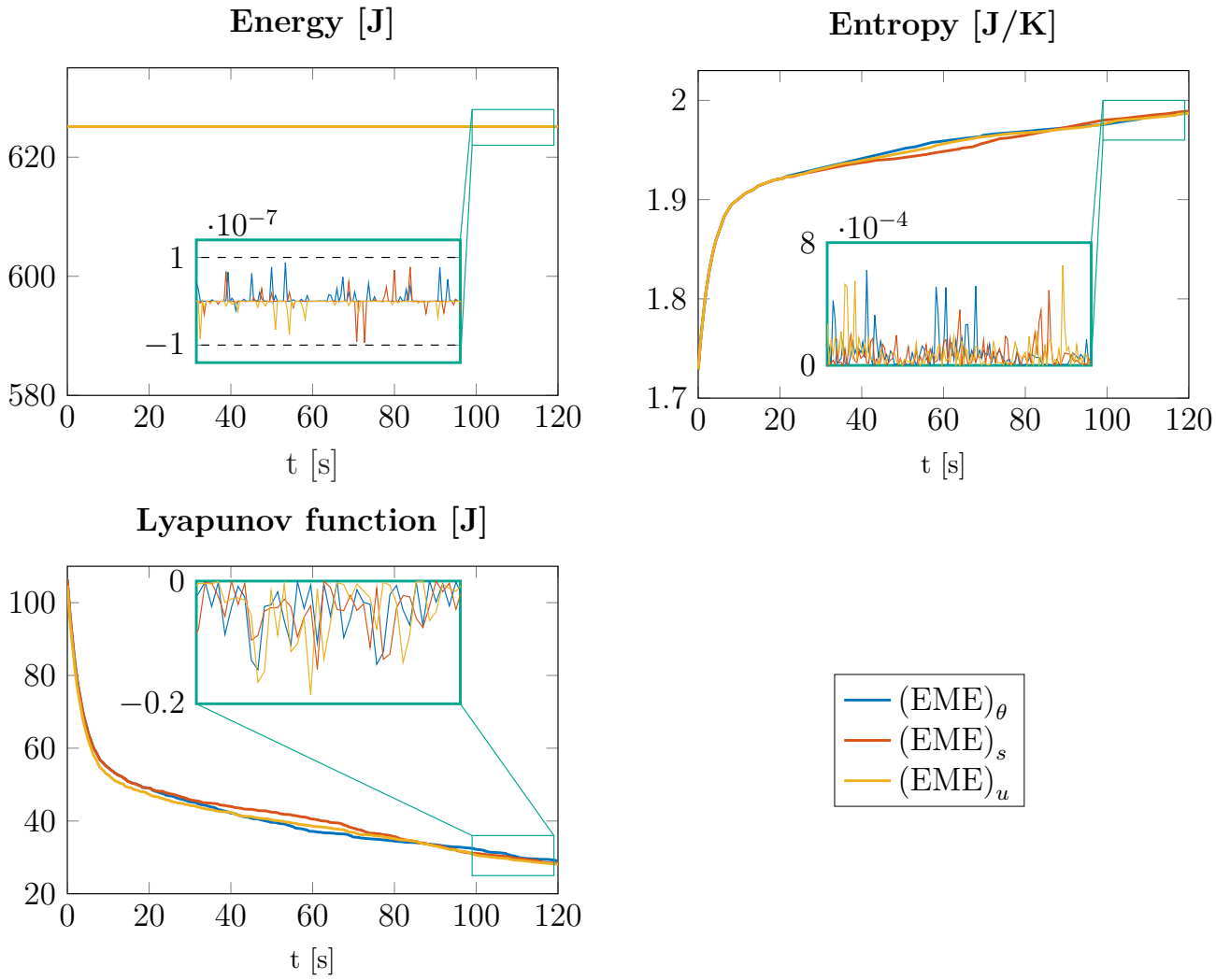

Fig. 4: Numeric results of the EME integrators that display the course of the total energy, the total entropy and the Lyapunov function as well as their respective incremental changes.

deformations. The numeric stability of the EME integrators follows from the monotonous decreasing course of the Lyapunov function.

The incorporation of the constraint functions g_1 and g_2 is evaluated in Fig. 5 for the (EME)$_\theta$ integrator. As mentioned before the constraint on the position vector is workless and hence inherits the GENERIC's thermodynamic consistency. However, the constraint on the temperature leads to a heat flux over the system's boundary, leading to a decay of the energy and entropy. Still, the (EME)$_\theta$ integrator yields a numeric stable behaviour, as depicted by the decreasing Lyapunov function.

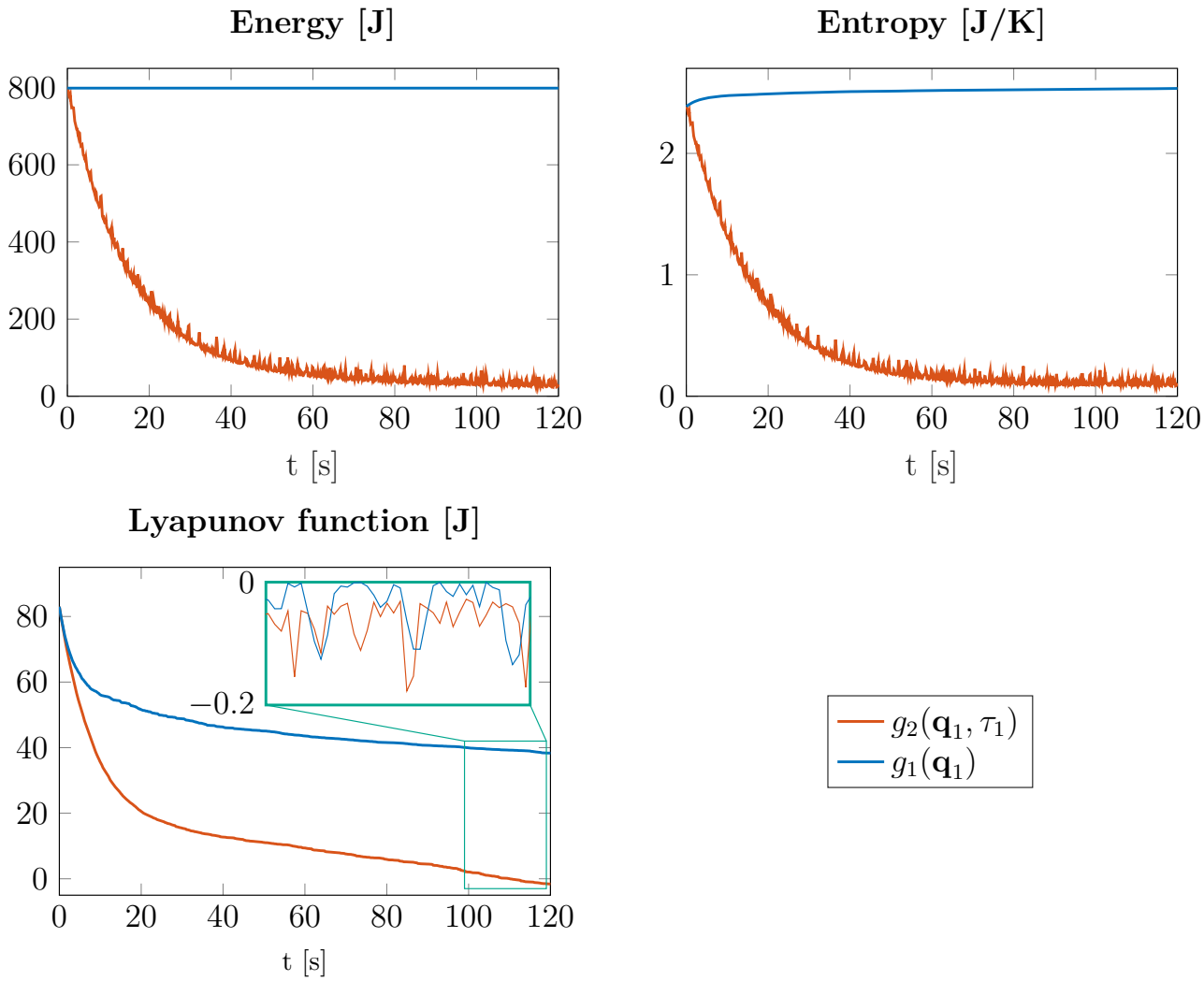

Fig. 5: Numeric results of the (EME)$_\theta$ integrator for the incorporation of the constraint functions $g_1(\mathbf{q}_1)$ and $g_2(\mathbf{q}_1, \tau_1)$, showing the course of the total energy and entropy, as well as the Lyapunov function and its incremental change.

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