A temperature-based thermodynamically consistent integration scheme for discrete thermo-elastodynamics

Sergio Conde Martín , Peter Betsch , Juan Carlos García Orden

ABSTRACT

The formulation of thermodynamically consistent (TC) time integration methods was introduced by a general procedure based on the GENERIC form of the evolution equations for thermo-mechanical problems. The use of the entropy was reported to be the best choice for the thermodynamical variable to easily provide TC integrators. Also the employment of the internal energy was proved to not involve excessive complications. However, attempts towards the use of the temperature in the design of GENERIC-based TC schemes have so far been unfruitful. This paper complements the said procedure to attain TC integrators by presenting a TC scheme based on the temperature as thermodynamical state variable. As a result, the problems which arise due to the use of the entropy are overcome, mainly the definition of boundary conditions. What is more, the newly proposed method exhibits the general enhanced numerical stability and robustness properties of the entropy formulation.

1. Introduction

The concept of thermodynamically consistent (TC) time integration methods encompasses any numerical integration method intended to solve thermodynamical systems in such a way that the laws of thermodynamics are discretely satisfied by construction. The practical engineering interest that thermodynamical systems have together with the success of the energy–momentum time integrators for Hamiltonian (conservative) systems, see [1,2], motivated many works towards this end, such as [3–5]. However, these methods – unlike the Hamiltonian case – were not developed within a uniform procedure.

It was not until the works of Romero [6–8] that TC schemes were devised in a general procedure for any thermodynamical system. This generalization was made possible by the use of GENERIC form of the evolution equations of the thermodynamical system at hand. The acronym GENERIC stands for "*General Equation for the Non-Equilibrium Reversible Irreversible Coupling*" and was introduced by Öttinger and co-workers [9]. This framework provides the evolution equations of any thermodynamical system by separating its reversible and irreversible parts. While the reversible part is connected to the derivative of the total energy of the system, the irreversible one depends on the derivative of the total entropy. For the particular case of reversibility the GENERIC formalism simplifies to the Hamiltonian one, as pointed out in [6], so that it can be interpreted as a natural generalization of the latter.

The design of the procedure to systematically attain TC integration schemes relies on the use of the discrete gradient operator which is a second order approximation of the standard gradient operator evaluated at midpoint, and satisfies two important

properties: *directionality* and *consistency*, see [10–13]. This key ingredient makes TC integrators share some of the appealing properties derived from conservation of structure, such as the conservation of the symmetries.

In theory, the thermodynamical state of any system can be described either by the absolute temperature or by the entropy or by the internal energy or by any other quantity that is a combination of these three. Due to its intuitive physical interpretation, temperature is often used as the variable for the thermodynamical state, see [4,5]. However, the use of the entropy as thermodynamical state variable has been reported to be the most suitable choice to yield TC integrators, see for instance [6–8,14]. Although therein the entropy was successfully employed, additional restrictions had to be assumed such as the necessity for material models to enable the analytical provision of its potentials in terms of the entropy. In addition, many of the thermodynamical problems of practical interest require Dirichlet boundary conditions which can only be defined by means of the temperature, concluding that the entropy choice does not allow or at least substantially hinders the solution of a wide range of problems.

The search for GENERIC form of the evolution equations has so far become cumbersome when the temperature was considered, consequently preventing the formulation of a corresponding TC integrator in the sense of Romero [6]. Recently, Mielke [15] has thoroughly elaborated a systematic procedure to reach the GENERIC form departing from any thermodynamic variable, demonstrating that a GENERIC form in terms of temperature may be achieved for dissipative thermo-mechanical systems. However, its application to any particular system remains non-trivial at all and, therefore, the way to formulate a temperature-based TC integrator has so far been an issue. In this work we successfully resolve this issue, proving that the election of the temperature as state variable does not involve a complex GENERIC form to deal with and hence facilitating the design of a new temperature-based TC integrator. On a related note, [15] contains the GENERIC representation for the limit case of isothermal dissipative systems which could be of interest to derive TC integrators for isothermal viscoelasticity or plasticity, as has profusely been addressed based on different approaches in [4,16–18].

Furthermore, the election of the temperature as thermodynamical state variable offers advantages from the analytical and numerical point of view. In this way, as the temperature can be directly measured, it is normally the preferable variable to work with in the material modelling community, see for instance [19–23]. The use of any thermodynamical variable other than the temperature would automatically involve the redefinition of the thermo-mechanical potentials such that they are expressed in terms of that other variable. For realistic models this step could become cumbersome or even impossible from an analytical point of view, so that a full implementation would then require a numerical strategy which would complicate in excess the formulation without any doubt. This factor along with the general necessity of imposing Dirichlet boundary conditions in continuous approaches (normally based on the FE method) motivated the search for a TC integrator in terms of the temperature.

This article is organized as follows. In Section 2, we summarize the thermodynamical system used for the formulation of the TC integrator based on the temperature as state variable. Subsequently, we outline the GENERIC formalism for finite dimensional systems and elaborate a temperature-based GENERIC form of the evolution equations. This is the departing point to formulate the TC integrator in Section 3, where we also perform a detailed comparison of the novel scheme with those previously obtained in the literature. Then, the numerical examples in Section 4 illustrate the performance of this method in comparison with traditional implicit methods and the entropy-based TC integrator. Finally, in Section 5 we outline the main conclusions derived from this work.

2. Model problem: thermo-spring system

This section summarizes the fundamental features of the thermodynamical system used to formulate a TC integrator based on the temperature. In particular, we consider the simple but meaningful model problem of a thermoelastic double pendulum which was first proposed by Romero [6], see also [24]. Therein, the problem was fully defined and its thermodynamical soundness was demonstrated as well.

2.1. The initial value problem

The thermoelastic double pendulum is an insulated system consisting of two point masses m_1 and m_2 connected with thermo-springs as depicted in Fig. 1. The first spring connects m_1 to the ground and the second spring connects m_2 to m_1. The positions of the particles are given by the vectors $\mathbf{q}_1$ and $\mathbf{q}_2$ relative to the inertial reference frame $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. The two thermo-springs have a natural length of λ_1^0 and λ_2^0, respectively, and exchange heat according to a unidimensional Fourier's law of the form

$$h = k(\theta_2 - \theta_1), \tag{1}$$

θ_α being the absolute temperature of the spring α and $k \geq 0$ being the coefficient of thermal conductivity.

According to the main goal of the present work the spring temperatures are considered as the variables to describe the thermodynamical state of the system. Then, each spring behaves according to a Helmholtz free-energy function $\Psi_\alpha(\lambda_\alpha, \theta_\alpha)$, which accounts for the thermo-mechanical coupling behaviour. It should be noted that this function is naturally defined in terms of the temperature. In addition, the elastic responses of the springs depend on their lengths, which are expressed in terms
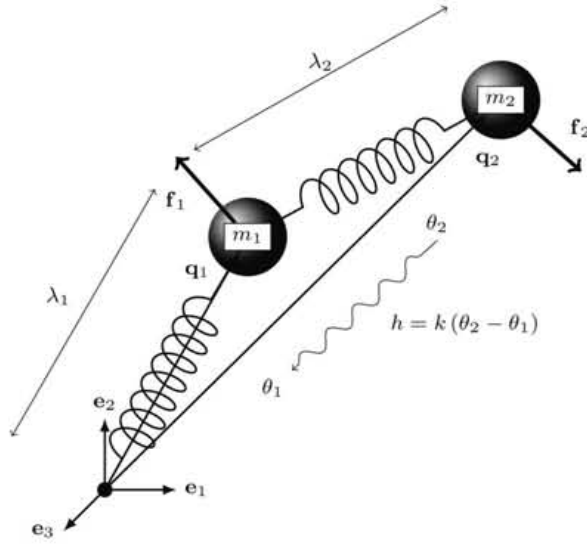
Fig. 1. Thermo-spring system.

of the position vectors as

$$\lambda_1(\mathbf{q}_1) = \|\mathbf{q}_1\| = \sqrt{\mathbf{q}_1 \cdot \mathbf{q}_1},$$
$$\lambda_2(\mathbf{q}_1, \mathbf{q}_2) = \|\mathbf{q}_2 - \mathbf{q}_1\| = \sqrt{(\mathbf{q}_2 - \mathbf{q}_1) \cdot (\mathbf{q}_2 - \mathbf{q}_1)} \tag{2}$$

The internal energy of each spring follows from the application of the Legendre transform to the above free-energy function, see [25], yielding

$$e_\alpha(\lambda_\alpha, s_\alpha(\lambda_\alpha, \theta_\alpha)) = \Psi_\alpha(\lambda_\alpha, \theta_\alpha) - \theta_\alpha \frac{\partial \Psi_\alpha(\lambda_\alpha, \theta_\alpha)}{\partial \theta_\alpha}, \tag{3}$$

which has also been expressed in terms of the temperature. In this connection, the entropy of each spring is identified to be

$$s_\alpha(\lambda_\alpha, \theta_\alpha) = -\frac{\partial \Psi_\alpha(\lambda_\alpha, \theta_\alpha)}{\partial \theta_\alpha} \tag{4}$$

The linear momentum and energy balance lead to the evolution equations of the system. By defining the associated momenta $\mathbf{p}_\alpha = m_\alpha \dot{\mathbf{q}}_\alpha$, the classical Newtonian approach, can be employed to derive the linear momentum balance for each spring

$$\dot{\mathbf{p}}_\alpha = -\sum_{\beta=1}^{2} \frac{\partial \Psi_\beta(\lambda_\beta, \theta_\beta)}{\partial \lambda_\beta} \frac{\partial \lambda_\beta}{\partial \mathbf{q}_\alpha} + \mathbf{f}_\alpha, \tag{5}$$

$\mathbf{f}_\alpha$ being external forces applied to the particles.

On the other hand, the energy balance of each spring establishes that the power of the force exerted on it is employed to change its internal energy or transfer heat

$$\frac{\partial \Psi_1}{\partial \lambda_1} \dot{\lambda}_1 = \dot{e}_1(\lambda_1, \theta_1) - h,$$
$$\frac{\partial \Psi_2}{\partial \lambda_2} \dot{\lambda}_2 = \dot{e}_2(\lambda_2, \theta_2) + h, \tag{6}$$

which, after using (3) along with the chain rule and some algebra, leads to the local energy balance in entropy form

$$\dot{s}_1(\lambda_1, \theta_1) = k\left(\frac{\theta_2}{\theta_1} - 1\right),$$
$$\dot{s}_2(\lambda_2, \theta_2) = k\left(\frac{\theta_1}{\theta_2} - 1\right) \tag{7}$$

For more details on this entropy form of the energy balance the reader is referred to [24].

It is worth mentioning that the above equations can as well be derived by applying a variational approach, see [26] for further details.

It only remains to set initial conditions for the positions $\mathbf{q}_\alpha^0$, the momenta $\mathbf{p}_\alpha^0$ and the temperatures θ_α^0 to complete the initial value problem given by (5), (7) along with the relation $\mathbf{p}_\alpha = m_\alpha \dot{\mathbf{q}}_\alpha$.

In what follows, we will conveniently work with the evolution equations in terms of the internal energy and entropy functions, given in (3) and (4). To this end, relationship (3) is used in the linear momentum balance (5). Furthermore, the energy balance of the two thermo-spring system may be rewritten so that the rate of temperature explicitly appears. It suffices to apply the chain rule to the function $\dot{s}_\alpha(\lambda_\alpha, \theta_\alpha)$ expressed in terms of positions via (2), to give

$$\dot{\theta}_\alpha = \left(\frac{\partial s_\alpha}{\partial \theta_\alpha}\right)^{-1}\left(\frac{h}{\theta_\alpha} - \sum_{\beta=1}^{2}\frac{\partial s_\alpha}{\partial \lambda_\alpha}\frac{\partial \lambda_\alpha}{\partial \mathbf{q}_\beta} \cdot \dot{\mathbf{q}}_\beta\right) \tag{8}$$

Remark 2.1. In the traditional calorimetry approach, the partial derivatives appearing in (8) are linked to the spring specific heat capacity

$$c_\alpha = \frac{\partial e_\alpha}{\partial \theta_\alpha} = \theta_\alpha \frac{\partial s_\alpha}{\partial \theta_\alpha} > 0, \tag{9}$$

and the spring latent heat

$$\nu_\alpha = \theta_\alpha \frac{\partial s_\alpha}{\partial \lambda_\alpha} \tag{10}$$

Note that the specific heat capacity indicates the amount of energy required to produce unit increase in the temperature while keeping the deformation fixed, and the latent heat accounts for the thermo-mechanical coupling, see for instance [27].

Then, taking into account the above considerations the following equivalent set of evolution equations is obtained

$$\begin{aligned}
\dot{\mathbf{q}}_\alpha &= \frac{\mathbf{p}_\alpha}{m_\alpha} \\
\dot{\mathbf{p}}_\alpha &= -\left[\sum_{\beta=1}^{2}\left(\frac{\partial e_\beta}{\partial \lambda_\beta} - \theta_\beta \frac{\partial s_\beta}{\partial \lambda_\beta}\right)\frac{\partial \lambda_\beta}{\partial \mathbf{q}_\alpha}\right] + \mathbf{f}_\alpha \\
\dot{\theta}_1 &= \left(\frac{\partial e_1}{\partial \theta_1}\right)^{-1}\left[-\theta_1 \frac{\partial s_1}{\partial \lambda_1}\frac{\partial \lambda_1}{\partial \mathbf{q}_1} \cdot \dot{\mathbf{q}}_1 + k(\theta_2 - \theta_1)\right] \\
\dot{\theta}_2 &= \left(\frac{\partial e_2}{\partial \theta_2}\right)^{-1}\left[-\theta_2 \sum_{\beta=1}^{2}\frac{\partial s_2}{\partial \lambda_2}\frac{\partial \lambda_2}{\partial \mathbf{q}_\beta} \cdot \dot{\mathbf{q}}_\beta + k(\theta_1 - \theta_2)\right]
\end{aligned} \tag{11}$$

2.2. GENERIC formalism for finite dimensional systems

We outline next the GENERIC formalism described in Öttinger [9] for finite dimensional systems as was advocated by Romero for the design of TC schemes in [6]. As previously indicated, the GENERIC formalism provides the evolution equations of a thermodynamical system based on an additive decomposition into reversible and irreversible parts. In this way, the reversible part is associated with the derivative of the total energy, whereas the irreversible part relies on the derivative of the total entropy.

Formally, given a state space $\mathcal{S}$ which contains all the mechanical, thermal, chemical, etc., variables required to fully represent the thermodynamical system so that its total energy $E : \mathcal{S} \to \mathbb{R}$ and total entropy $S : \mathcal{S} \to \mathbb{R}$ can thoroughly be obtained, the time-evolution of the state variables collected in $\mathbf{z} \in \mathcal{S}$ may be expressed by the following initial value problem

$$\dot{\mathbf{z}} = \mathbf{L}(\mathbf{z})\nabla E(\mathbf{z}) + \mathbf{M}(\mathbf{z})\nabla S(\mathbf{z}), \quad \mathbf{z}(0) = \mathbf{z}_0. \tag{12}$$

$\nabla(\bullet)$ being the gradient operator with respect to the state space vector, $\mathbf{z}_0$ containing the prescribed initial conditions and $\mathbf{L}, \mathbf{M} : \mathcal{S} \to \mathbb{R}^{\dim(\mathbf{z})\times\dim(\mathbf{z})}$ being the so-called Poisson matrix, which must be skew-symmetric, and the Dissipative matrix, which is required to be symmetric and positive semi-definite, respectively. In addition, these two matrices must satisfy the following degeneracy or non-interaction conditions

$$\nabla S^\mathsf{T}\mathbf{L} = \mathbf{0}, \quad \nabla E^\mathsf{T}\mathbf{M} = \mathbf{0} \tag{13}$$

The introduced requirements for the Poisson and Dissipative matrices together with the non-interaction conditions (13) ensure the fulfilment of laws of thermodynamics, as one can straightforwardly verify by computing both the rate of the total energy and total entropy of the system

$$\dot{E} = \nabla E \cdot \dot{\mathbf{z}} = \nabla E^\mathsf{T}\mathbf{L}\nabla E + \nabla E^\mathsf{T}\mathbf{M}\nabla S = 0, \tag{14}$$

$$\dot{S} = \nabla S \cdot \dot{\mathbf{z}} = \nabla S^\mathsf{T}\mathbf{L}\nabla E + \nabla S^\mathsf{T}\mathbf{M}\nabla S \geq 0, \tag{15}$$

where use has been made of (12).

In the described formalism (12)–(15), the definition of the Poisson and Dissipative matrices plays a crucial role since they contain the reversible/irreversible structure of the thermodynamical evolution of the system. Their obtention in terms of the

state variables chosen determines the particular thermodynamical system. In that way, the work of Mielke [15] is quite valuable as it provides a systematic procedure to obtain these matrices for a wide range of problems of practical interest, in particular, dissipative mechanical systems.

2.3. Temperature-based GENERIC form of the initial value problem

The GENERIC form of the two thermo-spring system in terms of either the entropy or the internal energy can be found in [6]. Here, we complement these two formulations with the one based on the temperature, which can be also found in a more abstract form in [15]. To do so, let us consider a state vector which includes the temperatures of the springs as the thermodynamical variables

$$\mathbf{z} = [\mathbf{q}_1, \mathbf{q}_2, \mathbf{p}_1, \mathbf{p}_2, \theta_1, \theta_2]^\mathsf{T},\tag{16}$$

so the state space is hence defined by

$$\mathcal{S} = \{\mathbf{z} \in (\mathbb{R}^3, \mathbb{R}^3, \mathbb{R}^3, \mathbb{R}^3, \mathbb{R}^+, \mathbb{R}^+), \mathbf{q}_1 \neq \mathbf{0}, \mathbf{q}_2 \neq \mathbf{q}_1\}\tag{17}$$

The total energy of the two thermo-spring system is the sum of the kinetic energy of the point masses, the internal energy of the springs and the potential of the conservative external forces. This is mathematically expressed in terms of the above state vector (16) as

$$E(\mathbf{z}) = K(\mathbf{z}) + \sum_{\beta=1}^{2} [e_\beta(\lambda_\beta, \theta_\beta) - V_\beta(\mathbf{q}_\beta)],\tag{18}$$

$K : \mathcal{S} \to \mathbb{R}$ being the kinetic energy given by

$$K(\mathbf{z}) = \frac{1}{2} \sum_{\beta=1}^{2} \frac{\mathbf{p}_\beta \cdot \mathbf{p}_\beta}{m_\beta}\tag{19}$$

Remark 2.2. If the spring entropies are used in the state vector instead of the spring temperatures, the obtention of the function $e_\alpha(\lambda_\alpha, s_\alpha)$ explicitly expressed in terms of the entropy is required, see [6,14,24]. This requirement has to be viewed as important technical restriction to the applicability of specific thermoelastic models. This issue will be illustrated with the example presented in Section 4.

The total entropy of the system is obtained as the sum of the spring entropy, which is expressed in terms of the state vector by (4) as

$$S(\mathbf{z}) = \sum_{\alpha=1}^{2} s_\alpha(\lambda_\alpha, \theta_\alpha) = \sum_{\alpha=1}^{2} -\frac{\partial \Psi_\alpha(\lambda_\alpha, \theta_\alpha)}{\partial \theta_\alpha}\tag{20}$$

Thus, the first step to find the GENERIC form is the computation of the gradient of the total energy and total entropy with respect to the state vector (16). Accordingly,

$$\nabla E = \begin{bmatrix} \dfrac{\partial e_1}{\partial \lambda_1} \dfrac{\partial \lambda_1}{\partial \mathbf{q}_1} + \dfrac{\partial e_2}{\partial \lambda_2} \dfrac{\partial \lambda_2}{\partial \mathbf{q}_1} - \mathbf{f}_1 \\[2mm] \dfrac{\partial e_2}{\partial \lambda_2} \dfrac{\partial \lambda_2}{\partial \mathbf{q}_2} - \mathbf{f}_2 \\[2mm] \dfrac{\mathbf{p}_1}{m_1} \\[2mm] \dfrac{\mathbf{p}_2}{m_2} \\[2mm] \dfrac{\partial e_1}{\partial \theta_1} \\[2mm] \dfrac{\partial e_2}{\partial \theta_2} \end{bmatrix}, \nabla S = \begin{bmatrix} \dfrac{\partial s_1}{\partial \lambda_1} \dfrac{\partial \lambda_1}{\partial \mathbf{q}_1} + \dfrac{\partial s_2}{\partial \lambda_2} \dfrac{\partial \lambda_2}{\partial \mathbf{q}_1} \\[2mm] \dfrac{\partial s_2}{\partial \lambda_2} \dfrac{\partial \lambda_2}{\partial \mathbf{q}_2} \\[2mm] 0 \\[2mm] 0 \\[2mm] \dfrac{\partial s_1}{\partial \theta_1} \\[2mm] \dfrac{\partial s_2}{\partial \theta_2} \end{bmatrix}\tag{21}$$

The associated Poisson and Dissipative matrices required to recast the evolution equations (11) in the GENERIC form (12) are given by

$$
\mathbf{L}(\mathbf{z}) = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & L_{11} & L_{12} \\ 0 & -1 & 0 & 0 & 0 & L_{22} \\ 0 & 0 & \tilde{L}_{11} & 0 & 0 & 0 \\ 0 & 0 & \tilde{L}_{21} & \tilde{L}_{22} & 0 & 0 \end{bmatrix}, \quad \text{with} \quad \mathbf{L}_{\alpha\beta} = -\tilde{\mathbf{L}}_{\beta\alpha}^{\mathsf{T}} = \left(\frac{\partial s_\beta}{\partial \theta_\beta} \right)^{-1} \frac{\partial s_\beta}{\partial \lambda_\beta} \frac{\partial \lambda_\beta}{\partial \mathbf{q}_\alpha}. \tag{22}
$$

$$
\mathbf{M}(\mathbf{z}) = \theta_1 \theta_2 \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & M_{11} & M_{12} \\ 0 & 0 & 0 & 0 & M_{21} & M_{22} \end{bmatrix}, \quad \text{with} \quad M_{\alpha\beta} = (-1)^{\alpha+\beta} k \left(\frac{\partial e_\alpha}{\partial \theta_\alpha} \right)^{-1} \left(\frac{\partial e_\beta}{\partial \theta_\beta} \right)^{-1} \tag{23}
$$

Due to the state vector including the temperatures, the GENERIC form provides the evolution equations in the form (11). However, the form in (5) and (7) could easily be recovered by the inverse way performed in Section 2.1. Interestingly, this feature will be also inherited by the discrete counterpart presented in Section 3.

It is worth mentioning that, as a result of the use of the positions $\mathbf{q}_\alpha$ and the momenta $\mathbf{p}_\alpha$ as mechanical variables, the Poisson matrix comprises the Hamiltonian canonical symplectic matrix [28] plus additional terms which take into account the thermo-mechanical coupling. Such terms are not present if the spring entropies are used as state variables. However, similar ones appear when the internal energies are considered in the state vector, see [6], demonstrating that the temperature election is not much more involved than the other common choices, as also demonstrated in [15].

2.4. First and second laws of thermodynamics

It can be easily verified that matrices (22) and (23) satisfy the important structural properties stated in Section 2.2: leading to the fulfilment of the first law of thermodynamics (14).

The second law of thermodynamics is obtained for this case using the particular form of Dissipative matrix (23) along with the gradient $(21)_2$, leading to the rate of entropy

$$
\dot{S}(\mathbf{z}) = \nabla S \cdot \dot{\mathbf{z}} = \nabla S^{\mathsf{T}} \mathbf{M} \nabla S = k \frac{(\theta_2 - \theta_1)^2}{\theta_1 \theta_2} \geq 0, \tag{24}
$$

that demonstrates the two thermo-spring system is thermodynamically sound.

2.5. Symmetries

In a general thermomechanical system, a symmetry is the action of a Lie group on the state space that preserves both energy and entropy. Noether's theorem indicates that associated with these actions are momentum maps that are constant along the solution. A detailed description of the purely Hamiltonian case can be found in [29], and in [9] within the GENERIC framework. In our model the symmetries may be translational or rotational and the conserved quantities would be linear and angular momentum, defined respectively as:

$$
\mathbf{L} = \sum_{\alpha=1}^{2} \mathbf{p}_\alpha, \quad \mathbf{J} = \sum_{\alpha=1}^{2} \mathbf{q}_\alpha \times \mathbf{p}_\alpha \tag{25}
$$

Conservation of these momenta when the resultant applied force and torque vanish is a classic result, and the proofs are omitted.

3. Thermodynamically consistent discrete GENERIC form

In this section we resort to the methodology proposed by Romero [6] to formulate the novel TC integration scheme based on the temperature as thermodynamical state variable.

The methodology relies on the classical partition of the time integration interval $[0, T]$ into constant subintervals, for the sake of simplicity, as $\Delta t = |\mathcal{I}_{n+1}|$ with $\mathcal{I}_{n+1} = [t_{n+1}, t_n]$, such that the state vector at certain instants of time t_i can be approximated as $\mathbf{z}_i \simeq \mathbf{z}(t_i)$. In addition, the discrete preservation of the thermodynamical structure rests on the discrete gradient operator in the sense of Gonzalez [10].

Thus, the GENERIC form for finite dimensional systems can be approximated by the following monolithic implicit second order accurate scheme

$$\frac{\mathbf{z}_{n+1} - \mathbf{z}_n}{\Delta t} = \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n) + \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n), \tag{26}$$

where the operator $\mathrm{D}(\bullet)(\mathbf{z}_{n+1}, \mathbf{z}_n)$ is the discrete gradient and $\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n)$, $\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n)$ are second order approximations of the continuous Poisson and Dissipative matrices evaluated at midpoint

$$\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{L}(\mathbf{z}_{n+\frac{1}{2}}) + \mathcal{O}(\mathbf{z}_{n+1} - \mathbf{z}_n)^2, \tag{27}$$

$$\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{M}(\mathbf{z}_{n+\frac{1}{2}}) + \mathcal{O}(\mathbf{z}_{n+1} - \mathbf{z}_n)^2 \tag{28}$$

In analogy to the continuous case the discrete Poisson matrix $\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n)$ has to be skew-symmetric, while the discrete Dissipative matrix $\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n)$ has to be symmetric and positive semi-definite. Additionally, discrete versions of the Poisson and Dissipative matrices must satisfy the degeneracy or non-interaction conditions in the following form

$$\mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n)^\mathsf{T} \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{0}, \quad \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n)^\mathsf{T} \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = \mathbf{0} \tag{29}$$

The use of the discrete gradient operator is justified due to its directionality property that is responsible for the laws of thermodynamics to be discretely fulfilled. Such property thus enables the total energy balance in any time step to be expressed by

$$E_{n+1} - E_n = \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot (\mathbf{z}_{n+1} - \mathbf{z}_n) \tag{30}$$

Using (26) this can be further elaborated to give

$$E_{n+1} - E_n = \Delta t \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n)^\mathsf{T} \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n) + \Delta t \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n)^\mathsf{T} \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n) = 0 \tag{31}$$

This result can be directly deduced from the skew-symmetry of the discrete Poisson matrix together with the non-interaction conditions. Similarly, the total entropy balance results in

$$\begin{aligned} S_{n+1} - S_n &= \mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n) \cdot (\mathbf{z}_{n+1} - \mathbf{z}_n) \\ &= \Delta t \mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n)^\mathsf{T} \mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n) + \Delta t \mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n)^\mathsf{T} \mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) \mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n) \geq 0 \end{aligned} \tag{32}$$

Accordingly, the total entropy is always non-decreasing because of the symmetry and positive semi-definiteness of the discrete Dissipative matrix together with the non-interaction conditions. These results are the proof for the discrete setting given by (26) to satisfy the laws of thermodynamics.

3.1. Temperature-based TC integrator scheme

For the thermodynamical system presented in Section 2, the discrete gradient applied to the total energy (18) and total entropy (20) can be elaborated by using the partitioned definition of the discrete gradient operator to give

$$\mathrm{D}E(\mathbf{z}_{n+1}, \mathbf{z}_n) = \begin{bmatrix} \mathrm{D}_{\mathbf{q}_1} E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\mathbf{q}_2} E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\mathbf{p}_1} E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\mathbf{p}_2} E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\theta_1} E(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\theta_2} E(\mathbf{z}_{n+1}, \mathbf{z}_n) \end{bmatrix} = \begin{bmatrix} \mathrm{D}_{\mathbf{q}_1} e_1 + \mathrm{D}_{\mathbf{q}_1} e_2 - \tilde{\mathbf{f}}_1 \\ \mathrm{D}_{\mathbf{q}_2} e_2 - \tilde{\mathbf{f}}_2 \\ \mathrm{D}_{\mathbf{p}_1} K \\ \mathrm{D}_{\mathbf{p}_2} K \\ \mathrm{D}_{\theta_1} e_1 \\ \mathrm{D}_{\theta_2} e_2 \end{bmatrix}, \tag{33}$$

$$\mathrm{D}S(\mathbf{z}_{n+1}, \mathbf{z}_n) = \begin{bmatrix} \mathrm{D}_{\mathbf{q}_1} S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\mathbf{q}_2} S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\mathbf{p}_1} S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\mathbf{p}_2} S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\theta_1} S(\mathbf{z}_{n+1}, \mathbf{z}_n) \\ \mathrm{D}_{\theta_2} S(\mathbf{z}_{n+1}, \mathbf{z}_n) \end{bmatrix} = \begin{bmatrix} \mathrm{D}_{\mathbf{q}_1} s_1 + \mathrm{D}_{\mathbf{q}_1} s_2 \\ \mathrm{D}_{\mathbf{q}_2} s_2 \\ \mathbf{0} \\ \mathbf{0} \\ \mathrm{D}_{\theta_1} s_1 \\ \mathrm{D}_{\theta_2} s_2 \end{bmatrix}, \tag{34}$$

where $\mathrm{D}_k f$ might be interpreted as the second order accurate discrete counterpart to the respective partial derivative of the function f at midpoint; details about its computation are summarized in Appendix A. Furthermore, the terms $\tilde{\mathbf{f}}_\alpha$ are second order accurate approximations to the external forces $\mathbf{f}_\alpha$.

In addition to that we define the following discrete versions of the Poisson and Dissipative matrices to be

$$
\mathbf{L}(\mathbf{z}_{n+1}, \mathbf{z}_n) =
\begin{bmatrix}
0 & 0 & 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
-1 & 0 & 0 & 0 & \dfrac{D_{\mathbf{q}_1}s_1}{D_{\theta_1}s_1} & \dfrac{D_{\mathbf{q}_1}s_2}{D_{\theta_2}s_2} \\
0 & -1 & 0 & 0 & 0 & \dfrac{D_{\mathbf{q}_2}s_2}{D_{\theta_2}s_2} \\
0 & 0 & -\dfrac{D_{\mathbf{q}_1}s_1^{\mathsf{T}}}{D_{\theta_1}s_1} & 0 & 0 & 0 \\
0 & 0 & -\dfrac{D_{\mathbf{q}_1}s_2^{\mathsf{T}}}{D_{\theta_2}s_2} & -\dfrac{D_{\mathbf{q}_2}s_2^{\mathsf{T}}}{D_{\theta_2}s_2} & 0 & 0
\end{bmatrix}
\tag{35}
$$

$$
\mathbf{M}(\mathbf{z}_{n+1}, \mathbf{z}_n) = k\theta_1^*\theta_2^*
\begin{bmatrix}
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & (D_{\theta_1}e_1)^{-2} & -(D_{\theta_1}e_1)^{-1}(D_{\theta_2}e_2)^{-1} \\
0 & 0 & 0 & 0 & -(D_{\theta_2}e_2)^{-1}(D_{\theta_1}e_1)^{-1} & (D_{\theta_2}e_2)^{-2}
\end{bmatrix}
\tag{36}
$$

It can be easily verified that definitions (35) and (36) do satisfy the crucial structural properties stated above. In particular, the conditions for the discrete Dissipation matrix (36) hold independent of the specific choice for the algorithmic temperatures θ_1^* and θ_2^*. For example, one could choose the midpoint temperatures $\theta_\alpha^* = (\theta_{\alpha,n} + \theta_{\alpha,n+1})/2$ to arrive at a second-order accurate thermodynamically consistent scheme. Instead we prefer to introduce the algorithmic temperature

$$
\theta_\alpha^* = \frac{D_{\theta_\alpha}e_\alpha}{D_{\theta_\alpha}s_\alpha},
\tag{37}
$$

that also leads to a second order thermodynamically consistent scheme, as the results provided in Section 4 confirm. Definition (37) of the algorithmic temperature can be viewed as canonical choice that provides a unique discrete counterpart of the specific heat capacity (9) given by

$$
c_\alpha^* = D_{\theta_\alpha}e_\alpha = \theta_\alpha^* D_{\theta_\alpha}s_\alpha > 0
\tag{38}
$$

Now, inserting relationships (33) through (37) into the discrete GENERIC form (26), we arrive at the following representation of the TC scheme formulated in terms of the temperature

$$
\begin{aligned}
\frac{\mathbf{q}_{\alpha,n+1} - \mathbf{q}_{\alpha,n}}{\Delta t} &= D_{\mathbf{p}_\alpha}K \\
\frac{\mathbf{p}_{\alpha,n+1} - \mathbf{p}_{\alpha,n}}{\Delta t} &= -\sum_{\beta=1}^{2}(D_{\mathbf{q}_\alpha}e_\beta - \theta_\beta^* D_{\mathbf{q}_\alpha}s_\beta) + \tilde{\mathbf{f}}_\alpha \\
\frac{\theta_{1,n+1} - \theta_{1,n}}{\Delta t} &= (D_{\theta_1}e_1)^{-1}\left[-\theta_1^* D_{\mathbf{q}_1}s_1^{\mathsf{T}}D_{\mathbf{p}_1}K + k(\theta_2^* - \theta_1^*)\right] \\
\frac{\theta_{2,n+1} - \theta_{2,n}}{\Delta t} &= (D_{\theta_2}e_2)^{-1}\left[-\theta_2^* \sum_{\beta=1}^{2} D_{\mathbf{q}_\beta}s_2^{\mathsf{T}}D_{\mathbf{p}_\beta}K + k(\theta_1^* - \theta_2^*)\right]
\end{aligned}
\tag{39}
$$

It can be easily observed that the newly developed TC scheme (39) clearly resembles its continuous counterpart (11), where the continuous partial derivatives have been replaced by its discrete counterparts and the temperatures have been consistently evaluated in the sense of (37). Note also that due to the fact that the kinetic energy is merely a quadratic function of the momenta we obtain

$$
D_{\mathbf{p}_\alpha}K = \frac{\mathbf{p}_{\alpha,n+\frac{1}{2}}}{m_\alpha}
\tag{40}
$$

What is more, the directionality property of the discrete gradient enables the last two equations in (39) to be recast in the form

$$
\begin{aligned}
\frac{s_1(\lambda_{1,n+1}, \theta_{1,n+1}) - s_1(\lambda_{1,n}, \theta_{1,n})}{\Delta t} &= k\left(\frac{\theta_2^*}{\theta_1^*} - 1\right), \\
\frac{s_2(\lambda_{2,n+1}, \theta_{2,n+1}) - s_2(\lambda_{2,n}, \theta_{2,n})}{\Delta t} &= k\left(\frac{\theta_1^*}{\theta_2^*} - 1\right),
\end{aligned}
\tag{41}
$$

Note that (41) can be viewed as discrete version of the energy balance in entropy form given by (7).

Remark 3.1. The newly devised temperature-based TC scheme (39) emanating from the underlying discrete GENERIC form (26) can be obtained as well by discretizing the evolution equations (11). This procedure relies on the application of a mid-point-type discretization of (11) in which the mid-point gradients are replaced by discrete gradient operators. In addition to that, definition (37) for the algorithmic temperature has to be substituted for the mid-point temperature. This observation may be helpful to formulate temperature-based TC integrators for more general thermo-mechanical coupling problems even if the GENERIC form may not be reachable.

Remark 3.2. The thermodynamical consistency of (39) algorithmically relies on the application of the discrete gradient to both the internal energy and the entropy functions. In contrast to that, the entropy-based approach [6] requires only to apply the discrete gradient to the internal energy function expressed in terms of the entropy. Therefore, the newly proposed temperature-based TC method involves more computational cost which is the price to be paid in order to overcome the problems pointed out in Remark 2.2.

Remark 3.3. It is possible to show that the proposed temperature-based TC scheme (39) also preserves the translational and rotational symmetries of the continuous evolution problem. These symmetries lead to the conservation of the discrete linear and angular momentum for a force-free motion. Details of the proof are omitted but closely follow the ones provided in [14].

Lastly, it is worth commenting that, due to the construction of the discrete version of the Poisson and Dissipative matrices according to (35) and (36), the conservation of energy as well as the production of entropy are guaranteed. It only remains to compute the increment of the entropy in each time step which follows from (32)

$$S_{n+1} - S_n = \Delta t k \frac{(\theta_2^* - \theta_1^*)^2}{\theta_1^* \theta_2^*} \geq 0, \tag{42}$$

and can be viewed as the discrete counterpart of (24).

4. Numerical simulations

In this section the performance of the novel temperature-based TC integration scheme is illustrated and compared to the performance exhibited by the previously developed entropy-based TC scheme. For that purpose, we use numerical examples previously proposed in Romero [6] and Krüger et al. [24]. In addition, we consider a new example to further explore the use of the new formulation in a case impossible to be solved by current existing TC schemes based on the entropy. The solution of this new example has also been obtained with the classical midpoint and trapezoidal schemes implemented in terms of the temperature.

For every simulation, we consider the following Helmholtz free-energy function

$$\Psi_\alpha(\lambda_\alpha, \theta_\alpha) = \frac{C_\alpha(\theta_\alpha)}{2} \log^2 \frac{\lambda_\alpha}{\lambda_\alpha^0} - \beta_\alpha(\theta_\alpha - \theta_{\text{ref}}) \log \frac{\lambda_\alpha}{\lambda_\alpha^0} + c_{0,\alpha} \left(\theta_\alpha - \theta_{\text{ref}} - \theta_\alpha \log \frac{\theta_\alpha}{\theta_{\text{ref}}} \right), \tag{43}$$

where $C_\alpha(\theta_\alpha)$ is the possibly temperature-dependent spring stiffness, β_α accounts for the thermo-mechanical coupling effects, $c_{0,\alpha}$ is the heat capacity and θ_{ref} is the reference temperature at which we define the unstressed deformation to be zero.

As pointed out in the above sections, one of the main advantages of the newly developed temperature-based approach is that general free-energy functions can be directly applied. As any free-energy function is naturally formulated in terms of the temperature, one merely needs to differentiate once to obtain

$$s_\alpha(\lambda_\alpha, \theta_\alpha) = -\frac{C_\alpha'(\theta_\alpha)}{2} \log^2 \frac{\lambda_\alpha}{\lambda_\alpha^0} + \beta_\alpha \log \frac{\lambda_\alpha}{\lambda_\alpha^0} + c_{0,\alpha} \log \frac{\theta_\alpha}{\theta_{\text{ref}}}, \tag{44}$$

$C_\alpha'(\theta_\alpha)$ being the absolute derivative of the function $C_\alpha(\theta_\alpha)$.

Then, according to the Legendre transform (3), the internal energy function can be directly obtained in terms of the temperature

$$e_\alpha(\lambda_\alpha, \theta_\alpha) = \frac{C_\alpha(\theta_\alpha) - \theta_\alpha C_\alpha'(\theta_\alpha)}{2} \log^2 \frac{\lambda_\alpha}{\lambda_\alpha^0} + \beta_\alpha \theta_{\text{ref}} \log \frac{\lambda_\alpha}{\lambda_\alpha^0} + c_{0,\alpha}(\theta_\alpha - \theta_{\text{ref}}) \tag{45}$$

Note that the entropy-based TC scheme requires the temperature to be expressed in terms of the entropy by inverting (44). This cannot be done analytically for some cases. For instance, that is the case when a non-linear temperature dependent function for the spring stiffness $C_\alpha(\theta_\alpha)$ is considered.

4.1. Validation and comparison with entropy-based TC scheme

We employ the first example in [6] to validate the proposed scheme and compare it with the entropy-based TC scheme. The example is based on the above free-energy function (43) considering constant spring stiffness C_α and the following data: $m_1 = 1$, $m_2 = 2$, $C_1 = 0.1$, $C_2 = 1$, $\lambda_1^0 = 2$, $\lambda_2^0 = 1$, $k = 300$, $\beta_1 = \beta_2 = 0.2$, $c_{0,1} = c_{0,2} = 5$ and $\theta_{\text{ref}} = 300$. Then, the newly proposed temperature-based TC method is used within the time interval $[0, 25]$ with constant time step size $\Delta t = 0.3$ and initial conditions:

$$\mathbf{q}_1^0 = \mathbf{e}_1, \quad \mathbf{p}_1^0 = 2\mathbf{e}_2, \quad \mathbf{q}_2^0 = 2.2\mathbf{e}_1, \quad \mathbf{p}_2^0 = \mathbf{e}_1, \quad \theta_1^0 = 380, \quad \theta_2^0 = 310$$
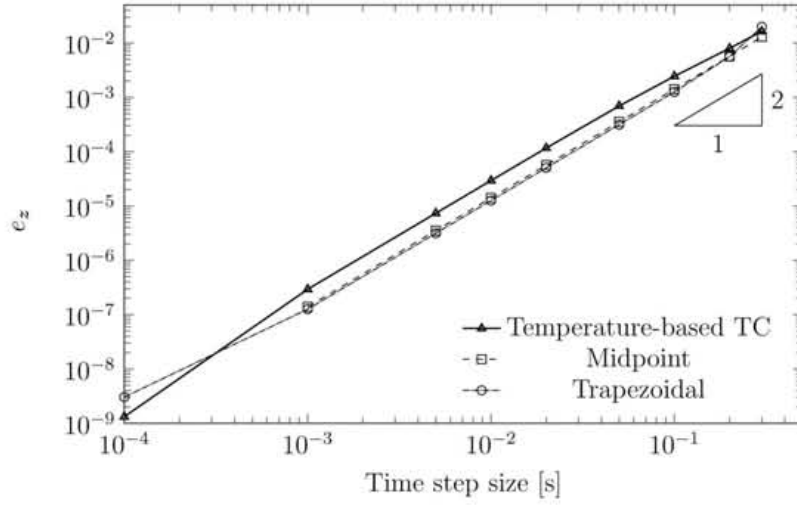
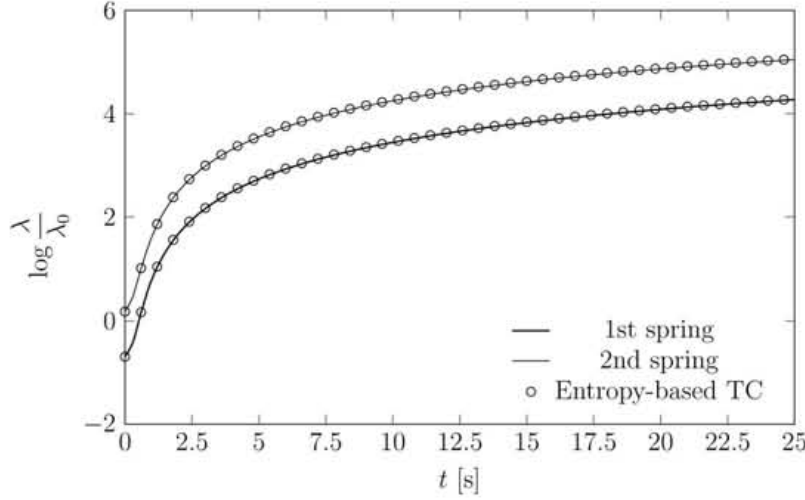**Fig. 2.** State vector relative error.

Fig. 3. Temperature-based TC scheme solution: strains.

To validate the novel method we have studied its order of accuracy based on this particular example by computing the relative error at different time step sizes with respect to a reference solution as

$$e_{\mathbf{z}} = \frac{||\mathbf{z} - \mathbf{z}_{\text{ref}}||}{||\mathbf{z}_{\text{ref}}||}. \tag{46}$$

$||\bullet||$ being the vector 2-norm, $\mathbf{z}$ being the solution at $t_f = 25$ and $\mathbf{z}_{\text{ref}}$ being the reference solution at the same instant t_f obtained with the midpoint method and time step size of $\Delta t = 10^{-4}$. The results obtained with the temperature-based TC, the midpoint and trapezoidal methods are plotted in Fig. 2. It shows the second order of accuracy of the temperature-based TC method, with an error constant which is very similar to the one of midpoint and trapezoidal method.

For comparison, Figs. 3 and 4 plot the evolution of the spring strains and the spring temperatures along with the results obtained with the entropy-based scheme reported by Romero [6]. They show that the newly proposed temperature-based TC integrator yields practically the same solution.

The energy evolution is depicted in Fig. 5 which clearly shows that the first law is fully satisfied as in the case of using spring entropies, confirming the theoretical results obtained in previous sections. Regarding the second law, Fig. 6 shows that each method produces different amounts of total entropy while being in accordance with the thermodynamics. It is worth mentioning, however, that this difference is appreciable due to the large time-step size used. It can be checked that they both produce the same amount as the time-step size is reduced. Interestingly, the reference solution provides the same final amount as the one provided by the entropy-based TC integrator for the time step size used of $\Delta t = 0.3$.
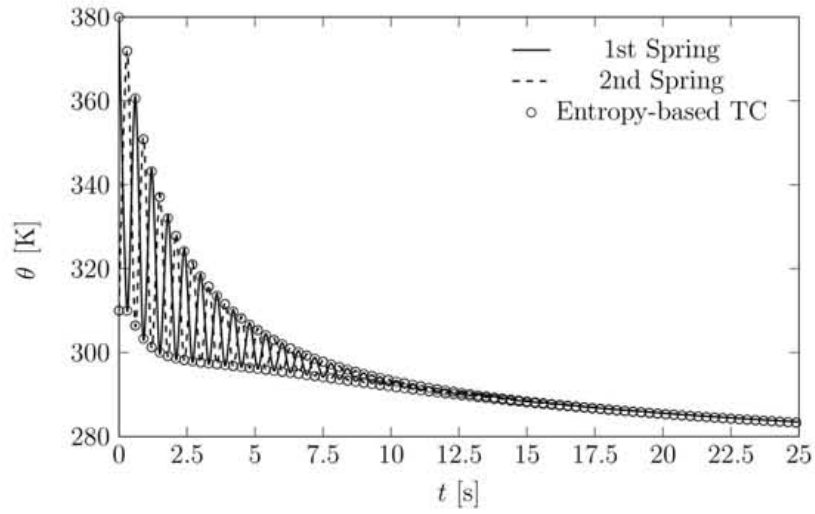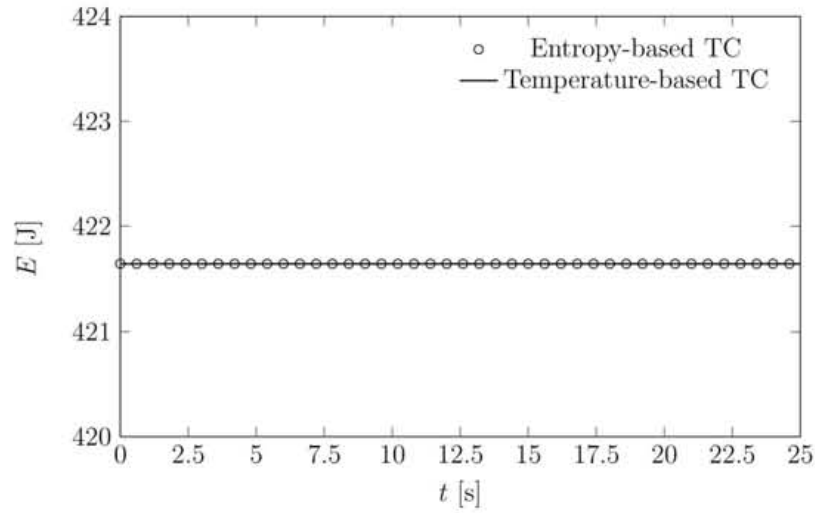
Fig. 4. Temperature.

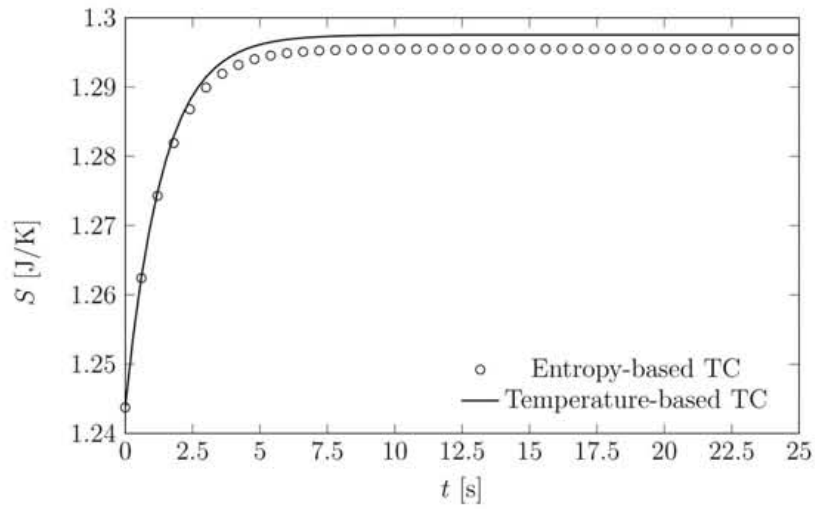**Fig. 5.** Total energy $E = K + U$.
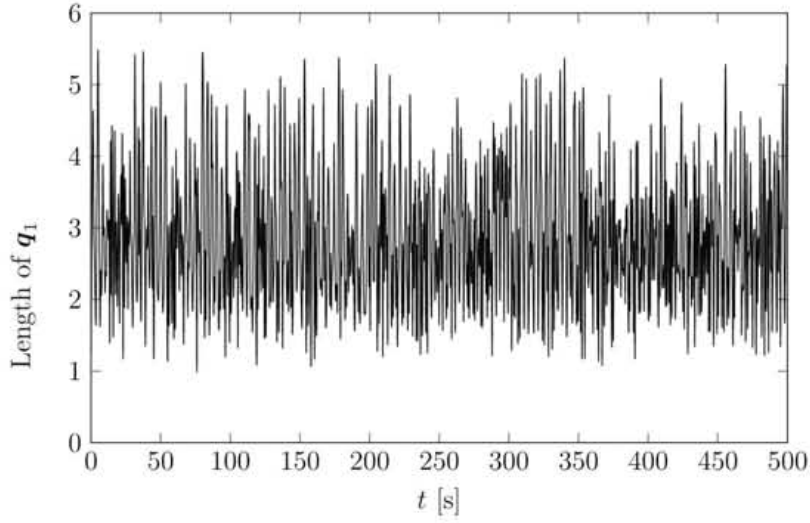

Fig. 6. Total entropy.

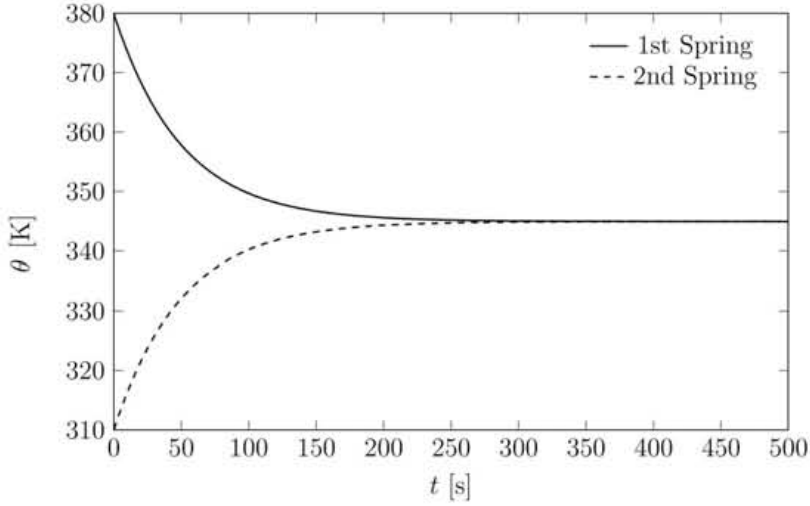**Fig. 7.** Temperature-based TC scheme solution: 1st spring elongation.

Fig. 8. Temperature-based TC scheme solution: evolution of the two thermo-spring temperatures.

For the second simulation, we explore the performance of the newly proposed temperature-based TC scheme with the example introduced by Krüger et al. [24]. This example is dominated by high frequencies and is based on constant spring stiffness parameter. In particular, the following data is used: $m_1 = 1$, $m_2 = 2$, $C_1 = 100$, $C_2 = 100$, $\lambda_1^0 = 2$, $\lambda_2^0 = 1$, $k = 10$, $\beta_1 = \beta_2 = 0.2$, $c_{0.1} = c_{0.2} = 1000$ and $\theta_{\text{ref}} = 300$.

The temperature-based TC scheme is used within the time interval [0, 500] with constant time step size $\Delta t = 0.1$ and initial conditions:

$$\mathbf{q}_{1.0} = 1\mathbf{e}_1, \mathbf{p}_{1.0} = 1\mathbf{e}_2, \mathbf{q}_{2.0} = 2.2\mathbf{e}_1, \mathbf{p}_{2.0} = 4.4\mathbf{e}_2, \theta_{1.0} = 380, \theta_{2.0} = 310$$

Figs. 7 and 8 show the obtained first spring stretch and the temperatures, respectively. They both coincide with the results reported by Krüger et al. [24]. In addition, the use of this time step with the temperature-based midpoint scheme leads to the same non-physical solution that was reported in the aforementioned work, see Fig. 9. Therefore, it is apparent that both the entropy-based and temperature-based schemes allow for larger time steps to provide a stable solution.

Fig. 10 shows the evolution of the energy compared to that obtained with the entropy-based scheme and allows to conclude that both implementations succeed in satisfying the first law of thermodynamics.

Interestingly, it can be seen in Fig. 11 that the productions of entropy provided by the two methods are indistinguishable and are in accordance with the second law of thermodynamics.
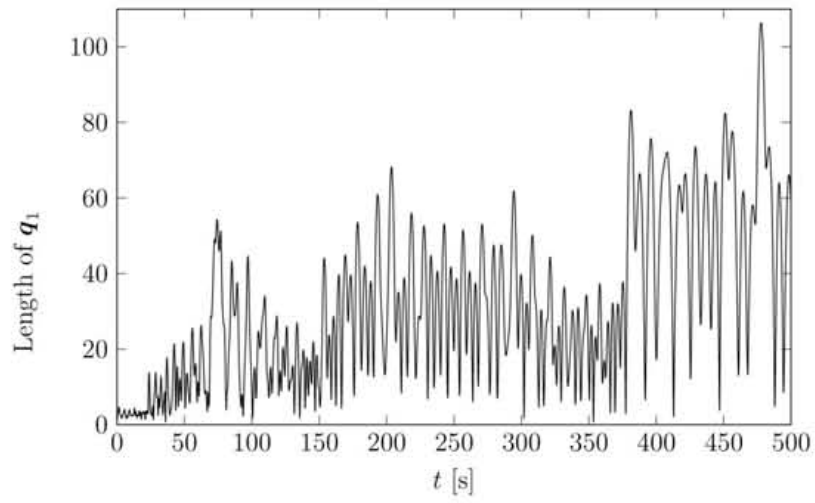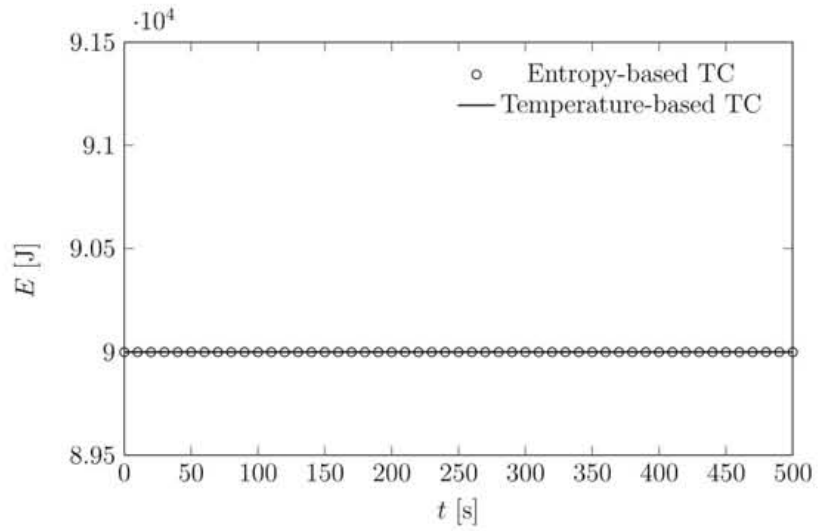
Fig. 9. Midpoint scheme solution: 1st spring elongation.

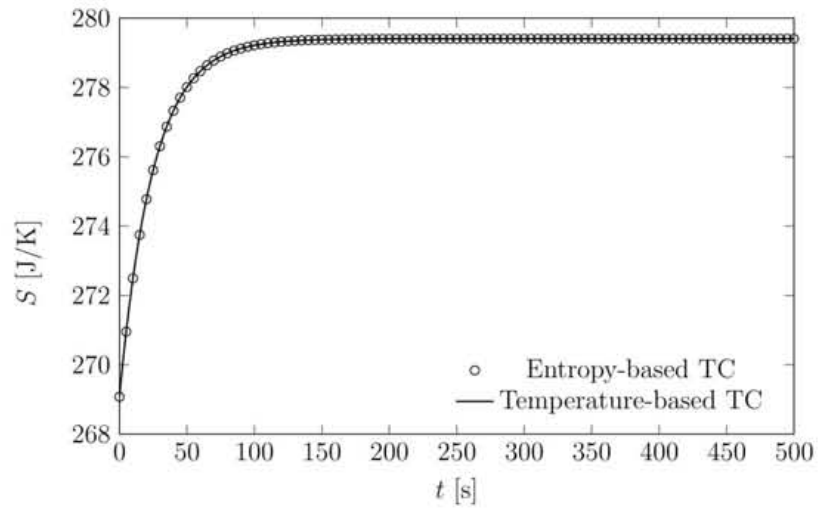**Fig. 10.** Evolution of the two thermo-spring system energy.

Fig. 11. Evolution of the two thermo-spring system entropy.
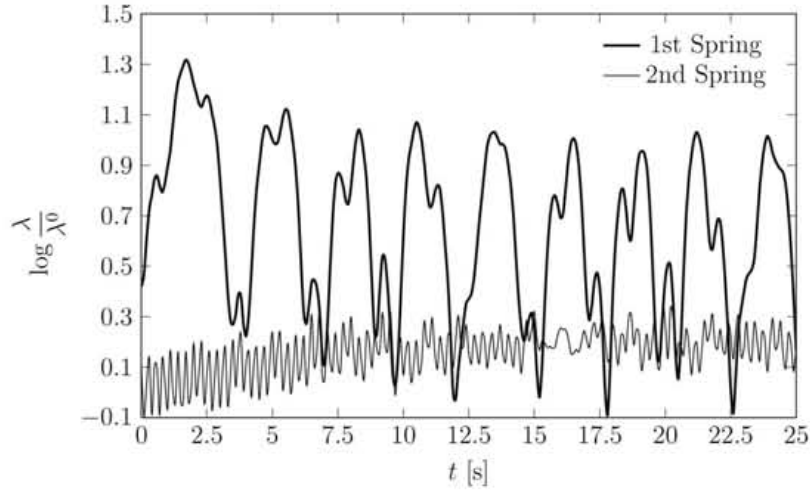
Fig. 12. Temperature-based TC scheme solution: stretches.
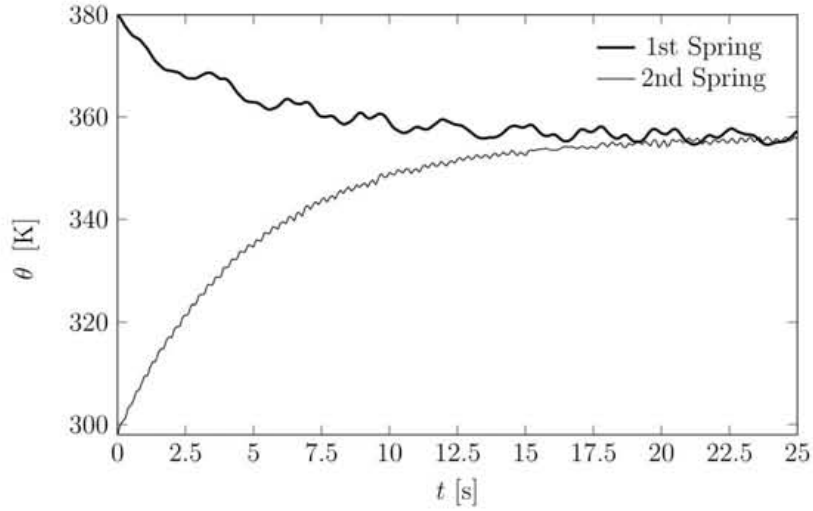

Fig. 13. Temperature-based TC scheme solution: temperature.

4.2. Non-linear temperature-dependent stiffness example

To emphasize the applicability of the novel TC formulation we introduce a new example considering a non-linear temperature-dependent function for the spring stiffness expressed by

$$C_\alpha(\theta_\alpha) = C_\alpha^0 - C_\alpha^1 \theta_{\text{ref}} \log\left(\frac{\theta_\alpha}{\theta_{\text{ref}}}\right) \tag{47}$$

It can be checked that this choice makes impossible the use of the entropy-based formulation since relationship (44) cannot be analytically solved to obtain the function $\theta_\alpha(\lambda_\alpha, s_\alpha)$. It should also be noted that the above logarithmic dependency has been chosen as an example of a non-linear function that does not spoil the free-energy attributes. Furthermore, for small changes in the temperature the above expression behaves as the linear one used in [14].

The data employed in the simulation is: $m_1 = 10$, $m_2 = 20$, $C_1^0 = 5 \cdot 10^3$, $C_2^0 = 10^4$, $C_1^1 = 50$, $C_2^1 = 60$, $\lambda_1^0 = 2$, $\lambda_2^0 = 1$, $k = 300$, $\beta_1 = \beta_2 = 20$, $c_{0,1} = 5000$, $c_{0,2} = 2000$ and $\theta_{\text{ref}} = 300$. The motion of the two thermo-spring system is integrated within the time interval $[0, 25]$ with constant time step size $\Delta t = 0.1$ and initial conditions:

$$\mathbf{q}_{1,0} = 3\mathbf{e}_1 + 0.5\mathbf{e}_3, \mathbf{q}_{2,0} = 3\mathbf{e}_1 + \mathbf{e}_2 + \mathbf{e}_3, \mathbf{p}_{1,0} = 10\mathbf{e}_2, \mathbf{p}_{2,0} = -20\mathbf{e}_3, \quad \theta_{1,0} = 380, \theta_{2,0} = 298.$$
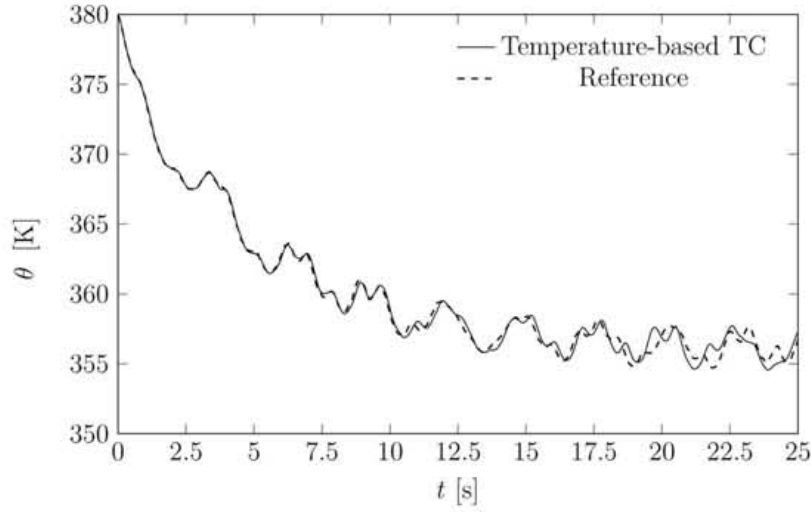
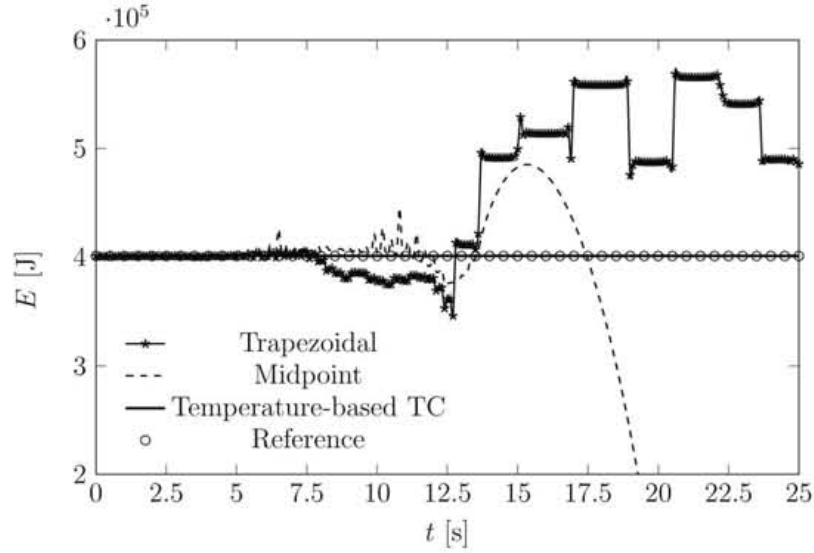**Fig. 14.** First spring temperature evolution.

Fig. 15. The two thermo-spring system total energy.

The solution of the evolution equations in temperature form is obtained with three methods: the midpoint rule, the trapezoidal rule and the temperature-based TC method using the same time step of $\Delta t = 0.1$. Moreover, a reference solution is computed with the midpoint rule with time step $\Delta t_{\mathrm{ref}} = 0.005$.

The 3D motion of the two masses is governed by the extraordinary high thermo-mechanic coupling. Moreover, the first spring stiffness is twice as much as the second spring one which altogether results in appreciable oscillations on the evolution of the temperatures and makes quite challenging for the standard methods to provide solutions for moderate time step sizes. This can be seen in the solution provided by the new consistent scheme depicted in Fig. 13. Note that a small oscillation appears on the second spring temperature due to its higher stiffness. This can be clearly seen in Fig. 12 that plots the stretches of the springs.

Fig. 14 contains the evolution of the first spring temperature provided by the newly proposed consistent scheme compared with the reference solution. The difference between both curves is sufficiently low so it can be concluded that the proposed scheme provides physically reliable solutions. The same conclusions can be reached if the temperature of the second spring (not shown) is plotted.

Figs. 15 and 16 show the incapability of the traditional methods to satisfy the laws of thermodynamics for moderate time step sizes. The midpoint rule yields unphysical results which eventually cause the failure of the iterative solution procedure. In case of the trapezoidal method Newton's method still finds a solution although the results are unphysical as well.
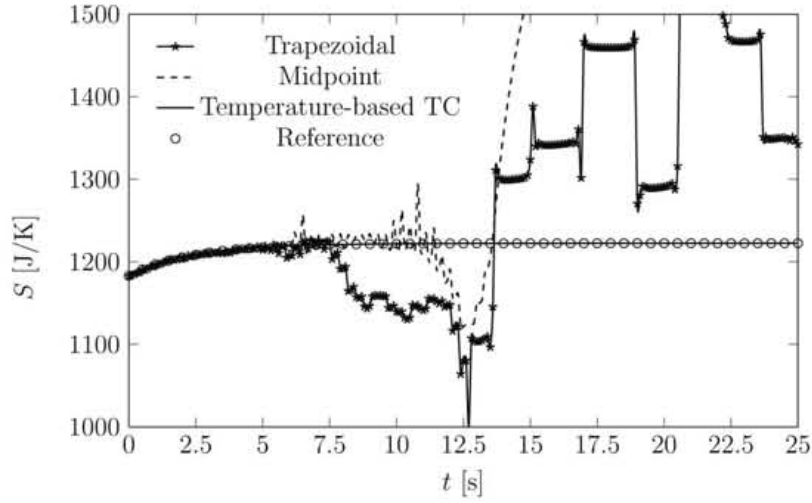
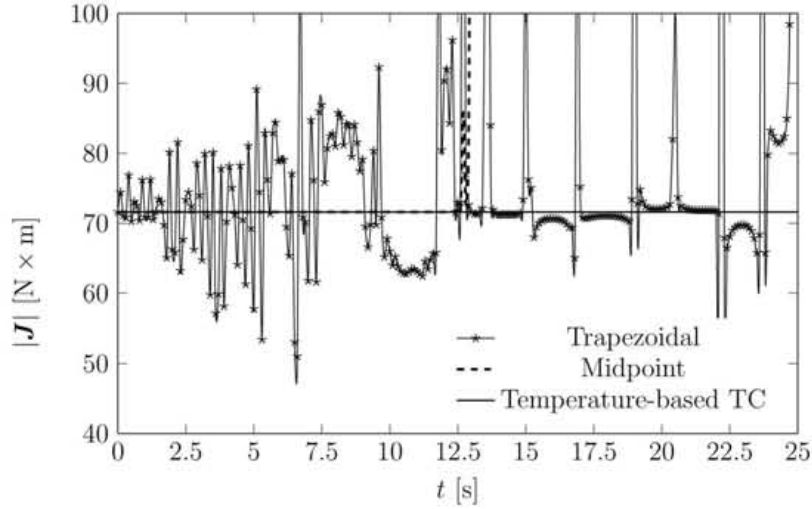**Fig. 16.** The two thermo-spring system total entropy.

Fig. 17. Evolution of the two thermo-spring system angular momentum.

It is obvious from Figs. 15 and 16 that the standard schemes fail to adhere to the two fundamental laws of thermodynamics. In addition to that it can be observed from Fig. 17 that the trapezoidal method also fails to conserve the angular momentum.

In contrast to the failure of the standard schemes, the temperature-based TC scheme provides solutions which strictly comply with both laws of thermodynamics. Additionally, the TC scheme inherits the conservation law for angular momentum from the underlying continuous description. As expected, the structure-preserving properties of the newly developed TC scheme yield superior numerical stability and robustness.

5. Conclusions

In this paper we have demonstrated that the methodology to formulate TC integration schemes suggested by Romero [6] can be used to devise a TC scheme relying on the temperature as the thermodynamical variable. Based on a representative thermodynamical model problem composed of two point masses linked by thermo-springs, we have first confirmed that a state vector including the spring temperatures can perfectly be used to express the GENERIC form of the evolution equations of such system, which is an essential requirement of the present approach. Subsequently, we have fully formulated a novel temperature-based TC integration scheme which is second order, implicit and monolithic. A first order staggered one can also be obtained by following the steps provided in [6], now departing from the presented GENERIC form in terms of the temperature. In this regard the present temperature-based approach complements the previously developed entropy-based method.

To achieve the design of a temperature-based TC scheme the discrete version of the GENERIC formalism had to be supplemented by a proper selection of the algorithmic temperature. Grounded on the fact that the resulting discrete scheme can restore

the discrete entropy form for the energy balance (41), we have suggested the use of an algorithmic temperature given by (37), which additionally makes it much more interpretable than any other option.

Despite relying on a simple finite dimensional system, the provided temperature-based formulation can be applied to general infinite dimensional systems as long as the description of the system in its GENERIC form can be achieved. What is more, the proposed temperature-based approach will enable the correct imposition of Dirichlet boundary conditions for the temperature that are commonly present in most of the applications of interest.

In essence, the newly proposed TC scheme relies on the notion of discrete gradient applied to the internal energy and entropy functions. It is worth noting, however, that the present approach requires about twice as much implementation effort and computational cost compared to the entropy-based approach that only needs the elaboration of the discrete gradient for the internal energy expressed in terms of entropy. Despite this, the present approach resolves the drawbacks resulting from the use of the entropy as state variable. Thus, common constitutive formulations in terms of the temperature can directly be applied. Moreover, as mentioned before, the extension to the continuous case makes possible to directly impose Dirichlet boundary conditions for the temperature.

As has been illustrated by the numerical examples of Section 4, the new TC scheme not only conserves angular and linear momentum, and the laws of thermodynamics, but considerably improves the numerical stability and enables the use of larger time steps compared to standard integration schemes.

Acknowledgements

Appendix A. Discrete gradient operator

The discrete gradient operator is a second order approximation of the standard derivative operator evaluated at midpoint. According to [10], for any smooth function $f : \mathbb{R} \to \mathbb{R}$, this second-order operator is given by

$$\mathrm{D}f(x, y) = \frac{f(x) - f(y)}{x - y} \tag{A.1}$$

For the limit case in which $x = y$ the discrete gradient operator collapses to

$$\mathrm{D}f(x, y) = \left. \frac{\mathrm{d}f}{\mathrm{d}x} \right|_{n+\frac{1}{2}} \tag{A.2}$$

In addition, if $f : \mathbb{R} \times \cdots \times \mathbb{R} \to \mathbb{R}$ $k \geq 1$ times, the discrete derivative operator is given by

$$\mathrm{D}f(\mathbf{x}, \mathbf{y}) \cdot (\mathbf{x} - \mathbf{y}) = \sum_{i=1}^{k} \mathrm{D}_i f(x_i, y_i)(x_i - y_i), \tag{A.3}$$

where the term $\mathrm{D}_i f(x_i, y_i)$ might be interpreted as the ith second order accurate discrete counterpart to the ith partial derivative of the function f at midpoint; for more details about its computation the reader is referred to [10].

The discrete gradient operator satisfies two important properties which are *directionality* and *consistency*

$$\mathrm{D}f(\mathbf{x}, \mathbf{y}) \cdot (\mathbf{x} - \mathbf{y}) = f(\mathbf{x}) - f(\mathbf{y}), \tag{A.4}$$

$$\mathrm{D}f(\mathbf{x}, \mathbf{y}) = \mathrm{D}f\left(\frac{\mathbf{x} + \mathbf{y}}{2}\right) + \mathcal{O}(\|\mathbf{x} - \mathbf{y}\|^2). \tag{A.5}$$

The first one holds the key to preserve discretely the evolution structure while the second one ensures the second order accuracy. Furthermore, another interesting property is a discrete version of the chain rule. That is, let $f : \mathbf{U} \to \mathbb{R}$ be a function and let π be an invariant of the motion, then let us denote as $\tilde{f} : \pi(\mathbf{U}) \to \mathbb{R}$ the associated reduced function defined by the expression $\tilde{f}(\pi(\mathbf{q})) = f(\mathbf{q})$, for all $\mathbf{q}$. If the invariant π is at most of degree two, in [10] is proved that

$$\mathrm{D}f(\mathbf{x}, \mathbf{y}) = \mathrm{D}\pi\left(\frac{\mathbf{x} + \mathbf{y}}{2}\right)^{\top} \mathrm{D}\tilde{f}(\pi(\mathbf{x}), \pi(\mathbf{y})). \tag{A.6}$$

Finally, let $\tau : \mathbb{R}_+ \times \mathbb{R}_+ \to \mathbb{R}$ be either the internal energy or the entropy, then the fully elaborated formulas required to the implementation of the temperature-based TC scheme are

$$\mathrm{D}_{\mathbf{q}_\alpha} \tau_\beta = \mathrm{D}_{\lambda_\beta^2} \tau_\beta \left(\frac{\partial \lambda_\beta^2}{\partial \mathbf{q}_\alpha} \right)_{n+\frac{1}{2}} \quad \text{with } \alpha, \beta = 1, 2 \tag{A.7}$$

$$\mathrm{D}_{\lambda^2} \tau = \frac{\tau(\lambda_{n+1}, \theta_{n+1}) - \tau(\lambda_n, \theta_{n+1}) + \tau(\lambda_{n+1}, \theta_n) - \tau(\lambda_n, \theta_n)}{2(\lambda_{n+1}^2 - \lambda_n^2)} \tag{A.8}$$

$$D_\theta \tau = \frac{\tau(\lambda_{n+1}, \theta_{n+1}) - \tau(\lambda_{n+1}, \theta_n) + \tau(\lambda_n, \theta_{n+1}) - \tau(\lambda_n, \theta_n)}{2(\theta_{n+1} - \theta_n)} \tag{A.9}$$

where indexes have been omitted where deemed unnecessary.

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