



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



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ARTICLE INFO

Article history:

Received 11 September 2014

Revised 15 May 2015

Accepted 4 August 2015

Available online 11 August 2015

Keywords:

Time integration

Structure preservation

Geometric integration

Thermodynamics

GENERIC formalism

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.

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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

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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

$$h = k(\theta_2 - \theta_1), \quad (1)$$

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

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