

PERFORMANCE ASSESSMENT OF VARIATIONAL INTEGRATORS FOR THERMOMECHANICAL PROBLEMS

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ABSTRACT: Structure-preserving integrators are in the focus of ongoing research because of their distinguished features of robustness and long time stability. In particular, their formulation for coupled problems that include dissipative mechanisms is still an active topic. Conservative formulations, such as the thermo-elastic case without heat conduction, fit well into a variational framework and have been solved with variational integrators, whereas the inclusions of viscosity and heat conduction are still under investigation. To encompass viscous forces and the classical heat transfer (Fourier's law), an extension of Hamilton's principle is required. In this contribution we derive variational integrators for thermo-viscoelastic systems with classical heat transfer. Their results are compared for two discrete model problems vs. energy-entropy-momentum methods.

KEY WORDS: Variational integrators, energy-entropy-momentum methods, viscoelasticity, thermomechanical coupling, heat transfer.

1 INTRODUCTION

The simulation of large deformations, such as crash-tests, is on the cutting edge of research in mechanical engineering. Due to its geometric nonlinearity, which often coincides with material nonlinearities and thermomechanical coupling, there is no hope for analytical solutions of real world problems and even many model problems. Consequently numerical methods are the only choice to obtain results and insight. Due to their nonuniqueness and parameter sensitivity these systems are hard to validate thoroughly in experiments, thus preservation of their physical structure deserves more attention. This article compares two prominent structure-preserving approaches for the transient simulation of thermomechanical systems: Variational Integrators (VI) and Energy-Entropy-Momentum (EEM) methods. In mechanics, VI

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and Energy-Momentum (EM) methods are the current state of the art in structure-preserving time-integration. Both of these families of methods have been used for over two decades in many applications and have consistently demonstrated their ability to solve evolution equations in a robust and accurate manner. Although completely different in their genesis and background, they pursue the same goal of accurate structure preservation, and compete as they are applied to ever more general theories.

The concept of VI was introduced by Cadzow [1] in the seventies and comprehensively developed by the group at Caltech, who worked out many special cases (see the overview [2]). The basic idea is to start the discretization directly from the variational principle, thus skipping the formulation of differential equations and leading to one-step maps, which are implicitly determined by algebraic equations. Originally developed for conservative systems, their extension to dissipative effects is currently being researched (c.f. the recent works [3, 4]). Viscosity and heat transfer are such effects of technical relevance in order to account for damping and temperature effects. The geometric consequence of dissipation is the loss of symplecticity, however the performance of VIs does not deteriorate. They are robust and by design at least second-order accurate. Typical applications are in astronomy and molecular dynamics, and increasingly in robotics, where VIs offer practical advantages for feedback control.

EEM methods were introduced by Romero [5] and utilize the discrete derivative operator [6], initially developed for the Energy-Momentum method (EM) [7], to build thermodynamically consistent algorithms from the *geometric* structure revealed by the GENERIC formalism [8]. Such formalism enables a unified expression of the evolution equations of any isolated thermodynamic system to be generated from the addition of the reversible and irreversible parts, which are directly related to the gradient of the total energy and the total entropy of the system in terms of the state vector, respectively. Due to the key properties of the discrete derivative operator, the resulting methods are automatically second-order accurate, energy-preserving and entropy-producing by design. In addition, first order accurate staggered methods could also be formulated in terms of entropy in such a way that each step remains thermodynamically consistent, see also [5]. Within this approach, different thermomechanical systems have successfully been addressed in terms of the so called entropy-based formulation, i.e using entropy as thermodynamic state variable, such as discrete thermo-elasticity [5], discrete thermo-viscoelasticity [9] and continuous nonlinear thermoelasticity [10, 11] with heat transfer. Very recently, a temperature-based formulation for discrete thermo-elasticity has been proposed in [12], overcoming the problems associated to the use of the entropy and hence fully complementing the GENERIC-based approach.

The purpose of this contribution is the assessment of the precision and robustness of variational integrators, in comparison to EEM methods and focusing on their conservation properties. To this end, the paper is structured as follows. In Section 2 the problem of thermomechanical systems is defined in general. In Section 3 the time discretization is described, namely a VI and two EEM schemes, namely the energy-entropy-momentum method in entropy and in temperature formulation. In Section 4 these integrators are compared with each other at two discrete systems, a planar single and a spatial double pendulum. Section 5 concludes this performance assessments.

2 PROBLEM DEFINITION

In this article we consider thermo-viscoelastic models possessing a Lagrangian

$$(1) \quad L = T(\mathbf{q}, \dot{\mathbf{q}}) - \psi(\lambda, \gamma, \vartheta),$$

where T denotes kinetic coenergy (the distinction between kinetic energy and coenergy is in the spirit of Crandall [13]) and ψ , the free energy function (Helmholtz free energy). The structure of the free energy

$$(2) \quad \psi(\lambda, \gamma, \vartheta) = (1 + \beta_c)\psi_e + \mu\gamma^2 - \beta_c\gamma\frac{\partial\psi_e}{\partial\lambda}$$

is adopted from Holzapfel and Simo [14]. This kind of models are referred to as generalized Maxwell-elements and may be represented as rheological model of a thermo-elastic spring (main spring), characterized by the free energy $\psi_e(\lambda, \vartheta)$, in parallel with a combination of another thermo-elastic spring in series with a dashpot (see Fig. 1). Sometimes it is also referred to as Poynting-element by some authors [15]. Equation (2) fulfills all requirements from thermodynamics. It may be used either as infinitesimal line element for the construction of a continuum model or as component of a discrete model. This element is described by three state variables, namely, the total stretch λ , the viscous stretch γ and its temperature ϑ . The total stretch is a function of the generalized coordinates $\mathbf{q}$ and its internal variable γ by their time history. For the temperature it will turn out useful for VIs to formulate it as time derivative $\vartheta = \dot{\alpha}$ of a quantity called thermacy α , which is also referred to as “thermal displacement”, since temperature $\vartheta = \dot{\alpha}$ is related with the averaged velocity of atoms (strictly speaking their averaged kinetic energy). The corresponding momenta are the mechanical momentum $\mathbf{p}$ and the entropy s

$$(3a) \quad \mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}},$$

$$(3b) \quad s = \frac{\partial L}{\partial \dot{\alpha}} = -\frac{\partial \psi}{\partial \dot{\alpha}}.$$

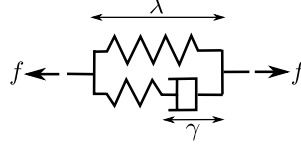


Fig. 1. Generalized Maxwell-element.

Due to the similarities of these two definitions, the entropy is sometimes referred to as “thermal momentum”. The viscous stretch is related with a vanishing momentum variable, since its time derivative $\dot{\gamma}$ does not enter the Lagrangian. With thermacy it is the other way round, only its time derivative enters the Lagrangian for classical heat transfer. In rare cases of non-classical heat transfer, such as Green & Naghdi type II [16], thermacy would occur in the Lagrangian.

The quantities conjugated to the deformation variables are the total internal force f and its viscous component g

$$(4a) \quad f = \frac{\partial \psi}{\partial \lambda},$$

$$(4b) \quad g = -\frac{\partial \psi}{\partial \gamma}.$$

The internal energy

$$(5) \quad e(\lambda, \gamma, \dot{\alpha}) = \psi + \dot{\alpha} s$$

is obtained by the Legendre transformation of the free energy ψ with respect to the temperature $\dot{\alpha}$. Further relations that will be utilized later are

$$(6a) \quad \dot{\mathbf{q}} = \frac{\partial \tilde{T}}{\partial \mathbf{p}},$$

$$(6b) \quad \dot{\alpha} = \frac{\partial \tilde{e}}{\partial s},$$

where $\tilde{T}(\mathbf{q}, \mathbf{p})$ is the kinetic energy and $\tilde{e}(\lambda, \gamma, s)$ denotes the internal energy as a function of (λ, γ, s) .

3 TIME DISCRETIZATION

The problems addressed in this paper are nonlinear in nature, and usually only numerical solutions can be obtained. Three structure-preserving time integration schemes will be described in this section: a VI, an EEM method in entropy formulation (EEM-Gs) and in temperature formulation (EEM-GT). All of them aim at good longtime behavior and improved numerical stability in comparison to standard methods for ordinary differential equations.

3.1 VARIATIONAL INTEGRATORS

Variational integrators are based on a discrete version of Hamilton's principle of stationary action. To formulate them, the essential step is thus to write the action functional, from which the method follows naturally. For conservative mechanical problems, this choice is standard. However, the inclusion of dissipative effects (viscosity and Fourier's heat transfer) requires the use of incremental potentials [17] or the use of D'Alembert terms [18]. In this article we follow the latter option.

In this section we introduce the extended Hamilton principle which encompasses thermomechanics. Based on this principle, variational integrators are constructed in a systematic fashion. More specifically, the action is approximated with a discrete action evaluated as a quadrature based on the midpoint rule (MP). The resulting method, which we refer to as "variational mid-point", is not to be mistaken with the conventional mid-point quadrature rule. The generalization to higher order integrators will be outlined at the end of this section.

3.1.1 VARIATIONAL FORMULATION

The classical Hamilton Principle reads

$$(7) \quad \delta S = \delta \int_{t_0}^{t_1} L \, dt = \delta \int_{t_0}^{t_1} (T - V) \, dt = 0,$$

where L, T, V are, respectively, the Lagrangian, the kinetic, and the potential energies. The extension of this principle to thermoelasticity is obtained by replacing the potential energy $V(\mathbf{q})$ by the free energy $\psi(\lambda, \gamma, \vartheta)$ [19]. The use of thermacy as variable makes the resulting Euler–Lagrange equations of the thermal problem to take the same mathematical structure as the mechanical one

$$(8a) \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{\mathbf{q}}} - \frac{\partial L}{\partial \mathbf{q}} = 0,$$

$$(8b) \quad \frac{d}{dt} \frac{\partial L}{\partial \dot{\alpha}} - \frac{\partial L}{\partial \alpha} = 0.$$

These equations refer to the conservative case. In order to include nonconservative generalized forces, Hamilton's principle is enhanced by D'Alembert terms [18]

$$(9) \quad \delta \int_{t_0}^{t_1} L \, dt + \int_{t_0}^{t_1} \delta W^{\text{nc}} \, dt = 0,$$

where δW^{nc} splits into mechanical and thermal contributions

$$(10) \quad \delta W_{\text{mech}}^{\text{nc}} = \mathbf{f} \cdot \delta \mathbf{q}, \quad \delta W_{\text{therm}}^{\text{nc}} = \dot{s} \delta \alpha.$$

These terms account for mechanical forces such as external forcing or damping and for entropy fluxes, also called “thermal forces” that stem from heat production (external source) or from heat transfer by Fourier’s law. They enter eqs. (8a) and (8b) on the right-hand side, replacing the zeros. In the first example, in section 4.1, will be demonstrated how the well-known equations for thermomechanics and heat transfer are recovered from this extension of Hamilton’s principle.

3.1.2 CONSTRUCTION OF VARIATIONAL INTEGRATORS

The construction of a variational integrator starts directly from the variational principle. It consists of two steps. Firstly, the functions of the generalized coordinates $\mathbf{q}(t)$ are discretized by interpolation functions $\mathbf{q}_d(t)$. Secondly, a quadrature rule for the evaluation of the action integral is applied. For the sake of simplicity the following explanations refer exemplarily to linear interpolation

$$(11a) \quad \mathbf{q}(t) \approx \mathbf{q}_d(t) = \frac{t^{k+1} - t}{t^{k+1} - t^k} \mathbf{q}^k + \frac{t - t^k}{t^{k+1} - t^k} \mathbf{q}^{k+1},$$

$$(11b) \quad \dot{\mathbf{q}}(t) \approx \dot{\mathbf{q}}_d(t) = \frac{\mathbf{q}^{k+1} - \mathbf{q}^k}{t^{k+1} - t^k} \text{ for } t \in [t^k, t^{k+1}],$$

and numerical integration by the midpoint rule

$$(12) \quad \int_{t^k}^{t^{k+1}} L(\mathbf{q}_d(t), \dot{\mathbf{q}}_d(t)) dt \approx \underbrace{h L(\mathbf{q}_d(t^{k+1/2}), \dot{\mathbf{q}}_d(t^{k+1/2}))}_{L_d(\mathbf{q}^k, \mathbf{q}^{k+1})},$$

where $h = t^{k+1} - t^k$ denotes the time step size, $t^{k+1/2} = t^k/2 + t^{k+1}/2$ half-time and L_d is called discrete Lagrangian. As a result of this step, the continuous variational problem is turned into a discrete one, one requiring the stationarity of the discrete action sum

$$(13) \quad S_d = (\mathbf{q}^0, \dots, \mathbf{q}^N) = \sum_{k=0}^{N-1} L_d(\mathbf{q}^k, \mathbf{q}^{k+1})$$

plus discrete D’Alembert terms

$$(14a) \quad \delta W^{nc} = \int_{t_1}^{t_2} \mathbf{f}_d \cdot \delta \mathbf{q} + \dot{s} \delta \alpha dt$$

$$(14b) \quad \approx \sum_{k=0}^{N-1} h (\mathbf{f} \cdot \delta \mathbf{q} + \dot{s} \delta \alpha)|_{t=t_k+1/2} = \delta W_d^{nc}$$

to vanish. The discrete forces, likewise the discrete Lagrangian, are obtained by numerical integration. If again the midpoint rule is applied to the time integral, now of the virtual work, then the force during one time step is split into discrete values, one at the beginning and the other at the end of the time step. Thus at each time point, except the first and the last one, two forces enter the equation, one originating from the previous time step and the other from the next time step

$$(15a) \quad \mathbf{f}_d^+(\mathbf{q}^{k-1}, \mathbf{q}^k) = \int_{t^{k-1}}^{t^k} \mathbf{f}(t) \frac{\partial \mathbf{q}_d(t)}{\partial \mathbf{q}^k} dt = \frac{h \mathbf{f}(t^{k-1/2})}{2},$$

$$(15b) \quad \mathbf{f}_d^-(\mathbf{q}^k, \mathbf{q}^{k+1}) = \int_{t^k}^{t^{k+1}} \mathbf{f}(t) \frac{\partial \mathbf{q}_d(t)}{\partial \mathbf{q}^k} dt = \frac{h \mathbf{f}(t^{k+1/2})}{2},$$

as deduced from the discrete D'Alembert principle [18]. Evaluating the stationarity condition (9)

$$(16) \quad 0 = \sum_{k=0}^{N-1} \delta L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) + \sum_{k=0}^{N-1} \delta W_d^{nc}(\mathbf{q}^k, \mathbf{q}^{k+1})$$

results in N discrete Euler–Lagrange equations for all admissible positions $\mathbf{q}^1 \dots \mathbf{q}^N$. The shorthand symbol D_i will be used in the following to denote derivation with respect to the i th argument, i.e. $D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) = \frac{\partial L_d}{\partial \mathbf{q}^k}$. At first the numerical scheme must connect to the given initial conditions. For the initial position $\mathbf{q}(t^0) = \mathbf{q}^0$ this is trivial and for the initial velocity $\dot{\mathbf{q}}(t^0) = \dot{\mathbf{q}}^0$ the definition of the corresponding momentum is inserted into the first step

$$(17) \quad D_2 L(\mathbf{q}^0, \dot{\mathbf{q}}^0) = -D_1 L_d(\mathbf{q}^0, \mathbf{q}^1) - \mathbf{f}_d^-(\mathbf{q}^0, \mathbf{q}^1)$$

determining $\mathbf{q}^1$. While for $k = 1 \dots N - 1$ the remaining positions $\mathbf{q}^{k+1}$ follow recursively from

$$(18) \quad 0 = D_2 L_d(\mathbf{q}^{k-1}, \mathbf{q}^k) + \mathbf{f}_d^+(\mathbf{q}^{k-1}, \mathbf{q}^k) + D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) + \mathbf{f}_d^-(\mathbf{q}^k, \mathbf{q}^{k+1}).$$

Introducing the following definitions:

$$(19a) \quad \mathbf{p}^k = -D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) - \mathbf{f}_d^-(\mathbf{q}^k, \mathbf{q}^{k+1}),$$

$$(19b) \quad \mathbf{p}^{k+1} = +D_2 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) + \mathbf{f}_d^+(\mathbf{q}^k, \mathbf{q}^{k+1}),$$

results in the position-momentum form. This name is justified, because the $\mathbf{p}^k$ are the discrete analogues to momenta and fulfill a discrete version of Noether's theorem [2]. Equation (19a) is then solved iteratively with tangent matrix

$$(20) \quad \mathbf{T} = D_2 D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1}) - D_2 \mathbf{f}_d^-(\mathbf{q}^k, \mathbf{q}^{k+1})$$

by a Newton scheme. The resulting $\mathbf{q}^{k+1}$ are just inserted into eq. (19b) in order to update the momentum. Then the procedure repeats for the next time step.

Remark: Higher order of the approximation increases the number of unknowns. For instance, quadratic polynomials

$$(21a) \quad q_d(t) = at^2 + bt + q^0 \quad \text{and} \quad \dot{q}_d(t) = 2at + bt \quad \text{with}$$

$$(21b) \quad a = \frac{2q^0 + 2q^1 - 4q^{1/2}}{h^2},$$

$$(21c) \quad b = \frac{4q^{1/2} - 3q^0 - q^1}{h},$$

have as unknowns $q^{1/2}$ and q^1 , since the value q^0 at the beginning of the time step is known. A matching numerical integration is given by Simpson's rule

$$(22) \quad L_d = \frac{h}{6} (L|_{t=t^k} + 4L|_{t=t^{k+1/2}} + L|_{t=t^{k+1}}).$$

Evaluation of the variation results in the same number of Euler-Lagrange equations as the number of unknowns, here for the conservative part

$$(23a) \quad \mathbf{0} = D_3 L_d(\mathbf{q}^{k-1}, \mathbf{q}^{k-1/2}, \mathbf{q}^k) + D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1/2}, \mathbf{q}^{k+1}),$$

$$(23b) \quad \mathbf{0} = D_2 L_d(\mathbf{q}^{k-1}, \mathbf{q}^{k-1/2}, \mathbf{q}^k).$$

Including nonconservative forces and expressing in position-momentum form yields the resulting equation system

$$(24a) \quad \mathbf{p}^k = -D_1 L_d(\mathbf{q}^k, \mathbf{q}^{k+1/2}, \mathbf{q}^{k+1}) - \mathbf{f}_d^k,$$

$$(24b) \quad \mathbf{0} = +D_2 L_d(\mathbf{q}^k, \mathbf{q}^{k+1/2}, \mathbf{q}^{k+1}) + \mathbf{f}_d^{k+1/2},$$

$$(24c) \quad \mathbf{p}^{k+1} = +D_3 L_d(\mathbf{q}^k, \mathbf{q}^{k+1/2}, \mathbf{q}^{k+1}) + \mathbf{f}_d^{k+1},$$

consisting of a nonlinear part, eqns. (24a)-(24b), which must be solved iteratively and an update equation (24c). While the first and last equation enforce continuity of momentum from one time step to the next, the second equation expresses the stationarity condition of the action during one time step. Combining quadratic approximations with a Lobatto quadrature formula of third-order leads to a forth-order

accurate VI scheme whereas the combination of linear approximation and mid-point rule is second-order accurate.

The state variables $\mathbf{q}$, $\mathbf{p}$ are calculated directly by the variational integrator. In contrast to mechanical position, thermacy is merely used for the derivation of the time stepping scheme, its absolute values are barely of interest and hence not stored in simulations. In order to obtain dependent quantities, i.e. velocity and temperature, their definitions by eqs. (6a)-(6b) are rather evaluated than the time derivatives of their approximations. These values are better in terms of structure preservation than the interpolations, whose time-derivatives are not necessarily continuous at the time nodes. Similarly the kinetic energy T and internal energy e are evaluated as functions of the state variables $\mathbf{q}$, $\mathbf{p}$. If these relations cannot be evaluated analytically, e.g. the Legendre transform does not provide an analytical expression for the velocities as function of the momenta, they still can be evaluated numerically.

One of the most important aspects of variational integrators is backward error analysis. It predicts the characteristics of the discrete-time path rather than the rate of convergence. Considering the discretization of a Hamiltonian system by a variational integrator results in discrete states that are the exact solutions to a nearby Hamiltonian system [20]

$$(25) \quad \tilde{H}(\mathbf{q}, \mathbf{p}) = H(\mathbf{q}, \mathbf{p}) + \frac{h^2}{2!} g_1(\mathbf{q}, \mathbf{p}) + \frac{h^4}{4!} g_2(\mathbf{q}, \mathbf{p}) + \dots,$$

where H denotes the original Hamiltonian. The functions g_i can be determined using the method of modified equations [21]. Even though the conservation of the original Hamiltonian is incompatible with symplecticity, the energy error remains bounded. Variational integrators are symplectic as long as the time steps are equidistant [20].

Note that, besides conservative forces variational integrators can handle both external forcing and dissipation [2] and proved well suited for practical applications in robotics [22] and also to be demonstrated by the following examples in this paper.

3.2 ENERGY-ENTROPY-MOMENTUM METHODS

For general, finite-dimensional isolated thermodynamic systems, the state variables are arranged in the vector $\mathbf{z}$, in purely mechanical systems it used to be $\mathbf{z} = [\mathbf{q}, \mathbf{p}]^T$ for thermomechanical system it is either (33) or (34). Their time-evolution may be expressed by the following initial-value problem:

$$(26) \quad \dot{\mathbf{z}} = \mathbf{L}(\mathbf{z}) \nabla E(\mathbf{z}) + \mathbf{M}(\mathbf{z}) \nabla S(\mathbf{z}), \quad \mathbf{z}(0) = \mathbf{z}_0$$

E being the total energy and S being the total entropy, $\nabla(\bullet)$ being the gradient operator with respect to the state space vector, $\mathbf{z}_0$ containing the prescribed initial

conditions and $\mathbf{L}, \mathbf{M}$ being the so-called Poisson matrix and the Dissipative matrix, respectively. The evolution equations (26) will be in accordance with the laws of thermodynamics provided that the Poisson and Dissipative matrices are skew-symmetric and symmetric, positive semi-definite, respectively, and satisfy the degeneracy conditions

$$(27) \quad \nabla S^T \mathbf{L} = \mathbf{0}, \quad \nabla E^T \mathbf{M} = \mathbf{0}.$$

The proof is straightforward and can be found in [12].

Following the guidelines in Romero [5], the discrete derivative operator, denoted as $D(\bullet)(\mathbf{z}^{k+1}, \mathbf{z}^k)$, is employed to arrive at the following monolithic implicit second order accurate method:

$$(28) \quad \frac{\mathbf{z}^{k+1} - \mathbf{z}^k}{h} = \mathbf{L}(\mathbf{z}^{k+1}, \mathbf{z}^k) DE(\mathbf{z}^{k+1}, \mathbf{z}^k) + \mathbf{M}(\mathbf{z}^{k+1}, \mathbf{z}^k) DS(\mathbf{z}^{k+1}, \mathbf{z}^k),$$

where the $\mathbf{L}(\mathbf{z}^{k+1}, \mathbf{z}^k)$, $\mathbf{M}(\mathbf{z}^{k+1}, \mathbf{z}^k)$ are second order approximations of the above Poisson and Dissipative matrices and, therefore, have their respective properties. Particularly, the degeneracy conditions are fulfilled in the following way:

$$(29a) \quad \mathbf{0} = DS(\mathbf{z}^{k+1}, \mathbf{z}^k)^T \mathbf{L}(\mathbf{z}^{k+1}, \mathbf{z}^k),$$

$$(29b) \quad \mathbf{0} = DE(\mathbf{z}^{k+1}, \mathbf{z}^k)^T \mathbf{M}(\mathbf{z}^{k+1}, \mathbf{z}^k).$$

The *discrete* laws of thermodynamics are thus satisfied due to these properties and the directionality property of the discrete derivative operator that allows to express the balance of any function in any time-step as

$$(30) \quad E^{k+1} - E^k = DE(\mathbf{z}^{k+1}, \mathbf{z}^k) \cdot (\mathbf{z}^{k+1} - \mathbf{z}^k)$$

that can be further elaborated using (28) to give

$$(31) \quad E^{k+1} - E^k = h DE(\mathbf{z}^{k+1}, \mathbf{z}^k)^T \mathbf{L}(\mathbf{z}^{k+1}, \mathbf{z}^k) DE(\mathbf{z}^{k+1}, \mathbf{z}^k) + h DE(\mathbf{z}^{k+1}, \mathbf{z}^k)^T \mathbf{M}(\mathbf{z}^{k+1}, \mathbf{z}^k) DS(\mathbf{z}^{k+1}, \mathbf{z}^k) = 0.$$

Similarly, the total entropy balance results in

$$(32) \quad S^{k+1} - S^k = DS(\mathbf{z}^{k+1}, \mathbf{z}^k) \cdot (\mathbf{z}^{k+1} - \mathbf{z}^k) = h DS(\mathbf{z}^{k+1}, \mathbf{z}^k)^T \mathbf{L}(\mathbf{z}^{k+1}, \mathbf{z}^k) DE(\mathbf{z}^{k+1}, \mathbf{z}^k) + h DS(\mathbf{z}^{k+1}, \mathbf{z}^k)^T \mathbf{M}(\mathbf{z}^{k+1}, \mathbf{z}^k) DS(\mathbf{z}^{k+1}, \mathbf{z}^k) \geq 0.$$

The method (28) also ensures the conservation of quadratic momentum maps if the discrete derivative is modified to account for the symmetries in the system. Details and proofs of this statement can be found in [5].

When specifying the presented approach, the Poisson and Dissipative matrices need to be fully defined. In doing so, a crucial issue in the formulation raises regarding the choice for the thermodynamic variables. Thus, in the very beginning of EEM methods the use of entropy variables was favored, as it easily provides the matrices and, therefore, thermodynamically consistent methods were straightforwardly achieved, although assuming significant restrictions in the formulation, such as difficulties for temperature boundary conditions. The recent work [23] concluded that a temperature-based formulation can also provide the GENERIC matrices, facilitating the formulation of thermodynamically consistent methods based on temperature variables, see [12], and thus overcoming the mentioned restrictions. In the following subsections we summarize the main aspects of both formulations for the model presented in Section 2.

3.2.1 ENERGY-ENTROPY-MOMENTUM METHODS IN ENTROPY FORMULATION

As previously pointed out, the GENERIC formulation only applies to isolated systems, i.e. the element and the environment with which it exchanges heat must be considered as the thermodynamic system. To this end, the easiest way is to consider the environment to have a constant temperature ϑ_∞ . Thus the system is thermomechanically determined by means of five independent variables, among which both element and environment entropies s and s_∞ must be included to achieve an entropy-based formulation, that is

$$(33) \quad \mathbf{z} = [\mathbf{q}, \mathbf{p}, \gamma, s, s_\infty] .$$

This choice simplifies the Poisson matrix to be the classical symplectic one, see [24], and the Dissipative matrix gets not too involved, enabling such a straightforward formulation that it was achieved in [9] with no need for the GENERIC form to reveal the structure meant to be preserved. Examples of the algorithmic matrices $\mathbf{L}(\mathbf{z}^{k+1}, \mathbf{z}^k)$, $\mathbf{M}(\mathbf{z}^{k+1}, \mathbf{z}^k)$ are worked out in the detailed description of the EEM-integrator in entropy formulation [5]. In the following this integrator will be abbreviated as EEM-Gs.

However, this formulation is valid provided that the relations $\vartheta = \vartheta(\lambda, \gamma, s)$ could be analytically found. For standard temperature-based free energy functions [25], this consideration limits the thermo-elastic parameters of the model to be at most linearly temperature-dependent.

3.2.2 ENERGY-ENTROPY-MOMENTUM METHODS IN TEMPERATURE FORMULATION

To avoid this issue, a temperature-based formulation becomes crucial, for which the element and the environment temperatures should be considered as state variables

$$(34) \quad \mathbf{z} = [\mathbf{q}, \mathbf{p}, \gamma, \vartheta, \vartheta_\infty].$$

Note that this choice implies the environment temperature ϑ_∞ to be non-constant so that the environment internal energy in terms of it, $\epsilon(\vartheta_\infty): \mathbb{R}^+ \rightarrow \mathbb{R}$, can be defined. With this consideration, the GENERIC matrices become more intricate but affordable, thus allowing to formulate a temperature-based thermodynamically consistent counterpart which overcomes the restrictions related to the entropy formulation pointed out before. This integrator will be referred to as EEM-GT in the next sections.

4 NUMERICAL EXAMPLES

The two classes of integrators introduced in the previous section, variational integrators and EEM methods, are now applied to model problems from the literature: a planar thermo-viscoelastic single pendulum [9] and a spatial thermo-elastic double pendulum [12]. The former compares a second-order accurate VI with a second-order accurate EEM method in entropy formulation whereas the latter compares the same VI with an EEM method in temperature formulation. Both model problems have many features, such as strongly nonlinear dynamics, thermoelastic coupling and heat transfer, in common with challenging real world problems. Integrators that perform well with these low-dimensional model problems, are expected to perform well with large-scale models of many degrees of freedom and similar nonlinearities.

4.1 PLANAR THERMO-VISCOELASTIC SINGLE PENDULUM WITH CLASSICAL HEAT CONDUCTION WITH THE ENVIRONMENT

This planar pendulum shown in Fig. 2 is taken from the literature [9]. Its kinetic coenergy is

$$(35) \quad T = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2)$$

and the length of the massless pendulum rod

$$(36) \quad \lambda = \sqrt{x^2 + y^2}$$

depends on the position $\mathbf{q} = [x, y]^T$ of the attached mass. The evolution equation of the dashpot is assumed to be linear

$$(37) \quad \eta \dot{\gamma} = g,$$

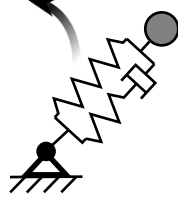


Fig. 2. Example 1: a mass attached to a massless thermo-viscoelastic spring with heat transfer with the environment.

where γ denotes stretch of the dashpot and g the corresponding viscous force (4b). The free energy, defined generally by eq. (2), is specified by thermo-elastic springs with

$$(38) \quad \psi_e(\lambda, \dot{\alpha}) = \frac{k}{2} \log^2 \left(\frac{\lambda}{\lambda_0} \right) - \beta_t (\dot{\alpha} - \vartheta_r) \log \left(\frac{\lambda}{\lambda_0} \right) + c \left[\dot{\alpha} - \vartheta_r - \dot{\alpha} \log \left(\frac{\dot{\alpha}}{\vartheta_r} \right) \right],$$

where k denotes the elasticity coefficient, which is related with stiffness, of the main spring, β_t the thermomechanical coupling parameter, which is related with thermal expansion, and c the heat capacity. This free energy function allows for large strains and Gough-Joule coupling. It has been successfully validated in experiments [26–28] and its purely mechanical form is available in commercial codes. All parameters entering the simulation are summarized in Table 1 for convenience.

The thermal part is the heat transfer between spring and environment and the heat generated by the dashpot. The heat flux follows from Fourier's law

$$(39) \quad \phi = -\kappa(\dot{\alpha} - \vartheta_\infty),$$

where the environment is assumed to be a thermal reservoir of constant temperature ϑ_∞ . Regarding the dashpot, it is assumed that all energy mechanically dissipated is completely converted into heat, which corresponds to the entropy production

$$(40) \quad \dot{s}_v = \frac{g\dot{\gamma}}{\dot{\alpha}}.$$

The expression for the virtual work of the nonconservative forces thus consists of three terms

$$(41) \quad \delta W^{nc} = -g\delta\gamma + \frac{g\dot{\gamma}}{\dot{\alpha}}\delta\alpha + \kappa \frac{\dot{\alpha} - \vartheta_\infty}{\dot{\alpha}}\delta\alpha = -\eta\dot{\gamma}\delta\gamma + \frac{\eta\dot{\gamma}^2}{\dot{\alpha}}\delta\alpha + \kappa \frac{\dot{\alpha} - \vartheta_\infty}{\dot{\alpha}}\delta\alpha$$

Table 1. Single pendulum parameters (example 1)

m	1	kg	mass
λ_0	1	m	unstretched length
$k(\vartheta)$	$k_0 - k_1(\vartheta - \vartheta_r)$		temperature-dependent elasticity coefficient
k_0	100	J	
k_1	0.5	J/K	
β_c	0.1		spring ratio
β_t	4	J/K	thermoelastic coupling
c	1	J/K	heat capacity
$\mu(\vartheta)$	$\mu_0 - \mu_1(\vartheta - \vartheta_r)$		temperature-dependent viscosity coefficient
μ_0	5	N/m	
μ_1	0.1	N/mK	
$\eta(\vartheta)$	$\eta_0 e^{a(1/\vartheta - 1/\vartheta_r)}$		temperature-dependent viscosity
η_0	100	Ns/m	
a	10	K	
κ	10	W/K	thermal conductivity
ϑ_r	300	K	reference temperature
ϑ_∞	300	K	environment temperature
$\mathbf{q}(0)$	[3, 0]	m	initial position
$\dot{\mathbf{q}}(0)$	[0, 1]	m/s	initial velocity
$\gamma(0)$	0	m	initial viscous stretch
$\vartheta(0)$	380	K	initial temperature
t_{sim}	20	s	simulation time
h	0.2	s	time step
ε	10^{-10}		Newton tolerance for Euclidean norm $ \Delta \mathbf{z} $

done by the viscous force of the dashpot, heat generated by the dashpot and heat conduction with the environment. Both energy and entropy of the environment are assumed zero initially. Since the extension of Hamilton's principle to thermo-viscoelasticity may seem unfamiliar to many readers, the classical expressions are recovered here in detail

$$(42a) \quad \delta \mathbf{q} : \quad \dot{\mathbf{p}} + \frac{\partial \psi}{\partial \lambda} \frac{\partial \lambda}{\partial \mathbf{q}} = 0$$

$$(42b) \quad \delta \gamma : \quad -\frac{\partial \psi}{\partial \gamma} = \eta \dot{\gamma}$$

$$(42c) \quad \delta \alpha : \quad \beta_t \left((1 + \beta_c) \frac{\dot{\lambda}}{\lambda} + \beta_c \gamma \frac{\dot{\lambda}}{\lambda^2} \right) + (1 + \beta_c) c \frac{\ddot{\alpha}}{\dot{\alpha}} = \frac{\eta \dot{\gamma}^2}{\dot{\alpha}} + \kappa \frac{\dot{\alpha} - \vartheta_\infty}{\dot{\alpha}}.$$

While the first and second equation represent a common equation of motion and an evolution equation for the internal variable, respectively, we have a closer look at the

third equation. Its meaning as energy balance gets evident, when written as

$$(43) \quad (1 + \beta_c)c\ddot{\alpha} = \eta\dot{\gamma}^2 + \kappa(\dot{\alpha} - \vartheta_\infty) - \dot{\alpha}\beta_t \left(1 + \beta_c \left[1 + \frac{\gamma}{\lambda}\right]\right) \frac{\dot{\lambda}}{\lambda}.$$

The first term on the right hand side corresponds to power of the dashpot, the second term to the heat flux from the environment into the springs and the third term to the thermomechanical coupling. Note that both springs of the generalized Maxwell-element (Fig. 1) are modeled as thermoelastic.

The free motion for given initial conditions is taken as example. The linearization around the unstretched position at rest and at reference temperature indicates free oscillations of period $t_{\text{period}} = 0.086$ s and gives an idea of the motions time scale.

Using the same time step $h = 0.2$ s as in the reference [9] results, after 3-4 Newton-iterations per time step, in trajectories and time histories of position and temperature that are indistinguishable.

Thus the focus is now on the conservation properties. Fig. 3 a) shows how the numerically obtained total energy deviates from the exact value that is known to be constant on physical grounds. As expected the EEM scheme outperforms the variational integrator in terms of energy as listed in Table 3. The entropy is, as usual for diffusion processes in which temperatures level out, a monotonically increasing function asymptotically approaching its upper bound. Fig. 3 b) shows the deviations of the total entropy compared to a reference trajectory much finer discretized than the other results ($h = 0.005$ s), both integrators show oscillatory deviations settling to the final value. The entropy rates are not shown additionally, as they are in accor-

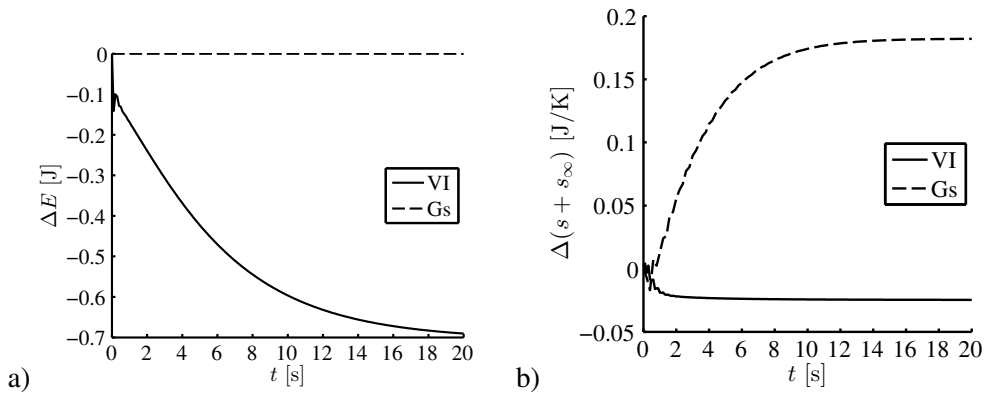


Fig. 3. Example 1: a) error in total energy ($E = \text{const.} = 1704$ J) vs. time, b) error in total entropy ($s + s_\infty = 5.4258 \dots 5.4613$ J/K) vs. time for the variational integrator (VI) and the Energy-Entropy-Momentum method (EEM-Gs).

dance with the second law, i.e. strictly increasing for all the simulations, which is an inherent characteristic of both schemes.

Both integrators calculate the angular momentum, which is to be constant in this model, within Newton-tolerance.

Comparisons with standard solvers are not feasible, since they do not converge to a solution for this step size as documented in [9].

4.2 SPATIAL THERMO-ELASTIC DOUBLE PENDULUM WITH CLASSICAL HEAT CONDUCTION BETWEEN THE SPRINGS

This example, shown in Fig. 4, is taken from Conde [12]. The free energy of both springs has again structure (38), but in contrast to the previous example, their parameters are not only different in value but also in their functional dependencies, as listed in Table 2. Particularly the logarithmic term in the elasticity coefficient turns the relation between entropy s and temperature $\dot{\alpha}$ into a transcendental equation. This makes the decisive difference compared to the previous example, the Legendre transform gets more involved, since there is no more analytical expression for temperature as function of entropy. As a consequence, the EEM method in entropy formulation is ruled out.

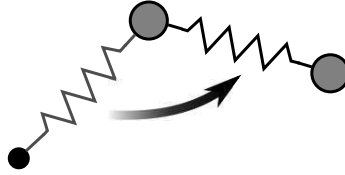


Fig. 4. Example 2: thermo-elastic double pendulum with heat transfer between the springs.

The thermal system contains heat transfer between the springs but not with the environment. The heat fluxes from spring 1 into spring 2 and vice versa are again modeled by Fourier's law

$$(44a) \quad \phi_1 = -\kappa(\vartheta_1 - \vartheta_2) = -\kappa(\dot{\alpha}_1 - \dot{\alpha}_2),$$

$$(44b) \quad \phi_2 = -\phi_1.$$

Thus, the double pendulum forms an isolated system and its total energy $E = T + e$ is to be conserved.

The system linearized around the state of rest in vertical hanging position and at average temperature indicates a minimum period of free oscillations $t_{\text{period}} = 0.17$ s, which gives an orientation for setting the time step.

Using the same time step $h = 0.1$ s as Conde [12] makes the trajectories coincide in the beginning but diverge at about half-time ($t = 12.5$ s). This divergence

Table 2. Double pendulum parameters (example 2)

m_1	10	kg	mass
m_2	20	kg	mass
$\lambda_{0,1}$	2	m	unstretched length, spring 1
$\lambda_{0,2}$	1	m	unstretched length, spring 2
$k_i(\vartheta)$	$k_{0i} - k_{1i}\vartheta_r \log(\vartheta_i/\vartheta_r)$		temperature-dependent elasticity coefficient
k_{01}	5000	J	
k_{11}	50	J/K	
k_{02}	10000	J	
k_{12}	60	J/K	
β_{t1}	20	J/K	thermoelastic coupling, spring 1
β_{t2}	20	J/K	thermoelastic coupling, spring 2
c_1	5000	J/K	heat capacity, spring 1
c_2	2000	J/K	heat capacity, spring 2
κ	300	W/K	thermal conductivity between springs
ϑ_r	300	K	reference temperature
$\mathbf{q}_1(0)$	$[3, 0, 0.5]^T$	m	initial position
$\mathbf{q}_2(0)$	$[3, 1, 1]^T$	m	initial position
$\mathbf{p}_1(0)$	$[0, 10, 0]^T$	kg m/s	initial momentum
$\mathbf{p}_2(0)$	$[0, 0, -20]^T$	kg m/s	initial momentum
$\vartheta_1(0)$	380	K	initial temperature
$\vartheta_2(0)$	298	K	initial temperature
t_{sim}	25	s	simulation time
h	0.1	s	time step
ε	10^{-10}		Newton tolerance for Euclidean norm $ \Delta \mathbf{z} $

is probably rather due to the chaotic behavior of the mechanical system than to the integrator. The temperatures shown in Fig. 5 a) coincide well until the diverging mechanical behavior affects the temperatures by the relatively strong thermal coupling in this example. Thus, the focus is more set on energetic quantities. Fig. 5 b) shows total energy, which should be constant on physical grounds. As expected the EEM scheme outperforms the variational integrator.

The entropy in the discrete solution increases as it should in an isolated system. A reference solution is taken to be a trajectory obtained with a very small time step size ($h = 0.005$ s). Fig. 6 a) shows that the variational integrator is closer to this reference trajectory than the EEM method. Both integrators are in accordance with the second law of thermodynamics by design.

As the VI inherently preserves momentum maps, it is supposed to perform better in the balance of momentum. For the double pendulum the angular momentum with respect to the pivot is to be preserved and indeed in Fig. 6 b) only the error of the EEM

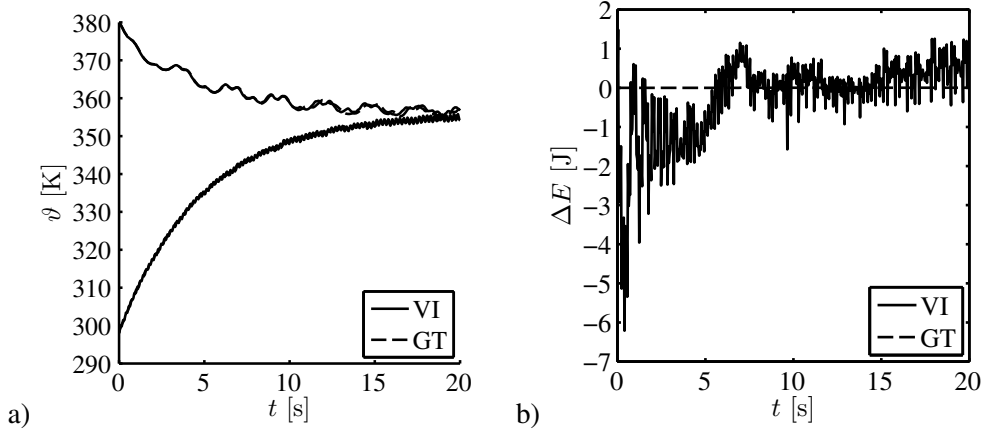


Fig. 5. Example 2: a) temperatures of spring 1 and 2 vs. time, b) energy error ($E = \text{const.} = 4 \cdot 10^5 \text{J}$) vs. time for the variational integrator (VI) and the Energy-Entropy-Momentum method (EEM-GT).

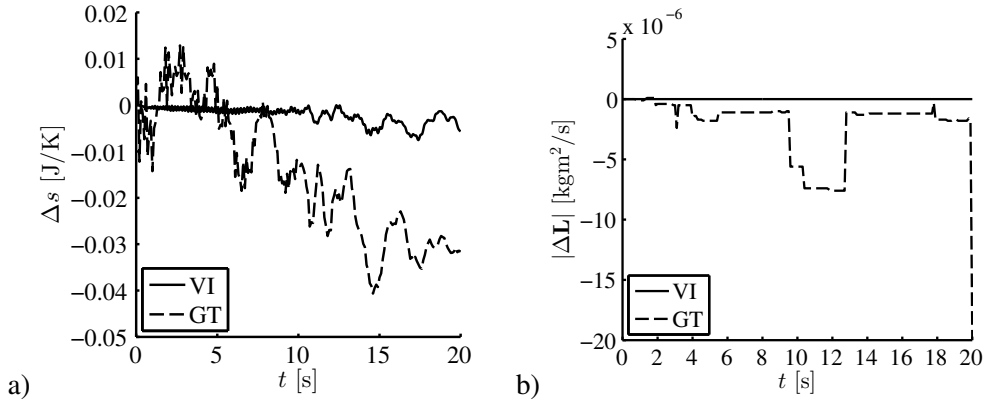


Fig. 6. Example 2: a) entropy ($s = 1183 \dots 1222 \text{J/K}$) error vs. time, b) error in angular momentum ($|\mathbf{L}| = \text{const.} = 71.6 \text{kgm}^2/\text{s}$) vs. time for the variational integrator (VI) and the Energy-Entropy-Momentum method (EEM-GT).

scheme is visible, while the variational integrator stays within Newton-tolerance. In average, the variational integrator required one Newton iteration (3-4 iterations) less then the EEM-integrator (4-5 iterations). We note that a standard solver (mid-point rule with fixed step size) would have needed a time step size of less than $h = 0.01 \text{ s}$ in order to stably integrate the motion. The relative errors for the simulations of both examples, single pendulum and double pendulum, are listed in Table 3.

Table 3. Relative errors in examples 1 and 2 computed as ratio between maximal deviation from the reference trajectory divided by the mean value of the reference trajectory

	energy	entropy	momentum
example 1: VI	$4 \cdot 10^{-4} \%$	$5 \cdot 10^{-4} \%$	$1 \cdot 10^{-14} \%$
example 1: EEM-Gs	$3 \cdot 10^{-15} \%$	$3 \cdot 10^{-3} \%$	$1 \cdot 10^{-15} \%$
example 2: VI	$1 \cdot 10^{-3} \%$	$6 \cdot 10^{-4} \%$	$7 \cdot 10^{-11} \%$
example 2: EEM-GT	$1 \cdot 10^{-12} \%$	$3 \cdot 10^{-3} \%$	$3 \cdot 10^{-5} \%$

5 SUMMARY AND OUTLOOK

Variational integrators (VI) have been extensively employed for approximating the evolution of Hamiltonian systems, leading to time integration schemes with remarkable, well-known, features. Similarly to Energy-Entropy-Momentum (EEM) methods, they demonstrate that structure preservation leads to time stepping schemes that are more robust than standard ones, especially in stiff problems. Both time discretizations, VI and EEM methods, can employ time step sizes which are too large for standard solvers, and their long term behavior is much more accurate. In comparison to EEM methods, particularly in entropy formulation, the implementation of VIs poses no restrictions on boundary conditions and parameter dependencies for the time stepping itself. However, the postprocessing still may require further numerical evaluations.

Thermo-viscoelasticity is not covered by classical Hamiltonian Mechanics. However, we have shown that viscous forces and heat transfer can be incorporated to the Hamiltonian action using D'Alembert terms. Comparison of the results for the discrete examples produced by same time steps shows the advantage of VI over EEM in momentum preservation, including entropy balance, on the one hand, and the disadvantage of worse energy conservation on the other hand. This is not surprising, since EEMs are by design energy consistent and VIs known to preserve momentum maps exactly. In addition it is observed for VI methods that they not get worse when applied to dissipative systems, i.e. when extended by the discrete D'Alembert principle, where symplecticity is lost.

As disadvantage both families of methods, VI and EEM, share the strong interlocking between physics and numerics that makes their implementations problem specific.

Further works aim at algorithmic speedup and simplification by separating and modularizing these integrators as much as possible. Yet another possible line of improvement is the development of splitting methods that separate the governing equations of the problem into implicit and explicit blocks.

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