Variational time integrators for finite dimensional thermo-elasto-dynamics without heat conduction

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SUMMARY

This paper focuses on the formulation of variational integrators (VI) for finite dimensional thermo-elastic systems without heat conduction. The dynamics of these systems happen to have a Hamiltonian structure, after thermal displacements are introduced. It is then possible to formulate integrators by taking advantage of standard methods in VI. The class of integrators we construct have some remarkable features: (a) they are symplectic, (b) they exactly conserve the entropy of the system, or in other words, they exactly satisfy the second-law of the thermodynamics for reversible adiabatic processes, (c) they nearly exactly conserve the value of the energy for very long times, and (d) they exactly conserve linear and angular momentum. We first describe how to adapt any VI for classical mechanical systems to integrate adiabatic thermo-elastic ones, and then formulate three new types of integrators. The first class, based on a generalized trapezoidal rule, gives rise to two first-order, explicit integrators, and a second-order, implicit one. By composing then the two first-order integrators we construct a second-order, explicit one. Finally, we formulate a fourth-order, implicit integrator, which is a symplectic partitioned Runge-Kutta method. The performance of these new algorithms is showcased through numerical examples. Copyright © 2000 John Wiley & Sons, Ltd.

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1. Introduction

Early approaches toward the creation of time integrators for the dynamics of deformable bodies consisted in constructing a discretization of the momentum balance equations, without

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accounting for additional structure these equations might have had; see for example Ch. 9 of [1] or Ch. 9 and 10 of [2].

Pioneering contributions in the development of the so-called *conserving schemes* are for example [3, 4], among others. Conspicuous among these are the energy-momentum algorithms by Simo et al. [5, 6], which conserve energy as well as linear and angular momentum. These have been further extended to consider mechanical problems described by partial differential equations, such as encountered in the nonlinear dynamics of solids [7], rods [8, 9], and shells [10]. The list of contributions in this area is long, with for example [11, 12, 13, 14, 15] among others.

Variational integrators constitute a more recent approach toward the creation of structure-preserving integrators. The construction of VI is rooted in the formulation of a discrete analog to Hamilton’s variational principle. These ideas were first developed in the context of integrable systems in mechanics by Veselov [16] and Moser and Veselov [17], who constructed a suitable approximation of the action integral named the discrete action sum. Stationary points of this functional are then the discrete-in-time trajectories of the mechanical system, and can be proved to approximate the exact trajectories as the time-step goes to zero. Furthermore, the resulting integrator is symplectic, and if the discrete action sum preserves the symmetries of the original mechanical system, then discrete versions of the conjugate momenta will be conserved by the discrete trajectories. This is also known as a discrete version of Noether’s theorem, see e.g. [18, 19, 20]. Finally, an appealing aspect of VI is that they display outstanding energy behavior without explicitly enforcing it. More precisely, the energy of the discrete trajectories remains close to its initial value for very long times, provided the time step is small enough, see e.g. [21, 22].

A thorough account on symplectic methods can be found in [21, 22], and about the essential aspects of VI in [18]. Applications and extensions of this basic theory to different fields are numerous, such as to mechanical problems with multi-symplectic geometry [23], to the construction of asynchronous integration methods in solid mechanics and field theories [19, 20, 24, 25, 26], to problems with contact [27, 28, 29, 30], problems with oscillatory solutions [31], stochastic differential equations [32], constrained and forced problems [18], and to problems where the configuration space is a nonlinear manifold [33, 34, 35], among many others.

As noted in [36], VI and energy-momentum schemes have been formulated based on exploiting the underlying Hamiltonian structure of conservative problems. Some energy-momentum algorithms have been formulated for problems that do not possess this structure, such as involving plastic dissipation [37, 38] or, more recently, thermo-elastic materials with heat conduction [39]. The use of a discrete version of Lagrange-D’Alembert principle enables the extension of VI to include non-conservative generalized forces. This is advantageous in mildly dissipative systems, since by adopting a VI integrator for the conservative part very little numerical dissipation is included, and hence accurate solutions at relatively large time steps are recovered, see [39]. However, when non-conservative forces play a dominant role in the dynamics of the system, the use of Lagrange-d’Alembert principle does not seem to offer any particular advantages.

The formulation of time integrators for thermo-mechanical systems presents a unique set of requirements over purely mechanical systems. Of course, conserved quantities associated to symmetries of the system should be respected, but what makes integrators for thermo-mechanical systems special is whether the computed trajectories satisfy the first
(energy conservation) and second (non-decreasing entropy of an isolated system) laws of thermodynamics. More precisely, for an isolated system the energy of the system should remain constant, and the entropy of the system should not decrease. If additionally the system is adiabatic (no heat conduction) then the entropy should remain constant. Integrators whose trajectories satisfy this property are sometimes said to be thermodynamically consistent.

Thermo-elastic systems are likely the simplest thermo-mechanical systems. They are also relevant systems for some applications. This is why these are the systems of choice towards testing ideas for the formulation of thermodynamically consistent integrators, see e.g. [36, 40, 41, 42, 43]. Of course, a crucial difficulty is that thermo-elastic systems with an arbitrary constitutive behavior for heat conduction do not posses a Hamiltonian structure. In particular, and crucially, when Fourier’s law of heat conduction is adopted the resulting evolution equations do not derive from an autonomous Lagrangian (or equivalently, an autonomous Hamiltonian). Alternative variational principles other than a Hamiltonian structure have been proposed instead, e.g., [44, 45, 46, 47, 48, 49, 50].

A particularly appealing formulation of thermo-elasticity is obtained by introducing the concept of thermacy, or thermal displacements, created apparently early in the last century and extensively discussed by Maugin [51, 52, 53] and Green and Naghdi [54, 55, 56, 57]. In this formulation the thermal displacements are analogs to the mechanical displacements. Similarly, the temperatures, as the time derivatives of the thermal displacements, are analogs to the velocities. Furthermore, the entropy is the conjugate momentum to the temperature, inasmuch the linear momentum is the conjugate momentum to the velocities. For adiabatic thermo-elasticity, i.e., no heat conduction, the introduction of the thermal displacements unveils a Hamiltonian structure for the evolution equations. The Hamiltonian structure can be still conserved by considering a different type of heat conduction, which depends on the gradient of the thermal displacements rather than the temperature, analog to the dependence of the stress on the gradient of the displacements or strains [52, 54]. Of course, such structure is lost when classical Fourier’s heat conduction is considered, as mentioned earlier.

A number of different integration algorithms have been proposed for thermo-elastic systems, see [58, 59, 60, 61, 62, 63, 64, 65, 66] to name a few. Closely related to the discussion in this paper are the integration algorithms by Romero [36, 67]. These are energy-momentum methods that are thermodynamically consistent even with heat conduction. Notably, this contribution suggests that energy-momentum algorithms can be adapted to a more general class of systems other than those with a Hamiltonian structure: systems based on the so-called GENERIC formalism [68].

Time-integration algorithms for thermo-elastic systems with the Hamiltonian structure considered here have been proposed by Bargmann and Steinmann [40, 41, 42]. In [43] an incremental formulation, in part obtained with the help of an adequate discretization of Hamilton’s principle, is introduced. However, the resulting integration schemes do not preserve any type of constant of motion of the system, and no further advantage is taken of the Hamiltonian structure of the problem.

As a starting point towards the formulation of variational integrators for bodies made of thermo-elastic materials, in this paper we formulate VI for a class of finite-dimensional thermo-elastic systems. These are systems formed by point masses connected by nonlinear thermo-elastic springs. This class of systems share many features with the finite-dimensional thermo-mechanical systems obtained after introducing a finite element discretization of a body. In this paper we restrict our attention to the adiabatic case in which there is no heat conduction.
The introduction of the special heat conduction formulated by Green and Naghdi \cite{54} is rather simple, and we shall discuss it elsewhere. The methodology to include Fourier’s heat conduction is, however, less clear.

The formulation of VI is made possible by taking advantage of the Hamiltonian structure unveiled by the introduction of the thermal displacements. We review the basic aspects of this theory in \S\textsuperscript{2} and show examples of the type of thermo-elastic systems under consideration in \S\textsuperscript{3}. We see, for example, that in the absence of heat conduction the constancy of the entropy of each spring is a consequence of the symmetry of the system upon rigid translations of each one of the thermal displacements. We therefore identify that, for adiabatic evolutions, the Lagrangian of classical mechanics is the Lagrangian resulting from a Routh reduction of this symmetry \S\textsuperscript{2,3}.2.

We construct the integrators by utilizing the tools and results available from the theory of variational integrators, which we review in \S\textsuperscript{4,4}. The remarkable aspects of the resulting integrators are:

1. The algorithms are symplectic in an extended phase space that now includes the thermal displacements and the entropies.
2. The discrete Euler-Lagrange equations are discrete analogs to Newton’s second-law and, most importantly in this context, the second-law of thermodynamics for reversible adiabatic evolutions of the system. Therefore, the constancy of the entropy of each spring is strongly imposed as one of the equations that define the algorithm. This has to be contrasted to other possible ways to define the discrete thermodynamic evolution of the system, such as by imposing the conservation of energy or first law of thermodynamics.
3. The energy of the system is nearly exactly conserved for very long times, as it is the case with variational integrators for classical mechanics. Consequently, the first law of thermodynamics is satisfied without explicitly imposing it, only as a consequence of the symplecticity of the integrators.
4. The discrete trajectories exactly conserve the momenta conjugate to the symmetries of the system, such as linear and angular momentum, and in this case, the entropy of each spring as well.

We construct three classes of time integrators. However, before that, we describe how to adapt variational integrators for classical mechanical systems to thermo-elastic ones without heat conduction. This procedure is based on the reduced Lagrangian obtained from the translational symmetry of the thermal displacements, see \S\textsuperscript{4.2}. In this case, if the initial value of the entropy of each spring is adopted as a parameter, then the a Lagrangian for a classical mechanical system is recovered. Therefore, any standard variational integrator for classical mechanics can be utilized to integrate its trajectories. As an example, we reproduce the central differences or Newmark’s second-order explicit discrete Lagrangian, but others such as Asynchronous Variational Integrators \cite{20} function equally well. The distinguishing aspects of these integrators are that they heavily rely on the fact that the entropy is constant for their formulation, and that no approximation of the temperature or thermal displacements is needed. The temperature is computed a posteriori given the discrete mechanical displacements and the parametric values for the entropies of the springs.

The new integrators we construct are instead based on the thermo-elastic Lagrangian. In \S\textsuperscript{4.3,1} we formulate integrators through a generalized trapezoidal rule, the most elementary type of variational time integrator. Among the integrators in this class there is one that
is second-order but implicit, and two that are first-order and explicit, identified as the two
variants of symplectic Euler applied to this system [69]. In a purely mechanical problem the
second-order integrator would be explicit as well. However, a crucial difference in the thermo-
elastic setting is that in general the Lagrangian does not depend quadratically on the thermal
velocities (or temperatures), as it does in classical mechanics. Consequently, the formulation
of a second-order explicit integrator is not so straightforward. To address this issue, in [114] we
turn instead to the standard procedure in time integration of elevating the order of an algorithm
through composition, see e.g. [22]. By composing the two first-order, explicit algorithms we
obtain a second-order, explicit algorithm. The composition algorithm happens to be a non-
trivial rephrasing in terms of the thermal displacements of Newmark’s explicit second-order
algorithm adapted to adiabatic thermo-elastic systems, as described above. Consequently, the
composition provides a way to obtain this last algorithm directly from the thermo-elastic
Lagrangian, instead of resorting to a priori prescribing that the entropy is constant.

Along the way (§4.3.2), we construct a fourth-order implicit integrator by making use of
piecewise quadratic polynomials to describe the mechanical and thermal trajectories in time.
This is also a symplectic partitioned Runge-Kutta method, see [18].

2. Lagrangian and Hamiltonian formulations

2.1. Description of the systems

We consider the dynamics of systems formed by a spatial arrangement of \( N \) masses connected
by \( M \) thermo-elastic springs, such as those shown in Fig. 1. Despite their simplicity, these systems retain important features of continuum mechanics systems, such as geometric
nonlinearities and coupled thermo-elasticity in finite dimensions.

Following some of the ideas in [52], it is possible to obtain the dynamics of these systems from Hamilton’s principle. This formulation relies crucially on the introduction of the so-called thermal displacements of the system. These thermal displacements play the role of
the mechanical displacements but on the thermal evolution of the system. The temperatures
of each one of the springs are recovered as the thermal velocities, or the time derivatives of the
thermal displacements. We introduce these concepts next.

The spatial position of the masses at time \( t \) is described by means of the generalized

Figure 1. (a) Triple thermo-elastic pendulum. (b) Spatial net.
displacements
\[ \mathbf{q}(t) = (q^1(t), \ldots, q^P(t)) \in \mathcal{Q}, \tag{1} \]
where \( \mathcal{Q} \) is the mechanical configuration manifold. The generalized velocities follow as \( \mathbf{v} = \dot{\mathbf{q}} \), and \( (\mathbf{q}, \dot{\mathbf{q}}) \in T\mathcal{Q} \). Additionally, each thermo-elastic spring is assigned a thermal displacement \( \Phi^i \in \mathbb{R} \) such that, for any time evolution \( \Phi^i(t) \), the empirical temperatures \( \theta^i(t) \) follow as
\[ \theta^i = \frac{d\Phi^i}{dt}, \quad i \in \{1, \ldots, M\}. \tag{2} \]
We denote all thermal displacements and (empirical) temperatures of the system by
\[ \Phi = (\Phi^1, \ldots, \Phi^M) \quad \text{and} \quad \theta := (\theta^1, \ldots, \theta^M), \tag{3} \]
where \( \Phi \in \mathbb{R}^M \) and \( (\Phi, \theta) \in T\mathbb{R}^M \). The configuration of the system is fully specified as a point \( (\mathbf{q}, \Phi) \in \mathcal{G} := \mathcal{Q} \times \mathbb{R}^M \), the configuration manifold of the system. Similarly, points in state space are given by \( (\mathbf{q}, \Phi, \dot{\mathbf{q}}, \theta) \in T\mathcal{G} := T\mathcal{Q} \times T\mathbb{R}^M \).

The thermo-elastic behavior of each spring is assumed to be described by a Helmholtz free-energy function
\[ A_i(\mathbf{q}, \theta^i), \quad i \in \{1, \ldots, M\}, \]
so that the Helmholtz free energy of the system \( A : T\mathcal{G} \rightarrow \mathbb{R} \) follows as
\[ A(\mathbf{q}, \theta) = \sum_{i=1}^M A_i(\mathbf{q}, \theta^i). \tag{4} \]
For simplicity, we shall henceforth assume that for each value of the mechanical displacements \( \mathbf{q} \) the function \( A(\mathbf{q}, \cdot) \) is convex. Of course, this precludes important phenomena such as some phase transitions, but additional care should be exercised to analyze algorithms in that case.

2.2. Lagrangian formulation

We now obtain the equations of motion of the system from Hamilton’s principle. To this end, the Lagrangian of the system, \( L : T\mathcal{G} \rightarrow \mathbb{R} \) is constructed as
\[ L(\mathbf{q}, \dot{\mathbf{q}}, \Phi, \theta) = K(\mathbf{q}, \dot{\mathbf{q}}) - A(\mathbf{q}, \theta), \tag{5} \]
where the kinetic energy \( K : T\mathcal{G} \rightarrow \mathbb{R} \) is given by
\[ K(\mathbf{q}, \dot{\mathbf{q}}) = \frac{1}{2} \dot{\mathbf{q}} \cdot \mathbf{m}(\mathbf{q}) \dot{\mathbf{q}}. \tag{6} \]
Here \( \mathbf{m}(\mathbf{q}) \) is the symmetric and positive definite mass matrix of the system, which in generalized coordinates can be configuration-dependent.

Once the Lagrangian has been defined, the equations of motion of the system follow as the Euler-Lagrange equations of Hamilton’s principle. Even though this is standard, we include the derivation below for completeness.

We consider the set \( \mathcal{C} \) of all (smooth enough) trajectories \( (\mathbf{q}(\cdot), \Phi(\cdot)) : [t_a, t_b] \rightarrow \mathcal{G} \) of the system, as well as the action \( \mathcal{S} : \mathcal{C} \rightarrow \mathbb{R} \)
\[ \mathcal{S}[\mathbf{q}(\cdot), \Phi(\cdot)] = \int_{t_a}^{t_b} L(\mathbf{q}, \dot{\mathbf{q}}, \Phi, \theta) dt. \tag{7} \]
Hamilton’s principle states that the trajectory of the system is a stationary point of the action under all variations in \( C \) that leave the end-points of the trajectory fixed, i.e.,
\[
\delta q(t_a) = \delta q(t_b) = 0 \quad \text{and} \quad \delta \Phi(t_a) = \delta \Phi(t_b) = 0.
\]
The trajectory \((q(\cdot), \Phi(\cdot))\) should then satisfy the Euler-Lagrange equations
\[
\frac{\partial L}{\partial q^I} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^I} \right) = 0, \quad I \in \{1, \ldots, P\},
\]
(8a)
\[
\frac{\partial L}{\partial \Phi^i} - \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{\Phi}^i} \right) = 0, \quad i \in \{1, \ldots, M\}.
\]
(8b)

Particularizing the above equations for the Lagrangian (5) gives the following Euler-Lagrange equations:
\[
\frac{d}{dt} (m \ddot{q}) = \frac{1}{2} (\nabla_q m) : \dot{q} \otimes \dot{q} - \nabla_q A = \nabla_q L,
\]
(9a)
\[
\frac{d}{dt} (\nabla_\theta A) = 0.
\]
(9b)

To define the trajectory, these equations need to be supplemented with appropriate boundary conditions: (i) \( q(t_a) = q_a \), (ii) \( \Phi(t_a) = \Phi_a \), (iii) \( \dot{q}(t_a) = v_a \) and (iv) \( \theta(t_a) = \theta_a \).

Several remarks are appropriate:

i. Equation (9a) is the statement of Newton’s second law for a thermo-elastic system. In this case the Helmholtz free energy function is the potential for the thermo-elastic forces acting on the system, i.e.,
\[
f = -\nabla_q A(q, \theta).
\]
(10)

ii. A classical result from thermodynamics (e.g., [70]) identifies the Helmholtz free energy function as a potential for the vector of entropies as well, i.e.,
\[
\eta(q, \theta) = -\nabla_\theta A(q, \theta).
\]
(11)

Therefore, the Euler-Lagrange equation (9b) implies that the entropy of each spring stays constant in time. In other words, the invariance of the entropy in each spring is obtained as a stationarity condition for the action. The total entropy of the system is obtained as
\[
\eta^t = \sum_{i=1}^{M} \eta_i.
\]

iii. Given \( \eta \) and \( q \), it is possible to solve (11) for the vector of temperatures of the system.

We denote the resulting function with \( \dot{\theta}(q, \eta) \). Therefore, if the vector of entropies of the system at time \( t_a \) is \( \eta_0 \), the temperatures of the spring at any time \( t \) are computed as
\[
\theta(t) = \dot{\theta}(q(t), \eta_0).
\]
(12)

The function \( \dot{\theta} \) is well-defined due to the assumed convexity of \( A \) with respect to \( \theta \).

iv. Equation (9b) is the statement of the second law of thermodynamics for reversible, adiabatic evolutions.

v. Additionally, if the coordinates \( q \) are such that the resulting mass matrix is configuration independent, Eqs. (9a) and (9b) reduce to
\[
m \ddot{q} = -\nabla_q A,
\]
\[
\dot{\eta} = 0.
\]

2.3. Hamiltonian formulation

Alternatively, it is possible to work directly with the Hamiltonian point of view of the problem. The Hamiltonian $H : T^*G \to \mathbb{R}$ follows as the Legendre transform of the Lagrangian in the velocity and temperature variables, namely,

$$H(q, p, \Phi, \eta) = \inf_{\dot{q}, \dot{\theta}} \{ p \cdot \dot{q} + \eta \cdot \dot{\theta} - L(q, \dot{q}, \Phi, \theta) \};$$

and carrying out the minimization yields the following definition of the mechanical and thermal momenta:

$$p = \nabla_q L = m \dot{q},$$

$$\eta = \nabla_\theta L = -\nabla_\theta A.$$  

Notice that the thermal momentum coincides with the constitutive entropy (see (11)) and therefore, the use of the concept of thermal displacements establishes a complete analogy between the mechanical and thermal parts of the problem, as summarized in Table I. The phase space $T^*G$ has then coordinates $(q, \Phi, p, \eta)$.

<table>
<thead>
<tr>
<th>Mechanical</th>
<th>q</th>
<th>q</th>
<th>p</th>
</tr>
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<tbody>
<tr>
<td>Thermal</td>
<td>\Phi</td>
<td>\theta</td>
<td>\eta</td>
</tr>
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</table>

The Hamiltonian can be compactly written after introducing the internal energy $U(q, \eta)$, i.e., the Legendre transform of the Helmholtz free energy with respect to the vector of temperatures

$$A(q, \dot{q}(q, \eta)) + \eta \cdot \dot{\theta}(q, \eta) = U(q, \eta) = \sum_{i=1}^{M} U_i(q, \eta_i),$$

where $U_i = A_i + \eta_i \theta_i, i \in \{1, \ldots, M\}$ is the internal energy of each spring. The internal energy then constitutes a potential for the internal forces and the temperatures, namely,

$$f = -\nabla_q U(q, \eta), \quad \theta = \nabla_\eta U(q, \eta) = \dot{\theta}(q, \eta).$$

The Hamiltonian can then be explicitly written as

$$H(q, p, \Phi, \eta) = K(q, p) + U(q, \eta),$$

and Hamilton’s equations of motion become

$$\dot{q} = \nabla_p H(q, p, \Phi, \eta) = m^{-1} p,$$

$$\dot{\Phi} = \nabla_\eta H(q, p, \Phi, \eta) = \nabla_\eta U(q, \eta),$$

$$\dot{p} = -\nabla_q H(q, p, \Phi, \eta) = -\nabla_q (K(q, p) + U(q, \eta)),$$

$$\dot{\eta} = -\nabla_\Phi H(q, p, \Phi, \eta) = 0.$$

These equations are equivalent to the Euler-Lagrange equations (9a)-(9b).

Finally, if we denote a point in $T^*G$ with $z \equiv (q, \Phi, p, \eta)$, then it is possible to rewrite these equations in canonical form as

$$\dot{z} = J \nabla_z H(z),$$

where $J$ is the canonical symplectic matrix $[71]$.
2.3.1. Conservation properties. Due to the fact that the problem possesses a Hamiltonian structure, a number of conserved quantities can be identified.

(i) Energy conservation.
The Hamiltonian, or the total energy, is constant throughout any trajectory of the system, satisfying in this way the first law of thermodynamics. This can be seen as either a consequence of the time-translation symmetry of the system, or by directly computing the time derivative of H along solution trajectories:

\[
\dot{H} = \nabla_z H(z) \cdot \dot{z} = \nabla_z H(z) \cdot J \nabla_z H(z) = 0, \quad (20)
\]

since J is skew-symmetric.

(ii) Symplecticity of the flow.
Hamiltonian systems generate flows in \( T^*G \) that are symplectic, i.e., for each time \( t \) the map \((q(0), p(0), \Phi(0), \theta(0)) \mapsto (q(t), p(t), \Phi(t), \eta(t)) \) is symplectic, so it preserves area elements in \( T^*G \) (see [22] pp. 184–185, and [19]). In this case the canonical symplectic form preserved by the flow is

\[
\Omega = dq^I \wedge dp_I + d\Phi^i \wedge d\eta_i, \quad (21)
\]

where repeated indices in the same term indicate sum over all mechanical or thermal coordinates.

(iii) Symmetries: conservation of total linear and angular momentum.
Noether’s theorem states that each symmetry of the Lagrangian leads to a conjugate conserved momentum. In particular, the invariance of the Lagrangian under the action of rigid displacements or rigid rotations in space lead to the conservation of the linear or angular momenta of the system, respectively.

(iv) Conservation of each spring’s entropy.
In addition to the possible symmetries upon the action of rigid body motions, the Lagrangian in (5) is also symmetric under translations of each thermal displacement. The conjugate conserved momentum is the entropy of each spring. We expand on this next.

Clearly the conservation of the entropy of each spring along trajectories is a direct consequence of the Euler-Lagrange equation (9b). To see this as a symmetry of the Lagrangian (5), we note that

\[
\frac{d}{de} L(q, \dot{q}, \Phi + e, \theta) = \frac{\partial L}{\partial \Phi^i} = 0.
\]

Thus it follows from (8b) that

\[
\frac{d}{dt} \frac{\partial L}{\partial \Phi^i} = \dot{\eta}_i = 0, \quad i \in \{1, \ldots, M\}.
\]
2.3.2. The simplest entropy-conserving Lagrangian. Taking into account that Eq. (9b) ensures entropy conservation, it is possible to write a Lagrangian $L^\eta : TQ \to \mathbb{R}$ expressed in terms of $\eta_0$ regarded as a vector of constant parameters i.e.

$$L^{\eta_0}(q, \dot{q}) := K(q, \dot{q}) - U^{\eta_0}(q),$$

where

$$U^{\eta_0}(q) = U(q; \eta_0) = \sum_{k=1}^{M} U_k(q; \eta_0 k).$$

Alternatively, $L^{\eta_0}$ can be seen as the Lagrangian obtained after a Routh reduction of the symmetry on $\Phi$.

Eq. (24) implies that neither $\Phi$ nor $\theta$ play an essential role in the dynamics, and the temperature in each thermo-elastic spring is obtained from (16). The Euler-Lagrange equations of the reduced system are

$$\frac{d}{dt}(m\dot{q}) - \frac{1}{2}(\nabla_q m) : \dot{q} \otimes \dot{q} = -\nabla_q U^{\eta_0},$$

as expected.

3. Examples

We next give two simple examples of the thermo-elastic systems under consideration.

3.1. Thermo-Elastic pendulum

Let $(r, \varphi)$ be the polar coordinates describing the kinematics of the thermo-elastic pendulum shown in Fig. 2. Additionally, the system has associated a thermal displacement $\Phi$. The corresponding kinetic energy is $K = \frac{1}{2}m(\dot{r}^2 + (r\dot{\varphi})^2)$ while the Helmholtz free energy of the spring is assumed to be

$$A(r, \theta) = \frac{E}{2r_0}(r - r_0)^2 - \beta(\theta - \theta_0)(r - r_0) - \frac{C_0}{2\theta_0}(\theta - \theta_0)^2 - (\theta - \theta_0)\eta_0,$$

where $\theta$ and $\theta_0$ are the current and reference temperature, $\eta_0$ is a reference entropy, $r_0$ is a reference length, $E$ is the elastic modulus, $C_0$ a specific heat and $\beta$ is a parameter coupling the thermal and mechanical behaviors. Therefore, from (10), (11) and (15) the following relations

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are obtained:

\[ f_r = -\frac{\partial A}{\partial r} = -\frac{E}{r_0}(r - r_0) + \beta(\theta - \theta_0), \]  

(27a)

\[ \eta = -\frac{\partial A}{\partial \theta} = \frac{C_0}{\theta_0}(\theta - \theta_0) + \beta(r - r_0) + \eta_0, \]  

(27b)

\[ \theta = \hat{\theta}(r, \eta) = \frac{\theta_0}{C_0}(\eta - \eta_0 - \beta(r - r_0)) + \theta_0, \]  

(27c)

\[ U(r, \eta) = \frac{E}{2r_0}(r - r_0)^2 + \frac{\theta_0}{2C_0}(\eta - \eta_0 - \beta(r - r_0))^2 + \eta_0. \]  

(27d)

Eqs. (27a) and (27b) are the constitutive relations for the modulus of the radial force and entropy in the spring, which couple the mechanical and thermal parts. Eq. (27c) is the inverse of (27b) for each \( r \) and determine the temperature. Finally, Eq. (27d) is the internal energy.

The configuration manifold is \( G = \mathbb{R}^2 \times \mathbb{R} \), which corresponds to the position of the mass and the thermal displacement. The E-L equations (9a) and (9b) become

\[ \ddot{r} - r\dot{\varphi}^2 + \frac{E}{m r_0}(r - r_0) - \frac{\beta}{m}(\theta - \theta_0) = 0, \]  

(28a)

\[ \dot{\varphi} = \frac{p_{\varphi}}{m r^2}, \]  

(28b)

\[ \dot{\theta} = \frac{C_0}{\theta_0} \dot{\eta} + \dot{\beta} = 0, \]  

(28c)

which have to be complemented with appropriate initial conditions. The second and third equations are statements of the conservation of the angular momentum and entropy, respectively.

The corresponding conjugate momenta are \( p_r = m\dot{r} \), \( p_\varphi = m r^2 \dot{\varphi} \) and \( \eta \) in (27d). The Hamiltonian function is given by

\[ H = \frac{1}{2m}(p_r^2 + \frac{p_{\varphi}^2}{r^2}) + U(r, \eta), \]  

(29)

and then the balance equations in Hamiltonian form are obtained as

\[ \dot{r} = \frac{\partial H}{\partial p_r} = \frac{p_r}{m}, \]  

\[ \dot{\varphi} = \frac{\partial H}{\partial p_\varphi} = \frac{p_\varphi}{m r^2}, \]  

\[ \dot{\theta} = \frac{\partial H}{\partial \eta} = \theta, \]  

(30a)

\[ \dot{p}_r = -\frac{\partial H}{\partial r} = \frac{p_{\varphi}^2}{m r^3} + f_r, \]  

\[ \dot{p}_\varphi = \frac{\partial H}{\partial r} = 0, \]  

\[ \dot{\eta} = \frac{\partial H}{\partial \Phi} = 0. \]  

(30b)

Eqs. (30b) and (30b) are the conserved quantities associated to the invariance of the Lagrangian with respect to rigid body rotations in the plane and rigid body thermal displacements.

### 3.2. Chain of \( N \) masses

The next example consists of a chain of \( N \) masses connected in series by means of thermo-elastic springs, sketched in Fig. 3.

In the following \( \mathbf{q}_i^j \in \mathbb{R}^3 \) denotes the position of mass \( i \), and by convention, \( \mathbf{q}_0^0 \) is a fixed point in \( \mathbb{R}^3 \). Each spring has a thermal displacement \( \Phi^i \) and empirical temperature \( \theta^i \). The
Figure 3. Chain of \( N \) masses connected in series by means of thermo-elastic springs.

position vector, the vector of thermal displacements and the vector of temperatures of the system are denoted by

\[
\mathbf{q} = (q^1, ..., q^N) \in \mathbb{R}^{3N}, \quad \mathbf{Φ} = (\Phi^1, ..., \Phi^N) \in \mathbb{R}^N \quad \text{and} \quad \mathbf{θ} = (\theta^1, ..., \theta^N) \in \mathbb{R}^N,
\]

respectively. The configuration manifold is \( G \equiv \mathbb{R}^{(3+1)N} \) and the Helmholtz free energy of each spring is assumed to be

\[
F(l, \theta) = \frac{c}{2} \ln \left( \frac{l}{l_0} \right) - \beta(\theta - \theta_0) \ln \left( \frac{l}{l_0} \right) + C_0 \left( \theta - \theta_0 - \theta \ln \left( \frac{l}{\theta_0} \right) \right), \tag{31}
\]

where \( l/l_0 \) is the quotient between the length of the spring and a reference length \( l_0 \), \( c \) and \( \theta_0 \) are an elastic constant and a reference temperature, \( \beta \) is a thermo-mechanical coupling parameter and \( C_0 \) is the heat capacity.

Then, the following relations are obtained:

\[
\begin{align*}
& f_l = -\frac{\partial F}{\partial l} = -\frac{c}{l} \ln(l/l_0) + \frac{\beta}{l} (\theta - \theta_0), \quad (32a) \\
& \eta = -\frac{\partial F}{\partial \theta} = \beta \ln(l/l_0) + C_0 \ln(\theta/\theta_0), \quad (32b) \\
& \theta = \theta_0 \exp \left[ \frac{\eta - \beta \ln(l/l_0)}{C_0} \right], \quad (32c) \\
& U(l, \eta) = \frac{c}{2} \ln^2(l/l_0) + \beta \theta_0 \ln(l/l_0) + C_0 \theta_0 \left( \exp \left[ C_0^{-1} \left( \eta - \beta \ln(l/l_0) \right) \right] - 1 \right). \quad (32d)
\end{align*}
\]

In this way, the Helmholtz free energy, internal energy and entropy of the system are

\[
A(\mathbf{q}, \mathbf{θ}) = \sum_{i=1}^{N} F(l_i, \theta^i), \quad U(\mathbf{q}, \mathbf{η}) = \sum_{i=1}^{N} U(l_i, \eta^i) \quad \eta^i = \sum_{i=1}^{N} \eta_i,
\]

where \( l_j = \| \mathbf{q}^j - \mathbf{q}^{j-1} \|, \quad j = 1, ..., N \). Here \( \| \cdot \| \) is the Euclidean norm in \( \mathbb{R}^3 \).

The kinetic energy \( K : T\mathcal{Q} \to \mathbb{R} \) is given by

\[
K(\mathbf{q}) = \frac{1}{2} \sum_{j=1}^{N} m_j \mathbf{q}^j \cdot \mathbf{q}^j, \tag{33}
\]
and the Lagrangian follows as

\[ L(q, \dot{q}, \Phi, \theta) = K(\dot{q}) - A(q, \theta) = \sum_{j=1}^{N} \left[ \frac{1}{2} m_j \dot{q}_j \cdot \dot{q}_j - F(l_j, \theta^j) \right]. \]  

(34)

The Euler-Lagrange equations for each spring and mass of the system are

\[ m_j \ddot{q}_j = -\nabla_{q_j} A, \]  

(35a)

\[ \dot{\eta}_j = 0, \]  

(35b)

for \( j \in \{1, ..., N\} \), which have to be supplemented with adequate initial conditions on the mechanical displacements, velocities and temperatures.

4. Variational integrators

Variational integrators provide a methodology for constructing integrators which automatically have a number of properties: (i) they are symplectic, (ii) they exactly preserve the momenta associated to symmetries, (iii) and they have excellent longtime energy behavior (see [19, 20, 22, 39]). In this section we begin by reviewing the method, and then use it to construct integrators in two ways: (i) by adapting integrators for classical mechanical systems to thermoelastic ones in the absence of heat conduction, and (ii) by directly constructing variational integrators for the thermo-elastic Lagrangian [15]. In the first case, as an example we adapt Newmark’s explicit second–order algorithm. In the second case, a polynomial interpolation of the mechanical and thermal displacements is combined with Lobatto quadrature rules to construct discrete Lagrangians. The resulting numerical maps correspond to the standard Lobatto IIIA-IIIB symplectic partitioned Runge-Kutta methods, as explained in §3.6.6 of [18]. Finally, we utilize composition to elevate the order of two first-order, explicit variational integrators into a second-order, explicit one, and find that we recover the adapted Newmark’s explicit second-order algorithm. For simplicity, throughout this section we assume that the mass is independent of the configuration.

4.1. Summary of the method

We begin by partitioning the time interval of interest \([t_a, t_b]\) into equally spaced time intervals of length \(h = (t_b - t_a)/N_t\), and set \( t^k = t_a + kh \) for \( k = 0, \ldots, N_t \). In the following, we use \([\cdot]^k\) to denote the numerical approximation to the time varying quantity \([\cdot]\) evaluated at \( t^k \).

The method is based on constructing a discrete Lagrangian \( L_d \), which approximates the action integral over the time interval \([t^k, t^{k+1}]\) as

\[ L_d(z^k, z^{k+1}) \approx \int_{t^k}^{t^{k+1}} L(z(t), \dot{z}(t)) dt, \]  

(36)

where \( z(t) : [t^k, t^{k+1}] \rightarrow G \) is the solution of the Euler-Lagrange equations satisfying \( z(t^k) = z^k \) and \( z(t^{k+1}) = z^{k+1} \), in a sense made precise in [18]. The discrete Lagrangian then leads to the construction of the discrete action sum

\[ S_d(z^0, ..., z^{N_t}) = \sum_{k=0}^{N_t-1} L_d(z^k, z^{k+1}). \]  

(37)
The integrator then follows from a discrete version of Hamilton’s principle, namely the variation of the action sum $\delta S_d$ should be equal to zero among all variations of $z^1, \ldots, z^{N_t - 1}$. The stationarity conditions, or discrete Euler-Lagrange (DEL) equations, are then

$$D_2 L_d(z^{k-1}, z^k) + D_1 L_d(z^k, z^{k+1}) = 0, \quad k \in \{1, \ldots, (N_t - 1)\},$$

where $D_1 L_d$ denotes the partial derivative of $L_d$ with respect the $i$th slot. The momentum of the system $\Pi$ is defined by

$$\Pi^k = -D_1 L_d(z^k, z^{k+1}),$$

for $k = 0, 1, \ldots, N_t - 1$, from where the DEL equations can be equivalently expressed as

$$\Pi^{k+1} = D_2 L_d(z^k, z^{k+1}),$$

for $k = 0, 1, \ldots, N_t - 1$. Equations (39) and (40) constitute what is called the position-momentum form of the algorithm. They define a map $(z^k, \Pi^k) \mapsto (z^{k+1}, \Pi^{k+1})$, which constitutes the integrator. The method consist in solving (39) for $z^{k+1}$, and then replacing it in Eq. (40) to obtain $\Pi^{k+1}$.

The integrator is initialized by setting $(z^0, \Pi^0) = (z(t^0), \Pi(t^0))$. If only the initial velocity $\dot{z}(t^0)$ is known instead, then $\Pi^0$ is computed from

$$\Pi^0 = \nabla_z L(z(t^0), \dot{z}(t^0)).$$

A convergence result on variational integrators in [18] roughly states that if the approximation of the action in (36) is of order $h^{r+1}$, $r > 1$, and some standard smoothness conditions on $L$ are satisfied, then $z^{T/h} \to z(T)$ and $\Pi^{T/h} \to \Pi(T)$ as $h \to 0$ with an error that decays at least as $h^r$. Therefore, higher-order approximations in (36) result in correspondingly higher-order integrators.

### 4.2. Classical mechanics integrators for thermo-elastic systems without heat conduction

Perhaps the simplest strategy for the construction of time-integrators for adiabatic thermo-elastic systems is to use the reduced Lagrangian [24]. Due to the fact that in this case the Lagrangian is parametrized in terms of the entropies of the springs, the constancy of each spring’s entropy is automatically satisfied.

Since for each value of $\eta$ the reduced Lagrangian is that of a classical mechanical system, the mechanical displacements can be approximated by any variational integrator for classical mechanics. The approximate temperatures are computed a posteriori, once the approximate displacements are known.

We illustrate these ideas with the adaptation of the central differences or Newmark’s explicit second-order algorithm to this setting. The discrete Lagrangian is:

$$L_{d}^{\eta_0}(q^0, q^1) = h \left[ K_d(q^0, q^1) - \frac{1}{2} U^{\eta_0}(q^0) - \frac{1}{2} U^{\eta_0}(q^1) \right],$$

where

$$K_d(q^0, q^1) = \frac{1}{2} \left( \frac{q^1 - q^0}{h} \right) \cdot m \left( \frac{q^1 - q^0}{h} \right).$$

The DEL equations (38) are then

$$\frac{m}{h^2}(q^{k+1} - 2q^k + q^{k-1}) = \nabla_q U^{\eta_0}(q^k), \quad k \in \{1, \ldots, N_t - 1\},$$

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which, as mentioned earlier, correspond to the central difference approach for finite dimensional mechanical problems.

The position-momentum form of the algorithm given by (39) and (40), which defines the conjugate momenta, follows as

\[ p_k = m \left( q_{k+1} - q_k \right) - \frac{1}{2} h \nabla_q U_{\eta_0}(q_k), \]  
\[ p_{k+1} = m \left( q_{k+1} - q_k \right) - \frac{1}{2} h \nabla_q U_{\eta_0}(q_{k+1}). \]

The algorithmic steps for each update are:

(i) Solve (44a) for \( q_{k+1} \).
(ii) Update \( p_{k+1} \) using (44b).
(iii) Compute the temperature as \( \theta_{k+1} = \nabla_\eta U(q_{k+1}, \eta_0) = \hat{\theta}(q_{k+1}, \eta_0) \).

which only adds the last step to a classical integrator.

The resulting algorithms are the trivial extension of variational integrators to adiabatic thermo-elasticity. Among other characteristics it is worth mentioning that

- It is simple to construct discrete Lagrangians so that the resulting integrators conserve linear and angular momentum, if the exact trajectories do. Additionally, all variational algorithms are symplectic and display very good long term energy behavior, with the Hamiltonian given by (17). The central differences scheme above has all of these features.
- Higher order algorithms can be easily constructed as well, see [18].
- Even when the resulting algorithms inherit these desirable characteristics, they heavily make use of the fact that \( \eta \) is constant. Consequently, it is not possible to extend them to problems including heat conduction (\( \dot{\eta}_i > 0 \)).

4.3. Variational integrators based on the thermo-elastic Lagrangian

In the following we concentrate on the formulation of variational time integrators based on the Lagrangian (5), so we discretize both mechanical and thermal displacements. A key motivation to do it is that they open a door for a future extension of these ideas to the case with heat conduction.

4.3.1. Generalized trapezoidal rule. We consider first the perhaps most commonly used discrete Lagrangians, namely, \( L_d^\alpha \) given by

\[ L_d^\alpha = \alpha L_d^0 + (1 - \alpha) L_d^1, \]  

where \( \alpha \in [0, 1] \) and

\[ L_d^0(q^0, q^1, \Phi^0, \Phi^1) = h \left[ K_d(q^0, q^1) - A \left( q^0, \frac{\Phi^1 - \Phi^0}{h} \right) \right], \]  
\[ L_d^1(q^0, q^1, \Phi^0, \Phi^1) = h \left[ K_d(q^0, q^1) - A \left( q^1, \frac{\Phi^1 - \Phi^0}{h} \right) \right]. \]
Then, the following expressions for the DEL equations are obtained:

\[
\begin{align*}
\frac{m}{h^2}(q^{k+1} - 2q^k + q^{k-1}) &= \alpha f^{k+1} + (1 - \alpha) f^k, \quad (47a) \\
\alpha \Gamma^{k+1} + (1 - \alpha) \Gamma^{(k+1)-} &= \alpha \Gamma^{(k+1)-} + (1 - \alpha) \Gamma^{k-}. \quad (47b)
\end{align*}
\]

where

\[
\begin{align*}
f^{k+} &= -\nabla_q A\left(q^k, \frac{\Phi^{k+1} - \Phi^k}{h}\right), \\
f^{k-} &= -\nabla_q A\left(q^k, \frac{\Phi^k - \Phi^{k-1}}{h}\right), \\
\Gamma^{k+} &= -\nabla_{\theta} A\left(q^k, \frac{\Phi^{k+1} - \Phi^k}{h}\right), \\
\Gamma^{k-} &= -\nabla_{\theta} A\left(q^k, \frac{\Phi^k - \Phi^{k-1}}{h}\right).
\end{align*}
\]

Equation (47a) is a discrete analog to Newton’s second law for mechanical displacements, while (47b) establishes a discrete form of entropy conservation.

The position-momentum form is

\[
\begin{align*}
p^k &= \frac{m}{h}(q^{k+1} - q^k) - ahf^{k+} \quad (48a) \\
p^{k+1} &= \frac{m}{h}(q^{k+1} - q^k) + (1 - \alpha)hf^{(k+1)-}. \quad (48b) \\
\eta^k &= \alpha \Gamma^{k+} + (1 - \alpha) \Gamma^{(k+1)-} \quad (48c) \\
\eta^{k+1} &= \alpha \Gamma^{k+} + (1 - \alpha) \Gamma^{(k+1)-}, \quad (48d)
\end{align*}
\]

where \(\eta^k\) and \(\eta^{k+1}\) are the approximations to the entropy at \(t^k\) and \(t^{k+1}\), respectively. Explicit expressions for (47a), (48a) and (48b) for the case of a configuration-dependent mass matrix are given in Appendix 7.

It follows from (47b), (48c) and (48d) that

\[
\eta^{k+1} = \eta^k, \quad (48e)
\]

which is a statement of algorithmic entropy conservation.

Different integrators are obtained for each value \(\alpha\):

1. Setting \(\alpha = 0\) or \(\alpha = 1\) yield first-order algorithms with explicit updating rules for \(q\) in (47a). The entropy equation (47b) together with (48d) reduce to

\[
\eta^k = -\nabla_{\theta} A\left(q^k, \frac{\Phi^{k+1} - \Phi^k}{h}\right), \quad (49)
\]

for \(\alpha = 0\), and to

\[
\eta^k = -\nabla_{\theta} A\left(q^k, \frac{\Phi^{k+1} - \Phi^k}{h}\right), \quad (50)
\]

for \(\alpha = 1\). These updating rules are also explicit, as we discuss later. These algorithms are sometimes called symplectic Euler.
2. If $0 < \alpha < 1$, both $q$ and $\Phi$ have to be updated by means of simultaneously solving (47a) and (47b). These are all first-order algorithms, except for the one obtained for $\alpha = 1/2$, which is second order. In this last case the entropy equation (47b) together with (48d) reduce to

$$\eta^k = -\frac{1}{2} \left[ \nabla_\theta A \left( q^k, \frac{\Phi^{k+1} - \Phi^k}{h} \right) + \nabla_\theta A \left( q^{k+1}, \frac{\Phi^{k+1} - \Phi^k}{h} \right) \right].$$

Remark. In connection with the higher-order integrators described later in §4.3.2, the integrators constructed in this section can be seen as a result of choosing continuous trajectories for $(q, \Phi)$ which restricted to $[t^k, t^{k+1}]$ are affine, together with quadrature rules with quadrature points $t^k$ and $t^{k+1}$. With this perspective, the velocity and temperature vectors are piecewise constant in each time interval, but not necessarily continuous across time interval boundaries, see Fig. 4. In fact, it is possible to define the two one-sided limits

$$\lim_{t \to t^k^+} (\dot{q}(t), \theta(t)) = (\dot{q}^{k+}, \theta^{k+}) \quad \text{and} \quad \lim_{t \to t^k^-} (\dot{q}(t), \theta(t)) = (\dot{q}^{k-}, \theta^{k-}),$$

which serve to motivate and interpret the notation $f_{\pm}$ and $\Gamma_{\pm}$ above.

Figure 4. The integrators in this section can be constructed by assuming a piecewise affine evolution of the thermal and mechanical displacements, sketched in (a), together with suitable quadrature rules. Under these conditions, the temperatures are piecewise constant, and possibly discontinuous across time-interval boundaries, as sketched in (b).

Notes on implementation. A practical way to implement the algorithm is through the position-momentum form. Each time step consists in: Given $(q, \Phi, p, \eta)^k$, $\alpha \in [0, 1]$ and $h$, find $(q, \Phi, p, \eta)^{k+1}$ such that (48a) to (48d) are satisfied up to a certain tolerance. This involves

i. Determining $q^{k+1}$ and $\Phi^{k+1}$ by solving the (implicit) relations given in (48a) and (48c). If implicit, the solution of these equations can be carried out with a Newton-Raphson method.

ii. Computing $p^{k+1}$ and $\eta^{k+1}$ by using (48b) and (48d).

iii. If of interest, compute $\theta^{k+1} = \nabla_\eta U(q^{k+1}, \eta^{k+1})$. 


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As mentioned earlier, explicit algorithms are obtained for the $\alpha = 0, 1$. We detail next the steps for the update in these cases.

**When $\alpha = 0$,** we compute

\[
\begin{align*}
q^{k+1} & = q^k + hm^{-1}p^k, \\
\Phi^{k+1} & = \Phi^k + h\nabla_\eta U(q^{k+1}, \eta^k), \\
p^{k+1} & = p^k + hf^{(k+1)} - 1, \\
\eta^{k+1} & = \eta^k.
\end{align*}
\]

which follow from (49) and (16).

By rewriting $f^{(k+1)}$ in terms of $(q^{k+1}, \eta^k)$ in (51c), we recover the classical structure of the symplectic-Euler $A$ method as presented in [21, 22, 69] and revisited in the context of VI for classical mechanics in [18]. More precisely, we have that

\[
\begin{align*}
f^{(k+1)} = -\nabla_q A \left( q^{k+1}, \frac{\Phi^{k+1} - \Phi^k}{h} \right) = -\nabla_q U(q^{k+1}, \eta^k),
\end{align*}
\]

where we have used the expression for $h^{-1}(\Phi^{k+1} - \Phi^k)$ obtained from (51f).

**When $\alpha = 1$**, we compute

\[
\begin{align*}
\Phi^{k+1} & = \Phi^k + h\nabla_\eta U(q^k, \eta^k), \\
p^{k+1} & = p^k + hf^{k+}, \\
q^{k+1} & = q^k + hm^{-1}p^{k+1}, \\
\eta^{k+1} & = \eta^k.
\end{align*}
\]

which follow from (50) and (16). Analogously, by rewriting $f^{k+}$ in (52b) in terms of $(q^k, \eta^k)$, taking advantage of the expression for $h^{-1}(\Phi^{k+1} - \Phi^k)$ obtained from (52a), it is possible to recognize the classical structure of the symplectic-Euler $B$ method [18, 21, 22, 69].

**Error analysis and convergence.** The convergence of these algorithms for $\alpha = 0, 1, 1/2$ is proved in [18, pp. 402], by computing the order of these discrete Lagrangians. Of course, some standard conditions on the smoothness of $A$ need to be satisfied. As stated earlier, when $\alpha = 0, 1$ only first order convergence is obtained, while second-order convergence happens for $\alpha = 1/2$. From the results therein, or by simply computing the consistency error, it is not hard to prove that the algorithms are first order for all other values of $\alpha$ as well.

**4.3.2. Higher-order algorithms.** The formulation of higher order variational integrators is straightforward, as detailed in [18]. This methodology is equivalent to constructing both continuous Galerkin methods in time and a family of symplectic partitioned Runge-Kutta methods (see theorem 2.6.1 and 2.6.2 in [18]). The main idea consists in considering continuous trajectories that are polynomials of a certain degree in each time interval. The discrete Lagrangian is obtained by numerically integrating its exact counterpart for each discrete trajectory. This is accomplished by selecting an appropriate set of quadrature points and weights.
More precisely, let $\mathbb{P}^K([0,h])$ be the space of polynomials of degree $K$ in $[0,h]$, and $\{t^g\}_{g=1}^n \subseteq [0,h]$ and $\{w^g\}_{g=1}^n$ be a set of quadrature points and suitable quadrature weights for polynomials of degree $K$, respectively. The class of variational integrators considered here stem from the discrete Lagrangian

$$L_d(z^0, z^1) = \inf_{z(t) \in [\mathbb{P}^K([0,h])]^{N_G}} \left[ \sum_{g=1}^{N_G} w_g L(z(t^g), z(t^g)) \right].$$

where $N_G$ is the dimension of the configuration manifold $G$.

We now formulate time integrators by adopting second degree polynomials in each time interval, so trajectories in $G$ can be written as

$$\Phi_i(t^k + \tau) = N_1(\tau)\Phi^k + N_2(\tau)\Phi^{k+\frac{1}{2}} + N_3(\tau)\Phi^{k+1},$$

$$q(t^k + \tau) = N_3(\tau)q^k + N_2(\tau)q^{k+\frac{1}{2}} + N_3(\tau)q^{k+1},$$

for each $k = 0, 1, \ldots$, where $\tau \in [0,h]$ and $N_i : [0,h] \to \mathbb{R}$, $i \in \{1, 2, 3\}$, are the set of basis functions for $\mathbb{P}^2([0,h])$ which, for convenience, satisfy $N_i(\tau_j) = \delta_{ij}$ for $\tau_j \in \{0, h/2, h\}$.

For the quadrature we chose a full Lobatto rule with weights $\{\frac{1}{3}, \frac{2}{3}, \frac{1}{3}\}$ and quadrature point coordinates $\{0, h/2, h\}$. In [53], $\{q^k, \Phi^k\} \in G$ for $k = 0, 1/2, 1, 3/2, \ldots$, which are the coefficients that define the continuous piecewise polynomial trajectory in time.

To construct the discrete Lagrangian, we first define the unoptimized discrete Lagrangian

$$L_u^d(q^0, q^\frac{1}{2}, q^1, \Phi^0, \Phi^\frac{1}{2}, \Phi^1) = \frac{h}{6}(L^0 + 4L^\frac{1}{2} + L^1),$$

where

$$L^0 = K_d(v^0) - A(q^0, \theta^0),$$

$$L^\frac{1}{2} = K_d(v^\frac{1}{2}) - A(q^\frac{1}{2}, \theta^\frac{1}{2}),$$

$$L^1 = K_d(v^1) - A(q^1, \theta^1),$$

and

$$\theta^0 = h^{-1}(4\Phi^\frac{1}{2} - 3\Phi^0 - \Phi^1), \quad \theta^\frac{1}{2} = h^{-1}(\Phi^1 - \Phi^0), \quad \theta^1 = h^{-1}(\Phi^0 - 4\Phi^\frac{1}{2} + 3\Phi^1),$$

$$v^0 = h^{-1}(4q^\frac{1}{2} - 3q^0 - q^1), \quad v^\frac{1}{2} = h^{-1}(q^1 - q^0), \quad v^1 = h^{-1}(q^0 - 4q^\frac{1}{2} + 3q^1),$$

which denote the values of the temperatures and velocities at the quadrature points $\tau = 0, h/2, h$. The discrete Lagrangian follows as

$$L_d(q^0, \Phi^0, q^1, \Phi^1) = \inf_{q^\frac{1}{2}, \Phi^\frac{1}{2}} L_u^d(q^0, q^\frac{1}{2}, q^1, \Phi^0, \Phi^\frac{1}{2}, \Phi^1).$$

The conditions for the infimum in (55) in the time interval $[t^k, t^{k+1}]$ are

$$\frac{4m}{h^2}(q^k - 2q^{k+\frac{1}{2}} + q^{k+1}) = f^{k+\frac{1}{2}},$$

$$\Gamma^{k+} - \Gamma^{(k+1)-} = 0,$$

while the discrete Euler-Lagrange equations then follow as

$$\frac{m}{h^2}(-q^{k+1} + 8q^{k+\frac{1}{2}} - 14q^k + 8q^{k-\frac{1}{2}} - q^{k-1}) = \frac{1}{2}(f^{k+} + f^{k-}),$$

$$\Gamma^{(k+1)-} - 4\Gamma^{k+\frac{1}{2}} - 3\Gamma^{k+} + 3\Gamma^{k-} + 4\Gamma^{k-\frac{1}{2}} - \Gamma^{(k-1)+} = 0,$$
where

\[ \begin{align*}
\mathbf{f}^{k+} &= -\nabla_q A(q^k, -3\Phi^k + 4\Phi^{k+\frac{1}{2}} - \Phi^{k+1}) \\
\mathbf{f}^k &= -\nabla_q A(q^k, \Phi^{k-1} - 4\Phi^{k-\frac{1}{2}} + 3\Phi^k), \\
\mathbf{f}^{k+\frac{1}{2}} &= -\nabla_q A(q^{k+\frac{1}{2}}, \Phi^{k+1} - \Phi^k), \\
\Gamma^{k+} &= -\nabla_\theta A(q^k, -3\Phi^k + 4\Phi^{k+\frac{1}{2}} - \Phi^{k+1}), \\
\Gamma^k &= -\nabla_\theta A(q^k, \Phi^{k-1} - 4\Phi^{k-\frac{1}{2}} + 3\Phi^k), \\
\Gamma^{k+\frac{1}{2}} &= -\nabla_\theta A(q^{k+\frac{1}{2}}, \Phi^{k+1} - \Phi^k).
\end{align*} \]

Together, (57a)-(57d) provide enough equations to solve for \((q^{k+\frac{1}{2}}, q^{k+1}, \Phi^{k+\frac{1}{2}}, \Phi^{k+1})\) given \((q^{k-\frac{1}{2}}, q^k, \Phi^{k-\frac{1}{2}}, \Phi^k)\). Expressions for the case of configuration dependent mass can be found in appendix 7.

The conjugate momenta are given by

\[ \begin{align*}
p^k &= \frac{m}{3h} (8q^{k+\frac{1}{2}} - 7q^k - q^{k+1}) - \frac{h}{6} \mathbf{f}^k, \\
p^{k+1} &= \frac{m}{3h} (q^k - 8q^{k+\frac{1}{2}} + 7q^{k+1}) + \frac{h}{6} \mathbf{f}^{(k+1)-}, \\
\eta^k &= \frac{3}{6} \Gamma^{k+} - \frac{1}{6} \Gamma^{(k+1)-} + \frac{4}{6} \Gamma^{k+\frac{1}{2}}, \\
\eta^{k+1} &= \frac{3}{6} \Gamma^{(k+1)-} - \frac{1}{6} \Gamma^{k+} + \frac{4}{6} \Gamma^{k+\frac{1}{2}}. 
\end{align*} \]  

Subtracting Eq. (58c) from (58d) and using (57a) it is clear that

\[ \eta^{k+1} = \eta^k, \tag{59} \]

and therefore, the numerically computed entropy is exactly conserved.

Regarding the order of convergence, for an arbitrary quadrature rule the convergence rate might only be cubic, but since this is a symmetric method (i.e., equal to its adjoint, see [22]), then the convergence rate should be even. The algorithm is fourth-order.

**Notes on implementation.** The algorithm consists in determining \((q^{k+1}, \Phi^{k+1})\), and \((p^{k+1}, \eta^{k+1})\) given \((q^k, \Phi^k)\) and \((p^k, \eta^k)\). To this end, the midpoint variables \((q^{k+\frac{1}{2}}, \Phi^{k+\frac{1}{2}})\) have to be simultaneously solved for. The solution procedure is summarized in the following two steps:

(i) Solve simultaneously (57a), (57b), (58a) and (58c) for \((q^{k+\frac{1}{2}}, \Phi^{k+\frac{1}{2}}, q^{k+1}, \Phi^{k+1})\) with, for example, a Newton-Raphson scheme.

(ii) Use (58b) and (58d) to update \(p^{k+1}\) and \(\eta^{k+1}\).
4.4. Composition methods

In previous sections we have formulated time integrators presenting second or higher accuracy order which are always implicit. The only explicit integrators we formulated so far were those in section 4.3.1 after selecting $\alpha = 0, 1$, and these are only first-order accurate. For some problems explicit algorithms exhibiting second order of accuracy are very attractive.

An alternative to formulate a second-order algorithm is by composing a first-order integrator with its adjoint, see [22, Ch. 2]. More precisely, an integrator defines a map $F_{L_d}^h : T^* G \rightarrow T^* G$, parameterized by $h$, such that $(z^{k+1}, \Pi^{k+1}) = F_{L_d}^h(z^k, \Pi^k)$. The idea then is to construct another integrator defined by the map

$$\hat{F}_h = F_{L_d}^{h/2} \circ F_{L_d}^{-h/2},$$  

(60)

where $F_{L_d}^h$ is the adjoint method to $F_{L_d}^h$. For VI the following relation [18] holds between a method and its adjoint

$$F_{L_d}^* = F_{L_d}^h,$$  

(61)

for all $z^k \equiv (q^k, \Phi^k) \in G$, $k = 0, 1$. In (62) the arguments of $L_d$ have been augmented, now including $h$ to highlight its role in the computation of the discrete Lagrangian of the adjoint method.

For the discrete Lagrangian given in (45) and the algorithms given in (51a) to (52d) the following relations are obtained

$$\left(L_d^0\right)^* = L_d^1$$ and $$\left(L_d^1\right)^* = L_d^0,$$

(63)

and taking into account (60) and (61), the following second-order maps can be constructed

$$\hat{F}_h^{01} = F_{L_d}^{(h/2)} \circ F_{L_d}^{*-h/2} = \Gamma_{L_d}^{(h/2)} \circ \Gamma_{L_d}^{-h/2},$$

$$\hat{F}_h^{10} = F_{L_d}^{(h/2)} \circ F_{L_d}^{*-h/2} = \Gamma_{L_d}^{h/2} \circ \Gamma_{L_d}^0,$$

(64)

(65)

The explicit form for the $F_{L_d}^{01}$ map is given by

$$\Phi^{k+1/2} = \Phi^k + \frac{h}{2} \nabla U(q^k, \eta^k),$$

$$p^{k+1/2} = p^k - \frac{h}{2} \nabla A(q^k, \frac{\Phi^{k+1/2} - \Phi^k}{h/2}),$$

$$q^{k+1} = q^k + h m^{-1} p^{k+1/2},$$

$$\Phi^{k+1} = \Phi^{k+1/2} + \frac{h}{2} \nabla U(q^{k+1}, \eta^k),$$

$$p^{k+1} = p^{k+1/2} - \frac{h}{2} \nabla A(q^{k+1}, \frac{\Phi^{k+1} - \Phi^{k+1/2}}{h/2}),$$

$$\eta^{k+1} = \eta^k.$$
The discrete Lagrangian for this integrator is

\[
\mathcal{L}_{01}^{01}(q^0, q^1, \Phi^0, \Phi^1) = \inf_{(q, \Phi)} \left[ \frac{h}{2} \mathcal{L}_d(q^0, q^1, \Phi^0, \Phi^1, h/2) + \frac{h}{2} \mathcal{L}_d(q^0, q^1, \Phi^0, \Phi^1, h/2) \right]. \tag{67}
\]

The equations for \(\mathcal{F}_{10}^{01} h\) are obtained following the same procedure, and from the discrete Lagrangian that results from commuting the order in which \(\mathcal{L}_d^0\) and \(\mathcal{L}_d^1\) are used to approximate the action over \([0, h/2]\) and \([h/2, h]\). Even though \(\mathcal{F}_{10}^{01}\) and \(\mathcal{F}_{10}^{10}\) differ only in the order of application of the maps \(\mathcal{F}^{(h/2)}_d\) and \(\mathcal{F}^{(h/2)}_d\), they in fact constitute different algorithms of the same order.

The algorithm \(\mathcal{F}_{10}^{01}\) coincides exactly with that presented in [4.2] as it can be verified after identifying the relations (66a) and (66d) with the Legendre transform given in (16) and replacing in the rest of the equations of the method. So this section provides the formulation of that algorithm directly from the thermo-elastic Lagrangian, without a priori using the fact that the entropy is constant in time.

It is interesting to note that in the context of a separable Lagrangian such as the one for classical mechanics in Cartesian coordinates, the discrete Lagrangians (67) and (45) with \(\alpha = 1/2\) are exactly the same ones. This is why in that case the composition of the two symplectic Euler methods results in Newmark’s explicit second-order algorithm, also known as Störmer-Verlet [69]. This is not the case for thermo-elastic Lagrangians, because the free-energy depends on the thermal velocities.

5. Numerical examples

In this section two numerical examples showcase the performance and main features of the formulated algorithms are presented.

5.1. Three-dimensional motion of a chain of thermo-elastic springs and masses

The first example correspond to the simulation of the dynamics of a chain of three thermo-elastic springs and masses in \(\mathbb{R}^3\). See Fig. 5. The free-energy of all springs is that in (31), with constants \(\beta = 0.2, C_0 = 5.0, \ell_0 = 1, c = 100\) and \(\theta_0 = 300\). The initial momenta (in components in a Cartesian basis) and initial temperature are summarized in Table II. The initial positions are those shown in Fig. 5.

![Figure 5. Chain composed by three thermo-elastic springs and masses.](image)

5.1.1. Order of convergence of the algorithms. We first examine the numerical order of convergence of the algorithms introduced in sections 4.3.1, 4.3.2 and 4.4. Henceforth we shall...
Mass & $m$ & $p_1(0)$ & $p_2(0)$ & $p_3(0)$ & Spring & $\theta(0)$
--- & --- & --- & --- & --- & --- & ---
1 & 1.0 & 20.0 & 10.0 & 10.0 & 1 & 800.0
2 & 2.0 & 10.0 & 20.0 & 10.0 & 2 & 1200.0
3 & 1.5 & 0.0 & 10.0 & 0.0 & 3 & 400.0

Table II. Mechanical properties, initial temperature and Cartesian components of the initial momenta of the system.

refer to them as \textit{GTR} for generalized trapezoidal rule, \textit{HO4} for higher-order, and \textit{CO2} for composition, respectively. For the GTR algorithms we set $\alpha$ to $\{0.0, 0.5, 1.0\}$, as discussed earlier, and label them GTR-0, GTR-1/2 and GTR-1.

We simulated the dynamics of this system with these algorithms and evaluate errors at time $t = 1$, with the goal of numerically verifying their order of convergence. The errors at this time were measured for positions, momenta and temperatures separately. We show the rate of convergence by computing the square root of the sum of the square of the error in each Cartesian component of each mass, for the algorithmic positions $q_h(1)$ or algorithmic momenta $p_h(1)$. For the algorithmic temperatures $\theta_h(1)$ (obtained with (18b)), we compute the square root of the sum of the square of the error in the temperature of each spring instead. In the absence of an analytical solution, we computed a reference solution with HO4 by setting $h = 10^{-4}$. This time step yields the precise computation of 10 decimal digits in all variables, so we adopted it as a proxy for the exact solution, and errors were computed with respect to it. Simulations were carried out for all or a subset of the following time steps, depending on the integrator: $0.1$, $0.05$, $0.025$, $0.0125$, $0.00625$, $0.003125$, $0.0015625$, $0.00078125$ and $0.000390625$.

Figures 6 to 8 show the convergence curves. As expected, the curves show first-order convergence in all variables for GTR-0 and GTR-1, second-order convergence for GTR-1/2 and CO2, and fourth-order convergence for HO4. A remarkable feature is that the accuracy of the implicit algorithm GTR-1/2, and of the explicit algorithm CO2, seem to be the same. This might be a good reason to prefer the latter, CO2. The higher-order algorithm HO4 is more accurate than the rest for all tested time steps.

Regarding the computational performance, Fig. 9 shows the computing time as a function of the the magnitude of the error in position at $t = 100$, for each one of the algorithms. Analogous results are obtained when the computing time is plotted as a function of the errors in momentum or temperature. No particular emphasis has been placed in optimizing the code for each algorithm, so these results could change upon a more careful implementation.

As expected, for lower accuracy simulations the lower order algorithms (GTR-0, GTR-1, GTR-1/2 and CO2) are somewhat more advantageous when compared against the higher order algorithm HO4. However, if higher accuracy is required, HO4 becomes a lot more convenient. Finally, notice that throughout the whole range of computing times CO2 is more accurate than GTR-1/2, which makes it more attractive.

5.1.2. Long-term energy behavior and conserved quantities. We next showcase the behavior of the algorithms for long times. We simulate the evolution of the system up to $t = 100$, with a time step length $h = 0.01$, so a complete simulation involves $10^4$ time steps.

We first show parts of the trajectories and temperatures, as computed with CO2. Figures 10 and 11 show the projections of the motion of each mass in the $e_1$–$e_2$ and $e_1$–$e_3$ planes, where $\{e_i\}_{i=1,2,3}$ is the Cartesian basis in Fig. 5. The motion of the masses is clearly non-trivial and...
fully three-dimensional, with very large stretches of each one of the springs which induces large fluctuations of temperature and potential energy in the system. The evolution of the former is shown in Fig. 12.

In following the results obtained with CO2 is compared with those from HO4. Of course, by design both the entropy and the angular momentum of the system are conserved up to machine precision. This is shown in Figures 13 and 14. In both figures the curves obtained from each one of the two algorithms superposes exactly.

Figure 6. Convergence curve for the positions.

Figure 7. Convergence curves for the linear momenta.
Finally the total angular momentum at $t^k$ is computed as

$$A^k := \sum_{i}^{N} (q^i \times p^i)^k,$$

and the energy of the system by

$$H^k = \frac{1}{2} p^k \cdot m^{-1} p^k + U(q^k, \eta^k).$$
Figure 10. Trajectories of the masses in the $e_1$–$e_2$ plane. Here $q^i$ is the coordinate along the $e_i$ direction.

Figure 11. Trajectories of the masses in the $e_1$–$e_3$ plane. Here $q^i$ is the coordinate along the $e_i$ direction.

Figure 12. Evolution of the temperatures of the springs through 10,000 time steps.

The total energy trajectories computed with CO2 and HO4 is shown in Figure 15. When examined at full scale, Fig. 15(a), it is evident that (i) the energy is essentially conserved by both algorithms, and (ii) both algorithms are perceived as identical at this scale. Only when the vertical scale is small enough can the differences between the second- and fourth-order...
5.2. The dynamics of a simple thermo-elastic net

To conclude, we show the behavior of the CO2 algorithm in a slightly different example, the thermo-elastic system shown in Fig. 16. This examples also showcase the conservation of linear momentum. Each spring has the constitutive behavior defined by (31), with $C_0 = 5$, $\beta = 0.2$, $l_0 = 1$ and $\theta_0 = 300$. Initially the springs form an equilateral triangle with side length 1, with the masses located at the vertices. The stiffness of each spring, as well as its initial temperature and the initial momentum of each mass are shown in Table III. The simulation was performed up to a final time $t = 10$, with time step $h = 0.001$.

Projections of the three-dimensional trajectories of mass 1 in the $e_1$–$e_3$ and $e_1$–$e_2$ planes are shown in Fig. 17 where $\{e_i\}_{i=1,2,3}$ is the Cartesian basis shown in Fig. 16. Figure 18 shows the time histories of temperature and strain in spring 2, with strain defined as $\ln(l/l_0)$. Finally, Fig. 19 displays the evolution of the system’s energy, total entropy and total linear and angular momentum about $e_2$. The last three are conserved within machine precision, and the energy
Figure 15. (a) Evolution of the energy of the system through 10,000 time steps, shown at a full scale in the energy axis. (b) The fact that the energy oscillates around a constant value can only be seen by selecting a smaller scale for the energy axis. The oscillations in the higher-order algorithm need a yet smaller scale to be apparent, as shown in (c).

Figure 16. Thermo-elastic net for the second numerical example.

Table III. Mechanical properties and initial temperature of each spring, and mass and Cartesian components of the initial momentum of each mass.
oscillates around a constant value for the duration of the simulation.

![Figure 17. Projections of the trajectory of mass 1 in the $e_1$-$e_3$ and $e_1$-$e_2$ planes. Here $q^i$ denotes the coordinate along the $e_i$-direction.](image)

![Figure 18. Evolution of the strain and the temperature in the thermo-elastic spring 2.](image)

![Figure 19. Numerical conservation of the energy and momenta of the system.](image)
6. Conclusions

The construction of variational integrators for adiabatic thermo-elastic systems followed a standard procedure. These same ideas will soon be extended to continuum media, with the special heat conduction of Green and Naghdi \[53\]. The challenge of extending these structure-preserving integrators to the presence of Fourier’s heat conduction remains. A key property we would like to satisfy in that case is that, if the thermo-elastic system is isolated from the external world, so that there are no heat sources or sinks, then the energy of the system should be conserved. This has been explicitly enforced in the energy-momentum method in \[36\]. Since for this case the equations no longer have a Hamiltonian structure, then the good long-term energy behavior of variational integrators cannot be directly exploited.

7. Appendix

The explicit expression for the DEL equations given in (67a) for the case of configuration-dependent mass matrix is

$$\frac{1}{h^2} \left( m^{k+\alpha} q^{k+1} - (m^{k+\alpha} + m^{k-1+\alpha})q^k + m^{k-1+\alpha} q^{k-1} \right) =$$

$$= \frac{1}{2h^2} \nabla q m^k : \mathbf{Y}^{k+1-\alpha} + (1-\alpha) f^{k-} + \alpha f^{k+},$$  \hspace{1cm} (68)

where

$$m^{k+\alpha} = \alpha m^k + (1-\alpha)m^{k+1},$$

$$\mathbf{Y}^{k+1-\alpha} = \alpha \mathbf{Y}^{k+1} + (1-\alpha)\mathbf{Y}^k,$$

$$\mathbf{Y}^{k+1} = (q^{k+1} - q^k) \otimes (q^{k+1} - q^k).$$

The corresponding mechanical momentum maps are

$$p^k = h^{-1} m^{k+\alpha} (q^{k+1} - q^k) + \alpha [h f^{k+} + h^{-1} \nabla q m^k : \mathbf{Y}^{k+1}],$$  \hspace{1cm} (69a)

$$p^{k+1} = h^{-1} m^{k+\alpha} (q^{k+1} - q^k) - (1-\alpha) [h f^{(k+1)-} + h^{-1} \nabla q m^{k+1} : \mathbf{Y}^{k+1}].$$  \hspace{1cm} (69b)

Similarly, the explicit form of Eqs. (67a) for the case of configuration-dependent mass is

$$-m_a q^{k+1} + 4m_a q^{k+\frac{1}{2}} - m_a q^k + 4m_d q^{k-\frac{1}{2}} q^{k-\frac{1}{2}} - m_c q^{k-1} =$$

$$= \frac{1}{2} \nabla q m^k : (\Theta^{k+} + \Theta^{k-}) + h^2 (f^{k+} + f^{k-}),$$  \hspace{1cm} (70)

where

$$m_a = 3m^k - 4m^{k+\frac{1}{2}} + 3m^{k+1},$$

$$m_b = 3m^k + m^{k+1},$$

$$m_c = m^{k+1} + 4m^{k+\frac{1}{2}} + 18m^k + 4m^{k-\frac{1}{2}} + m^{k-1},$$

$$m_d = m^{k-1} + 3m^k,$$

$$m_e = 3m^{k-1} - 4m^{k-\frac{1}{2}} + 3m^k,$$

$$\Theta^{k+} = (-3q^k + 4q^{k+\frac{1}{2}} - q^{k+1}) \otimes (-3q^k + 4q^{k+\frac{1}{2}} - q^{k+1}),$$

$$\Theta^{k-} = (q^{k-1} - 4q^{k-\frac{1}{2}} + 3q^k) \otimes (q^{k-1} - 4q^{k-\frac{1}{2}} + 3q^k).$$
Moreover, the analogue of (57a) is given by
\[ \mathbf{m}/q^k - (\mathbf{m}_f + \mathbf{m}_g)q^{k+\frac{1}{2}} + \mathbf{m}_g q^{k+1} = h^2 f^{k+\frac{1}{2}} + \frac{1}{2} \nabla q^k \mathbf{m}^{k+\frac{1}{2}} : \Theta^{k+\frac{1}{2}}, \quad (71) \]
where
\[ \begin{align*}
\mathbf{m}_f &= 3\mathbf{m}^k + \mathbf{m}^{k+1}, \\
\mathbf{m}_g &= \mathbf{m}^k + 3\mathbf{m}^{k+1}, \\
\Theta^{k+\frac{1}{2}} &= (q^{k+1} - q^k) \otimes (q^{k+1} - q^k).
\end{align*} \]

Additionally, explicit expressions for the mechanical momenta are
\[ \begin{align*}
p^k &= \frac{1}{6h} \left[ -m_h q^k + 4m_g q^{k+\frac{1}{2}} + m_j q^{k+1} - h^2 f^{k+\frac{1}{2}} - \frac{1}{2} \nabla q^k \mathbf{m}^k : \Theta^{k+\frac{1}{2}} \right], \\
p^{k+1} &= \frac{1}{6h} \left[ -m_h q^k - 4m_g q^{k+\frac{1}{2}} + m_j q^{k+1} + h^2 f^{(k+1)-} + \frac{1}{2} \nabla q^k \mathbf{m}^{k+1} : \Theta^{(k+1)-} \right]. \quad (72a)
\end{align*} \]
where
\[ \begin{align*}
m_h &= 9\mathbf{m}^k + 4\mathbf{m}^{k+\frac{1}{2}} + \mathbf{m}^{k+1}, \\
m_i &= -3\mathbf{m}^k + 4\mathbf{m}^{k+\frac{1}{2}} - 3\mathbf{m}^{k+1}, \\
m_j &= \mathbf{m}^k + 4\mathbf{m}^{k+\frac{1}{2}} + 9\mathbf{q}^{k+1}.
\end{align*} \]

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