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THERMODYNAMICALLY CONSISTENT TIME INTEGRATORS FOR THERMO-ELASTIC SYSTEMS WITH HEAT CONDUCTION

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We formulate a new class of structure-preserving, thermodynamically consistent time integrators for finite-dimensional thermo-elastic systems with heat conduction of Fourier type. The Hamiltonian structure of the adiabatic problem is used to develop standard variational integrators. We include heat transfer as an irreversible perturbation applied to the entropy balance equation. Variational methods are then formulated by means of the application of the discrete D'Alembert principle [4]. The resulting algorithms are (i) structure-preserving i.e. they are momentum-conserving (if the original problem posses symmetries) and (ii) they are thermodynamically consistent in the sense that for isolated systems, the total energy of the system is nearly exactly conserved for a very long time and the total entropy is non-decreasing and, (iii) they behave as symplectic integrators in the non-conductive case.

We consider an arrangement of N mases connected by M thermo-elastic springs [1, 2, 3] such as those shown in Figure 1. The spatial position of the masses at time t is described by a vector of generalized displacements $\mathbf{q}(t)$. Moreover, each thermo-elastic spring is assigned with a *thermal displacement* $\Phi_i(t) \in \mathbb{R}$, $(i \in \{1, ..., M\})$ such that its time derivative corresponds to the temperature $\theta_i = \dot{\Phi}_i$. The Helmholtz free energy of the system, A, corresponds to the sum of the contributions of each thermo-elastic spring

$$\mathsf{A}(\mathbf{q}, \boldsymbol{\theta}) = \sum_{i=1}^{M} \mathsf{A}_i(\mathbf{q}, \theta^i),$$

and the kinetic energy is taken as $\mathsf{K} = \frac{1}{2}\mathbf{m}\dot{\mathbf{q}} \cdot \dot{\mathbf{q}}$ where $\mathbf{m}$ is a mass matrix. Then, the Lagrangian is defined as $\mathsf{L}(\mathbf{q}, \dot{\mathbf{q}}, \boldsymbol{\theta}) = \mathsf{K}(\mathbf{q}, \dot{\mathbf{q}}) - \mathsf{A}(\mathbf{q}, \boldsymbol{\theta})$ and the equations of motion of the system follow as the Euler-Lagrange equations of Hamilton's principle [1, 2].

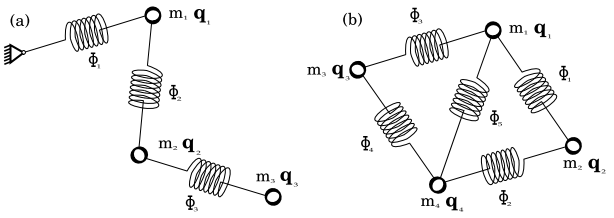

Figure 1: (a) Triple thermo-elastic pendulum. (b) Spatial net.

The Hamiltonian, H, follows as the Legendre transform of the Lagrangian in the velocity and temperature variables and the corresponding balance equations are

$$\dot{\mathbf{q}} = \nabla_{\mathbf{p}}\mathsf{H}(\mathbf{q},\mathbf{p},\boldsymbol{\Phi},\boldsymbol{\eta}), \qquad \dot{\boldsymbol{\Phi}} = \nabla_{\boldsymbol{\eta}}\mathsf{H}(\mathbf{q},\mathbf{p},\boldsymbol{\Phi},\boldsymbol{\eta}), \tag{1a}$$

$$\dot{\mathbf{p}} = -\nabla_{\mathbf{q}}\mathsf{H}(\mathbf{q},\mathbf{p},\boldsymbol{\Phi},\boldsymbol{\eta}), \qquad \dot{\boldsymbol{\eta}} = -\nabla_{\boldsymbol{\Phi}}\mathsf{H}(\mathbf{q},\mathbf{p},\boldsymbol{\Phi},\boldsymbol{\eta}) = \mathbf{0}. \tag{1b}$$

where $\mathbf{p}$ is the vector of mechanical momenta and $\boldsymbol{\eta}$ corresponds to the vector of thermal momenta which coincides with the vector of entropies of the system. The above equations describe the evolution of a thermo-elastic system with symmetries following a reversible adiabatic process. In order to allow for heat conduction, $(1b)_2$ has to be modified adding an entropy flux vector of Fourier type as

$$\dot{\eta}_i = \mathrm{f}_i = \kappa \sum_j \frac{(\theta_i - \theta_j)}{\theta_i}, \qquad i \in \{1, ..., M\},$$

where κ is a conductivity parameter. The system remains being energy and momentum-conserving but the total entropy now increases and the system is no longer Hamiltonian. From the numerical point of view, a discrete form of D'Alembert principle is used to formulate a class of second-order accurate, momentum-conserving time integrators. Numerical evidence shows that proposed algorithms are thermodynamically consistent.

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