



A novel variational formulation for thermoelastic problems



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ABSTRACT

A novel variational formulation for thermoelasticity is proposed in this paper. The formulation is based on the Hamilton–Pontryagin principle and the concept of temperature displacement. Although there are many other papers that have a similar goal, most of the proposed approaches are quite complicated, and contain assumptions that curtail their applicability. The proposed variational principle in this paper is straightforward with no extra assumptions and it is in conformity with the Clausius–Duhem inequality as a statement of the second law of thermodynamics. Conservation laws for linear momentum and energy, and the constitutive equation for thermoelasticity are consequences of this variational formulation.

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1. Introduction

A variational description of a physical system consists of a statement that the variation of a specified functional is equal to some fixed value, which can be customarily chosen to be zero. Attempts to state variational principles for natural laws date back in history and the development of such variational principles have received attention due to their elegance and the advantages they exhibit when solving practical problems. Various variational formulations for thermomechanical problems have been suggested both for discrete and continuous systems in the past decades and authors have usually introduced new variables and quantities in stating the principle from their respective viewpoints.

Many of the pioneering works in this direction have been due to M.A. Biot, who has published many significant papers in this area [1–7]. In his variational principle, Biot introduced a quantity called the *entropy displacement vector* \bar{S} , in addition to the common displacement vector u , to describe the thermal part of his formulation. This quantity is defined by the following equation,

$$\frac{\partial \bar{S}}{\partial t} = \frac{1}{\theta_r} \frac{\partial \bar{H}}{\partial t}, \quad (1)$$

where $\frac{\partial \bar{H}}{\partial t}$ is the rate of the heat flow \bar{H} , and θ_r is the temperature of the environment, that is assumed to be constant. He also introduced a non-negative quadratic dissipation function in terms of generalized velocities that is proportional to the entropy production. From these, he obtained a variational formulation, which yielded Euler–Lagrange equations that

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Nomenclature

i, j, k, \dots	indices in continuum mechanics
\mathbf{b}	Body force per unit volume
\mathbf{e}	the strain tensor
\mathbf{p}	the momentum vector
\mathbf{p}_u	mechanical momentum
\mathbf{p}_τ	thermal momentum
\mathbf{q}	thermomechanical generalized coordinate vector
\mathbf{t}	the stress tensor
\mathbf{u}	mechanical displacement vector
\mathbf{v}	the velocity vector
\mathbf{w}	mechanical velocity vector
r	rate of heat supply
t	time
\mathbf{F}	deformation gradient tensor
\bar{S}	entropy displacement vector
\bar{H}	heat flow
$\bar{\mathbf{K}}$	heat conductivity tensor
\mathbf{Q}	heat flux vector
$Q_{i,i}$	divergence of heat flux vector
$\bar{\mathbf{P}}$	first Piola stress tensor
θ	instantaneous temperature
θ_0	initial temperature
θ_r	temperature of environment
$\hat{\theta}$	dimensionless temperature
τ	temperature displacement
ρ_0	the density in reference configuration
η	entropy function
ψ	Helmholtz free energy

describe thermomechanical systems [6]. Biot's formulation was applied to heat conduction [8], and some nonlinear problems in heat transfer [9].

Kermidas and Ting [10] used temperature-based variables instead of entropy displacement. They assumed a linear relation between entropy and a dimensionless temperature that is defined to be

$$\hat{\theta} = \frac{\theta - \theta_0}{\theta_0}, \quad (2)$$

where θ and θ_0 are instantaneous and initial absolute temperatures, respectively. These linear constitutive relations limit the applicability of the approach to a local region of validity.

Some authors have suggested the futility of developing variational formulations for thermomechanical problems and have proposed the use of other methods, like Galerkin projection, for approximating thermomechanical systems [11]. He et al. [12] obtained a variational principle for coupled thermoelasticity with finite displacement using the semi-inverse method for the field equations directly. To do this, they replaced the time derivative terms in the coupled heat conduction equations with finite-difference approximations. Sawada [13] derived a variational principle for nonlinear and non-steady (non-equilibrium) thermodynamic systems using the principle of maximum entropy production. He also applied this approach to simulate a chemical structure with a growing random pattern [14]. Maugin and Kalpakides [15] formulated a variational principle based on the inverse motion mapping and then explored the corresponding Euler–Lagrange equations. Subsequently, they also derived a Hamiltonian formulation from the Lagrangian formulation. Yang et al. [16] developed a variational formulation for general dissipative solids, where they made a distinction between the external temperature and the equilibrium temperature. Apostolakis and Dargush [17] used the mixed variational principle for thermoelastic materials. Their resulting relations are only valid for problems in the linear regime because they assumed that the temperature was constant in the energy equation.

In the present work, a new variational formulation for thermoelastic problems is proposed. This formulation contains no *a priori* assumptions which limit its validity except for the most commonly accepted assumptions in thermoelasticity. In the next section, we will review the necessary constraints on the thermomechanical responses to ensure that the second law of thermodynamics is satisfied. In addition, the energy equation for thermoelasticity is also stated. In the third part, the Lagrangian and Hamiltonian for a thermomechanical problem are derived. In the fourth section, the Hamilton–Pontryagin principle is presented and finally, the variational formulation is proposed in the last section using this principle.

2. Admissible thermodynamic processes in the context of thermoelasticity

It is well established that the second law of thermodynamics imposes certain constraints on thermodynamic processes. In thermoelasticity, it is a common constitutive assumption that the Helmholtz free energy is a function of the deformation gradient tensor and temperature, and that the heat flux vector is a linear function of the temperature gradient via the heat conduction tensor. The second law of thermodynamics, expressed in terms of the Clausius–Duhem inequality [18], constrains the set of allowable material constitutive relations. The following material constitutive relations,

$$\hat{\mathbf{P}}(\mathbf{F}, \theta) = \rho_0 D_{\mathbf{F}} \hat{\psi}(\mathbf{F}, \theta), \tag{3a}$$

$$\hat{\eta}(\mathbf{F}, \theta) = -D_{\theta} \hat{\psi}(\mathbf{F}, \theta), \tag{3b}$$

$$\mathbf{a} \cdot \hat{\mathbf{K}}(\mathbf{F}, \theta) \mathbf{a} \geq 0, \quad \text{for all } \mathbf{a} \tag{3c}$$

satisfy the inequality and are therefore thermodynamically allowable. Here, $\hat{\mathbf{P}}$ is the first Piola stress tensor which is a function of the deformation gradient tensor and the temperature. The Helmholtz free energy and entropy functions are denoted by $\hat{\psi}$ and $\hat{\eta}$, respectively, and ρ_0 is the density in the reference configuration. In the third equation, $\hat{\mathbf{K}}$ is the heat conduction coefficient tensor, and the equation expresses the condition that the heat conduction coefficient tensor is positive-definite. These constraints together with the following statement of energy balance,

$$\dot{\eta} \theta = -Q_{i,i} + r \tag{4}$$

constitute the basis for thermoelasticity. In the above equation, η and θ are the specific entropy and temperature, respectively. The rate of heat supply is denoted by r and $Q_{i,i}$ is the divergence of the heat flux vector.

3. Thermal displacement as an appropriate thermal variable

A thermomechanical system is composed of elements and subsystems that interact with each other through the exchange of energy. This energy exchange between elements and subsystems can be expressed in terms of physical variables like force, velocity, momentum, entropy, temperature, etc. The exchanged power is equal to the product of two variables that each of them is power conjugate of the other one. One of these power variables is assumed to be the effort and its conjugate, as the flow. This approach to modeling of interconnections as power ports serves as the basis of the port-Hamiltonian approach [19] for modeling the interconnection of Hamiltonian systems.

There is no canonical choice of effort and flow variables, and one can choose, as a matter of convenience, to view one as the effort and the other as the flow. The time integral of effort and flow are defined to be the generalized momentum and generalized displacement, respectively. In thermal systems, the power is equal to the product of temperature θ , and time derivative of entropy $\dot{\eta}$. In this article, the time derivative of the entropy is chosen as the effort and the temperature as the flow. Therefore, the entropy is the generalized momentum and the time integral of temperature is the generalized displacement, which is referred to as the thermal displacement τ .

4. The Lagrangian and Hamiltonian for thermoelastic systems

In the variational formulation that is proposed in this paper, the temperature displacement is chosen as the thermal variable, and the time derivative of the temperature displacement corresponds to the temperature. Although this variable has no physical counterpart, it is shown that along with the ordinary displacement vector it can form a thermomechanical 4-vector that can conveniently be used in the formation of the Lagrangian and Hamiltonian for the thermoelastic system. This thermomechanical 4-vector is denoted by,

$$\mathbf{q} = (u_i, \tau) = (\mathbf{u}, \tau), \tag{5}$$

where u_i is the mechanical displacement vector and the temperature $\theta = \frac{d\tau}{dt}$.

The time derivative of this vector is,

$$\mathbf{v} = \dot{\mathbf{q}} = (\dot{\mathbf{u}}, \dot{\tau}) = (\mathbf{w}, \theta), \tag{6}$$

where $w_i = \frac{du_i}{dt}$ is the mechanical velocity vector.

The Lagrangian density is written as

$$L(\mathbf{q}, \dot{\mathbf{q}}) = K(u_i, w_i) - \psi(e_{ij}, \theta), \tag{7}$$

where K and ψ are the kinetic energy and the Helmholtz free energy, respectively, and e_{ij} is the strain tensor. Integrating the Lagrangian density over a spatial domain yields a Lagrangian in the usual sense. By performing a Legendre transformation of the Lagrangian, we obtain the Hamiltonian of the system that is given by

$$H(\mathbf{q}, \mathbf{p}) = \mathbf{p} \cdot \dot{\mathbf{q}} - L(\mathbf{q}, \dot{\mathbf{q}}), \tag{8}$$

where

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{q}}} = (m\mathbf{w}_i, \eta) \quad (9)$$

is the generalized 4-momentum vector. It includes the mechanical momentum as its first three components and the entropy as the fourth one.

The entropy can be regarded as the thermal momentum and it is given by,

$$\eta = \frac{\partial L}{\partial \theta} = -\frac{\partial \psi}{\partial \theta}. \quad (10)$$

5. The Hamilton–Pontryagin principle

The Hamilton–Pontryagin principle is used to state the new variational principle for thermoelasticity. This principle is explained completely in [20,21], and it can be viewed as a generalization of both Hamilton's and Hamilton's phase space variational principle. We will review this principle and the extension to forced systems in this section, and discuss the application of this variational principle to thermoelasticity in the next section.

The basic idea is to relax the condition that the time derivative of the 4-displacement vector is equal to the 4-velocity vector and then impose their equality through a Lagrange multiplier that will be the 4-momentum vector, i.e.,

$$\delta \int_{t_i}^{t_f} [L(\mathbf{q}(t), \mathbf{v}(t)) + \mathbf{p}(t) \cdot (\dot{\mathbf{q}}(t) - \mathbf{v}(t))] dt = 0, \quad (11)$$

where t_i and t_f are the initial and final times. This variational formulation produces the following implicit Euler–Lagrange equations,

$$\dot{\mathbf{q}} = \mathbf{v}, \quad (12a)$$

$$\dot{\mathbf{p}} = \frac{\partial L}{\partial \mathbf{q}}, \quad (12b)$$

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}}. \quad (12c)$$

For systems with external force \mathbf{F} , the Lagrange–d'Alembert–Pontryagin principle applies,

$$\delta \int_{t_i}^{t_f} [L(\mathbf{q}(t), \mathbf{v}(t)) + \mathbf{p}(t) \cdot (\dot{\mathbf{q}}(t) - \mathbf{v}(t))] dt + \int_{t_i}^{t_f} \mathbf{F}(\mathbf{q}(t), \mathbf{v}(t)) \cdot \delta \mathbf{q}(t) dt = 0, \quad (13)$$

which results in the forced implicit Euler–Lagrange equations,

$$\dot{\mathbf{q}} = \mathbf{v}, \quad (14a)$$

$$\dot{\mathbf{p}} = \frac{\partial L}{\partial \mathbf{q}} + \mathbf{F}(\mathbf{q}, \mathbf{v}), \quad (14b)$$

$$\mathbf{p} = \frac{\partial L}{\partial \mathbf{v}}. \quad (14c)$$

In thermoelastic problems, the traction on the surface of the body and the heat conduction vector are considered as external forces.

6. Variational formulation for thermoelasticity

Using the Hamilton–Pontryagin principle allows us to derive the variational formulation without imposing any extra assumptions. Prior to presenting our approach, we will first review some of the approaches adopted in prior work.

Prior variational formulations. Some authors like Biot [6] and Yang [16] have used a variable related to entropy to describe the thermal part of the problem. For nonlinear irreversible processes and a system composed of K elements, Biot introduced a fundamental non-classical collective potential V , excess temperature $\bar{\theta}_K$ of element K , and generalized dissipative forces \mathbf{X} , that are given by,

$$V = \sum_K U_K - \sum_K \theta_K \eta_K, \quad (15a)$$

$$\bar{\theta}_K = \theta_K - \theta_r = \frac{\partial V_K}{\partial \eta_K}, \quad (15b)$$

$$\sum_i X_i \delta u_i = \sum_K \theta_K \delta \eta_K^*, \quad (15c)$$

where U_K, θ_K, η_K and η_K^* denote the internal energy, temperature, entropy, and entropy production of element K of system, θ_r is the constant temperature of a big thermal source (thermal well) and u_i is the generalized coordinate. Consequently, the principle of virtual dissipation as a generalization of d'Alembert's principle is used to derive Lagrange's equations with generalized coordinates [6].

Yang et al. [16] assumed the internal energy density U and the absolute temperature θ to be functions of the deformation gradient and the entropy per unit undeformed volume,

$$U = U(\mathbf{F}, \eta), \tag{16a}$$

$$\theta = \theta(\mathbf{F}, \eta). \tag{16b}$$

By distinguishing between the equilibrium temperature θ corresponding to the state (\mathbf{F}, η) , which is given by the equilibrium relation,

$$\theta = \partial_\eta U \tag{17}$$

and the external temperature field θ_r , they presented a weak form of the desired final rate equations and after some mathematical manipulation, they obtained the variational formulation for general dissipative solids.

Eliminating the time derivative in the heat conduction equation and using finite-differences to approximate the derivatives, He et al. [12] obtained a variational formulation by applying the semi-inverse method. It should be noted that the final relations are only applicable for small finite displacements due to the approximation of the derivatives.

Kermidas and Ting [10] assumed a linear relation between the dimensionless temperature $\hat{\theta}$ and the entropy η , and consequently, their results apply only to linear problems. Apostolakis and Dargush [17] assumed the temperature in (4) to be constant. Then, the final formulation is applicable only valid for problems in which the temperature variations are small. Maugin and Kalpakides [15] use the thermal displacement to describe the thermal field of the body as well. By first assuming the inverse motion mapping, they have derived Euler–Lagrange equations for their problem, and from this they derived a Hamiltonian form of the equations.

Proposed Hamilton–Pontryagin variational formulation. In contrast to the approaches described in the abovementioned works, the proposed variational principle stated in the paper is straightforward and with no extra assumptions. The use of the Hamilton–Pontryagin principle is critical as it provides a means of addressing the degeneracy of the problem. In contrast with many works that tacitly employ isothermal processes in their derivations, which limit the applicability of their results, this work does not suffer from this deficiency.

In what follows, a Hamilton–Pontryagin variational formulation of thermoelasticity is presented. The Lagrangian density for a thermoelastic body is given by,

$$L(\mathbf{q}, \dot{\mathbf{q}}) = K(u_i, w_i) - \psi(e_{ij}, \theta). \tag{18}$$

Applying the Lagrange–d'Alembert–Pontryagin principle (13), we obtain,

$$\begin{aligned} \delta \int_{t_i}^{t_f} \int_V [K(u_i, w_i) - \psi(e_{ij}, \theta) + p_{u_i}(\dot{u}_i - w_i) + p_\tau(\dot{\tau} - \theta)] dV dt \\ + \int_{t_i}^{t_f} \int_{\partial V} t_{ij} n_j \delta u_i dAdt + \int_{t_i}^{t_f} \int_V (b_i \delta u_i + \frac{r}{\theta} \delta \tau) dV dt - \int_{t_i}^{t_f} \int_V \frac{Q_{i,i}}{\theta} \delta \tau dV dt = 0, \end{aligned} \tag{19}$$

where t_{ij} is the stress tensor on the surface with outward unit normal n_j . The body force per unit volume is denoted by b_i , and r is the specific rate of heat supply. $Q_{i,i}$ is the divergence of the heat flux vector and $\frac{Q_{i,i}}{\theta}$ is regarded as an external thermal load.

Computing the variations yield the following expression

$$\begin{aligned} \int_{t_i}^{t_f} \int_V \left[\left(\frac{\partial K}{\partial u_i} - \dot{p}_{u_i} + t_{ijj} + b_i \right) \delta u_i + \left(\frac{\partial K}{\partial w_i} - p_{u_i} \right) \delta w_i + \left(-\frac{\partial \psi}{\partial e_{ij}} + t_{ij} \right) \delta e_{ij} \right. \\ \left. + (\dot{u}_i - w_i) \delta p_{u_i} + \left(-\dot{p}_\tau + \frac{r}{\theta} - \frac{Q_{i,i}}{\theta} \right) \delta \tau + \left(-\frac{\partial \psi}{\partial \theta} - p_\tau \right) \delta \theta + (\dot{\tau} - \theta) \delta p_\tau \right] dV dt = 0. \end{aligned} \tag{20}$$

From the fundamental theorem of the calculus of variations, the coefficients of the independent variations vanish, from which we obtain the following final relations,

$$\frac{\partial K}{\partial u_i} - \dot{p}_{u_i} + t_{ijj} + b_i = 0, \tag{21a}$$

$$\frac{\partial K}{\partial w_i} - p_{u_i} = 0, \tag{21b}$$

$$-\frac{\partial \psi}{\partial e_{ij}} + t_{ij} = 0, \tag{21c}$$

$$\dot{u}_i - w_i = 0, \tag{21d}$$

$$-\dot{p}_\tau + \frac{r}{\theta} - \frac{Q_{i,i}}{\theta} = 0, \tag{21e}$$

$$-\frac{\partial \psi}{\partial \theta} - p_\tau = 0, \quad (21f)$$

$$\dot{\tau} - \theta = 0. \quad (21g)$$

The first equation is the conservation of linear momentum. The second and sixth equations are the definitions of mechanical and thermal momentum. The third equation is the constitutive relation for thermoelasticity. The fourth and the seventh equations are the constraint equations. And finally, the fifth equation is the balance of energy for a thermoelastic body. Given these equations, all balance laws in the context of thermomechanical theory, including the equality relations implied by the second law of thermodynamics are satisfied. The only remaining constraint is the requirement that the heat conduction coefficient tensor must be positive-definite. It should be emphasized since no extra assumptions were imposed, the formulation is valid in the context of nonlinear thermoelasticity.

7. Conclusion

In this work, a variational formulation for thermoelasticity was proposed using the Lagrange–d’Alembert–Pontryagin principle. As a consequence of this formulation, all balance laws, including equality constraints implied by the second law of thermodynamics for a thermoelastic body were derived.

This work is of theoretical interest and providing an elegant derivation of the equations of motion of thermoelastic systems. In addition, it also paves the way towards geometric structure-preserving discretizations of thermoelastic problems based on variational integrators. The application of Hamilton–Pontryagin variational integration techniques [22] to our variational characterization of thermoelasticity will be the subject of a subsequent paper.

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