FINITE ELEMENT FORMULATIONS VIA THE THEOREM OF EXPENDED POWER IN THE LAGRANGIAN, HAMILTONIAN AND TOTAL ENERGY FRAMEWORKS

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Traditionally, variational principles and variational methods have been employed in describing finite element formulations for elastodynamics applications. Here we present alternative avenues emanating from the theorem of expended power, using the differential calculus directly.

We focus on scalar representations under three distinct frameworks: Lagrangian mechanics, Hamiltonian mechanics, and a new framework involving a built-in measurable quantity, called the total energy in the configuration space. All three frameworks are derivable from each other, since they represent the same physics as Newton's second law; however, the total energy framework which we advocate inherits features that are comparable and competitive to the usual Newtonian based finite element formulations, with several added advantages ideally suited for conducting numerical discretization.

The present approach to numerical space-time discretization in continuum elastodynamics provides physical insight via the theorem of expended power and the differential calculus involving the distinct scalar functions: the Lagrangian $\mathcal{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}) : TQ \to \mathbb{R}$, the Hamiltonian $\mathcal{H}(\boldsymbol{p}, \boldsymbol{q}) : T^*Q \to \mathbb{R}$, and the total energy $\mathcal{E}(\boldsymbol{q}, \dot{\boldsymbol{q}}) : TQ \to \mathbb{R}$. We show that in itself the theorem of expended power naturally embodies the weak form in space, and after integrating over a given time interval yields the weighted residual form in time. Hence, directly emanating from the theorem of expended power, this approach yields three differential operators: a discrete Lagrangian differential operator, a Hamiltonian differential operator, and a total energy differential operator.

The semidiscrete ordinary differential equations in time derived with our approach can be readily shown to preserve the same physical attributes as the corresponding continuous systems. This contrasts with traditional approaches, where such proofs are nontrivial or are not readily tractable.

The modeling of complicated structural dynamical systems such as a rotating bar and the Timoshenko beam are shown for illustration.

1. Introduction

Variational concepts have long played a significant role in the development of numerical discretization techniques. First, variational principles in physics and mechanics have been used to derive the governing differential equations from which numerical discretizations are routinely conducted. The principles — including Hamilton's principle in dynamics, in the electromagnetic and gravitational fields, and even in quantum mechanics; the principle of stationary potential energy and the Hu–Washizu's variational principle in continuum statics; Fermat's principle of least time leading to Snell's law in optics; Maupertuis' principle of least action, Jacobi and Lagrange's principle of least action in dynamics again; and Gurtin's

variational principles [1964a; 1964b] for initial value problems such as wave and transient heat transfer in lieu of Hamilton's principle — have been considered in engineering and science as an indispensable branch of mathematics to derive the differential equations, namely, the Euler–Lagrange equations. At the same time, variational methods such as the Rayleigh–Ritz method, the principle of virtual work, the Galerkin weighted residual method, the Kantorovitch method, and the Trefftz method have played a critical role in finding approximate solutions to the governing equations.

Thus, whether via the variation principle or the variational method, the notion of variation is ubiquitous. But the question arises: Can the differential formulation be used as an alternative to the variation formulation? This is the focus of this paper.

As mentioned, the calculus of variations, founded by Euler and Lagrange, has been used extensively to derive governing differential equations, especially for mechanical systems. It has been the focus of philosophical controversies and some misinterpretations due to the perception that it seems to bring a purpose to the flow of natural events. Both approaches are concerned with infinitesimal changes in physical quantities. However, in a sense the differential calculus uses the real quantity, while the variational calculus employs the imaginary quantity. The notion of variation is imaginary, but the notion of differential is real!

The biggest advantage of the variation over the differential seems to arise from problems described as *rheonomic systems*. Recall that holonomic systems where Lagrange's equations of motion and Hamilton's principle are true were classified by Boltzmann into scleronomic and rheonomic systems [Lanczos 1970]. In rheonomic systems, the direction of the differential differs from that of the variation, due to the presence of the partial derivative of any physical quantity with respect to time depending on time explicitly. The introduction of the variation enables one to eliminate the time partial derivative term. However, it is an imaginary and a mathematical abstract quantity.

Most engineering and science applications do not fall into the class of rheonomic systems [Castro 2000]. In scleronomic systems, the direction of the differential is identical to that of the variation. Therefore, for such applications, the variational approach is not indispensable in deriving governing equations or in finding approximate solutions. Fortunately, this is the case of most engineering and science problems.

In particular, the solid mechanics, elastodynamics and continuum mechanics problems to which the finite element formulations are usually applied are generally scleronomic. Variational formulations are not indispensable to such applications, and differential formulations also play an important role, as we now describe.

Contributions of the present approach. Traditional practices for finite element discretization tend to employ the Newtonian framework. They mostly start from the Cauchy equations of motion and invoke the variational calculus, leading to the weak form or, equivalently, the principle of virtual work. In contrast, we have previously provided alternate developments via Hamilton's law of varying action as a starting point which is also based on the concept of variations [Har and Tamma 2009]. Unlike all these past developments, in this paper we employ the differential calculus and frameworks involving scalar representations, namely, the Lagrangian $\mathscr{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}) : TQ \to \mathbb{R}$, the Hamiltonian $\mathscr{H}(\boldsymbol{p}, \boldsymbol{q}) : T^*Q \to \mathbb{R}$, and the total energy $\mathscr{E}(\boldsymbol{q}, \dot{\boldsymbol{q}}) : TQ \to \mathbb{R}$.

To our knowledge, this use of the differential calculus in describing finite element discretizations is novel. It provides alternate viewpoints and helps deepen physical insight.

For approximation procedures like the finite element formulation, the basic issue with the conventional approaches for continuum dynamics is that there is no notion of a *scalar function*, say energy, that is readily built-in or directly available. The procedure mostly relies upon numerical discretization of the governing equations with dependent variables in terms of vector quantities such as displacement, velocity, acceleration, etc. This gives rise to two issues:

(a) To deal with a physical quantity such as total energy in a finite element computation, or to interpret the results from a Newtonian viewpoint, one often resorts to introducing the well known scalar functions typical of the Lagrangian or the Hamiltonian, even though one is not working in the Lagrangian or Hamiltonian framework.

(b) To establish that the semidiscretized equations (which are of focus here) inherit the same physics as the continuous governing equations in space and time can be difficult in traditional frameworks, since no obvious scalar function is available for capitalizing on Noether's theorem and the like. In our framework involving scalar representations, by contrast, one can readily establish the symmetries for the continuous as well as the discrete scalar representations for the total energy, Lagrangian, and the Hamiltonian. (Proofs of the symmetries of $\mathscr{E}$ are given in [Har and Tamma 2009], while those for $\mathscr{L}(\boldsymbol{q}, \dot{\boldsymbol{q}})$ and $\mathscr{H}(\boldsymbol{p}, \boldsymbol{q})$ appear in the standard literature.) In other words, we propose a new space-discrete finite element formulation that circumvents the weak-form Cauchy equations and the principle of virtual work. Although it must yield the same semidiscretized equations on physical grounds, the new formulation leads more easily to proofs that the discrete system preserves the physical attributes of the continuum system, via the scalar representations that are invariant. In summary, if the continuum system obeys the conservation laws, establishing the symmetries for the semidiscretized system also ensures the same physical attributes as in the continuum system.

The role of symmetries. Noether's theorem relates the invariance properties of the Lagrangian to the conservation laws of physics [Noether 1918; Byers 1996; 1999]. Thus, the spatial translational invariance of the Lagrangian in configuration space gives rise to conservation of linear momentum, its rotational invariance to conservation of angular momentum, and the autonomous Lagrangian has invariance in time. The Hamiltonian in phase space shares the same invariance properties, by the Hamiltonian version of Noether's theorem; see [Simo et al. 1992], for example. It turns out that the autonomous total energy (which is not the Hamiltonian, nor it is in the same configuration space as that of the Hamiltonian) also possesses the three invariances. Hence it can be viewed as a total energy version of Noether's theorem [Har and Tamma 2009].

Conservation laws can be extended to the balance laws of mechanical systems, such as the linear momentum balance law, the angular momentum balance law, and the energy balance law in continuum mechanics [Marsden and Hughes 1983; Holzapfel 2000; Malvern 1969]. Newton's law for N-body dynamical systems or Cauchy's equations of motion for continuous-body dynamical systems can be obtained from the linear momentum balance law. We believe that, as the fundamental equation for N-body dynamical systems, d'Alembert's principle [Goldstein et al. 2002; Hand and Finch 1998] or the d'Alembert–Lagrange principle [Arnold 1989] or the generalized d'Alembert principle [Meirovitch 2003] or the Lagrangian form of d'Alembert's principle [Greenwood 1977] or the first form of the

fundamental equation [Pars 1965] result from the conceptual amalgamation of the linear momentum balance law and the principle of virtual work. Note that Lagrange's equations of motion can be derived from d'Alembert's principle; further, Hamilton's equations of motion can be deduced from Lagrange's equations of motion and the Legendre transformation. Thus the linear momentum balance law is at the origin of all these equations governing motion.

At the same time, it is known that Hamilton's principle has a logical inconsistency for handling transient initial value problems [Gurtin 1964a; 1964b; Tonti 1973; 1984; Bailey 1975; Simkins 1981; Carini and Genna 1998]. Hamilton's law of varying action, which is not a variational principle, circumvents this deficiency and is more appropriate to use. *However, both approaches use the notion of variation, and with respect to scalar representations of the governing equations of motion, they are, so to speak, secondary developments; Lagrange's equations of motion in configuration space are the first equations encountered in the logical derivation under these approaches.* It is from them that one obtains Hamilton's equations in phase space, by applying the Legendre transformation. Unlike the above, the theorem of expended power first yields naturally the so-called total energy representation of the equations of motion in the logical derivation in configuration space. Thereafter, employing a particular transformation that is not a Legendre transformation, one can then define the standard Lagrange equations of motion in configuration space. Through a Legendre transformation one is then led to Hamilton's equation in phase space.

As an alternative to the Lagrangian and the Hamiltonian frameworks, we proposed in [Har and Tamma 2009] a framework based on the directly measurable built-in scalar quantity called the total energy $\mathcal{E}(q, \dot{q}) : TQ \to \mathbb{R}$. The total energy has the same translation, rotation, and time invariance properties. The total energy we use here is the kinetic energy plus the potential energy for N-body systems and the kinetic energy plus the total potential energy for continuous-body systems.

Figure 1 summarizes the main quantities and equations in the total energy framework, as well as the traditional Lagrangian and Hamiltonian frameworks, for an N-body system. The figure also indicates the
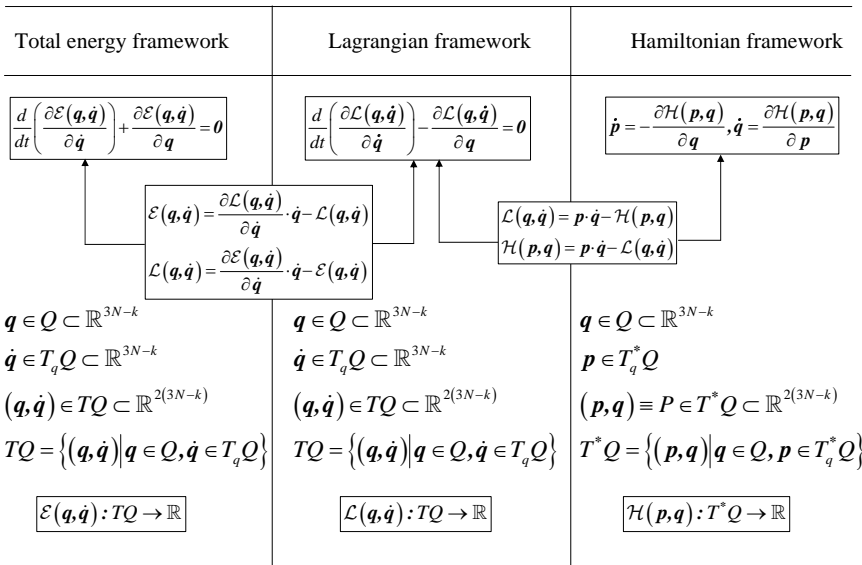

Figure 1. Comparison of the autonomous Lagrangian, Hamiltonian, and Total Energy frameworks for the N-body problem.

equivalence between the three. As discussed, all three scalar functions (in configuration or phase space as appropriate) possess spatial invariance under translations and rotations, and also translational time invariance in the autonomous case. This holds equally for finite- and infinite-dimensional dynamical systems.

Via Hamilton's principle, the total energy framework can be viewed as a third perspective (the first and second being the Lagrangian and the Hamiltonian), providing meaningful insight. The total energy has a direct physical interpretation and practical utility, in contrast to the somewhat abstract scalar quantity that is the Lagrangian $\mathscr{L}(\boldsymbol{q}, \dot{\boldsymbol{q}}) : TQ \to \mathbb{R}$ in configuration space. The second-order ordinary differential system arising from the total energy framework after space discretization offers the same features that apply to the Newtonian description for continuum mechanics, including considerations for designing time stepping algorithms. By contrast, the Hamiltonian $\mathscr{H}(\boldsymbol{p}, \boldsymbol{q}) : T^*Q \to \mathbb{R}$ (which, as we recall, does not in general represent energy directly) is not as popular for numerical discretization in the computational mechanics community, because the resulting first-order system requires altogether a different form of time discretization.

Remark. A different alternative to traditional finite element practices, called the cell method and amounting to a direct discrete formulation of field laws, can be found in the literature [Tonti 2001a; 2001b]. Without resorting to differential governing equations, the discretization procedure is carried out directly from physical laws using physical variables such as configuration, source, and energy variables. For most simplex elements, the stiffness matrices obtained by the formulation coincide with the one obtained by traditional finite element practices. Likewise, our proposed formulation also yields the same stiffness matrices (as well as the mass and damping matrices, and load vectors) reached by traditional practices.

Outline of paper. In Section 2 we discuss the theorem of expended power — the starting point of our formulation — in the context of discrete N-body systems; the treatment is extended in Section 3 to continua. Section 4 is devoted to the consequences to the second law of thermodynamics. In Section 5 we use the theorem of expended power to provide scalar description formalisms of Lagrangian, Hamiltonian, and total energy representations equivalent to the Cauchy equations of motion. The application of the proposed formulation to nonholonomic or nonconservative systems is the subject of Section 6. We turn in Section 7 to the space-discrete finite element formulation, both in the traditional approaches and in the new total energy approaches. Section 8 contains numerical examples and illustrations. An Appendix discusses in detail the space discretization via density formalisms and the finite element formulation.

2. N-body dynamical systems: theorem of expended power

For an illustration of the basic concepts, we focus first on a dynamical system of N particles moving in three-dimensional Euclidean space. Newton's equations of motion state that the rate of the total linear momentum of the constrained system is the total resultant acting on the system:

$$\boldsymbol{M}\ddot{\boldsymbol{x}} = \boldsymbol{F}_{\text{con}} + \boldsymbol{F}_{\text{nc}} + \boldsymbol{C}, \qquad \ddot{\boldsymbol{x}} = (\ddot{\boldsymbol{x}}^1, \dots, \ddot{\boldsymbol{x}}^i, \dots, \ddot{\boldsymbol{x}}^N) : \mathbb{I} \to \mathbb{R}^{3N}, \quad t \in \mathbb{I} = [t_1, t_2], \tag{1}$$

where $\ddot{\boldsymbol{x}}$ represents a set of $\ddot{\boldsymbol{x}}^i$ acceleration vectors of the particles, $\boldsymbol{M}$ the total diagonal mass matrix, $\boldsymbol{F}_{\text{con}} \in \mathbb{R}^3$ the total conservative force, $\boldsymbol{F}_{\text{nc}}(t) : \mathbb{I} \to \mathbb{R}^{3N}$, $t \in \mathbb{I} = [t_1, t_2]$ the total nonconservative force, and $\boldsymbol{C} \in \mathbb{R}^3$ the total constraint force. When the inertia term on the left-hand side of (1) is moved to the right, we have d'Alembert's principle, saying that the system is dynamically in equilibrium:

$$\boldsymbol{F}_{\text{con}} + \boldsymbol{F}_{\text{nc}}(t) + \boldsymbol{C} - \boldsymbol{M}\ddot{\boldsymbol{x}}(t) = 0. \tag{2}$$

We assume that the constraints are scleronomic (whether holonomic or not), confining the motion to a smooth surface. Then the constraint force is orthogonal to the velocity, which means it does not contribute to the virtual work. (Nonconservative forces are sometimes the result of nonholonomic constraints.)

Multiplying both sides of (2) by the velocity $\dot{x}(t) : \mathbb{I} \to \mathbb{R}^{3N}$, $t \in \mathbb{I} = [t_1, t_2]$ we have

$$\left(F_{\mathrm{con}} + F_{\mathrm{nc}}(t) - M\ddot{x}(t) \right) \cdot \dot{x}(t) = 0, \tag{3}$$

which can be recast as

$$\dot{x}(t) \cdot M\ddot{x} = F_{\mathrm{con}} \cdot \dot{x}(t) + F_{\mathrm{nc}}(t) \cdot \dot{x}(t). \tag{4}$$

By invoking the kinetic energy $\mathcal{K}(\dot{x}) : \mathbb{R}^3 \to \mathbb{R}$, the potential energy $\mathcal{U}(x) : \mathbb{R}^3 \to \mathbb{R}$, and the power input $\mathcal{P}_{\mathrm{input}}$ for the N-body system, Equation (4) can be expressed in terms of the total energy $\mathcal{E}(\dot{x}, x)$ as

$$\frac{d\mathcal{E}(\dot{x}, x)}{dt} = \mathcal{P}_{\mathrm{input}}, \qquad \mathcal{E}(\dot{x}, x) = \mathcal{K}(\dot{x}) + \mathcal{U}(x), \qquad \mathcal{P}_{\mathrm{input}} = F_{\mathrm{nc}}(t) \cdot \dot{x}(t), \tag{5}$$

where the kinetic energy and the potential energy are defined as

$$\mathcal{K}(\dot{x}) = \tfrac{1}{2}\dot{x}(t) \cdot M\dot{x}(t), \qquad F_{\mathrm{con}} = -\frac{\partial \mathcal{U}}{\partial x} = -\nabla \mathcal{U}(x). \tag{6}$$

Equation (5) corresponds to the principle of balance of energy for the N-body mechanical system.

Suppose the system is subject to k independent algebraic constraints. The constraints reduce the number of degrees of freedom to $n_{\mathrm{dof}} = 3N - k$, and can be written in terms of the positions of N particles as

$$f_i(x^1, \ldots, x^N) = 0, \quad i = 1, \ldots, k. \tag{7}$$

Invoking generalized coordinates $q = (q^1, \ldots, q^{n_{\mathrm{dof}}})$ belonging to a local configuration space $Q \subset \mathbb{R}^{n_{\mathrm{dof}}}$, the velocity in the Cartesian coordinate system can be expressed as

$$\dot{x}(q(x)) = \frac{\partial x}{\partial q} \cdot \dot{q}, \qquad q(x) = (q^1(x), \ldots, q^{n_{\mathrm{dof}}}(x)). \tag{8}$$

Then, (4) can be rewritten in terms of generalized velocities, as

$$(M\ddot{x} - F_{\mathrm{con}}) \cdot \frac{\partial x}{\partial q} \cdot \dot{q} = \mathcal{P}_{\mathrm{input}}. \tag{9}$$

This equation can be regarded as an analogue of the first form of the fundamental equation or d'Alembert's principle. We have

$$M\ddot{x} \cdot \frac{\partial x}{\partial q} = \frac{d}{dt}\left(M\dot{x} \cdot \frac{\partial x}{\partial q} \right) - M\dot{x} \cdot \frac{\partial \dot{x}}{\partial q} = \frac{d}{dt}\left(M\dot{x} \cdot \frac{\partial \dot{x}}{\partial \dot{q}} \right) - M\dot{x} \cdot \frac{\partial \dot{x}}{\partial q}. \tag{10}$$

In view of (6), we have the generalized force given as

$$Q = F_{\mathrm{con}} \cdot \frac{\partial x}{\partial q} = -\nabla \mathcal{U}(q). \tag{11}$$

In terms of the kinetic energy $\mathcal{K}(q, \dot{q})$ and potential energy $\mathcal{U}(q)$, Equation (9) can be rewritten as

$$\left(\frac{d}{dt} \frac{\partial \mathcal{K}(q, \dot{q})}{\partial \dot{q}} - \frac{\partial \mathcal{K}(q, \dot{q})}{\partial q} + \frac{\partial \mathcal{U}(q)}{\partial q} \right) \cdot \dot{q} = \mathcal{P}_{\mathrm{input}}. \tag{12}$$

If the system is scleronomic, the kinetic energy must be quadratic in the generalized velocities [Green-wood 1977] and have no explicit time dependence. As a consequence, in terms of the autonomous total energy, (12) gives

$$\left(\frac{d}{dt}\frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} + \frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} - 2\frac{\partial \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}}\right)\cdot \dot{\boldsymbol{q}} = \mathcal{P}_{\text{input}}, \tag{13}$$

and in terms of the autonomous Lagrangian $\mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}}) : TQ \to \mathbb{R}$, (12) also leads to

$$\left(\frac{d}{dt}\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} - \frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}}\right)\cdot \dot{\boldsymbol{q}} = \mathcal{P}_{\text{input}}. \tag{14}$$

Suppose that there is no external power input. Since the generalized velocities are arbitrary, the governing equations of motion can be obtained as

$$\frac{d}{dt}\frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} + \frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} - 2\frac{\partial \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} = 0 \quad \text{or} \quad \frac{d}{dt}\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} - \frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} = 0. \tag{15}$$

In the special case that the kinetic energy does not depend on the generalized coordinates, we have

$$\frac{d}{dt}\frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} + \frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} = 0. \tag{16}$$

Integrating both sides of (12) over the given time interval $\mathbb{I} = [t_1, t_2]$, we have

$$\int_{t_1}^{t_2}\left\{\frac{d}{dt}\left(\frac{\partial \mathcal{K}}{\partial \dot{\boldsymbol{q}}}\cdot \dot{\boldsymbol{q}} - \mathcal{K} + \mathcal{U}\right)\right\}dt = \int_{t_1}^{t_2}\mathcal{P}_{\text{input}}\,dt. \tag{17}$$

For conservative systems, we have no external power input. Then, (17) implies that

$$\left(\frac{\partial \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}}\cdot \dot{\boldsymbol{q}} - \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}}) + \mathcal{U}(\boldsymbol{q})\right)\bigg|_{t=t_1} = \left(\frac{\partial \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}}\cdot \dot{\boldsymbol{q}} - \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}}) + \mathcal{U}(\boldsymbol{q})\right)\bigg|_{t=t_2} = \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}}). \tag{18}$$

In terms of the Lagrangian, this equation can be rewritten as

$$\left(\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}}\cdot \dot{\boldsymbol{q}} - \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})\right)\bigg|_{t=t_1} = \left(\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}}\cdot \dot{\boldsymbol{q}} - \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})\right)\bigg|_{t=t_2} = \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}}). \tag{19}$$

The term in big parentheses, called Jacobi's integral [Pars 1965, p. 82; Greenwood 1977], is identical to the autonomous total energy, which remains constant. Within the Hamiltonian framework, the preceding equation can be rewritten as

$$\left(\boldsymbol{p}\cdot \dot{\boldsymbol{q}} - \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})\right)\big|_{t=t_1} = \left(\boldsymbol{p}\cdot \dot{\boldsymbol{q}} - \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})\right)\big|_{t=t_2} = \mathcal{H}(\boldsymbol{q},\boldsymbol{p}). \tag{20}$$

We thus arrive at the governing equations of motion in each of the three formalisms:

$$\frac{d\mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{dt} = \left(\frac{d}{dt}\frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} + \frac{\partial \mathcal{E}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} - 2\frac{\partial \mathcal{K}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}}\right)\cdot \dot{\boldsymbol{q}} = 0,$$

$$\frac{d}{dt}\left[\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}}\cdot \dot{\boldsymbol{q}} - \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})\right] = \left(\frac{d}{dt}\frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} - \frac{\partial \mathcal{L}(\boldsymbol{q},\dot{\boldsymbol{q}})}{\partial \boldsymbol{q}}\right)\cdot \dot{\boldsymbol{q}} = 0, \tag{21}$$

$$\frac{d\mathcal{H}(\boldsymbol{p},\boldsymbol{q})}{dt} = \left(\dot{\boldsymbol{p}} + \frac{\partial \mathcal{H}(\boldsymbol{p},\boldsymbol{q})}{\partial \boldsymbol{q}}\right)\cdot \dot{\boldsymbol{q}} - \left(\dot{\boldsymbol{q}} - \frac{\partial \mathcal{H}(\boldsymbol{p},\boldsymbol{q})}{\partial \boldsymbol{p}}\right)\cdot \dot{\boldsymbol{p}} = 0.$$

Integrating over time we reach the Galerkin time weighted-residual form for N-body dynamical systems under each formalism. For example, for the total energy formalism,

$$\int_{t_1}^{t_2} \left\{ \frac{d}{dt} \left(\frac{\partial \mathscr{E}(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} + \frac{\partial \mathscr{E}(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} - 2 \frac{\partial \mathscr{K}(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} \right) \cdot \dot{\boldsymbol{q}} \right\} dt = 0. \tag{22}$$

3. Continuous-body dynamical systems: theorem of expended power

The focus next is on elastodynamics, where a continuous body is parametrized by a simply connected and bounded open set $\mathscr{B}$, called the reference configuration, assumed to have a piecewise smooth boundary $\partial \mathscr{B}$. The smooth motion of the body may be described by a mapping $\boldsymbol{\varphi}(\boldsymbol{X}, t) : \mathscr{B} \times \mathbb{I} \to \mathbb{R}^3$ such that for each $t \in \mathbb{I}$ the restriction to $\mathscr{B} \times \{t\}$ is one-to-one and smooth; its image $\mathscr{S}$ for a given t is called the current configuration. The set of all such maps is called the configuration space:

$$\mathscr{C} = \left\{ \boldsymbol{\varphi}(\boldsymbol{X}, t) : \mathscr{B} \times \mathbb{I} \to \mathbb{R}^3 \mid \boldsymbol{\varphi} \text{ is of class } C^{2m} \ (m \geq 1) \text{ in } \boldsymbol{X} \text{ and } t, \ |\nabla \boldsymbol{\varphi}| > 0, \text{ and } \boldsymbol{\varphi}|_{\Gamma_{\partial \mathscr{B}_{\boldsymbol{\varphi}}}} = \overline{\boldsymbol{\varphi}} \right\}, \tag{23}$$

where $\overline{\boldsymbol{\varphi}}$ denotes the prescribed quantity on the prescribed-displacement boundary. Hence, continuous-body dynamical systems are holonomic. The configuration space is a smooth infinite-dimensional manifold. In the nonpolar case, when distributed body or surface couples are not prescribed, the power input $\mathscr{P}_{\text{input}}$ (the rate at which the external surface tractions and body forces are doing actual work) is defined as

$$\mathscr{P}_{\text{input}} = \int_{\mathscr{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\partial \mathscr{B}_{\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dA, \tag{24}$$

where $\rho_0(\boldsymbol{X}) : \mathscr{B} \to \mathbb{R}$ denotes the referential density, $\overline{\boldsymbol{T}}(\boldsymbol{X}, t) : \mathscr{B} \times \mathbb{I} \to \mathbb{R}^3$ the prescribed traction on the boundary $\partial \mathscr{B}$, $\boldsymbol{B}(\boldsymbol{X}, t) : \mathscr{B} \times \mathbb{I} \to \mathbb{R}^3$ the body force, and dA, dV the Lebesgue measures on the prescribed–traction boundary $\partial \mathscr{B}_{\sigma}$ and in the body $\mathscr{B}$. Notice that the body forces are not prescribed, and the external forces are not dead loads.

Next, invoking Cauchy's law $\overline{\boldsymbol{T}}(\boldsymbol{X}, t) = \boldsymbol{P}(\boldsymbol{X}, t) \cdot \hat{N}(\boldsymbol{X}, t)$ and Gauss's theorem, we rewrite (24) as

$$\mathscr{P}_{\text{input}} = \int_{\mathscr{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\mathscr{B}} \nabla \cdot (\boldsymbol{P} \cdot \dot{\boldsymbol{\varphi}}) \, dV, \tag{25}$$

where $\boldsymbol{P}(\boldsymbol{X}, t)$ denotes the first Piola–Kirchhoff stress tensor (see [Marsden and Hughes 1983], for example) in the reference configuration. Recall the product rule

$$\nabla \cdot (\boldsymbol{P} \cdot \dot{\boldsymbol{\varphi}}) = (\nabla \cdot \boldsymbol{P}) \cdot \dot{\boldsymbol{\varphi}} + \boldsymbol{P} \because (\nabla \dot{\boldsymbol{\varphi}}) = (\nabla \cdot \boldsymbol{P}) \cdot \dot{\boldsymbol{\varphi}} + \boldsymbol{P} \because \dot{\boldsymbol{F}}, \tag{26}$$

where $\dot{\boldsymbol{F}}$ denotes the total time derivative of the deformation gradient tensor, $\boldsymbol{F}$. Using (26), the power input can be expressed as

$$\mathscr{P}_{\text{input}} = \int_{\mathscr{B}} \left\{ \nabla \cdot \boldsymbol{P} + \rho_0 \boldsymbol{B}(\boldsymbol{X}, t) \right\} \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) dV + \int_{\mathscr{B}} \boldsymbol{P} \because \dot{\boldsymbol{F}} \, dV. \tag{27}$$

By virtue of Cauchy's equations of motion, the power input can be expressed as

$$\mathscr{P}_{\text{input}} = \int_{\mathscr{B}} \rho_0 \ddot{\boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\mathscr{B}} \boldsymbol{P} \because \dot{\boldsymbol{F}} \, dV. \tag{28}$$

The first term on the right is the rate of the system's kinetic energy; the second is known as the stress power. As a consequence of (24) and (28), we have the theorem of expended power [Gurtin 1972, p. 110]:

$$\frac{d\mathcal{K}}{dt} + \int_{\mathcal{B}} \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} \, dV = \int_{\mathcal{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dA. \tag{29}$$

This holds whether the system is mechanical or thermomechanical. In addition, by use of Cauchy's law, the theorem of expended power can be readily rewritten as the modified Bubnov–Galerkin weighted residual form [Mikhlin 1964]

$$\int_{\mathcal{B}} (\nabla \cdot \boldsymbol{P} + \rho_0 \boldsymbol{B} - \rho_0 \ddot{\boldsymbol{\varphi}}) \cdot \dot{\boldsymbol{\varphi}} \, dV + \int_{\partial \mathcal{B}_\sigma} (\overline{\boldsymbol{T}} - \boldsymbol{P} \cdot \hat{\boldsymbol{N}}) \cdot \dot{\boldsymbol{\varphi}} \, dA = 0, \tag{30}$$

where $\hat{\boldsymbol{N}}$ denotes the unit vector outward normal to the surface of the body. Thus, we observe that the theorem of expended power leads to the modified Bubnov–Galerkin weighted residual form, where the weighting function is the generalized velocity. Note that the traction boundary conditions (Cauchy's law) were applied to (24) and Cauchy's equations were imposed upon (27).

The first law of thermodynamics states that

$$\frac{d\mathcal{K}}{dt} + \frac{dU}{dt} =$$
$$\int_{\mathcal{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dA + \int_{\mathcal{B}} \rho_0 R(\boldsymbol{X}, t) \, dV - \int_{\mathcal{B}} \nabla \cdot \boldsymbol{Q}(\boldsymbol{X}, t) \, dV, \tag{31}$$

where U is the internal energy of the thermomechanical system, $\boldsymbol{Q}(\boldsymbol{X}, t) : \mathcal{B} \times \mathbb{I} \to \mathbb{R}^3$ the heat flux vector, and $R(\boldsymbol{X}, t) : \mathcal{B} \times \mathbb{I} \to \mathbb{R}$ the specific distributed internal heat supply. By Cauchy's law, (31) leads to

$$\int_{\mathcal{B}} (\rho_0 \ddot{\boldsymbol{\varphi}} - \nabla \cdot \boldsymbol{P} - \rho_0 \boldsymbol{B}) \cdot \dot{\boldsymbol{\varphi}} \, dV + \int_{\mathcal{B}} \left(\rho_0 \frac{\partial \bar{U}}{\partial t} - \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} - \rho_0 R + \nabla \cdot \boldsymbol{Q} \right) dV = 0, \tag{32}$$

which contains two governing equations: Cauchy's equations of motion and Kirchhoff's energy equations. Here $\bar{U}$ denotes the specific internal energy density in the reference configuration. Thus, for thermomechanical systems, the two governing equations are coupled; but for mechanical systems Kirchhoff's equation of energy implies that the rate of the internal energy is identical to the stress power, namely,

$$\rho_0 \frac{\partial \bar{U}}{\partial t} = \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}}. \tag{33}$$

Since the second integral in (32) vanishes owing to Kirchhoff's equation of energy, we obtain the Bubnov–Galerkin weighted residual form. Thus, we have the relation between the stress power and the specific internal energy density in mechanical systems as shown in (33).

4. Continuous-body dynamical systems and the second law of thermodynamics

According to the second law of thermodynamics, the rate of the total entropy of the thermomechanical system is equal to or greater than the entropy input rate:

$$\frac{d}{dt} \int_{\mathcal{B}} \rho_0(\boldsymbol{X}) S(\boldsymbol{X}, t) \, dV \geq \int_{\mathcal{B}} \rho_0(\boldsymbol{X}) \frac{R(\boldsymbol{X}, t)}{\Theta(\boldsymbol{X}, t)} \, dV - \int_{\partial \mathcal{B}} \frac{\hat{\boldsymbol{N}} \cdot \boldsymbol{Q}(\boldsymbol{X}, t)}{\Theta(\boldsymbol{X}, t)} \, dA, \tag{34}$$

where $S(X, t)$ is the specific entropy and $\Theta(X, t)$ is the absolute temperature. This relation is often called the Clausius–Duhem inequality. In an adiabatic process without heat sources, the total entropy should be nonnegative:

$$\frac{d}{dt} \int_{\mathcal{B}} \rho_0(X) S(X, t) \, dV \geq 0. \tag{35}$$

An application of Gauss's theorem yields the local form of the principle of entropy inequality:

$$\rho_0(X) \frac{\partial S(X, t)}{\partial t} - \rho_0(X) \frac{R(X, t)}{\Theta(X, t)} + \nabla \frac{Q(X, t)}{\Theta(X, t)} \geq 0. \tag{36}$$

The sum of terms on the left-hand side is the rate of entropy production. Use of Kirchhoff's equation of energy yields

$$\boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} - \rho_0 \frac{\partial \bar{U}}{\partial t} + \rho_0(X) \Theta(X, t) \frac{\partial S(X, t)}{\partial t} - \frac{\boldsymbol{Q}(X, t) \cdot \nabla \Theta(X, t)}{\Theta(X, t)} \geq 0. \tag{37}$$

Since the entropy production by heat flux should be positive [Coleman and Noll 1963], we have

$$-\frac{\boldsymbol{Q}(X, t) \cdot \nabla \Theta(X, t)}{\Theta(X, t)} \geq 0. \tag{38}$$

Hence (37) can be rewritten as

$$\mathscr{D}_{\text{int}} = \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} - \rho_0 \frac{\partial \bar{U}}{\partial t} + \rho_0(X) \Theta(X, t) \frac{\partial S(X, t)}{\partial t} \geq 0; \tag{39}$$

here $\mathscr{D}_{\text{int}}$, the internal dissipation, vanishes if and only if the process is reversible. In view of (39), for mechanical systems only, the internal dissipation can be rewritten as

$$\int_{\mathcal{B}} \mathscr{D}_{\text{int}} \, dV = \mathscr{P}_{\text{input}} - \frac{dE}{dt}, \tag{40}$$

where $E = \mathcal{K} + U$ is the sum of the kinetic energy and the internal energy. In the literature, E is called the total energy, but we reserve this term for a more comprehensive quantify; see (50).

In a thermomechanical system, the Helmholtz free energy Ψ satisfies

$$\frac{\partial \Psi}{\partial \Theta} = -S. \tag{41}$$

Via the Legendre transformation, this equation leads to the relation between the specific internal energy function and the Helmholtz free energy:

$$\bar{U}(\Phi, S) = \Psi(\Phi, \Theta) + \Theta S, \tag{42}$$

where Φ denotes an internal state variable. Substituting (42) into (39) leads to

$$\mathscr{D}_{\text{int}} = \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} - \rho_0 \frac{\partial \Psi}{\partial t} - \rho_0 S(X, t) \frac{\partial \Theta(X, t)}{\partial t} \geq 0. \tag{43}$$

In the case of no entropy production or in an isothermal process, this reduces to

$$\mathscr{D}_{\text{int}} = \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} - \rho_0 \frac{\partial \Psi}{\partial t} \geq 0. \tag{44}$$

In a thermodynamic process, a material whose mechanical behavior shows no internal dissipation, is called perfect [Truesdell and Noll 2004, p. 303]. Then, we have the equality

$$\mathcal{D}_{\text{int}} = \boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} - \rho_0 \frac{\partial \Psi}{\partial t} = 0. \tag{45}$$

The first Piola–Kirchhoff stress tensor is the thermodynamics force work-conjugate to the deformation gradient tensor:

$$\boldsymbol{P} = \rho_0 \frac{\partial \Psi(\boldsymbol{F})}{\partial \boldsymbol{F}}. \tag{46}$$

In a reversible process this equation also holds, so for mechanical systems we have

$$\boldsymbol{P} \cdot\cdot \dot{\boldsymbol{F}} = \rho_0 \frac{\partial \Psi}{\partial t} = \rho_0 \frac{\partial U}{\partial t} = \frac{\partial W}{\partial t}, \tag{47}$$

where W stands for the elastic potential energy. Regardless of whether the system is thermomechanical or mechanical, (29) can be written as

$$\frac{d\mathcal{K}}{dt} + \int_{\mathcal{B}} \rho_0 \frac{\partial \Psi}{\partial t} \, dV = \int_{\mathcal{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dA. \tag{48}$$

Thus the sum of the rate of the kinetic energy and the rate of the internal energy equals the power input.

5. The theorem of expended power and scalar description formalisms equivalent to the Cauchy equations of motion: continuous-body dynamical systems

Still under the assumption of scleronomic systems, the power input is

$$\mathcal{P}_{\text{input}} = \int_{\mathcal{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV + \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dA = -\frac{d\Pi_{\text{ext}}}{dt}. \tag{49}$$

In such a system the external loads, including surface tractions and body forces, are dead loads. Therefore, the system is conservative in the sense that the total energy, which we defined as the sum of the kinetic energy $\mathcal{K}(\dot{\boldsymbol{\varphi}}) : \boldsymbol{T}_\varphi \mathcal{C} \to \mathbb{R}$ and the total potential energy $\mathcal{U}(\boldsymbol{\varphi}) : \mathcal{C} \to \mathbb{R}$, is conserved. The body forces and tractions above are prescribed; as a result, external potential energies do exist. In view of (48) and (49), the theorem of expended power for perfect continuum materials has the following expression in terms of a naturally defined total energy:

$$\frac{d\mathcal{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}})}{dt} = 0, \qquad \mathcal{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) = \mathcal{K}(\dot{\boldsymbol{\varphi}}) + \mathcal{U}(\boldsymbol{\varphi}), \qquad \mathcal{U} = \Pi_{\text{int}} + \Pi_{\text{ext}}. \tag{50}$$

Here $\mathcal{U}$ denotes the total potential energy and the internal and external potential energy are defined as

$$\Pi_{\text{int}} = \int_{\mathcal{B}} \rho_0 \Psi(\boldsymbol{F}) \, dV, \qquad \Pi_{\text{ext}} = -\int_{\mathcal{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}(\boldsymbol{X}, t) \, dV - \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}(\boldsymbol{X}, t) \, dA, \tag{51}$$

where $\Psi(\boldsymbol{F})$ is the Helmholtz free energy per unit mass in homogeneous materials. The autonomous total energy is defined on the tangent bundle to the configuration space, $\boldsymbol{T}\mathcal{C} := \big\{ (\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) \mid \boldsymbol{\varphi} \in \mathcal{C}, \dot{\boldsymbol{\varphi}} \in \boldsymbol{T}_\varphi \mathcal{C} \big\}$, and can be written as

$$\mathcal{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) = \int_{\mathcal{B}} \overline{\overline{\mathcal{E}}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F}) \, dV - \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}(\boldsymbol{X}, t) \, dA, \tag{52}$$
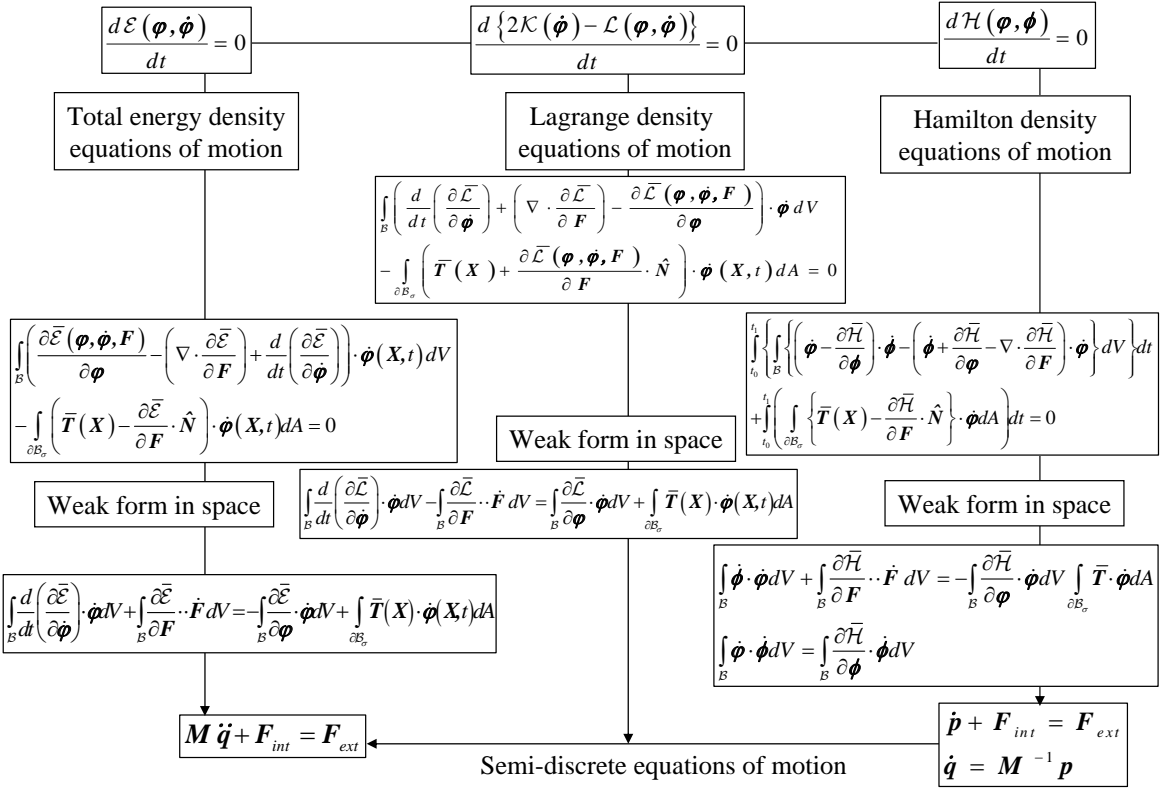
Figure 2. The theorem of expended power yields the strong and weak forms for elasto-dynamics; and their equivalence is shown within the Lagrangian, Hamiltonian, and Total Energy frameworks. (See also the Appendix.)

where the total energy density function $\overline{\mathcal{E}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F})$ is defined as

$$\overline{\mathcal{E}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F}) = \tfrac{1}{2}\rho_0 \dot{\boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} + \rho_0 \Psi(\boldsymbol{F}) - \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}. \tag{53}$$

Next, we derive the strong form representation from (50). We first give the scalar description formalism for deriving the total energy equation of motion from the theorem of expended power. By the chain rule, the rate of the total energy density function is

$$\frac{d\overline{\mathcal{E}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F})}{dt} = \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} + \frac{\partial \overline{\mathcal{E}}}{\partial \dot{\boldsymbol{\varphi}}} \cdot \ddot{\boldsymbol{\varphi}} + \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{F}} \cdots \dot{\boldsymbol{F}}. \tag{54}$$

The last term on the right can be represented as

$$\frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{F}} \cdots \dot{\boldsymbol{F}} = \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{F}} \cdots \nabla \dot{\boldsymbol{\varphi}} = \nabla \cdot \left(\dot{\boldsymbol{\varphi}} \cdot \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{F}} \right) - \left(\nabla \cdot \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{F}} \right) \cdot \dot{\boldsymbol{\varphi}}. \tag{55}$$

Besides, we have

$$\frac{\partial \overline{\mathcal{E}}}{\partial \dot{\boldsymbol{\varphi}}} \cdot \ddot{\boldsymbol{\varphi}} = \frac{d}{dt} \left(\frac{\partial \overline{\mathcal{E}}}{\partial \dot{\boldsymbol{\varphi}}} \cdot \dot{\boldsymbol{\varphi}} \right) - \frac{d}{dt} \left(\frac{\partial \overline{\mathcal{E}}}{\partial \dot{\boldsymbol{\varphi}}} \right) \cdot \dot{\boldsymbol{\varphi}} = \frac{d}{dt} \left(\frac{\partial \overline{\mathcal{E}}}{\partial \dot{\boldsymbol{\varphi}}} \right) \cdot \dot{\boldsymbol{\varphi}} \tag{56}$$

because the total energy density function is quadratic in $\dot{\boldsymbol{\varphi}}$. Substituting (55) and (56) into (54), we find

$$\frac{d\overline{\mathcal{E}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})}{dt} = \left(\frac{\partial\overline{\mathcal{E}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})}{\partial\boldsymbol{\varphi}} - \left(\nabla\cdot\frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\right) + \frac{d}{dt}\frac{\partial\overline{\mathcal{E}}}{\partial\dot{\boldsymbol{\varphi}}}\right)\cdot\dot{\boldsymbol{\varphi}} + \nabla\cdot\left(\dot{\boldsymbol{\varphi}}\cdot\frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\right). \tag{57}$$

By Gauss's theorem, the last term on the right yields

$$\int_{\mathcal{B}}\nabla\cdot\left(\dot{\boldsymbol{\varphi}}\cdot\frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\right)dV = \int_{\partial\mathcal{B}_\sigma}\dot{\boldsymbol{\varphi}}\cdot\frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\cdot\hat{\boldsymbol{N}}\,dA. \tag{58}$$

In view of (57) and (58), we obtain from (50)

$$\int_{\mathcal{B}}\left(\frac{\partial\overline{\mathcal{E}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})}{\partial\boldsymbol{\varphi}} - \left(\nabla\cdot\frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\right) + \frac{d}{dt}\frac{\partial\overline{\mathcal{E}}}{\partial\dot{\boldsymbol{\varphi}}}\right)\cdot\dot{\boldsymbol{\varphi}}(\boldsymbol{X},t)\,dV - \int_{\partial\mathcal{B}_\sigma}\left(\overline{\boldsymbol{T}}(\boldsymbol{X}) - \frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\cdot\hat{\boldsymbol{N}}\right)\cdot\dot{\boldsymbol{\varphi}}(\boldsymbol{X},t)\,dA = 0. \tag{59}$$

This equation takes the modified Bubnov–Galerkin weighted residual form [Mikhlin 1964] involving the strong form, namely, the governing equations and the natural boundary conditions are both included. Since the generalized velocities are arbitrary within the two open sets, we have the governing equations of motion in terms of the total energy density function as

$$\frac{d}{dt}\left(\frac{\partial\overline{\mathcal{E}}}{\partial\dot{\boldsymbol{\varphi}}}\right) = \left(\nabla\cdot\frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\right) - \frac{\partial\overline{\mathcal{E}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})}{\partial\boldsymbol{\varphi}}\quad\text{in } \boldsymbol{X}\in\mathcal{B}, \tag{60}$$

subject to the traction boundary condition

$$\overline{\boldsymbol{T}}(\boldsymbol{X}) - \frac{\partial\overline{\mathcal{E}}}{\partial\boldsymbol{F}}\cdot\hat{\boldsymbol{N}} = 0\quad\text{on } \boldsymbol{X}\in\partial\mathcal{B}_\sigma. \tag{61}$$

Within the Lagrangian framework, the theorem of expended power for perfect continuum materials reduces to

$$\frac{d\{2\mathcal{K}(\dot{\boldsymbol{\varphi}}) - \mathcal{L}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}})\}}{dt} = 0,\quad \mathcal{L}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}}) = \mathcal{K}(\dot{\boldsymbol{\varphi}}) - \mathcal{U}(\boldsymbol{\varphi}), \tag{62}$$

the term in braces being again Jacobi's integral. On the tangent bundle $T\mathcal{C} = \{(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}})\mid\boldsymbol{\varphi}\in\mathcal{C},\ \dot{\boldsymbol{\varphi}}\in T_\varphi\mathcal{C}\}$, the autonomous Lagrangian $\mathcal{L}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}}):T\mathcal{C}\to\mathbb{R}$ is defined as the kinetic energy minus the total potential energy, and so can be written

$$\mathcal{L}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}}) = \int_{\mathcal{B}}\overline{\mathcal{L}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})\,dV + \int_{\partial\mathcal{B}_\sigma}\overline{\boldsymbol{T}}(\boldsymbol{X})\cdot\boldsymbol{\varphi}(\boldsymbol{X},t)\,dA, \tag{63}$$

where the Lagrangian density function $\overline{\mathcal{L}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})$ is defined as

$$\overline{\mathcal{L}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F}) = \tfrac{1}{2}\rho_0\dot{\boldsymbol{\varphi}}\cdot\dot{\boldsymbol{\varphi}} - \rho_0\Psi(\boldsymbol{F}) + \rho_0\boldsymbol{B}(\boldsymbol{X})\cdot\boldsymbol{\varphi}. \tag{64}$$

Likewise, in terms of the Lagrangian density function, (62) can be rewritten as

$$\int_{\mathcal{B}}\left(\frac{d}{dt}\frac{\partial\overline{\mathcal{L}}}{\partial\dot{\boldsymbol{\varphi}}} + \nabla\cdot\frac{\partial\overline{\mathcal{L}}}{\partial\boldsymbol{F}} - \frac{\partial\overline{\mathcal{L}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})}{\partial\boldsymbol{\varphi}}\right)\cdot\dot{\boldsymbol{\varphi}}\,dV - \int_{\partial\mathcal{B}_\sigma}\left(\overline{\boldsymbol{T}}(\boldsymbol{X}) + \frac{\partial\overline{\mathcal{L}}(\boldsymbol{\varphi},\dot{\boldsymbol{\varphi}},\boldsymbol{F})}{\partial\boldsymbol{F}}\cdot\hat{\boldsymbol{N}}\right)\cdot\dot{\boldsymbol{\varphi}}(\boldsymbol{X},t)\,dA = 0. \tag{65}$$

Since the generalized velocities are arbitrary in the body and on the traction boundary surface, we have the governing equations in terms of the Lagrangian density function as

$$\frac{d}{dt}\frac{\partial \overline{\mathscr{L}}}{\partial \dot{\boldsymbol{\varphi}}} + \left(\nabla \cdot \frac{\partial \overline{\mathscr{L}}}{\partial \boldsymbol{F}}\right) - \frac{\partial \overline{\mathscr{L}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F})}{\partial \boldsymbol{\varphi}} = 0 \quad \text{in } \boldsymbol{X} \in \mathscr{B}, \tag{66}$$

subject to the traction boundary condition

$$\overline{\boldsymbol{T}}(\boldsymbol{X}) + \frac{\partial \overline{\mathscr{L}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F})}{\partial \boldsymbol{F}} \cdot \hat{\boldsymbol{N}} = 0 \quad \text{on } \boldsymbol{X} \in \partial \mathscr{B}_\sigma. \tag{67}$$

Equation (66) represents the Lagrangian density equations of motion, and is identical to Cauchy's equation of motion.

In addition, within the Hamiltonian framework involving the canonical momentum as a new dependent variable $\boldsymbol{\phi} \in T_\varphi^* \mathscr{C}$ belonging to the cotangent space, we have

$$\boldsymbol{\phi} = \frac{\partial \overline{\mathscr{L}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F})}{\partial \dot{\boldsymbol{\varphi}}} = \rho_0 \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t). \tag{68}$$

In view of this, we may define the Hamiltonian density function via the Legendre transformation

$$\overline{\mathscr{H}}(\boldsymbol{\varphi}, \boldsymbol{\phi}, \boldsymbol{F}) = \boldsymbol{\phi} \cdot \dot{\boldsymbol{\varphi}} - \overline{\mathscr{L}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F}), \tag{69}$$

where the Hamiltonian density function in view of (64) is given by

$$\overline{\mathscr{H}}(\boldsymbol{\varphi}, \boldsymbol{\phi}, \boldsymbol{F}) = \frac{1}{2\rho_0}\boldsymbol{\phi} \cdot \boldsymbol{\phi} + \rho_0 \Psi(\boldsymbol{F}) - \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}. \tag{70}$$

On the cotangent bundle (phase space) $T^*\mathscr{C} = \{(\boldsymbol{\varphi}, \boldsymbol{\phi}) \mid \boldsymbol{\varphi} \in \mathscr{C} \text{ and } \boldsymbol{\phi} \in T_\varphi^*\mathscr{C}\}$, an infinite-dimensional space, the autonomous Hamiltonian $\mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi}) : T^*\mathscr{C} \to \mathbb{R}$ can be defined as

$$\mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi}) = \int_\mathscr{B} \overline{\mathscr{H}}(\boldsymbol{\varphi}, \boldsymbol{\phi}, \boldsymbol{F})\, dV - \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}(\boldsymbol{X}, t)\, dA, \tag{71}$$

where the external forces are dead loads. Then, the theorem of expended power for perfect continuum materials yields

$$\frac{d\mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi})}{dt} = 0, \qquad \mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi}) = \mathscr{K}(\boldsymbol{\phi}) + \mathscr{U}(\boldsymbol{\varphi}). \tag{72}$$

For conservative systems, the Hamiltonian is the kinetic energy plus the total potential energy, just like the total energy that we previously described. However, the preceding equation is true if and only if the continuous-body dynamical system is scleronomic (otherwise, the Hamiltonian is not the total energy). In terms of the Hamiltonian density function, (72) can be rewritten as

$$\frac{d\mathscr{H}}{dt} = \int_\mathscr{B} \left(\left(\dot{\boldsymbol{\phi}} + \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\varphi}} - \nabla \cdot \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{F}} \right) \cdot \frac{d\boldsymbol{\varphi}}{dt} + \left(\frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\phi}} - \dot{\boldsymbol{\varphi}} \right) \cdot \frac{d\boldsymbol{\phi}}{dt} \right) dV - \int_{\partial \mathscr{B}_\sigma} \left(\overline{\boldsymbol{T}}(\boldsymbol{X}) - \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{F}} \cdot \hat{\boldsymbol{N}} \right) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t)\, dA$$

$$= 0. \tag{73}$$

In the Hamiltonian framework, generalized coordinates and generalized momentum are arbitrary. We readily observe that the rate of the autonomous Hamiltonian contains the strong form, namely, the Hamiltonian version of Cauchy's equations of motion and the traction boundary conditions:

$$\dot{\boldsymbol{\phi}} = -\frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\varphi}} + \left(\nabla \cdot \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{F}} \right), \qquad \dot{\boldsymbol{\varphi}} = \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\phi}} \quad \text{in } \boldsymbol{X} \in \mathscr{B} \tag{74}$$

subject to the traction boundary condition

$$\overline{\boldsymbol{T}}(\boldsymbol{X}) - \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{F}} \cdot \hat{\boldsymbol{N}} = 0 \quad \text{on} \quad \boldsymbol{X} \in \partial \mathscr{B}_\sigma. \tag{75}$$

Equation (74) represents the Hamiltonian density equations of motion; they are differential equations of the first order in time.

6. Application of the proposed formulation to nonholonomic/nonconservative systems

The rate of the total energy, Jacobi integral, and Hamiltonian presented in (50), (62) and (72), respectively, reflects geometric nonlinearity. However, when the material undergoes contact or impact deformation, the system is no longer holonomic due to nonlinear contact boundary conditions. Furthermore, if the external tractions are not dead loads and the body forces are prescribed, an external potential energy for the tractions cannot be defined and the system is no longer conservative. (The external potential energy for the body forces can still be defined).

For nonconservative systems (using elastoplastic contact/impact problems as an illustration), with time-independent body forces, the theorem of expended power for perfect materials leads to

$$\frac{d\mathscr{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}})}{dt} = \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}} \, dA, \qquad \mathscr{E} = \mathscr{K}(\dot{\boldsymbol{\varphi}}) + \mathscr{U}(\boldsymbol{\varphi}), \qquad \mathscr{U} = \Pi_{\text{int}} + \Pi_{\text{ext}} \tag{76}$$

with

$$\Pi_{\text{int}} = \int_{\mathscr{B}} \rho_0 \frac{\partial \Psi}{\partial t} \, dV, \qquad \Pi_{\text{ext}} = -\int_{\mathscr{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}(\boldsymbol{X}, t) \, dV;$$

that is, the autonomous total energy $\mathscr{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) : T\mathscr{C} \to \mathbb{R}$ is given by

$$\mathscr{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) = \int_{\mathscr{B}} \overline{\mathscr{E}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F}) \, dV, \qquad \overline{\mathscr{E}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F}) = \tfrac{1}{2} \rho_0 \dot{\boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} + \rho_0 \Psi(\boldsymbol{F}) - \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}. \tag{77}$$

External potential energies do not exist in the case of nonconservative forces; accordingly, the total energy in (76) is not conserved. Note that the total energy in (77) differs from the one in (52) in that the traction depends on time.

In the Lagrangian framework, the theorem of expended power for perfect materials becomes

$$\frac{d}{dt} \left[\int_{\mathscr{B}} \left(\frac{\partial \overline{\mathscr{L}}}{\partial \dot{\boldsymbol{\varphi}}} \cdot \dot{\boldsymbol{\varphi}} - \overline{\mathscr{L}} \right) dV \right] = \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}} \, dA, \quad \mathscr{L}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) = \mathscr{K}(\dot{\boldsymbol{\varphi}}) - \mathscr{U}(\boldsymbol{\varphi}), \quad \mathscr{U} = \Pi_{\text{int}} + \Pi_{\text{ext}} \tag{78}$$

with

$$\Pi_{\text{int}} = \int_{\mathscr{B}} \rho_0 \frac{\partial \Psi}{\partial t} \, dV, \qquad \Pi_{\text{ext}} = -\int_{\mathscr{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi} \, dV,$$

that is, the autonomous Lagrangian $\mathscr{L}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) : T\mathscr{C} \to \mathbb{R}$ is given by

$$\mathscr{L}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}) = \int_{\mathscr{B}} \overline{\mathscr{L}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F})\, dV, \qquad \overline{\mathscr{L}}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}}, \boldsymbol{F}) = \tfrac{1}{2}\rho_0 \dot{\boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} - \rho_0 \Psi(\boldsymbol{F}) + \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}. \tag{79}$$

Jacobi's integral of the system in (78) is not conserved. Note that the Lagrangian in (79) is different from the one in (63).

Finally, in the Hamiltonian framework, the theorem of expended power for perfect materials becomes

$$\frac{d\mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi})}{dt} = \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}\, dA, \qquad \mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi}) = \mathscr{K}(\boldsymbol{\phi}) + \mathscr{U}(\boldsymbol{\varphi}), \qquad \mathscr{U} = \Pi_{\text{int}} + \Pi_{\text{ext}}, \tag{80}$$

with

$$\Pi_{\text{int}} = \int_{\mathscr{B}} \rho_0 \frac{\partial \Psi}{\partial t}\, dV, \qquad \Pi_{\text{ext}} = -\int_{\mathscr{B}} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}(\boldsymbol{X}, t)\, dV;$$

that is, the autonomous Hamiltonian $\mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi}) : T^*\mathscr{C} \to \mathbb{R}$ is given by

$$\mathscr{H}(\boldsymbol{\varphi}, \boldsymbol{\phi}) = \int_{\mathscr{B}} \overline{\mathscr{H}}(\boldsymbol{\varphi}, \boldsymbol{\phi}, \boldsymbol{F})\, dV, \qquad \overline{\mathscr{H}}(\boldsymbol{\varphi}, \boldsymbol{\phi}, \boldsymbol{F}) = \frac{1}{2\rho_0}\boldsymbol{\phi} \cdot \boldsymbol{\phi} + \rho_0 \Psi(\boldsymbol{F}) - \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \boldsymbol{\varphi}. \tag{81}$$

For continuum dynamical systems with nonholonomic scleronomic constraints, the rate of the total energy, Jacobi's integral, and Hamiltonian is given by

$$\int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}\, dA + \int_{\partial \mathscr{B}_{\sigma_c}} \boldsymbol{\lambda} \cdot \frac{d\boldsymbol{g}}{dt}\, dA, \tag{82}$$

rather than 0 as in (50), (62) and (72). Here $\boldsymbol{\lambda}$ is the Lagrange multiplier, $\boldsymbol{g}$ is the impenetrability condition, and $\partial \mathscr{B}_{\sigma_c}$ is the contact boundary surface.

We briefly discuss next the elastoplastic contact/impact finite element formulation in the context of the total energy framework with the theorem of expended power. An illustrative example will demonstrate the applicability of the proposed formulation to a wide range of continuum-dynamic problems.

Suppose that we consider two bodies $\mathscr{B}^A$, $\mathscr{B}^B$ that are in contact: that is, the reference configuration is the open set $\mathscr{B} = \mathscr{B}^A \cup \mathscr{B}^B$, with $\partial \mathscr{B} = \partial \mathscr{B}^A \cup \partial \mathscr{B}^B$. The external loads are assumed to be dead loads. Each body has its own contact boundary surface respectively, namely, $\partial_{\sigma_c}\mathscr{B} = \partial_{\sigma_c}\mathscr{B}^A \cup \partial_{\sigma_c}\mathscr{B}^B$. As a salient feature of contact/impact problems, an impenetrability condition is imposed on the contact boundary surface, characterizing the contact boundary conditions as unknown and not prescribed. The impenetrability condition on the contact surface $\partial_{\sigma_c}\mathscr{B}^A$ can be written as

$$\big(\boldsymbol{\varphi}(\boldsymbol{X}_c^A, t) - \boldsymbol{\varphi}(\boldsymbol{X}_c^B, t)\big) \cdot \hat{\boldsymbol{N}}_c^A(\boldsymbol{X}_c^A, t) = 0, \tag{83}$$

where $\boldsymbol{\varphi}(\boldsymbol{X}_c^A, t) = \boldsymbol{X}_c^A + \boldsymbol{U}(\boldsymbol{X}_c^A, t)$, $\boldsymbol{U}(\boldsymbol{X}_c^A, t)$ being the displacement of the contact point on the body $\mathscr{B}^A$, and $\hat{\boldsymbol{N}}_c^A(\boldsymbol{X}_c^A, t)$ is the unit outward vector normal to the contact surface of $\mathscr{B}^A$.

In order to have an unconstrained variational formulation, we briefly consider the Lagrange multiplier method and the penalty method. For further details, see [Laursen 2002; Wriggers 2006].

In view of (83), the Lagrange multiplier method [Papadopoulos et al. 1995] leads to the following value for the rate of the total energy, Jacobi's integral, and Hamiltonian:

$$\int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}\, dA + \int_{\partial \mathscr{B}_c} \boldsymbol{\lambda} \cdot \hat{\boldsymbol{N}}_c^B(\boldsymbol{X}_c^A, t) \cdot \big(\dot{\boldsymbol{\varphi}}(\boldsymbol{X}_c^A, t) - \dot{\boldsymbol{\varphi}}(\boldsymbol{X}_c^B, t)\big)\, dA, \tag{84}$$

where $\boldsymbol{\lambda}$ is the Lagrange multiplier corresponding to the contact force vector.

In the penalty method, fairly popular in commercial hydro codes [Hallquist 1998; ABAQUS 2002], the impenetrability condition on the contact surface can be rewritten in terms of the stress tensor as

$$\left(\boldsymbol{P}_c^A(\boldsymbol{X}_c^A, t) - \boldsymbol{P}_c^B(\boldsymbol{X}_c^B, t)\right) \cdot \hat{\boldsymbol{N}}_c^A(\boldsymbol{X}_c^A, t) = \boldsymbol{T}_c^A(\boldsymbol{X}_c^A, t) + \boldsymbol{T}_c^B(\boldsymbol{X}_c^B, t) = 0, \tag{85}$$

where $\boldsymbol{P}_c^A(\boldsymbol{X}_c^A, t)$, $\boldsymbol{P}_c^B(\boldsymbol{X}_c^B, t)$ are the first Piola–Kirchhoff stress tensors and $\boldsymbol{T}_c^A(\boldsymbol{X}_c^A, t)$, $\boldsymbol{T}_c^B(\boldsymbol{X}_c^B, t)$ are the contact tractions, which can be calculated by use of some appropriate penalty parameter [Hallquist et al. 1985]. Then, Equation (84) for contact-impact problems with nonholonomic constraints gives the following value for the rate of the total energy, Jacobi's integral, and Hamiltonian:

$$\int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}} \, dA + \int_{\partial \mathcal{B}_c} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\boldsymbol{\varphi}} \, dA, \tag{86}$$

where $\boldsymbol{P}^A = -\overline{\mathscr{L}}/\partial \boldsymbol{F} = \overline{\mathscr{E}}/\partial \boldsymbol{F} = \overline{\mathscr{H}}/\partial \boldsymbol{F}$ on $\partial_{\sigma_c} \mathcal{B}^A$ and $\boldsymbol{P}^B = -\overline{\mathscr{L}}/\partial \boldsymbol{F} = \overline{\mathscr{E}}/\partial \boldsymbol{F} = \overline{\mathscr{H}}/\partial \boldsymbol{F}$ on $\partial_{\sigma_c} \mathcal{B}^B$, and $\hat{\boldsymbol{N}}_c^A = -\hat{\boldsymbol{N}}_c^B$.

If frictional contact on the contact surface is considered, the frictional contact force should be included in the external force on the right hand side. The contact forces can be obtained by several methods; for example we can consider the master-slave sideline algorithm [Hallquist et al. 1985] in the penalty method or the Lagrange multiplier in the Lagrange multiplier method [Papadopoulos et al. 1995].

Next, we often encounter material nonlinearity in contact/impact problems or in finite deformation problems [Simo and Hughes 1998]. For convenience, we consider hyperelastic-plastic material behavior [Belytschko et al. 2000; Simo and Hughes 1998], because we have used the total Lagrangian description [Hibbitt et al. 1970] in this work. From a phenomenological viewpoint, the multiplicative decomposition of the deformation gradient tensor [Lee and Liu 1967; Lee 1969; Simo and Hughes 1998; Nemat-Nasser 1982; Asaro and Lubarda 2006] has been used in the context of not only phenomenological polycrystalline plasticity, but also single crystal metal plasticity as follows:

$$\boldsymbol{F}(\boldsymbol{X}, t) = \boldsymbol{F}^e(\boldsymbol{X}, t) \cdot \boldsymbol{F}^p(\boldsymbol{X}, t). \tag{87}$$

This motivates one to introduce the intermediate configuration $\overline{\mathcal{B}}$ between the reference configuration $\mathcal{B}$ and the current configuration $\mathcal{S}$. In (87) the plastic part of the total deformation gradient tensor $\boldsymbol{F}^p(\boldsymbol{X}, t)$ characterizes the plastic flow in the body, while the elastic part $\boldsymbol{F}^p(\boldsymbol{X}, t)$ is the portion caused by stretching and rotation of the crystal lattice. The first Piola–Kirchhoff stress tensor in the intermediate configuration is

$$\bar{\boldsymbol{P}} = -\frac{\partial \overline{\mathscr{L}}}{\partial \boldsymbol{F}^e} = \frac{\partial \overline{\mathscr{E}}}{\partial \boldsymbol{F}^e} = \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{F}^e} = \rho_0 \frac{\partial \overline{\Psi}(\boldsymbol{F}^e)}{\partial \boldsymbol{F}^e} = \boldsymbol{F}^e \bar{\boldsymbol{S}}, \tag{88}$$

where $\bar{\boldsymbol{S}}$ stands for the second Piola–Kirchhoff stress tensor in the intermediate configuration. Then, the relation of the stress tensors between configurations can be obtained by the push-forward or pull-back operations. For instance, the second Piola–Kirchhoff stress tensor in the reference configuration is

$$\boldsymbol{S} = \boldsymbol{F}^{p-1} \bar{\boldsymbol{S}} \cdot \boldsymbol{F}^{p-T} = \boldsymbol{F}^{-1} \boldsymbol{P}. \tag{89}$$

In general, the radial return mapping scheme, as a stress update algorithm [Simo and Hughes 1998], can be employed to find the stress on the yield surface at every time step. Therefore, the internal force can be calculated by use of the updated stress.

7. Space-discrete finite element formulation in the three formalisms

We now present a novel numerical discretization approach that is significantly different from traditional practices for transient/dynamic applications. We must start by saying that from a practical point of view, it is impossible to choose the admissible trial functions satisfying both the natural boundary conditions (traction boundary conditions) and the essential boundary conditions. The weighted residual forms without natural boundary conditions are difficult to apply in practice, because the trial functions must satisfy both the essential and natural boundary conditions. The trial functions must fulfill this requirement because in the use of the weighted residual form the errors should be minimized in the satisfaction of the differential equations (governing equations) and boundary conditions. If the weighted residual form is given by the governing equations only, there is no mechanism by which errors in the satisfaction of the boundary conditions would be minimized. However, as shown in (59), (65) and (73), the rate of the total energy, Jacobi integral, and Hamiltonian presented in (50), (62) and (72) contains the weighted residual forms in terms of the governing equation and natural boundary conditions. Hence, as in the Ritz solution, which operates on the functional corresponding to the problem, the natural boundary conditions are contained implicitly in the functional; the rate equation contains implicitly both the governing equations and natural boundary conditions. In that sense, therefore, there is a mechanism by which the errors in the satisfaction of the governing equations and natural boundary conditions are minimized, when substituting the trial functions into the rate of the total energy, Jacobi integral, or Hamiltonian to discretize the space [Bathe 1982, p. 108; Cook et al. 2002, p. 136; Zienkiewicz et al. 2005, p. 61; Reddy 2006, p. 74]. As a consequence, the errors in the satisfaction of (59), (65) and (73) could be minimized by making use of the admissible trial functions satisfying the essential boundary conditions. Firstly, focusing on the total energy framework and the Lagrangian framework, the admissible trial functions $\tilde{\boldsymbol{\varphi}}$ are required to be piecewise continuous, but they should be continuous along the interelement boundaries. They may be represented by a linear combination of coordinate functions $N_i^h(X)$ and generalized coordinates $\tilde{\boldsymbol{\varphi}}_i^h(t)$:

$$
\begin{aligned}
\tilde{\boldsymbol{\varphi}}(X,t) &\equiv \tilde{\boldsymbol{\varphi}}^h(X,t) = \sum_{i=1}^{n_{\text{node}}} N_i^h(X)\tilde{\boldsymbol{\varphi}}_i^h(t) = \boldsymbol{N}\boldsymbol{q}, \\
\boldsymbol{q}(t) &= \left\{\tilde{\boldsymbol{\varphi}}_1^h(t)\dots\tilde{\boldsymbol{\varphi}}_{n_{\text{node}}}^h(t)\right\}^T \in Q \subset \mathbb{R}^{n_{\text{dof}}=3n_{\text{node}}}, \quad \boldsymbol{M} = \int_{\mathcal{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{N}\, dV.
\end{aligned}
\tag{90}
$$

Note that the trial functions depend on space and time.

In the Hamiltonian framework, the admissible trial functions $\tilde{\boldsymbol{\varphi}}$ and $\tilde{\boldsymbol{\phi}}$ are required to be piecewise continuous, but they must be continuous along the interelement boundaries. They may be represented by a combination of interpolation functions and nodal variables:

$$
\begin{aligned}
\tilde{\boldsymbol{\varphi}}(X,t) = \tilde{\boldsymbol{\varphi}}^h(X,t) = \sum_{i=1}^{n_{\text{node}}} N_i^h(X)\tilde{\boldsymbol{\varphi}}_i^h(t) = \boldsymbol{N}\boldsymbol{q}, \quad \tilde{\boldsymbol{\phi}}(X,t) = \tilde{\boldsymbol{\phi}}^h(X,t) = \sum_{i=1}^{n_{\text{node}}} N_i^h(X)\tilde{\boldsymbol{\phi}}_i^h(t) = \rho_0 \boldsymbol{N}\dot{\boldsymbol{q}}, \\
\boldsymbol{q}(t) = \left\{\tilde{\boldsymbol{\varphi}}_1^h(t)\dots\tilde{\boldsymbol{\varphi}}_{n_{\text{node}}}^h(t)\right\}^T \in Q \subset \mathbb{R}^{3n_{\text{node}}}, \quad \boldsymbol{p}(t) = \boldsymbol{M}\dot{\boldsymbol{q}}(t) \in T_q^* Q \subset \mathbb{R}^{3n_{\text{node}}}, \quad \boldsymbol{M} = \int_{\mathcal{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{N}\, dV.
\end{aligned}
\tag{91}
$$

In continuum dynamics, a body can be approximated by a finite number of subdomains, say finite elements. Therefore, the whole domain is assumed to consist of an assemblage of finite elements. Directly starting the discretization process via the rate given in (50), (62) and (72), we may choose the same admissible trial functions in (90) and (91) as the assumed displacement field functions, without involving

test or weighting functions when the discrete total energy or Lagrangian differential operator, which is discussed below, is employed to obtain the semidiscrete second order in time differential equations.

In addition, we may choose the same admissible trial functions in (91) as the assumed displacement and canonical momentum field functions, without involving test or weighting functions when the discrete Hamiltonian differential operator, which is also discussed below, is employed to obtain the semidiscrete first order in time differential equations. For simplicity, we introduce a phase space with generalized coordinates and canonical momenta, denoted by $T^*Q = \bigcup_{q \in Q} T_q^* Q$, that is,

$$T^*Q := \left\{ (\boldsymbol{q}, \boldsymbol{p}) \; \middle| \; \begin{array}{l} \boldsymbol{q}(t) = \left\{ \tilde{\boldsymbol{\varphi}}_1^h(t) \ldots \tilde{\boldsymbol{\varphi}}_{n_{\text{node}}}^h(t) \right\}^T \in Q \subset \mathbb{R}^{n_{\text{dof}} = 3n_{\text{node}}}, \\ \boldsymbol{p}(t) = \boldsymbol{M} \dot{\boldsymbol{q}}(t) \in T_q^* Q \subset \mathbb{R}^{n_{\text{dof}} = 3n_{\text{node}}}, \quad \boldsymbol{M} = \int_{\mathcal{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{N} \, dV \end{array} \right\}. \tag{92}$$

Upon substituting (90) into (50), the rate of the total energy can be discretized in space as follows

$$\frac{d\mathcal{E}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h)}{dt} = \frac{d}{dt} \left\{ \int_{\mathcal{B}} \rho_0 \dot{\tilde{\boldsymbol{\varphi}}}^h \cdot \dot{\tilde{\boldsymbol{\varphi}}}^h \, dV - \mathcal{L}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h) \right\} = 0, \tag{93}$$

where the autonomous space-discrete total energy for finite-dimensional systems is given by

$$\mathcal{E}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h) = \int_{\mathcal{B}} \overline{\mathcal{E}}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h, \tilde{\boldsymbol{F}}^h) \, dV - \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(X) \cdot \tilde{\boldsymbol{\varphi}}^h(X, t) \, dA = \mathcal{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}}), \tag{94}$$
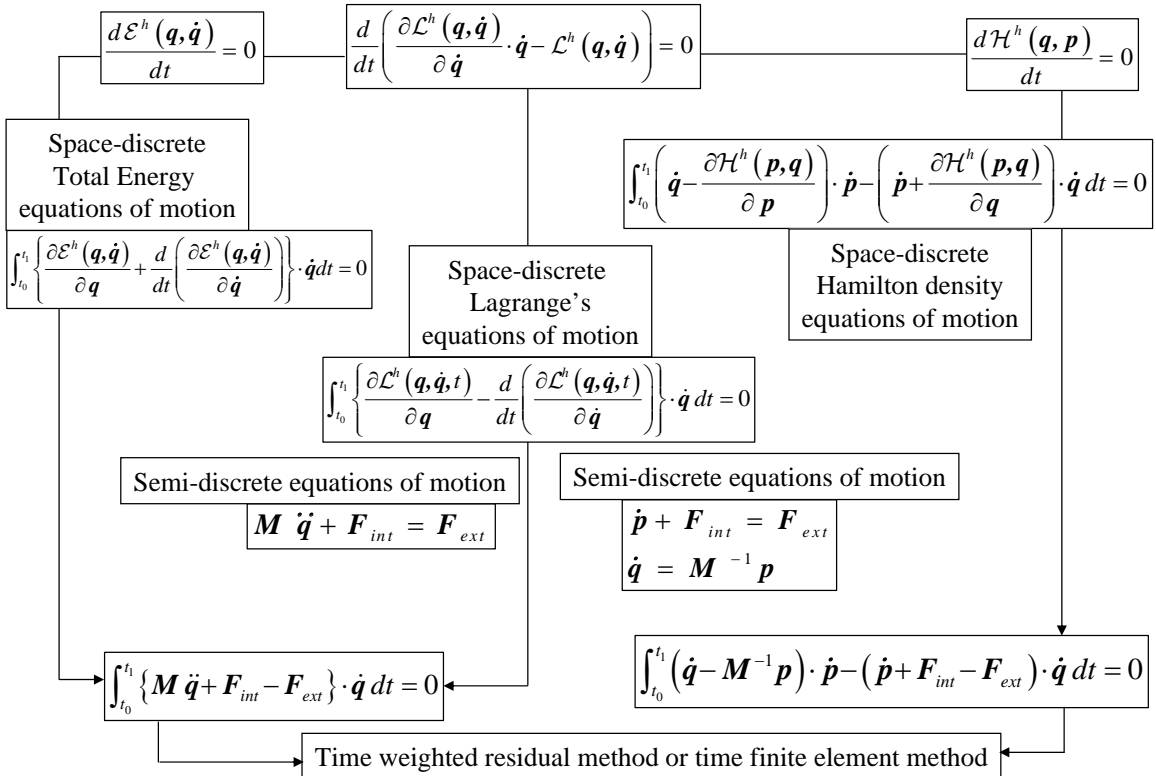

Figure 3. Space-discrete finite element formulation in the Lagrangian, Hamiltonian, and Total Energy frameworks, and their equivalence.

while the autonomous space-discrete Lagrangian for finite-dimensional systems is simply constructed as

$$\mathscr{L}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h) = \int_{\mathscr{B}} \overline{\mathscr{L}}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h, \tilde{\boldsymbol{F}}^h)\, dV + \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\tilde{\boldsymbol{\varphi}}}^h(\boldsymbol{X}, t)\, dA = \mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}}). \tag{95}$$

In terms of generalized coordinates within the total energy framework, (93) can be rewritten as

$$\frac{d\mathscr{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{dt} = \left\{ \frac{\partial \mathscr{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} + \frac{d}{dt}\left(\frac{\partial \mathscr{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} \right) \right\} \cdot \dot{\boldsymbol{q}} = 0, \tag{96}$$

where the space-discrete total energy in the direct notation is given by

$$\mathscr{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \tfrac{1}{2}\dot{\boldsymbol{q}} \cdot \boldsymbol{M}\dot{\boldsymbol{q}} + \Pi_{\text{int}}^h - \boldsymbol{q} \cdot \boldsymbol{F}_{\text{ext}}, \qquad \Pi_{\text{int}}^h = \int_{\mathscr{B}} \rho_0 \Psi(\boldsymbol{F}^h)\, dV \qquad \boldsymbol{M} = \int_{\mathscr{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{N}\, dV,$$

$$\frac{\partial \mathscr{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} = \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} \qquad \boldsymbol{F}_{\text{int}} = \int_{\mathscr{B}} \bar{\boldsymbol{B}}^T \boldsymbol{P}\, dV, \qquad \boldsymbol{F}_{\text{ext}} = \int_{\mathscr{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{B}\, dV + \int_{\partial \mathscr{B}_\sigma} \boldsymbol{N}^T \overline{\boldsymbol{T}}\, dA, \tag{97}$$

where $\bar{\boldsymbol{B}}$ denotes the strain matrix and $\boldsymbol{N}$ the interpolation matrix.

Within the Lagrangian framework, in lieu of (96), we have

$$\frac{d}{dt}\left\{ \frac{\partial \mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} \cdot \dot{\boldsymbol{q}} - \mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}}) \right\} = \left\{ \frac{\partial \mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} - \frac{d}{dt}\left(\frac{\partial \mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \dot{\boldsymbol{q}}} \right) \right\} \cdot \dot{\boldsymbol{q}}(t) = 0, \tag{98}$$

where the space-discrete autonomous Lagrangian is constructed as follows

$$\mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}}) = \tfrac{1}{2}\dot{\boldsymbol{q}} \cdot \boldsymbol{M}\dot{\boldsymbol{q}} - \Pi_{\text{int}}^h + \boldsymbol{q} \cdot \boldsymbol{F}_{\text{ext}}, \qquad \Pi_{\text{int}}^h = \int_{\mathscr{B}} \rho_0 \Psi(\boldsymbol{F}^h)\, dV, \qquad \boldsymbol{M} = \int_{\mathscr{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{N}\, dV,$$

$$\frac{\partial \mathscr{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial \boldsymbol{q}} = \boldsymbol{F}_{\text{ext}} - \boldsymbol{F}_{\text{int}}, \qquad \boldsymbol{F}_{\text{int}} = \int_{\mathscr{B}} \bar{\boldsymbol{B}}^T \boldsymbol{P}\, dV, \qquad \boldsymbol{F}_{\text{ext}} = \int_{\mathscr{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{B}\, dV + \int_{\partial \mathscr{B}_\sigma} \boldsymbol{N}^T \overline{\boldsymbol{T}}\, dA. \tag{99}$$

The admissible trial functions we used previously to discretize the rate of the total energy or Jacobi's integral are of class $C^{m-1}(\mathscr{B})$, like the trial functions applied to the principle of virtual work in (A.3). Because Equations (96) and (98) are equivalent to the discretization of the principle of virtual work in (A.3), discretizing the rate of the total energy or Jacobi's integral via admissible trial functions leads to the minimization of the errors arising from imposing the admissible trial functions into the weak form.

We next consider the Hamiltonian framework. Upon substituting (91) into (72), the rate of the Hamiltonian can be discretized in space as follows

$$\frac{d\mathscr{H}^h(\tilde{\boldsymbol{\varphi}}^h, \tilde{\boldsymbol{\varphi}}^h)}{dt} = 0, \tag{100}$$

where the space-discrete autonomous Hamiltonian for finite-dimensional systems can be simply constructed utilizing the Hamiltonian density function:

$$\mathscr{H}^h(\tilde{\boldsymbol{\varphi}}^h, \tilde{\boldsymbol{\varphi}}^h) = \int_{\mathscr{B}} \overline{\mathscr{H}}^h(\tilde{\boldsymbol{\varphi}}^h, \tilde{\boldsymbol{\varphi}}^h, \boldsymbol{F}^h)\, dV - \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \tilde{\boldsymbol{\varphi}}^h(\boldsymbol{X}, t)\, dA = \mathscr{H}^h(\boldsymbol{q}, \boldsymbol{p}). \tag{101}$$

In terms of the generalized coordinates and canonical momenta, (100) can be rewritten as

$$\frac{d\mathcal{H}^h(\boldsymbol{q}, \boldsymbol{p})}{dt} = \left(\dot{\boldsymbol{p}} + \frac{\partial \mathcal{H}^h}{\partial \boldsymbol{q}}\right) \cdot \dot{\boldsymbol{q}} - \left(\dot{\boldsymbol{q}} - \frac{\partial \mathcal{H}^h}{\partial \boldsymbol{p}}\right) \cdot \dot{\boldsymbol{p}} = 0, \tag{102}$$

where the space-discrete autonomous Hamiltonian consists of the space-discrete autonomous kinetic and potential energies:

$$\mathcal{H}^h(\boldsymbol{q}, \boldsymbol{p}) = \mathcal{K}^h(\boldsymbol{p}) + \mathcal{U}^h(\boldsymbol{q}), \qquad \mathcal{K}^h(\boldsymbol{p}) = \tfrac{1}{2}\boldsymbol{p} \cdot \boldsymbol{M}^{-1}\boldsymbol{p}, \qquad \mathcal{U}^h(\boldsymbol{q}) = \Pi^h_{\text{int}} - \boldsymbol{q} \cdot \boldsymbol{F}_{\text{ext}},$$

$$\Pi^h_{\text{int}} = \int_{\mathcal{B}} \rho_0 \Psi(\boldsymbol{F}^h) dV, \qquad \frac{\partial \mathcal{H}^h}{\partial \boldsymbol{q}} = \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}}, \qquad \boldsymbol{M} = \int_{\mathcal{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{N} \, dV, \tag{103}$$

$$\boldsymbol{F}_{\text{int}} = \int_{\mathcal{B}} \bar{\boldsymbol{B}}^T \boldsymbol{P} \, dV, \qquad \boldsymbol{F}_{\text{ext}} = \int_{\mathcal{B}} \rho_0 \boldsymbol{N}^T \boldsymbol{B} \, dV + \int_{\partial \mathcal{B}_\sigma} \boldsymbol{N}^T \bar{\boldsymbol{T}} \, dA.$$

Here $\boldsymbol{P}$ is the first Piola–Kirchhoff stress tensor, $\boldsymbol{B}$ the strain matrix, and $\boldsymbol{N}$ the interpolation matrix. Note that the admissible trial functions we used previously to discretize the rate of the Hamiltonian are of class $C^{m-1}(\mathcal{B})$ as the trial functions applied to the principle of virtual work in Equation (A.5) of the Appendix. We stress again that the discretization of the rate of the Hamiltonian as given in (100) corresponds to the discretization of the principle of virtual work in (A.6). Therefore, discretizing the rate of the Hamiltonian by the admissible trial functions automatically leads to the minimization of the errors arising from the approximating functions in association. The expression in (97), (99) and (103) holds regardless of whether material/geometric nonlinearity of the body exists or not.

In contrast to traditional practices (see the Appendix via the three formalisms but with "density forms of representation", instead of standard Newton-based Cauchy equations of motion, as a starting point), for space discretization we simply adopt the following procedure. In view of (96), we introduce the discrete total energy differential operator

$$\mathfrak{E}_D = \frac{d}{dt}\frac{\partial}{\partial \dot{\boldsymbol{q}}} + \frac{\partial}{\partial \boldsymbol{q}} \tag{104}$$

by which the space-discrete finite element equations of motion can be readily obtained after constructing the space-discrete total energy which only entails the use of trial functions. Upon substituting the space-discrete total energy into the discrete total energy differential operator, we obtain

$$\mathfrak{E}_D(\mathcal{E}^h) = 0 \Rightarrow \frac{d}{dt}\frac{\partial \mathcal{E}^h}{\partial \dot{\boldsymbol{q}}} + \frac{\partial \mathcal{E}^h}{\partial \boldsymbol{q}} = 0, \tag{105}$$

where the dependent state variable is the space-discrete total energy. Likewise, in view of (98), we first introduce the discrete Lagrangian differential operator

$$\mathfrak{L}_D = \frac{d}{dt}\frac{\partial}{\partial \dot{\boldsymbol{q}}} - \frac{\partial}{\partial \boldsymbol{q}}; \tag{106}$$

upon substituting this operator into the discrete Lagrangian differential operator, we obtain

$$\mathfrak{L}_D(\mathcal{L}^h) = 0 \Rightarrow \frac{d}{dt}\frac{\partial \mathcal{L}^h}{\partial \dot{\boldsymbol{q}}} - \frac{\partial \mathcal{L}^h}{\partial \boldsymbol{q}} = 0, \tag{107}$$

where the dependent state variable is the space-discrete Lagrangian. *The discrete total energy and Lagrangian differential operators above imply that errors associated with governing equations and natural boundary conditions are implicitly minimized when the admissible trial functions satisfying the essential boundary conditions are chosen.* Thus, we readily have the space discrete finite element equations of motion governing the mechanical dynamic behavior of the continuous-body within the total energy and Lagrangian frameworks:

$$M\ddot{q} + F_{\text{int}} - F_{\text{ext}} = 0. \tag{108}$$

In view of (102), we introduce the discrete Hamiltonian differential operators

$$\mathfrak{H}_{D1} = \dot{p} + \frac{\partial}{\partial q}, \quad \mathfrak{H}_{D2} = \dot{q} - \frac{\partial}{\partial p} \tag{109}$$

and use them to obtain the space-discrete finite element equations of motion can be after constructing the space-discrete Hamiltonian, which again only entails the use of trial functions. Upon substituting the space-discrete Hamiltonian into the discrete Hamiltonian differential operator, we have

$$\mathfrak{H}_{D1}(\mathcal{H}^h) = 0 \Rightarrow \dot{p} + \frac{\partial \mathcal{H}^h}{\partial q} = 0, \quad \mathfrak{H}_{D2}(\mathcal{H}^h) = 0 \Rightarrow \dot{q} - \frac{\partial \mathcal{H}^h}{\partial p} = 0, \tag{110}$$

where the dependent state variable is the space-discrete autonomous Hamiltonian. This discussion shows that *errors associated with governing equations and natural boundary conditions are implicitly minimized when the admissible trial functions satisfying the essential boundary conditions are chosen.* The space-discrete finite element equations of motion governing the mechanical dynamic behavior of the continuous-body within the Hamiltonian framework are then

$$\dot{p} + F_{\text{int}} - F_{\text{ext}} = 0, \quad \dot{q} - M^{-1}p = 0. \tag{111}$$

In contrast, for elastostatics, the corresponding discrete differential operators are simply $\mathfrak{E}_S = \partial/\partial q$, $\mathfrak{L}_S = -\partial/\partial q$, $\mathfrak{H}_S = \partial/\partial q$, and the finite element static equilibrium equations become

$$\mathfrak{E}_S(\mathcal{E}^h) = 0 \Rightarrow \frac{\partial \mathcal{E}^h}{\partial q} = 0, \quad \mathfrak{L}_S(\mathcal{L}^h) = 0 \Rightarrow -\frac{\partial \mathcal{L}^h}{\partial q} = 0, \quad \mathfrak{H}_S(\mathcal{H}^h) = 0 \Rightarrow \frac{\partial \mathcal{H}^h}{\partial q} = 0. \tag{112}$$

These equations describe the now familiar representation with the generalized coordinates corresponding to the Ritz coefficients. The same remark about optimization made after (110) applies.

Integrating both sides of (96), (98) and (102) over $t \in \mathbb{I} = [t_1, t_2]$, we have

$$\mathcal{E}^h(q, \dot{q})|_{t=t_1} - \mathcal{E}^h(q, \dot{q})|_{t=t_2} = \int_{t_1}^{t_2} (F_{\text{ext}} - F_{\text{int}} - M\ddot{q}) \cdot \dot{q}\, dt = 0, \tag{113}$$

$$\left(\frac{\partial \mathcal{L}^h(q, \dot{q})}{\partial \dot{q}} \cdot \dot{q} - \mathcal{L}^h(q, \dot{q}) \right)\Big|_{t=t_1} - \left(\frac{\partial \mathcal{L}^h(q, \dot{q})}{\partial \dot{q}} \cdot \dot{q} - \mathcal{L}^h(q, \dot{q}) \right)\Big|_{t=t_2} = \int_{t_1}^{t_2} (F_{\text{ext}} - F_{\text{int}} - M\ddot{q}) \cdot \dot{q}\, dt = 0,$$

$$\mathcal{H}^h(q, p)|_{t=t_2} - \mathcal{H}^h(q, p)|_{t=t_1} = \int_{t_1}^{t_2} \left((\dot{p} + F_{\text{int}} - F_{\text{ext}}) \cdot \dot{q} - (\dot{q} - M^{-1}p) \cdot \dot{p} \right) dt = 0.$$

The first two of these equations have the Bubnov–Galerkin weighted residual form in time, while the last has the hybrid weighted residual form in time. Instead of the virtual displacement, the equations in (113) take the generalized velocity as the weighting function. Hence, (113) can be used as a critical equation

to discretize the time domain. The first two equations in (113) may be regarded as an unconstrained generalized velocity formulation with a single dependent field variable in the time domain; thus we have the single-field generalized velocity problem within the total energy or Lagrangian framework. The last equation in (113) may be regarded as an unconstrained formulation with two dependent field variables in the time domain; thus we have the hybrid two-field problem within the Hamiltonian framework. In general, the time weighted-residual method [Tamma et al. 2000; Masuri et al. 2009a; 2009b] or the time finite element procedure [Simkins 1981; Aharoni and Bar-Yoseph 1992] can be applied to (113) for developing time stepping schemes.

In the presence of nonconservative forces such as contact forces on the contact boundary surfaces of nonholonomic systems, we have

$$\frac{d\mathcal{E}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h)}{dt} \text{ or } \frac{d}{dt}\left\{\int_{\mathcal{B}} \rho_0 \dot{\tilde{\boldsymbol{\varphi}}}^h \cdot \dot{\tilde{\boldsymbol{\varphi}}}^h dV - \mathcal{L}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h)\right\} \text{ or } \frac{d\mathcal{H}^h(\tilde{\boldsymbol{\varphi}}^h, \dot{\tilde{\boldsymbol{\varphi}}}^h)}{dt}$$
$$= \int_{\partial\mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\tilde{\boldsymbol{\varphi}}}^h(\boldsymbol{X}, t)\, dA + \int_{\partial\mathcal{B}_c} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\tilde{\boldsymbol{\varphi}}}^h\, dA. \quad (114)$$

Hence, Equations (96), (98) and (102) can be rewritten as

$$\frac{d\mathcal{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{dt} = \frac{d}{dt}\left(\frac{\partial\mathcal{E}^h}{\partial\dot{\boldsymbol{q}}}\right) + \frac{\partial\mathcal{E}^h}{\partial\boldsymbol{q}} = (\boldsymbol{F}_{\text{ext}} + \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}},$$

$$\frac{d}{dt}\left(\frac{\partial\mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial\dot{\boldsymbol{q}}} \cdot \dot{\boldsymbol{q}} - \mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})\right) = \left(\frac{\partial\mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial\boldsymbol{q}} - \frac{d}{dt}\frac{\partial\mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial\dot{\boldsymbol{q}}}\right) \cdot \dot{\boldsymbol{q}} = (\boldsymbol{F}_{\text{ext}} + \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}}, \quad (115)$$

$$\frac{d\mathcal{H}^h(\boldsymbol{q}, \boldsymbol{p})}{dt} = \left(\dot{\boldsymbol{p}} + \frac{\partial\mathcal{H}^h}{\partial\boldsymbol{q}}\right) \cdot \dot{\boldsymbol{q}} - \left(\dot{\boldsymbol{q}} - \frac{\partial\mathcal{H}^h}{\partial\boldsymbol{p}}\right) \cdot \dot{\boldsymbol{p}} = (\boldsymbol{F}_{\text{ext}} + \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}},$$

where $\boldsymbol{F}_{\text{contact}}$ denotes the contact force vector. Integrating for both sides of each equation over $t \in \mathbb{I} = [t_1, t_2]$ leads to

$$\mathcal{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})|_{t=t_2} - \mathcal{E}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})|_{t=t_1} = \int_{t_1}^{t_2} \left((\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{F}_{\text{int}}) \cdot \dot{\boldsymbol{q}}\right) dt = \int_{t_1}^{t_2} (\boldsymbol{F}_{\text{ext}} + \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}}\, dt,$$

$$\left(\frac{\partial\mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial\dot{\boldsymbol{q}}} \cdot \dot{\boldsymbol{q}} - \mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})\right)\bigg|_{t=t_2} - \left(\frac{\partial\mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})}{\partial\dot{\boldsymbol{q}}} \cdot \dot{\boldsymbol{q}} - \mathcal{L}^h(\boldsymbol{q}, \dot{\boldsymbol{q}})\right)\bigg|_{t=t_1}$$
$$= \int_{t_1}^{t_2} \left((\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{F}_{\text{int}}) \cdot \dot{\boldsymbol{q}}\right) dt = \int_{t_1}^{t_2} (\boldsymbol{F}_{\text{ext}} + \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}}\, dt, \quad (116)$$

$$\mathcal{H}^h(\boldsymbol{q}, \boldsymbol{p})|_{t=t_2} - \mathcal{H}^h(\boldsymbol{q}, \boldsymbol{p})|_{t=t_1} = \int_{t_1}^{t_2} \left((\dot{\boldsymbol{p}} + \boldsymbol{F}_{\text{int}}) \cdot \dot{\boldsymbol{q}} - (\dot{\boldsymbol{q}} - \boldsymbol{M}^{-1}\boldsymbol{p}) \cdot \dot{\boldsymbol{p}}\right) dt = \int_{t_1}^{t_2} (\boldsymbol{F}_{\text{ext}} + \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}}\, dt.$$

The first two of these equations above can be recast as

$$\int_{t_1}^{t_2} \left((\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} - \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}}\right) dt = 0, \quad (117)$$

which has the Bubnov–Galerkin weighted residual form in time. The weighting function is still the generalized velocity. Hence, (117) can be used as a critical equation to discretize the time domain.

Similarly, the last equation in (116) yields

$$\int_{t_1}^{t_2} \left((\dot{\boldsymbol{p}} + \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} - \boldsymbol{F}_{\text{contact}}) \cdot \dot{\boldsymbol{q}} - (\dot{\boldsymbol{q}} - \boldsymbol{M}^{-1}\boldsymbol{p}) \cdot \dot{\boldsymbol{p}} \right) dt = 0, \tag{118}$$

which has the hybrid weighted residual form in time. The weighting functions are the rates of the canonical coordinates. Hence, (118) can be also used as a critical equation to discretize the time domain [Aharoni and Bar-Yoseph 1992].

8. Numerical examples and illustrations

We consider two examples, the rotating bar and the Timoshenko beam, to illustrate the concepts discussed. We assume the systems are conservative and the materials undergo perfectly elastic deformations without producing entropy.

8.1. Rotating bar. Consider the dynamical behavior of a rotating bar described by the function $J(x)$, the polar moment of area about the center of the cross-section. As the dependent variable, we take the angle $\theta(x, t)$ of rotation about the axial axis. The kinetic energy is purely rotational:

$$\mathcal{K}(\dot{\theta}) = \frac{1}{2} \int_l \rho J(x) \dot{\theta}^2 \, dx. \tag{119}$$

Let G be the shear modulus. The torque $M_T(x, t)$ causing the bar to rotate can be written as

$$M_T(x, t) = G J(x) \theta'(x, t), \quad \theta'(x, t) = \frac{\partial \theta(x, t)}{\partial x}. \tag{120}$$

The total potential energy of the bar subject to the distributed torque $\bar{m}(x, t)$ is given by

$$\begin{aligned}
\mathcal{U}(\theta) &= \frac{1}{2} \int_l M_T(x, t) \theta'(x, t) \, dx - \int_l \bar{m}_T(x) \theta(x, t) \, dx \\
&= \frac{1}{2} \int_l G J(x) \big(\theta'(x, t)\big)^2 \, dx - \int_l \bar{m}_T(x) \theta(x, t) \, dx.
\end{aligned} \tag{121}$$

In view of (119) and (121), the Lagrangian is

$$\mathcal{L}(\theta, \dot{\theta}) = \int_l \overline{\mathcal{L}}(\theta, \dot{\theta}, \theta') \, dx + \int_l \bar{m}_T(x) \theta(x, t) \, dx, \tag{122}$$

where the Lagrangian density function is defined as

$$\overline{\mathcal{L}}(\theta, \dot{\theta}, \theta') = \tfrac{1}{2} \rho J(x) \dot{\theta}^2 - \tfrac{1}{2} G J(x) \big(\theta'(x, t)\big)^2. \tag{123}$$

The total energy is

$$\mathcal{E}(\theta, \dot{\theta}) = \int_l \overline{\mathcal{E}}(\theta, \dot{\theta}, \theta') \, dx - \int_l \bar{m}_T(x) \theta(x, t) \, dx, \tag{124}$$

where the total energy density function is defined as

$$\overline{\mathcal{E}}(\theta, \dot{\theta}, \theta') = \tfrac{1}{2} \rho J(x) \dot{\theta}^2 + \tfrac{1}{2} G J(x) \big(\theta'(x, t)\big)^2. \tag{125}$$

The total time derivative of the total energy is therefore

$$\frac{d\mathscr{E}(\theta, \dot{\theta}, \theta')}{dt} = \int_l \frac{d\overline{\mathscr{E}}(\theta, \dot{\theta}, \theta')}{dt} \, dx - \int_l \bar{m}_T(x)\theta(x, t) \, dx = 0, \tag{126}$$

or equivalently,

$$\frac{d\mathscr{E}(\theta, \dot{\theta}, \theta')}{dt} = \int_l \left(\frac{\partial\overline{\mathscr{E}}}{\partial\theta} + \frac{d}{dt}\frac{\partial\overline{\mathscr{E}}}{\partial\dot{\theta}} - \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{E}}}{\partial\theta'} - \bar{m}_T(x) \right)\dot{\theta} \, dx + \left.\frac{\partial\overline{\mathscr{E}}}{\partial\theta'}\dot{\theta}\right|_0^l = 0. \tag{127}$$

Therefore, the governing equation is

$$\frac{d}{dt}\frac{\partial\overline{\mathscr{E}}}{\partial\dot{y}} = \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{E}}}{\partial\theta'} - \frac{\partial\overline{\mathscr{E}}}{\partial\theta} + \bar{m}_T(x), \tag{128}$$

subject to the boundary condition

$$\left.\left(\frac{\partial\overline{\mathscr{E}}}{\partial\theta'}\dot{\theta}\right)\right|_0^l = 0. \tag{129}$$

Turning now to the Lagrangian framework, the rate of Jacobi's integral is

$$\int_l \left(\frac{d}{dt}\left(\frac{\partial\overline{\mathscr{L}}}{\partial\dot{\theta}}\right)\dot{\theta} - \frac{\partial\overline{\mathscr{L}}}{\partial\theta'}\dot{\theta}' \right) dx - \int_l \bar{m}_T(x)\dot{\theta} \, dx = 0, \tag{130}$$

or equivalently

$$\int_l \left(\frac{d}{dt}\frac{\partial\overline{\mathscr{L}}}{\partial\dot{\theta}} + \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{L}}}{\partial\theta'} - \bar{m}_T(x) \right)\dot{\theta} \, dx - \left.\frac{\partial\overline{\mathscr{L}}}{\partial\theta'}\dot{\theta}\right|_0^l = 0. \tag{131}$$

Therefore, the governing equation is

$$\frac{d}{dt}\frac{\partial\overline{\mathscr{L}}}{\partial\dot{\theta}} + \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{L}}}{\partial\theta'} - \bar{m}_T(x) = 0 \tag{132}$$

subject to the boundary condition

$$\left.\left(\frac{\partial\overline{\mathscr{L}}}{\partial\theta'}\dot{\theta}\right)\right|_0^l = 0. \tag{133}$$

Substituting the total energy or Lagrangian density function into the corresponding governing equations, we obtain the equation of motion

$$\rho J(x)\ddot{\theta} = \frac{\partial}{\partial x}\left(GJ(x)\frac{\partial\theta(x, t)}{\partial x} \right) + \bar{m}_T(x), \tag{134}$$

subject to the boundary condition

$$\left. GJ(x)\frac{\partial\theta(x, t)}{\partial x}\dot{\theta}(x, t) \right|_0^l = 0. \tag{135}$$

Within the Hamiltonian framework, the generalized momentum can be written

$$\phi = \frac{\partial\bar{L}}{\partial\dot{\theta}} = \rho J(x)\dot{\theta}. \tag{136}$$

We find the Hamiltonian density function by Legendre transformation:

$$\overline{\mathscr{H}}(\theta, \phi, \theta') = \phi\dot{\theta} - \overline{\mathscr{L}}(\theta, \dot{\theta}, \theta'). \tag{137}$$

The continuous Hamiltonian is therefore

$$\mathscr{H}(\theta, \phi) = \int_l \overline{\mathscr{H}}(\theta, \phi, \theta') \, dx - \int_l \bar{m}_T(x)\theta(x, t) \, dx. \tag{138}$$

and its total time derivative is

$$\frac{d\mathscr{H}(\theta, \phi)}{dt} = \int_l \frac{d\overline{\mathscr{H}}(\theta, \phi, \theta')}{dt} dx - \int_l \bar{m}_T(x)\theta(x, t) dx. \tag{139}$$

The total time derivative of the autonomous Hamiltonian can be rewritten as

$$\frac{d\mathscr{H}(\theta, \phi)}{dt} = \int_l \left\{ \left(\frac{\partial}{\partial x} \frac{\partial \overline{\mathscr{H}}}{\partial \theta'} - \frac{\partial \overline{\mathscr{H}}}{\partial \theta} - \frac{d\phi}{dt} + \bar{m}_T(x) \right) \dot{\theta} + \left(\dot{\theta} - \frac{\partial \overline{\mathscr{H}}}{\partial \phi} \right) \dot{\phi} \right\} dx + \left(\frac{\partial \overline{\mathscr{H}}}{\partial \theta'} \dot{\theta} \right) \Big|_0^l = 0. \tag{140}$$

Thus, the governing equations are

$$\frac{d\phi}{dt} = \frac{\partial}{\partial x} \frac{\partial \overline{\mathscr{H}}}{\partial \theta'} - \frac{\partial \overline{\mathscr{H}}}{\partial \theta} + \bar{m}_T(x), \quad \text{and} \quad \dot{\theta} - \frac{\partial \bar{H}}{\partial \phi} = 0, \tag{141}$$

subject to the boundary condition

$$\left(\frac{\partial \overline{\mathscr{H}}}{\partial \theta'} \dot{\theta} \right) \Big|_0^l = 0. \tag{142}$$

Substituting the Hamiltonian density function (137) into (141), we obtain the equations of motion, a set of first-order differential equations:

$$\dot{\phi} = \frac{\partial}{\partial x} \left(GJ(x) \frac{\partial \theta(x, t)}{\partial x} \right) + \bar{m}_T(x), \quad \dot{\theta} = \frac{\phi}{\rho J(x)}, \tag{143}$$

subject to the boundary condition

$$GJ(x) \frac{\partial \theta(x, t)}{\partial x} \dot{\theta}(x, t) \Big|_0^l = 0. \tag{144}$$

Next, we discuss the development of semidiscrete differential equations of motion in the three formalisms. The trial functions are approximated as

$$\theta^h(x, t) = N(x) \cdot q(t), \qquad \dot{\theta}^h(x, t) = N(x) \cdot \dot{q}(t), \qquad \frac{\partial \theta^h(x, t)}{\partial x} = B(x) \cdot q(t),$$

$$\phi^h(x, t) = \rho J(x) N(x) \cdot \dot{q}(t), \qquad M = \frac{1}{2} \int_l \rho J(x) N^T(x) N(x) dx, \tag{145}$$

$$q(t) = \left(\theta_1^h(t), \theta_2^h(t), \ldots, \theta_{n_{\text{node}}}^h(t) \right), \qquad \dot{q}(t) = \left(\dot{\theta}_1^h(t), \dot{\theta}_2^h(t), \ldots, \dot{\theta}_{n_{\text{node}}}^h(t) \right), \qquad p = M\dot{q}(t).$$

Then, we have the space-discrete kinetic and potential energies given by

$$\mathscr{K}^h(\dot{q}) = \frac{1}{2}\dot{q}(t) \cdot M\dot{q}(t) \text{ or } \mathscr{K}^h(p) = \frac{1}{2}p(t) \cdot M^{-1}p(t), \quad \mathscr{U}^h(q) = \frac{1}{2}q(t) \cdot K(x)q(t) - q(t) \cdot F_{\text{ext}}, \tag{146}$$

where the stiffness matrix and the external force are

$$K(x) = \int_l GJ(x)B^T(x)B(x) \, dx \quad \text{and} \quad F_{\text{ext}} = \int_l N^T(x)\bar{m}_T(x) \, dx. \tag{147}$$

Hence, the space-discrete autonomous Lagrangian, Hamiltonian and total energy are given by

$$\mathscr{L}^h(\boldsymbol{q},\dot{\boldsymbol{q}}) = \mathscr{K}^h(\dot{\boldsymbol{q}}) - \mathscr{U}^h(\boldsymbol{q}) = \tfrac{1}{2}\dot{\boldsymbol{q}}(t)\cdot\boldsymbol{M}\dot{\boldsymbol{q}}(t) - \tfrac{1}{2}\boldsymbol{q}(t)\cdot\boldsymbol{K}(x)\boldsymbol{q}(t) + \boldsymbol{q}(t)\cdot\boldsymbol{F}_{\text{ext}}, \qquad (148)$$

$$\mathscr{E}^h(\boldsymbol{q},\dot{\boldsymbol{q}}) = \mathscr{K}^h(\dot{\boldsymbol{q}}) + \mathscr{U}^h(\boldsymbol{q}) = \tfrac{1}{2}\dot{\boldsymbol{q}}(t)\cdot\boldsymbol{M}\dot{\boldsymbol{q}}(t) + \tfrac{1}{2}\boldsymbol{q}(t)\cdot\boldsymbol{K}(x)\boldsymbol{q}(t) - \boldsymbol{q}(t)\cdot\boldsymbol{F}_{\text{ext}}, \qquad (149)$$

$$\mathscr{H}^h(\boldsymbol{q},\boldsymbol{p}) = \mathscr{K}^h(\boldsymbol{p}) + \mathscr{U}^h(\boldsymbol{q}) = \tfrac{1}{2}\boldsymbol{p}(t)\cdot\boldsymbol{M}^{-1}\boldsymbol{p}(t) + \tfrac{1}{2}\boldsymbol{q}(t)\cdot\boldsymbol{K}(x)\boldsymbol{q}(t) - \boldsymbol{q}(t)\cdot\boldsymbol{F}_{\text{ext}}. \qquad (150)$$

Substituting $\mathscr{L}^h(\boldsymbol{q},\dot{\boldsymbol{q}})$ and $\mathscr{E}^h(\boldsymbol{q},\dot{\boldsymbol{q}})$ into the corresponding discrete differential operators given by (106) and (104) we get the semidiscrete equations of motion:

$$\mathfrak{L}_D(\mathscr{L}^h) \equiv \mathfrak{E}_D(\mathscr{E}^h) = 0 \Rightarrow \boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{K}\boldsymbol{q} - \boldsymbol{F}_{\text{ext}} = 0. \qquad (151)$$

Similarly, substituting $\mathscr{H}^h(\boldsymbol{q},\boldsymbol{p})$ into the discrete Hamiltonian differential operators defined by (109) yields the semidiscrete equations of motion

$$\mathfrak{H}_{D1}(\mathscr{H}^h) = 0 \Rightarrow \dot{\boldsymbol{p}} + \boldsymbol{K}\boldsymbol{q} - \boldsymbol{F}_{\text{ext}} = 0, \qquad \mathfrak{H}_{D2}(\mathscr{H}^h) = 0 \Rightarrow \dot{\boldsymbol{q}} - \boldsymbol{M}^{-1}\boldsymbol{p} = 0. \qquad (152)$$

8.2. Timoshenko beam. As an illustration typical of a more complicated numerical example in the class of structural dynamical systems, we consider the dynamical behavior of the Timoshenko beam with $A(x)$, the cross-sectional area and $I(x)$, the area moment per unit length about the neutral axis of the cross-section. It is governed by two differential equations, because of the presence of two dependent variables such as the transverse deflection $y(x,t)$ and the angle of rotation $\varphi(x,t)$ due to bending moment acting on the beam subject to transverse distributed load $\bar{\omega}(x)$. The reason for us to illustrate the Timoshenko beam problem is that the mechanics of the beam reflects the effect of rotary inertia of the beam mass as well as the translational kinetic motion effect. Thus, the proposed space-discrete formulation readily facilitates a simple and straightforward derivation of the space-discrete finite element equations of motion over the traditional principle of virtual work.

In matrix and vector notation, the continuous total energy of the Timoshenko beam can be written

$$\mathscr{E}(\boldsymbol{u},\dot{\boldsymbol{u}}) = \int_l \overline{\mathscr{E}}(\boldsymbol{u},\dot{\boldsymbol{u}},\boldsymbol{u}')\,dx - \int_l \bar{\omega}(x)\boldsymbol{a}\cdot\boldsymbol{u}\,dx, \quad \boldsymbol{u}'^T = \left(\frac{\partial y(x,t)}{\partial x}, \frac{\partial \varphi(x,t)}{\partial x}\right), \quad \boldsymbol{a}^T = (1,0), \quad (153)$$

where the total energy density function can be defined as

$$\overline{\mathscr{E}}(\boldsymbol{u},\dot{\boldsymbol{u}},\boldsymbol{u}') = \tfrac{1}{2}\dot{\boldsymbol{u}}\cdot\rho\dot{\boldsymbol{u}} + \tfrac{1}{2}\boldsymbol{\kappa}\cdot\boldsymbol{D}_b\boldsymbol{\kappa} + \tfrac{1}{2}\boldsymbol{\gamma}\cdot\boldsymbol{G}_s\boldsymbol{\gamma}, \qquad \boldsymbol{\kappa} = \left[\frac{\partial\varphi}{\partial x}\right], \qquad \boldsymbol{D}_b = [EI(x)],$$

$$\boldsymbol{\gamma} = \left[\frac{\partial y(x,t)}{\partial x} - \varphi(x,t)\right], \qquad \boldsymbol{G}_s = [\kappa GA(x)]. \tag{154}$$

In the context of the Lagrangian framework, the continuous Lagrangian of the Timoshenko beam is

$$\mathscr{L}(\boldsymbol{u},\dot{\boldsymbol{u}}) = \int_l \overline{\mathscr{L}}(\boldsymbol{u},\dot{\boldsymbol{u}},\boldsymbol{u}')\,dx + \int_l \bar{\omega}(x)\boldsymbol{a}\cdot\boldsymbol{u}\,dx, \qquad (155)$$

where the Lagrangian density function can be defined as

$$\overline{\mathscr{L}}(\boldsymbol{u},\dot{\boldsymbol{u}},\boldsymbol{u}') = \tfrac{1}{2}\dot{\boldsymbol{u}}\cdot\rho\dot{\boldsymbol{u}} - \tfrac{1}{2}\boldsymbol{\kappa}\cdot\boldsymbol{D}_b\boldsymbol{\kappa} - \tfrac{1}{2}\boldsymbol{\gamma}\cdot\boldsymbol{G}_s\boldsymbol{\gamma}. \qquad (156)$$

Then, the rate of the total energy gives

$$\frac{d\mathscr{E}(\boldsymbol{u}, \dot{\boldsymbol{u}})}{dt} = \int_l \frac{d\overline{\mathscr{E}}(\boldsymbol{u}, \dot{\boldsymbol{u}}, \boldsymbol{u}')}{dt}\, dx - \int_l \bar{\omega}(x)\boldsymbol{a} \cdot \dot{\boldsymbol{u}}\, dx = 0. \tag{157}$$

Within the Lagrangian framework, the rate of Jacobi's integral can be expressed

$$\frac{d}{dt}(2\mathscr{K}(\dot{\boldsymbol{u}}) - \mathscr{L}(\boldsymbol{u}, \dot{\boldsymbol{u}})) = \int_l \frac{d}{dt}\left\{ \frac{\partial\overline{\mathscr{L}}(\boldsymbol{u}, \dot{\boldsymbol{u}}, \boldsymbol{u}')}{\partial\dot{\boldsymbol{u}}} \cdot \dot{\boldsymbol{u}} - \overline{\mathscr{L}}(\boldsymbol{u}, \dot{\boldsymbol{u}}, \boldsymbol{u}') \right\} dx - \int_l \bar{\omega}(x)\boldsymbol{a} \cdot \dot{\boldsymbol{u}}\, dx = 0. \tag{158}$$

Consequently, (157) and (158) result in respectively

$$\int_l \left\{ \left(\frac{\partial\overline{\mathscr{E}}}{\partial\boldsymbol{u}} + \frac{d}{dt}\frac{\partial\overline{\mathscr{E}}}{\partial\dot{\boldsymbol{u}}} - \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{E}}}{\partial\boldsymbol{u}'} - \bar{\omega}(x)\boldsymbol{a} \right) \cdot \dot{\boldsymbol{u}} \right\} dx + \left(\frac{\partial\overline{\mathscr{E}}}{\partial\boldsymbol{u}'} \cdot \dot{\boldsymbol{u}} \right)\Big|_0^l = 0,$$

$$\int_l \left\{ \left(\frac{\partial\overline{\mathscr{L}}}{\partial\boldsymbol{u}} - \frac{d}{dt}\frac{\partial\overline{\mathscr{L}}}{\partial\dot{\boldsymbol{u}}} - \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{L}}}{\partial\boldsymbol{u}'} + \bar{\omega}(x)\boldsymbol{a} \right) \cdot \dot{\boldsymbol{u}} \right\} dx + \left(\frac{\partial\overline{\mathscr{L}}}{\partial\boldsymbol{u}'} \cdot \dot{\boldsymbol{u}} \right)\Big|_0^l = 0, \tag{159}$$

where both governing equations and natural boundary conditions are included. The governing equations in terms of the Lagrangian and total energy density functions are

$$\frac{\partial\overline{\mathscr{L}}}{\partial\boldsymbol{u}} - \frac{d}{dt}\frac{\partial\overline{\mathscr{L}}}{\partial\dot{\boldsymbol{u}}} - \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{L}}}{\partial\boldsymbol{u}'} + \bar{\omega}(x)\boldsymbol{a} = 0 \quad \text{and} \quad \frac{\partial\overline{\mathscr{E}}}{\partial\boldsymbol{u}} + \frac{d}{dt}\frac{\partial\overline{\mathscr{E}}}{\partial\dot{\boldsymbol{u}}} - \frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{E}}}{\partial\boldsymbol{u}'} - \bar{\omega}(x)\boldsymbol{a} = 0, \tag{160}$$

subject to the natural boundary conditions

$$\frac{\partial\overline{\mathscr{L}}}{\partial\boldsymbol{u}'} \cdot \dot{\boldsymbol{u}}\Big|_0^l = 0 \quad \text{and} \quad \left(\frac{\partial\overline{\mathscr{E}}}{\partial\boldsymbol{u}'} \cdot \dot{\boldsymbol{u}} \right)\Big|_0^l = 0. \tag{161}$$

In the Hamiltonian framework, the components of the canonical momenta $\boldsymbol{\phi}^T(x, t) = (\boldsymbol{\phi}_1(x, t), \boldsymbol{\phi}_2(x, t))$ are

$$\boldsymbol{\phi} = \frac{\partial\overline{\mathscr{L}}(\boldsymbol{u}, \dot{\boldsymbol{u}}, \boldsymbol{u}')}{\partial\dot{\boldsymbol{u}}}. \tag{162}$$

The Legendre transformation gives

$$\overline{\mathscr{H}}(\boldsymbol{u}, \boldsymbol{\phi}, \boldsymbol{u}') = \boldsymbol{\phi}(x, t) \cdot \dot{\boldsymbol{u}}(x, t) - \overline{\mathscr{L}}(\boldsymbol{u}, \dot{\boldsymbol{u}}, \boldsymbol{u}') = \tfrac{1}{2}\boldsymbol{\phi} \cdot \rho^{-1}\boldsymbol{\phi} + \tfrac{1}{2}\boldsymbol{\kappa} \cdot D_b\boldsymbol{\kappa} + \tfrac{1}{2}\boldsymbol{\gamma} \cdot G_s\boldsymbol{\gamma}. \tag{163}$$

Hence, the rate of the continuous Hamiltonian, which is autonomous, yields

$$\frac{d\mathscr{H}(\boldsymbol{u}, \boldsymbol{\phi})}{dt} = 0, \tag{164}$$

where the continuous Hamiltonian of the Timoshenko beam can be obtained as

$$\mathscr{H}(\boldsymbol{u}(x, t), \boldsymbol{\phi}(x, t)) = \int_l \overline{\mathscr{H}}(\boldsymbol{u}(x, t), \boldsymbol{\phi}(x, t), \boldsymbol{u}'(x, t))\, dx - \int_l \bar{\omega}(x)\boldsymbol{a} \cdot \boldsymbol{u}\, dx. \tag{165}$$

Hence, (164) leads to

$$\frac{d\mathscr{H}(\boldsymbol{u}, \boldsymbol{\phi})}{dt} = \int_l \left\{ \left(\dot{\boldsymbol{u}} - \frac{\partial\overline{\mathscr{H}}}{\partial\boldsymbol{\phi}} \right) \cdot \dot{\boldsymbol{\phi}} + \left(\frac{\partial}{\partial x}\frac{\partial\overline{\mathscr{H}}}{\partial\boldsymbol{u}'} - \frac{\partial\overline{\mathscr{H}}}{\partial\boldsymbol{u}} - \frac{d\boldsymbol{\phi}}{dt} + \bar{\omega}(x)\boldsymbol{a} \right) \cdot \dot{\boldsymbol{u}} \right\} dx - \frac{\partial\overline{\mathscr{H}}}{\partial\boldsymbol{u}'} \cdot \dot{\boldsymbol{u}}\Big|_0^l = 0, \tag{166}$$

where both governing equations and natural boundary conditions are included. The governing equations in terms of the Hamiltonian density function can be given by

$$\frac{\partial}{\partial x}\frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{u}'} - \frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{u}} - \frac{d\boldsymbol{\phi}}{dt} + \bar{\omega}(x)\boldsymbol{a} = 0, \qquad \dot{\boldsymbol{u}} - \frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{\phi}} = 0 \tag{167}$$

subject to the natural boundary conditions

$$\frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{u}'} \cdot \boldsymbol{u} \Big|_0^l = 0. \tag{168}$$

Consequently, we have shown the derivation of the two governing equations of motion with the traction boundary condition via the theorem of expended power. In contrast to following traditional practices, instead of substituting the admissible functions into the Bubnov–Galerkin weighted residual forms in (159) and (166), alternatively we construct first the space-discrete Lagrangian, Hamiltonian and total energy. The admissible trial functions are given by

$$y^h(x,t) = \boldsymbol{H}_y(x)\boldsymbol{q}(t), \quad \boldsymbol{\varphi}^h(x,t) = \boldsymbol{H}_\varphi(x)\boldsymbol{q}(t),$$
$$\boldsymbol{H}_y(x) = \begin{bmatrix} N_y(x) & 0 \end{bmatrix}, \quad \boldsymbol{H}_\varphi(x) = \begin{bmatrix} 0 & N_\varphi(x) \end{bmatrix},$$
$$\boldsymbol{u} = \boldsymbol{H}(x)\boldsymbol{q}(t), \quad \dot{\boldsymbol{u}} = \boldsymbol{H}(x)\dot{\boldsymbol{q}}(t), \quad \boldsymbol{H}^T(x) = \begin{bmatrix} \boldsymbol{H}_y^T(x) & \boldsymbol{H}_\varphi^T(x) \end{bmatrix}, \tag{169}$$
$$\boldsymbol{q}(t) = \left(y_1^h(t), y_2^h(t), \ldots, y_{n_{\text{node}}}^h(t), \boldsymbol{\varphi}_1^h(t), \boldsymbol{\varphi}_2^h(t), \ldots, \boldsymbol{\varphi}_{n_{\text{node}}}^h(t) \right),$$
$$\dot{\boldsymbol{q}}(t) = \left(\dot{y}_1^h(t), \dot{y}_2^h(t), \ldots, \dot{y}_{n_{\text{node}}}^h(t), \dot{\boldsymbol{\varphi}}_1^h(t), \dot{\boldsymbol{\varphi}}_2^h(t), \ldots, \dot{\boldsymbol{\varphi}}_{n_{\text{node}}}^h(t) \right).$$

The space-discrete Lagrangian, Hamiltonian and total energy may be written as

$$\mathcal{L}^h(\boldsymbol{q},\dot{\boldsymbol{q}}) = \tfrac{1}{2}\dot{\boldsymbol{q}}(t)\cdot\boldsymbol{M}\dot{\boldsymbol{q}}(t) - \tfrac{1}{2}\boldsymbol{q}(t)\cdot\boldsymbol{K}\boldsymbol{q}(t) + \boldsymbol{q}(t)\cdot\boldsymbol{F}_{\text{ext}},$$
$$\mathcal{E}^h(\boldsymbol{q},\dot{\boldsymbol{q}}) = \tfrac{1}{2}\dot{\boldsymbol{q}}(t)\cdot\boldsymbol{M}\dot{\boldsymbol{q}}(t) + \tfrac{1}{2}\boldsymbol{q}(t)\cdot\boldsymbol{K}\boldsymbol{q}(t) - \boldsymbol{q}(t)\cdot\boldsymbol{F}_{\text{ext}},$$
$$\mathcal{H}^h(\boldsymbol{q},\boldsymbol{p}) = \tfrac{1}{2}\boldsymbol{p}(t)\cdot\boldsymbol{M}^{-1}\boldsymbol{p}(t) + \tfrac{1}{2}\boldsymbol{q}(t)\cdot\boldsymbol{K}\boldsymbol{q}(t) - \boldsymbol{q}(t)\cdot\boldsymbol{F}_{\text{ext}},$$
$$\boldsymbol{M} = \frac{1}{2}\int_l \boldsymbol{H}(x)^T\rho\boldsymbol{H}(x)\,dx, \qquad \boldsymbol{p}(t) = \boldsymbol{M}\dot{\boldsymbol{q}}(t), \tag{170}$$
$$\boldsymbol{K}_b = \int_l \boldsymbol{B}_b^T(x)\boldsymbol{D}_b\boldsymbol{B}_b(x)dx, \qquad \boldsymbol{K}_s = \int_l \boldsymbol{B}_s^T(x)\boldsymbol{G}_s\boldsymbol{B}_s(x)dx, \qquad \boldsymbol{K} = \boldsymbol{K}_b + \boldsymbol{K}_s,$$
$$\boldsymbol{B}_b = \begin{bmatrix} \dfrac{\partial \boldsymbol{H}_\varphi(x)}{\partial x} \end{bmatrix}, \qquad \boldsymbol{B}_s = \begin{bmatrix} \dfrac{\partial \boldsymbol{H}_y(x)}{\partial x} - \boldsymbol{H}_\varphi(x) \end{bmatrix}, \qquad \boldsymbol{F}_{\text{ext}} = \int_l \bar{\omega}(x)\boldsymbol{H}_y^T(x)\,dx,$$

where E denotes Young's modulus, κ the shear correction factor, and G the shear modulus. Substituting the space-discrete Lagrangian total energy, and Hamiltonian into the corresponding discrete differential operators (104), (106), (109) leads to the space-discrete finite element equations of motion within the corresponding frameworks:

$$\mathcal{L}_D(\mathcal{L}^h) \equiv \mathfrak{E}_D(\mathcal{E}^h) = 0 \Rightarrow \boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{K}\boldsymbol{q} - \boldsymbol{F}_{\text{ext}} = 0.$$
$$\mathfrak{H}_{D1}(\mathcal{H}^h) = 0 \Rightarrow \dot{\boldsymbol{p}} + \boldsymbol{K}\boldsymbol{q} - \boldsymbol{F}_{\text{ext}} = 0, \qquad \mathfrak{H}_{D2}(\mathcal{H}^h) = 0 \Rightarrow \dot{\boldsymbol{q}} - \boldsymbol{M}^{-1}\boldsymbol{p} = 0. \tag{171}$$

9. Conclusions

In most renowned textbooks, and historically, the finite element method for elastodynamics applications has been explained in the sense of the principle of virtual work involving the concept of variations from various viewpoints. Traditional variational practices and Newton based formulations stemming from the Cauchy equations of motion cannot readily establish the various symmetries for the semidiscrete system. In contrast, alternate developments via differential calculus were described involving the theorem of expended power and scalar representations which provide an improved physical interpretation, and for also ensuring that the semidiscretized system also inherits the same physics as in the continuous system by capitalizing on theorems' such as Noether. In this work, we introduced and showed that the theorem of expended power involving three distinct frameworks, namely, the Total Energy, the Lagrangian, and the Hamiltonian density functions is a consistent and viable alternative for deriving the governing equations with boundary conditions for both N-body and continuous-body scleronomic dynamical systems. In addition, in contrast to traditional practices, which, after obtaining the model governing equations, seek to employ the weak form or principle of virtual work with trial and test functions to enacting the discretization process, we proposed a space-discrete Total Energy, Lagrangian, and Hamiltonian finite element formulation involving only trial functions to directly discretize the theorem of extended power, without resorting to traditional practices resulting in the space discrete finite element equations of motion for continuum-dynamical systems. Extensions to account for non-holonomic constraints were also described. The equivalence of the three frameworks in terms of the strong and weak forms were established in relation to describing Newton's second law and the underlying equation of motion, and illustrative examples of the rotating bar and Timoshenko beam were demonstrated to describe the basic ideas.

Appendix: Space discretization via density formalisms and finite element formulation

Alternatively, we herein describe the evolution of traditional practices using as a starting point, the theorem of expended power within the total energy density formalism and framework, followed by the Lagrangian and Hamiltonian frameworks via the corresponding density formalisms. In view of (54) and (56), the rate of the total energy easily yields the weak form in the sense of the space

$$\frac{d\mathscr{E}(\boldsymbol{\varphi}, \dot{\boldsymbol{\varphi}})}{dt} = \int_{\mathscr{B}} \frac{d}{dt}\left(\frac{\partial \overline{\mathscr{E}}}{\partial \dot{\boldsymbol{\varphi}}}\right) \cdot \dot{\boldsymbol{\varphi}} \, dV + \int_{\mathscr{B}} \frac{\partial \overline{\mathscr{E}}}{\partial \boldsymbol{F}} \cdot\cdot \, \dot{\boldsymbol{F}} \, dV + \int_{\mathscr{B}} \frac{\partial \overline{\mathscr{E}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} \, dV - \int_{\partial \mathscr{B}_{\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}} \, dA = 0. \quad \text{(A.1)}$$

We know that this equation can be obtained when the virtual displacement in the principle of virtual work is replaced by the generalized velocity. This is the so-called the single field problem; the dependent variable is the displacement, and one can follow traditional practices of discretization in space and time. Likewise, the rate of Jacobi's integral gives the weak form in terms of the Lagrangian density function

$$\int_{\mathscr{B}} \frac{d}{dt}\left(\frac{\partial \overline{\mathscr{L}}}{\partial \dot{\boldsymbol{\varphi}}}\right) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV - \int_{\mathscr{B}} \frac{\partial \overline{\mathscr{L}}}{\partial \boldsymbol{F}} \cdot\cdot \, \dot{\boldsymbol{F}} \, dV - \int_{\mathscr{B}} \frac{\partial \overline{\mathscr{L}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dV - \int_{\partial \mathscr{B}_{\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t) \, dA = 0. \quad \text{(A.2)}$$

Note that the essential boundary conditions become nodal position vectors on nodal points. This is the conventional process for the Galerkin finite element method [Hughes 1987; Reddy 2006]. Consequently,

substituting appropriate trial and test functions into (A.1) and (A.2), yields the semidiscrete second order in time differential equations of motion as

$$\sum_{i=1}^{n_{\text{elem}}} \left(\int_{\mathcal{B}_i} \rho \ddot{\tilde{\boldsymbol{\varphi}}}^h \cdot \dot{\boldsymbol{\varphi}}^h \, dV + \int_{\mathcal{B}_i} \tilde{\boldsymbol{P}}^h \cdot\cdot \dot{\tilde{\boldsymbol{F}}}^h \, dV - \int_{\mathcal{B}_i} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}^h \, dV - \int_{\partial \mathcal{B}_{i\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}^h \, dA \right) = 0, \quad \text{(A.3)}$$

where $\mathcal{B}_i$ stands for the i-th element domain. Notice that (A.3) gives a set of simultaneous N ordinary time differential equations to be discretized subsequently in time. Therefore, the weak form is the most important equation to which one must apply both the admissible trial functions $\tilde{\boldsymbol{\varphi}}(\boldsymbol{X}, t)$ and the admissible test functions $\dot{\boldsymbol{\varphi}}(\boldsymbol{X}, t)$ to discretize the domain of interest. From (A.3), we obtain the semidiscrete second order differential equations, that is, the finite element equations of motion resulting as follows for the total energy and Lagrangian frameworks:

$$\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} = 0. \tag{A.4}$$

In addition, within the Hamiltonian framework, the rate of the Hamiltonian yields the weak form in the sense of the space:

$$\int_{\mathcal{B}} \dot{\boldsymbol{\phi}} \cdot \dot{\boldsymbol{\varphi}} \, dV + \int_{\mathcal{B}} \frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{F}} \cdot\cdot \dot{\boldsymbol{F}} \, dV + \int_{\mathcal{B}} \frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} \, dV - \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}} \, dA = 0,$$

$$\int_{\mathcal{B}} \left(\dot{\boldsymbol{\varphi}} - \frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{\phi}} \right) \cdot \dot{\boldsymbol{\phi}} \, dV = 0. \tag{A.5}$$

Finally, substituting appropriate trial and test functions into (A.5), we obtain the semidiscrete first order differential equations of motion:

$$\sum_{i=1}^{n_{\text{elem}}} \left(\int_{\mathcal{B}_i} \dot{\tilde{\boldsymbol{\phi}}}^h \cdot \dot{\boldsymbol{\varphi}}^h \, dV + \int_{\mathcal{B}_i} \left(\frac{\partial \overline{\mathcal{H}}}{\partial \tilde{\boldsymbol{F}}} \right)^h \cdot\cdot \dot{\tilde{\boldsymbol{F}}}^h \, dV + \int_{\mathcal{B}_i} \left(\frac{\partial \overline{\mathcal{H}}}{\partial \boldsymbol{\varphi}} \right)^h \cdot \dot{\boldsymbol{\varphi}}^h \, dV - \int_{\partial \mathcal{B}_{i\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}^h \, dA \right) t = 0,$$

$$\sum_{i=1}^{n_{\text{elem}}} \left(\int_{\mathcal{B}_i} \dot{\tilde{\boldsymbol{\varphi}}}^h \cdot \dot{\boldsymbol{\phi}}^h \, dV - \int_{\mathcal{B}_i} \left(\frac{\partial \overline{\mathcal{H}}}{\partial \tilde{\boldsymbol{\varphi}}} \right)^h \cdot \dot{\boldsymbol{\phi}}^h \, dV \right) = 0 \tag{A.6}$$

which yields

$$\dot{\boldsymbol{p}} + \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} = 0, \qquad \dot{\boldsymbol{q}} - \boldsymbol{M}^{-1} \boldsymbol{p} = 0. \tag{A.7}$$

For nonholonomic or nonconservative systems involving contact, (A.1) and (A.2) should be modified:

$$\int_{\mathcal{B}} \frac{d}{dt} \left(\frac{\partial \overline{\mathcal{E}}}{\partial \dot{\boldsymbol{\varphi}}} \right) \cdot \dot{\boldsymbol{\varphi}} \, dV + \int_{\mathcal{B}} \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{F}} \cdot\cdot \dot{\boldsymbol{F}} \, dV + \int_{\mathcal{B}} \frac{\partial \overline{\mathcal{E}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} \, dV - \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}} \, dA = \int_{\partial \mathcal{B}_c} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\boldsymbol{\varphi}} \, dA,$$

$$\int_{\mathcal{B}} \frac{d}{dt} \left(\frac{\partial \overline{\mathcal{L}}}{\partial \dot{\boldsymbol{\varphi}}} \right) \cdot \dot{\boldsymbol{\varphi}} \, dV - \int_{\mathcal{B}} \frac{\partial \overline{\mathcal{L}}}{\partial \boldsymbol{F}} \cdot\cdot \dot{\boldsymbol{F}} \, dV - \int_{\mathcal{B}} \frac{\partial \overline{\mathcal{L}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} \, dV - \int_{\partial \mathcal{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}} \, dA = \int_{\partial \mathcal{B}_c} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\boldsymbol{\varphi}} \, dA.$$

The discretization of these equations gives

$$\sum_{i=1}^{n_{\text{elem}}} \left(\int_{\mathscr{B}_i} \rho \ddot{\tilde{\boldsymbol{\varphi}}}^h \cdot \dot{\boldsymbol{\varphi}}^h \, dV + \int_{\mathscr{B}_i} \tilde{\boldsymbol{P}}^h \cdot\cdot \dot{\tilde{\boldsymbol{F}}}^h \, dV - \int_{\mathscr{B}_i} \rho_0 \boldsymbol{B}(\boldsymbol{X}) \cdot \dot{\boldsymbol{\varphi}}^h \, dV - \int_{\partial \mathscr{B}_{i\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}^h \, dA \right)$$

$$= \sum_{i=1}^{n_{\text{elem}}} \left(\int_{\partial \mathscr{B}_{ic}} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\boldsymbol{\varphi}}^h \, dA \right) \quad \text{(A.8)}$$

which finally reduces to

$$\boldsymbol{M}\ddot{\boldsymbol{q}} + \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} = \boldsymbol{F}_{\text{contact}}. \quad \text{(A.9)}$$

Further, within the Hamiltonian framework, (A.5) should be modified to read

$$\int_{\mathscr{B}} \dot{\boldsymbol{\phi}} \cdot \dot{\boldsymbol{\varphi}} \, dV + \int_{\mathscr{B}} \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{F}} \cdot\cdot \dot{\boldsymbol{F}} \, dV + \int_{\mathscr{B}} \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\varphi}} \cdot \dot{\boldsymbol{\varphi}} \, dV - \int_{\partial \mathscr{B}_\sigma} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}} \, dA = \int_{\partial \mathscr{B}_c} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\boldsymbol{\varphi}} \, dA,$$

$$\int_{\mathscr{B}} \left(\dot{\boldsymbol{\varphi}} - \frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\phi}} \right) \cdot \dot{\boldsymbol{\phi}} \, dV = 0.$$

Discretization yields

$$\sum_{i=1}^{n_{\text{elem}}} \left(\int_{\mathscr{B}_i} \dot{\boldsymbol{\phi}}^h \cdot \dot{\boldsymbol{\varphi}}^h \, dV + \int_{\mathscr{B}_i} \left(\frac{\partial \overline{\mathscr{H}}}{\partial \tilde{\boldsymbol{F}}} \right)^h \cdot\cdot \dot{\tilde{\boldsymbol{F}}}^h \, dV + \int_{\mathscr{B}_i} \left(\frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\varphi}} \right)^h \cdot \dot{\boldsymbol{\varphi}}^h \, dV - \int_{\partial \mathscr{B}_{i\sigma}} \overline{\boldsymbol{T}}(\boldsymbol{X}, t) \cdot \dot{\boldsymbol{\varphi}}^h \, dA \right)$$

$$= \sum_{i=1}^{n_{\text{elem}}} \left(\int_{\partial \mathscr{B}_{ic}} (\boldsymbol{P}_c^A - \boldsymbol{P}_c^B) \cdot \hat{\boldsymbol{N}}_c^A \cdot \dot{\boldsymbol{\varphi}}^h \, dA \right) \quad \text{(A.10)}$$

and

$$\sum_{i=1}^{n_{\text{elem}}} \left(\int_{\mathscr{B}_i} \dot{\boldsymbol{\varphi}}^h \cdot \dot{\boldsymbol{\phi}}^h \, dV - \int_{\mathscr{B}_i} \left(\frac{\partial \overline{\mathscr{H}}}{\partial \boldsymbol{\phi}} \right)^h \cdot \dot{\boldsymbol{\phi}}^h \, dV \right) = 0, \quad \text{(A.11)}$$

which reduce to

$$\dot{\boldsymbol{p}} + \boldsymbol{F}_{\text{int}} - \boldsymbol{F}_{\text{ext}} = \boldsymbol{F}_{\text{contact}}, \qquad \dot{\boldsymbol{q}} - \boldsymbol{M}^{-1} \boldsymbol{p} = 0. \quad \text{(A.12)}$$

Equations (A.8), (A.10) and (A.11) represent the semidiscrete finite element equations of motion for nonholonomic or nonconservative systems with contact.

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