

Extended framework of Hamilton's principle for continuum dynamics



Jinkyu Kim^{a,*}, Gary F. Dargush^b, Young-Kyu Ju^a

^a School of Civil, Environmental and Architectural Engineering, Korea University, Anam-dong 5-ga 1, Seongbuk-goo 136-713, Republic of Korea

^b Department of Mechanical and Aerospace Engineering, SUNY at Buffalo, NY 14260, USA

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ABSTRACT

Hamilton's principle is the variational principle for dynamical systems, and it has been widely used in mathematical physics and engineering. However, it has a critical weakness, termed end-point constraints, which means that in the weak form, we cannot use the given initial conditions properly. By utilizing a mixed formulation and sequentially assigning initial conditions, this paper presents a novel extended framework of Hamilton's principle for continuum dynamics, to resolve such weakness. The primary applications lie in an elastic and a J_2 -viscoplastic continuum dynamics. The framework is simple, and initiates the development of a space–time finite element method with the proper use of initial conditions. Non-iterative numerical algorithms for both elasticity and J_2 -viscoplasticity are presented.

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1. Introduction

Hamilton (1834, 1835) formulated a variational method for dynamics, based upon the concept of stationary action, with action represented as the integral over time of the Lagrangian of the system. Despite its origin in conservative particle dynamics, Hamilton's principle has broad applicability (see Bretherton, 1970; Gossick, 1967; Landau and Lifshitz, 1975; Slawinski, 2003; Tiersten, 1967). For continuum dynamics, the action consists of a space–time integral for the Lagrangian density, and the stationarity of this action provides the equations of motion as its Euler–Lagrange equation. Thus, Hamilton's principle provides the theoretical basis for studying the dynamic behavior of materials in space–time. However, there are two main difficulties.

The first one is called the end-point constraints, which imply that the positions of the dynamical system are known at the beginning and at the end of the time interval. Considering that the primary objective in studying dynamical systems is to investigate how the system evolves in the future, the assumption that the position of the system at the end of a time interval is known is not appropriate. The second one is the restriction to conservative systems. Extending Hamilton's principle to embrace non-conservative systems requires another functional, Rayleigh's dissipation (Rayleigh, 1877), apart from a Lagrangian. While this is not a true variational method in a strict mathematical sense, it provides an

appropriate framework to accommodate non-conservative systems (Biot, 1955; Marsden and Rařiu, 1994).

Limiting our perspective within the application of a space–time finite element to dynamical systems, we can find original ideas in Argyris and Scharpf (1969) and Fried (1969). Since then, many other formulations (e.g., Hughes and Hulbert, 1988; Hughes and Marsden, 1978; Hulbert, 1992; Hulbert and Hughes, 1990; Jamet, 1978; John, 1977; Johnson, 1987; Johnson et al., 1984; Peters and Izadpanah, 1988) have been proposed and successfully implemented for engineering problems. However, finite-element methods in the temporal domain are still less popular than the classical time integration schemes, such as finite differences, Newmark, and Runge–Kutta have dominated. Furthermore, the finite-element methods in time suggested so far have had difficulty. The most common finite element methods in time are based on the time-discontinuous Galerkin's method (TDG: see Cannarozzi and Mancuso, 1995; Chien et al., 2003; Hughes and Hulbert, 1988; Hulbert, 1992; Li and Wiberg, 1996). However, there are inherent difficulties, such as (i) proper use of the initial conditions, (ii) freedom from the interference of the upwind information with respect to time, and (iii) the use of iterative algorithms due to the weak satisfaction of the initial conditions at each time-step. For example, Bottasso (1997) suggested bi-discontinuous and singly discontinuous temporal finite-element methods, where the time-boundary conditions (end-point constraints) are satisfied a priori, while allowing the momentum to have discontinuity at the beginning and at the end of a time interval (the bi-discontinuous method), or to have discontinuity at the beginning of a time interval (the singly discontinuous method).

* Corresponding author. Tel.: +82 2 3290 3833; fax: +82 2 921 2439.

E-mail addresses: jk295@korea.ac.kr, jk295@buffalo.edu (J. Kim), gdargush@eng.buffalo.edu (G.F. Dargush), tallsite@korea.ac.kr (Y.-K. Ju).

The main objective of the present work is to present a simple extension of Hamilton's principle to circumvent the first difficulty in continuum dynamics as well as the initiation of a space–time finite element method with the proper use of the initial conditions.

The remainder of the paper is organized as follows. In Section 2, the classical variational approach of Hamilton's principle is reviewed with single-degree-of-freedom oscillators as canonical examples. Section 3 presents the extended framework of Hamilton's principle to resolve the initial condition issues, and this is applied to elastic and J_2 -viscoplastic continuum dynamics. As we shall see, in each case, the new framework recovers all the governing differential equations along with the specified initial and boundary conditions. Section 4 is devoted to the numerical implementation of the new framework, where a space–time finite-element methodology is discussed. There, we also present non-iterative numerical algorithms for both elasticity and J_2 -viscoplasticity. Finally, the work is summarized and conclusions are drawn in Section 5.

2. Classical variational approaches

2.1. Hamilton's principle

Consider the harmonic oscillator displayed in Fig. 1, consisting of a mass m and linear spring having constant stiffness k . Let $u(t)$ represent the displacement of the mass from its equilibrium position, while

$$v(t) = \dot{u}(t) \tag{1}$$

denotes its velocity with the superposed dot indicating a derivative with respect to the time t .

The initial value problem associated with this system has the differential equation of motion

$$m\ddot{u} + ku = 0 \tag{2}$$

with the initial conditions

$$u(0) = u_0; \quad \dot{u}(0) = v_0 \tag{3}$$

Based upon a classical variational approach (e.g., Calkin, 1996; Fox, 1987; Gel'fand et al., 2000; Goldstein, 1980; Lanczos, 1970), we can define the Lagrangian L for this system as

$$L(u, \dot{u}; t) = T(\dot{u}; t) - U(u; t) \tag{4}$$

where kinetic energy T and elastic strain energy U are given by

$$T(\dot{u}; t) = \frac{1}{2} m[\dot{u}(t)]^2 \tag{5}$$

and

$$U(u; t) = \frac{1}{2} k[u(t)]^2 \tag{6}$$

The functional action A for the fixed time interval from t_0 to t is written

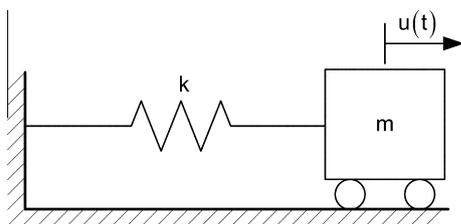


Fig. 1. Harmonic oscillator.

$$A(u, \dot{u}; t) = \int_{t_0}^t L(u, \dot{u}; \tau) d\tau \tag{7}$$

By the stationarity of the action, the first variation of (7) is

$$\delta A = -\delta \int_{t_0}^t L(u, \dot{u}; \tau) d\tau = 0 \tag{8}$$

or

$$\delta A = -\int_{t_0}^t \left[\frac{\partial L}{\partial \dot{u}} \delta \dot{u} + \frac{\partial L}{\partial u} \delta u \right] d\tau = 0 \tag{9}$$

and finally

$$\delta A = -\int_{t_0}^t [m\dot{u}\delta\dot{u} - k u \delta u] d\tau = 0 \tag{10}$$

Performing integration by parts to the first term in (10) leads to

$$\delta A = \int_{t_0}^t [m\ddot{u} + ku] \delta u d\tau - [m\dot{u}\delta u]_{t_0}^t = 0 \tag{11}$$

Following Hamilton (1834), in order to recover the governing equation of motion, we must invoke the condition of zero variation at the beginning and end of the time interval

$$\delta u(t_0) = 0; \quad \delta u(t) = 0 \tag{12}$$

Then, (11) changes into

$$\delta A = \int_{t_0}^t [m\ddot{u} + ku] \delta u d\tau = 0 \tag{13}$$

After allowing arbitrary variations δu between the end-points (t_0, t), we can recover the governing Eq. (2) for the harmonic oscillator from the stationarity of the action A . We can also derive (2) by invoking the Euler–Lagrange equation

$$\frac{d}{dt} \frac{\partial L}{\partial \dot{u}} - \frac{\partial L}{\partial u} = 0 \tag{14}$$

In either way, however, the time-boundary conditions (12) rather than the initial conditions (3) are used and this restriction is called the end-point constraints.

2.2. Rayleigh's dissipation

Rayleigh (1877) introduced a separate functional to account for non-conservative systems within the framework of Hamilton's principle. To illustrate this approach, let us consider the damped oscillator in Fig. 2, where the equation of motion and the initial conditions are

$$m\ddot{u} + c\dot{u} + ku = 0 \tag{15}$$

and

$$u(0) = u_0; \quad \dot{u}(0) = v_0 \tag{16}$$

The Rayleigh's dissipation φ for this system is defined as

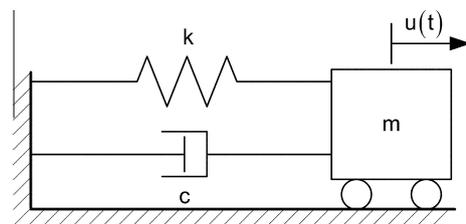


Fig. 2. Damped oscillator.

$$\varphi(\dot{u}; t) = \frac{1}{2}c[\dot{u}(t)]^2 \tag{17}$$

with the Lagrangian specified in (4)–(6).

The action itself can no longer be written in explicit form, and the first variation of A is defined as

$$\delta A = -\delta \int_{t_0}^t L(u, \dot{u}; \tau) d\tau + \int_{t_0}^t \frac{\partial \varphi(\dot{u}; \tau)}{\partial \dot{u}} \delta u d\tau = 0 \tag{18}$$

Then, from (11) and (12), we have

$$\delta A = -\int_{t_0}^t [m \dot{u} \delta \dot{u} - k u \delta u] d\tau + \int_{t_0}^t [c \dot{u}] \delta u d\tau = 0 \tag{19}$$

After applying integration by parts on the first term and end-point constraints (12), we recover the equation of motion (15) for the damped oscillator as the Euler–Lagrange equation.

While this approach is valid for arriving at the proper governing differential equation of motion, it is not completely satisfactory as a variational statement. In particular, the first variation of the dissipation (18) enters in an ad hoc manner.

3. Extended framework

To overcome the first difficulty in Hamilton’s principle, [Borri and Bottasso \(1993\)](#) suggest a general framework that correctly accounts for initial conditions within a displacement-based approach. In their approach, (i) displacement and momentum are primary variables, and (ii) the time-boundary conditions (end-point constraints) are satisfied a priori with weak satisfaction of momentum at the time-boundary. As we shall see in this Section, the new framework takes a somewhat opposite procedure to (ii) in such a general framework. Also, it utilizes a mixed formulation that has a number of computational and theoretical benefits.

3.1. The new perspective

The extension of Hamilton’s principle emanates from noticing the flaws in Hamilton’s principle, while viewing it sequentially as follows:

1. Define a Lagrangian: the dynamical system properties are defined.
2. Define an action: fix the time-window for the considered time duration.
3. Invoke stationary action $\delta A = 0$: consider all the cases where the dynamic system evolves arbitrarily from the initial to final time.
4. Enforce end-point constraints: find the dynamic evolution where the system has the known initial and final position.

Such a sequential viewpoint for Hamilton’s principle is valid, as examined through (4)–(13) for a harmonic oscillator.

Within this sequential viewpoint, Hamilton’s principle assigns end-point constraints to the dynamical system during the last step. Also, it considers all the dynamic evolution cases where the system has arbitrary (multiple) displacement and velocity at the initial and final time.

Thus, we may correctly account for the initial value problem in Hamilton’s principle, if Hamilton’s principle has the framework

1. Define a Lagrangian.
2. Define an action.
3. Invoke stationary action $\delta A_{NEW} = 0$: consider only the cases where the dynamical system evolves uniquely (but unspecified) from the initial to final time.
4. Assign the given initial conditions.

In other words, we extend the action variation as δA_{NEW} , and assign the given initial values to it. The last assigning process also has a sequence, and this is discussed next with a trivial example.

Consider a free particle whose mass is m and that moves on a frictionless surface with velocity $\dot{u}(t)$, as in [Fig. 3](#).

In the absence of a potential, the Lagrangian is simply equal to the kinetic energy

$$L(\dot{u}; t) = \frac{1}{2}m[\dot{u}(t)]^2 \tag{20}$$

The action of this system for time duration $[0, T]$ is written

$$A = \int_0^T L(\dot{u}; \tau) d\tau \tag{21}$$

In the new extended framework, we define the action variation for (21) as

$$\delta A_{NEW} = -\delta \int_0^T L(\dot{u}; \tau) d\tau + [m \hat{v}_T \delta \hat{u}_T - m \hat{v}_0 \delta \hat{u}_0] = 0 \tag{22}$$

to confine our focus to the unique dynamic evolution cases from unspecified value (\hat{v}_0, \hat{u}_0) at the initial and (\hat{v}_T, \hat{u}_T) at the final time.

The additional closed bracket terms in (22) are nothing but the counterparts to the terms without end-point constraints in Hamilton’s principle, and only the known initial values \bar{v}_0 and \bar{u}_0 are sequentially assigned to the undetermined reserved initial conditions \hat{v}_0 and \hat{u}_0 .

That is, (22) could be changed into

$$\begin{aligned} \delta A_{NEW} &= -\int_0^T \left(\frac{\partial L}{\partial \dot{u}} \delta \dot{u} + \frac{\partial L}{\partial u} \delta u \right) d\tau + [m \hat{v}_T \delta \hat{u}_T - m \hat{v}_0 \delta \hat{u}_0] \\ &= 0 \\ &= \int_0^T \left(\frac{d}{dt} \left(\frac{\partial L}{\partial \dot{u}} \right) - \frac{\partial L}{\partial u} \right) \delta u d\tau - \left[\frac{\partial L}{\partial \dot{u}} \delta u \right]_0^T \\ &\quad + [m \hat{v}_T \delta \hat{u}_T - m \hat{v}_0 \delta \hat{u}_0] \\ &= 0 \end{aligned} \tag{23}$$

and each term of closed brackets is matched as

$$\frac{\partial L}{\partial \dot{u}}(0) = m \hat{v}_0; \quad \delta u(0) = \delta \hat{u}_0; \quad \frac{\partial L}{\partial \dot{u}}(T) = m \hat{v}_T; \quad \delta u(T) = \delta \hat{u}_T \tag{24}$$

With (24), we can only consider the unique evolution cases for a particle motion.

Next, the unspecified initial value \hat{v}_0 is assigned to the given initial value

$$\hat{v}_0 = \bar{v}_0 \tag{25}$$

and successively, the unspecified initial value \hat{u}_0 has the given initial value

$$\delta \hat{u}_0 = \delta \bar{u}_0 = 0 \text{ or } \bar{u}_0 \text{ is given} \tag{26}$$

The subsequent zero-valued term (26) needs not appear explicitly in the new action variation, so that the new definition (22) with the sequential assigning process (25) and (26) can properly account for the initial value problems. It should be noted that the sequential assigning process takes somewhat opposite procedure to the previous framework by [Borri and Bottasso \(1993\)](#). In their framework, end-point constraints (displacement boundary condi-

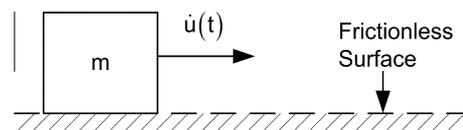


Fig. 3. Particle motion.

tions) are satisfied before the momentum boundary conditions (velocity boundary conditions) are applied while the new framework sequentially assigns the initial velocity and the initial displacement. Thus, compared to the previous framework, the new framework takes opposite procedure in assigning the initial conditions.

The extended framework is explained pictorially in Fig. 4, with a comparison to the original framework of Hamilton’s principle. To emphasize that only the known initial conditions are used, while leaving the final values uniquely unknown, the circle (displacement) and the tangent line (velocity) at each end are shown in different ways. There, the unique dynamic evolution is represented as

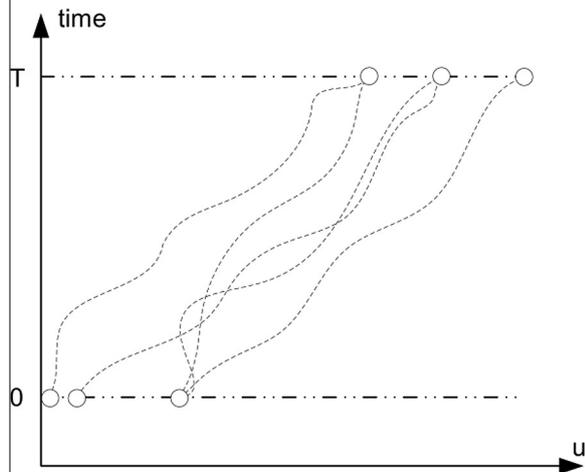
a solid-line while the multiple dotted lines represent that the trajectory of a particle is not unique.

3.2. Extension to continuum dynamics

Recent work by Sivaselvan and Reinhorn (2006), Lavan et al. (2009), Sivaselvan et al. (2009), Apostolakis and Dargush (2012, 2013) perceive a dynamical system as a collection of Euler–Lagrange equations in state variables, where each state variable such as displacements, internal stresses, and other variables can be treated uniformly with the adoption of a mixed Lagrangian formulation. Here, we continue along these lines, but propose a new

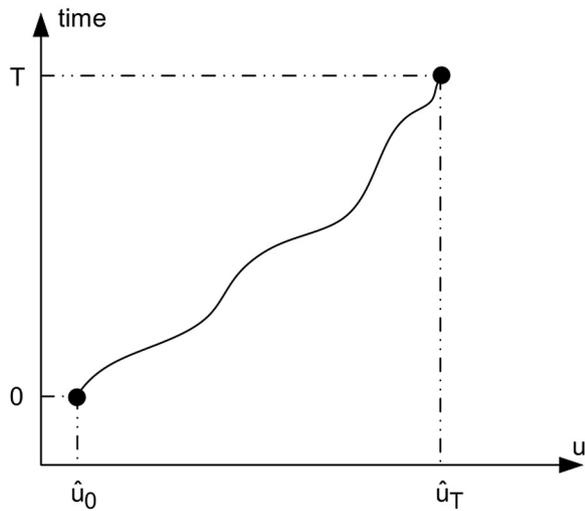
Framework of Hamilton’s Principle

1. Stationary of the action ($\delta A=0$)



Consider all the dynamic evolution cases where the displacement and velocity have arbitrary (multiple) values at initial/ final time.

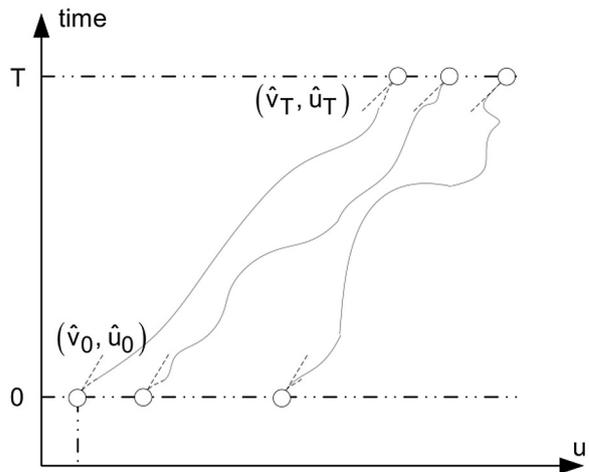
2. Invoke end-point constraints.



Find the true dynamic evolution where the system has the known initial and final displacement.

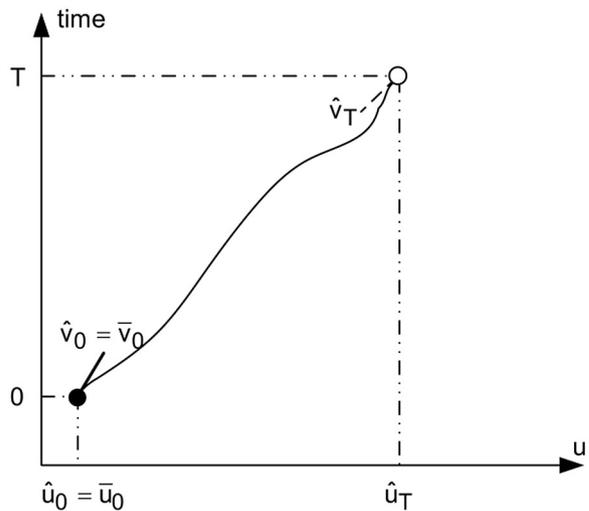
Extension Framework of Hamilton’s Principle

1. Stationary of the action ($\delta A_{NEW}=0$)



Consider only the unique dynamic evolution cases where the velocity and the displacement have unique unspecified value at initial/ final time.

2. Assign the given initial values.



Sequentially assign the given values \bar{v}_0 and \bar{u}_0 to \hat{v}_0 and \hat{u}_0 , and find the true dynamic evolution.

Fig. 4. Graphical view of the extended framework for Hamilton’s principle.

framework for continuum dynamics. The main objective here is to show how the extended framework can recover all the governing equations, with compatible initial and boundary conditions for an elastic and a viscoplastic continuum.

3.2.1. An elastic continuum

In the extended framework of Hamilton's principle, the action for the elastic continuum dynamics within the time duration $[0, T]$ is defined as

$$A = \int_0^T \int_{\Omega} l d\Omega d\tau + \int_0^T V d\tau \tag{27}$$

where, the Lagrangian density l and the applied force potential V are given by

$$l = \frac{1}{2} \rho \dot{u}_i \dot{u}_i + \frac{1}{2} A_{ijkl} \dot{J}_{ij} \dot{J}_{kl} - \dot{J}_{ij} \varepsilon_{ij} \tag{28}$$

and

$$V = \int_{\Omega} \hat{f}_i u_i d\Omega + \int_{\Gamma_t} \hat{t}_i u_i d\Gamma \tag{29}$$

In (28) and (29), ρ is the mass density and A_{ijkl} is the elastic constitutive tensor inverse to D_{ijkl} , the usual constitutive tensor for an anisotropic elastic medium, while $J_{ij}(t) = \int_0^t \sigma_{ij}(\tau) d\tau$ is an impulse of stress tensor σ_{ij} , and ε_{ij} is the strain tensor. Also, \hat{f}_i and \hat{t}_i represent the known body force density and the known traction of an elastic continuum occupying Ω in space, respectively. Here, the boundary conditions are defined such that $\Gamma_u \cup \Gamma_t = \Gamma$ and $\Gamma_u \cap \Gamma_t = \emptyset$.

The new action variation for elastodynamics is defined in terms of the generalized displacement field u_i and the generalized stress field $J_{ij}(= \sigma_{ij})$ as

$$\delta A_{NEW} = -\delta \int_0^T \int_{\Omega} l d\Omega d\tau - \delta \int_0^T V d\tau + \int_{\Omega} [\rho \hat{v}_i \delta \hat{u}_i]_0^T d\Omega = 0 \tag{30}$$

As in the previous particle example, (30) is defined by adding all the counterparts to the terms without end-point constraints in Hamilton's principle, and confining them to a unique but undetermined value at the initial and final time.

By substituting (28) and (29) into (30), (30) is written

$$\begin{aligned} \delta A_{NEW} = & - \int_0^T \int_{\Omega} [\rho \dot{u}_i \delta \dot{u}_i + A_{ijkl} \dot{J}_{ij} \delta \dot{J}_{kl} - \dot{J}_{ij} \delta \varepsilon_{ij}] d\Omega d\tau \\ & - \int_{\Omega} \int_0^T \hat{f}_i \delta u_i d\tau d\Omega - \int_{\Gamma_t} \int_0^T \hat{t}_i \delta u_i d\tau d\Gamma \\ & + \int_{\Omega} [\rho \hat{v}_i \delta \hat{u}_i]_0^T d\Omega \\ = & 0 \end{aligned} \tag{31}$$

After performing all of the temporal and spatial integration-by-parts operations on (31), we have

$$\begin{aligned} \delta A_{NEW} = & \int_0^T \int_{\Omega} (\rho \ddot{u}_i - \dot{J}_{ij,j} - \hat{f}_i) \delta u_i d\Omega d\tau \\ & + \int_0^T \int_{\Omega} (A_{ijkl} \ddot{J}_{ij} - \dot{\varepsilon}_{kl}) \delta J_{kl} d\Omega d\tau \\ & + \int_{\Omega} [(\varepsilon_{kl} - A_{ijkl} \dot{J}_{ij}) \delta J_{kl}]_0^T d\Omega \\ & + \int_0^T \int_{\Gamma} \hat{t}_i \delta u_i d\Gamma d\tau - \int_0^T \int_{\Gamma_t} \hat{t}_i \delta u_i d\Gamma d\tau \\ & + \int_{\Omega} [\rho \hat{v}_i \delta \hat{u}_i - \rho \dot{u}_i \delta \hat{u}_i]_0^T d\Omega = 0 \end{aligned} \tag{32}$$

While performing a spatial integration by parts on the term $\dot{J}_{ij} \delta \varepsilon_{ij}$ in (31), we make use of the symmetry of stresses J_{ij} and the Cauchy definition of surface traction, where $t_i = J_{ij} n_j$.

To satisfy $\delta A_{NEW} = 0$ in (32), we have not only the governing differential equations, representing linear momentum balance and elastic constitutive behavior, respectively

$$\rho \ddot{u}_i - \dot{J}_{ij,j} - \hat{f}_i = 0; \quad A_{ijkl} \ddot{J}_{ij} - \dot{\varepsilon}_{kl} = 0 \tag{33}$$

but also the compatibility equation at the initial and final time

$$\varepsilon_{kl} - A_{ijkl} \dot{J}_{ij} = 0 \tag{34}$$

More importantly, the new action variation (30) uses all the pertinent initial/boundary conditions in the last two lines of (32). That is, by expressing the displacement of an elastic continuum u_i as a function of position vector \vec{x} and time t as $u_i = u_i(\vec{x}, t)$, we can see that the given initial velocity condition

$$\dot{u}_i(\vec{x}, 0) = \hat{v}_i(\vec{x}, 0) = \bar{v}_i(\vec{x}, 0) \tag{35}$$

and successively the given initial displacement condition

$$u_i(\vec{x}, 0) = \hat{u}_i(\vec{x}, 0) = \bar{u}_i(\vec{x}, 0) \tag{36}$$

are properly used in the last line of (32).

Also, we have the boundary conditions

$$t_i = \hat{t}_i \text{ on } \Gamma_t \tag{37}$$

and

$$\delta u_i(\vec{x}, t) = 0 \text{ or } u_i(\vec{x}, t) = \tilde{u}_i(\vec{x}, t) \text{ on } \Gamma_u \tag{38}$$

in the fourth line of (32). In (38), $\tilde{u}_i(\vec{x}, t)$ is the given displacement boundary condition at the specified location \vec{x} .

3.2.2. A viscoplastic continuum

By applying Rayleigh's dissipation function to this framework, we can also account for non-conservative dynamical systems. Here, the Duvaut and Lions viscoplasticity (1976), where the dissipation function or flow potential that depends on the stress only through the J_2 invariant, is considered.

As described in Lubliner (1990) and Simo and Hughes (1998) well, the dissipation function of viscoplasticity, incorporating the Mises yield criterion and a J_2 flow potential, can be expressed in terms of a Macaulay bracket $\langle \bullet \rangle$ as

$$\varphi = \frac{1}{2\eta} \left\langle \sqrt{J_2} - \frac{\sigma_Y}{\sqrt{3}} \right\rangle^2 \tag{39}$$

where σ_Y and η represent the yield stress and viscosity, respectively.

This dissipation function is included in the new action variation for the time duration $[0, T]$ as

$$\int_0^T \int_{\Omega} \left[\dot{\varepsilon}_{kl}^{vp} = \frac{\partial \varphi}{\partial S_{kl}} = \frac{\partial \varphi}{\partial J_2} \frac{\partial J_2}{\partial S_{kl}} = \frac{1}{2\eta} \frac{\langle \sqrt{J_2} - \frac{\sigma_Y}{\sqrt{3}} \rangle}{\sqrt{J_2}} S_{kl} \right] \delta D_{kl} d\Omega d\tau \tag{40}$$

In (40), S_{kl} and δD_{kl} represent the deviatoric stress tensor, and the first variation of deviatoric impulse tensor, respectively. Also, the notation $\dot{\varepsilon}_{kl}^{vp}$ represents the rate-dependent plasticity or viscoplastic strain rate. The reason for introducing the first variation of deviatoric impulse δD_{kl} in (40) is that Rayleigh's method uses the first variation having less than one time differentiation value of the main variable in the dissipation potential. This was already examined in (18) for the damped oscillator.

However, whether using the first variation of deviatoric impulse tensor δD_{kl} , or the first variation of impulse δJ_{kl} in (40), does not make any difference, because the differentiation of the dissipation function with respect to the deviatoric stress (that is, $\partial \varphi / \partial S_{kl}$) and the differentiation of the dissipation function with respect to the stress ($\partial \varphi / \partial \sigma_{kl}$) are the same:

$$\frac{\partial \varphi}{\partial \sigma_{kl}} = \frac{\partial \varphi}{\partial J_2} \frac{\partial J_2}{\partial \sigma_{kl}}$$

where,
$$\frac{\partial J_2}{\partial \sigma_{kl}} = \frac{\partial (\frac{1}{2} S_{ij} S_{ij})}{\partial \sigma_{kl}} = \frac{\partial (\sigma_{ij} - \frac{1}{3} \sigma_{mm} \delta_{ij})}{\partial \sigma_{kl}} S_{ij} = \left(\delta_{ik} \delta_{jl} - \frac{1}{3} \delta_{mk} \delta_{ml} \delta_{ij} \right) S_{ij} = S_{kl} - \frac{1}{3} \delta_{kl} S_{ii} = S_{kl} \quad (41)$$

Thus, we can freely use δD_{kl} or δJ_{kl} in (40).

Combining the Rayleigh dissipation function (39) and its variational term (40), we define the new action variation for a viscoplastic continuum as

$$\begin{aligned} \delta A_{NEW} &= -\delta \int_0^T \int_{\Omega} l d\Omega d\tau - \delta \int_0^T \int_{\Omega} v d\tau + \int_0^T \int_{\Omega} [\hat{\epsilon}_{kl}^{vp}] \delta J_{kl} d\Omega d\tau \\ &+ \int_{\Omega} [\rho \hat{v}_i \delta \hat{u}_i]_0^T d\Omega - \int_{\Omega} [\hat{\epsilon}_{kl}^{vp} \delta J_{kl}]_0^T d\Omega \\ &= 0 \end{aligned} \quad (42)$$

where $\hat{\epsilon}_{kl}^{vp}$ represents the viscoplastic strain.

In terms of the mixed variables, such as u_i and J_{ij} , the governing differential equations for the viscoplastic continuum can be written

$$\rho \ddot{u}_i - \dot{J}_{ijj} - \hat{f}_i = 0; \quad A_{ijkl} \dot{J}_{ij} - \dot{\epsilon}_{kl} + \hat{\epsilon}_{kl}^{vp} = 0 \quad (43)$$

where they represent the equations of motion and rate-compatibility, respectively, valid at any time t . Note that the rate-compatibility equation $A_{ijkl} \dot{J}_{ij} - \dot{\epsilon}_{kl} + \hat{\epsilon}_{kl}^{vp} = 0$ is equivalent to the equation $\dot{\sigma}_{ij} - D_{ijkl} (\dot{\epsilon}_{kl} - \hat{\epsilon}_{kl}^{vp}) = 0$ with the usual elastic constitutive tensor D_{ijkl} .

Our objective is to show how the new action variation (42) recovers all of these governing relations (43) as the Euler–Lagrange equations for the viscoplastic continuum.

By substituting (28) and (29) into (42), (42) is written

$$\begin{aligned} \delta A_{NEW} &= - \int_0^T \int_{\Omega} [\rho \dot{u}_i \delta \dot{u}_i + A_{ijkl} \dot{J}_{ij} \delta J_{kl} - \epsilon_{ij} \delta J_{ij} - \dot{J}_{ij} \delta \epsilon_{ij}] d\Omega d\tau \\ &- \int_{\Omega} \int_0^T \hat{f}_i \delta u_i d\tau d\Omega - \int_{\Gamma_r} \int_0^T \hat{t}_i \delta u_i d\tau d\Gamma \\ &+ \int_{\Omega} [\rho \hat{v}_i \delta \hat{u}_i]_0^T d\Omega + \int_0^T \int_{\Omega} [\hat{\epsilon}_{kl}^{vp}] \delta J_{kl} d\Omega d\tau \\ &- \int_{\Omega} [\hat{\epsilon}_{kl}^{vp} \delta J_{kl}]_0^T d\Omega \\ &= 0 \end{aligned} \quad (44)$$

After applying temporal and spatial integration-by-parts to (44), we have

$$\begin{aligned} \delta A_{NEW} &= \int_0^T \int_{\Omega} (\rho \ddot{u}_i - \dot{J}_{ijj} - \hat{f}_i) \delta u_i d\Omega d\tau + \int_0^T \int_{\Omega} (A_{ijkl} \dot{J}_{ij} - \dot{\epsilon}_{kl} \\ &+ \hat{\epsilon}_{kl}^{vp}) \delta J_{kl} d\Omega d\tau + \int_{\Omega} [(\epsilon_{kl} - A_{ijkl} \dot{J}_{ij} - \hat{\epsilon}_{kl}^{vp}) \delta J_{kl}]_0^T d\Omega \\ &+ \int_0^T \int_{\Gamma} \hat{t}_i \delta u_i d\Gamma d\tau - \int_0^T \int_{\Gamma_r} \hat{t}_i \delta u_i d\Gamma d\tau \\ &+ \int_{\Omega} [\rho \hat{v}_i \delta \hat{u}_i - \rho \dot{u}_i \delta u_i]_0^T d\Omega \\ &= 0 \end{aligned} \quad (45)$$

In (45), we can explicitly have not only the governing differential equations (43) from the first two lines, but also the compatibility equation (the underlined terms). Furthermore, as in an elastic continuum, the new definition (44) uses all the pertinent initial/boundary conditions for a viscoplastic continuum, in the last two lines of (45).

3.3. Discussion of the extended framework

So far, we have shown how $\delta A_{NEW} = 0$ in the new framework finds the true dynamic evolution for elastic and viscoplastic continuum. Theoretically, $\delta A_{NEW} = 0$ holds because

1. It only considers unique dynamic evolution cases of the system, where the initial conditions are unspecified.
2. Among these unique cases, the true trajectory of the system is identified with sequentially assigning the known initial conditions.

Physically, this extends the principle of virtual work to dynamics in a mixed variational sense. For elastodynamics, by interpreting the first variations ($\delta u_i, \delta J_{kl}$) as virtual fields, and the independent field variables (u_i, J_{ij}) as real fields in (32), the Eq. (32) provides not only the equilibrium, but also the initial/boundary conditions and rate-compatibility/compatibility equations at the same time. Also, Eq. (45) can be viewed as the extension of the principle of virtual work in viscoplastic continuum dynamics with proper strong forms (43) and initial/boundary conditions (35)–(38).

The framework can be numerically implemented through applying a space–time Galerkin’s finite element. For elasticity, Eq. (31), which is equivalent to (32), provides the balanced continuity equation, since both u_i and J_{kl} in the real and virtual fields have C^0 time continuity, while u_i and J_{kl} in the real and virtual fields have C^0 and C^{-1} space continuity. Also, Eq. (44) provides the balanced continuity equation for the dynamics of a viscoplastic continuum.

4. A space–time finite element method from the extended framework

The implementation of space–time finite elements in the context of the extended framework is somewhat particular. The important issues are (i) the identification of the primary fields to use proper initial conditions, and (ii) numerical efficiency from the inherent disadvantage of mixed formulation. As we shall see in this Section, we resolve the first issue (i) by making the velocity at each time-end satisfy subsequent space–time continuity requirements. Also, to alleviate numerical efficiency somehow, (ii) we allow the mixed time-step algorithm, where the unknown velocity at the end of each time step cannot appear until the last time step.

4.1. Numerical implementation

By adopting Cartesian coordinates, each integration in (31) for elasticity can be written in vector and matrix form as:

$$J = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} & \frac{\partial z}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} & \frac{\partial z}{\partial \eta} \\ \frac{\partial x}{\partial \zeta} & \frac{\partial y}{\partial \zeta} & \frac{\partial z}{\partial \zeta} \end{bmatrix} \quad (46)$$

where (x, y, z) and (ξ, η, ζ) represent the global coordinate and natural coordinate. Also, the Jacobian determinant for each face of a certain element is written as J_f in INT4.

The integrations in the above tables are quite similar to those in the usual finite-element formulation, except that the independent fields, such as $\{\delta u_i\} = [\delta u_x \ \delta u_y \ \delta u_z]^T$ and $\{\delta J_{ij}\} = [\delta J_{xx} \ \delta J_{yy} \ \delta J_{zz} \ \delta J_{yz} \ \delta J_{zx} \ \delta J_{xy}]^T$, are functions of both space and time. Here, $\{\bullet\}$ and $[\bullet]$ represent column vector and row vector, respectively.

The constitutive matrix $[A_{ijkl}]$ in INT 6 is symmetric, and can represent isotropic or anisotropic material properties. For isotropic materials, $[A_{ijkl}]$ is written

$$\begin{bmatrix} \frac{1}{E} & -\frac{\nu}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & \frac{1}{E} & -\frac{\nu}{E} & 0 & 0 & 0 \\ -\frac{\nu}{E} & -\frac{\nu}{E} & \frac{1}{E} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{1}{G} & 0 & 0 \\ 0 & 0 & 0 & 0 & \frac{1}{G} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{G} \end{bmatrix} \quad (47)$$

where E is the Young's modulus, ν is the Poisson's ratio and G is the shear modulus. The shear modulus can be expressed in terms of the Young's modulus and Poisson's ratio as $G = \frac{E}{2(1+\nu)}$.

4.1.1. Numerical approximation of each field with the new notation

To avoid complication in the discretizing process while applying Galerkin's method to space-time, the new notations are deliberately contrived. That is, the notations related to the space of an independent field are placed at the right side, and those related to the time of an independent field are placed at the left side. In addition, the upper notations represent nodal values, and the lower notations represent approximation. For example, the space-time displacement field for the time duration $[t_{r-1}, t_r]$ of a certain element is approximated by

$$\begin{aligned} u_i \approx_r u_i &= \frac{1}{h} [t_r - t - t_{r-1} + t] \begin{Bmatrix} {}^{r-1}u_i \\ {}_r u_i \end{Bmatrix} \\ &= \frac{1}{h} [t_r - t - t_{r-1} + t] \begin{Bmatrix} \sum_p (N^{pr-1} u_i^p) \\ \sum_p (N^{pr} u_i^p) \end{Bmatrix} \end{aligned} \quad (48)$$

where $h = t_r - t_{r-1}$.

In (48), the linear shape function in time is adopted to satisfy the least temporal continuity requirements C^0 , whereas the shape functions in space N^p are not specified. No spatial element is specified to show the numerical implementation scheme of the new method in general.

Consequently, \dot{u}_i in the time duration $[t_{r-1}, t_r]$ is approximated by

$$\dot{u}_i \approx_r \dot{u}_i = \frac{1}{h} [-1 \ 1] \begin{Bmatrix} {}^{r-1}u_i \\ {}_r u_i \end{Bmatrix} = \frac{1}{h} [-1 \ 1] \begin{Bmatrix} \sum_p (N^{pr-1} u_i^p) \\ \sum_p (N^{pr} u_i^p) \end{Bmatrix} \quad (49)$$

Similarly, J_{ij} and Cauchy's stress \dot{J}_{ij} in the time duration $[t_{r-1}, t_r]$ are approximated by

$$\begin{aligned} J_{ij} \approx_r J_{ij} &= \frac{1}{h} [t_r - t - t_{r-1} + t] \begin{Bmatrix} {}^{r-1}J_{ij} \\ {}_r J_{ij} \end{Bmatrix} \\ &= \frac{1}{h} [t_r - t - t_{r-1} + t] \begin{Bmatrix} {}^{r-1}J_{ij}^{(p)} \\ {}_r J_{ij}^{(p)} \end{Bmatrix} \end{aligned} \quad (50)$$

and

$$\dot{J}_{ij} \approx_r \dot{J}_{ij} = \frac{1}{h} [-1 \ 1] \begin{Bmatrix} {}^{r-1}J_{ij} \\ {}_r J_{ij} \end{Bmatrix} = \frac{1}{h} [-1 \ 1] \begin{Bmatrix} {}^{r-1}J_{ij}^{(p)} \\ {}_r J_{ij}^{(p)} \end{Bmatrix} \quad (51)$$

Since J_{ij} requires C^{-1} space-continuity, letting J_{ij} have a representative value at a point in an element may be enough. The expression $\{p\}$ in (50) and (51) is used for consistency, and can be regarded as a dummy expression at this moment.

For viscoplasticity, the deviatoric stress S_{kl} in (40) could be numerically discretized by introducing deviatoric impulse D_{kl} . That is, D_{kl} is written

$$D_{kl}(t) = J_{kl}(t) - \frac{1}{3} J_{mm}(t) \delta_{kl} \quad (52)$$

Then, the deviatoric stress S_{kl} for the time duration $[t_{r-1}, t_r]$ is approximated by

$$S_{kl} = \dot{D}_{kl} \approx_r \dot{D}_{kl} = \frac{1}{h} [-1 \ 1] \begin{Bmatrix} {}^{r-1}D_{kl} \\ {}_r D_{kl} \end{Bmatrix} = \frac{1}{h} [-1 \ 1] \begin{Bmatrix} {}^{r-1}D_{kl}^{(p)} \\ {}_r D_{kl}^{(p)} \end{Bmatrix} \quad (53)$$

where the relation between ${}^r D_{kl}^{(p)}$ and ${}^r J_{kl}^{(p)}$ is also valid as (52) at any discrete time t_r .

Similarly, by replacing the real field nodal values in (48)–(51) with the virtual nodal values, each virtual field (continuity balanced to real fields) can be approximated.

With the approximation of (48)–(53) in both the real and virtual fields in Tables 1 and 2, we subsequently approximate \dot{v}_i at each time-end (INT 5 in Table 1) with the consideration of C^{-1} time continuity/ C^0 space continuity. This approach does not violate any continuity requirement of velocity, since the velocity in the integrand u_i is subsequently approximated with the C^{-1} time continuity requirement following the C^0 time continuity requirement on the displacement field and approximated with C^0 space continuity requirement following the C^0 space continuity requirement on the displacement field. Similarly, we approximate the viscoplastic strain $\hat{\epsilon}_{kl}^{vp}$ (INT9 in Table 2) by the representative value $\hat{\epsilon}_{kl}^{vp(p)}$. An initial version of this approach using low-order discrete time formulations leads toward development of higher-order time-stepping methods with much care about the initial conditions including impact problems in the future (see Farhat et al., 2003; Lorcher et al., 2007; Gassner et al., 2008; Petersen et al., 2009).

4.1.2. Implementation scheme for each space-time element

With the approximation scheme above, we can directly integrate individual space-time integration in Tables 1 and 2 firstly for the temporal domain by using Fubini's theorem. For example, doing the time-integration first for INT1 after substituting (49) into INT1 yields

$$\begin{aligned} \text{INT1} : & -\frac{\rho}{h} \\ & \times \int_{V_n} \left\{ \sum_m N^m (\delta^r u_i^m - \delta^{r-1} u_i^m) \right\}^T \left\{ \sum_p N^p ({}^r u_i^p - {}^{r-1} u_i^p) \right\} J dV_n \end{aligned} \quad (54)$$

Similarly, doing the time-integration first on the other integrations in Tables 1 and 2 yields

$$\begin{aligned} \text{INT2} : & \frac{1}{2} \\ & \times \int_{V_n} \left\{ \sum_m B^m \{ \delta^r u_i^m + \delta^{r-1} u_i^m \} \right\}^T \{ {}^r J_{ij}^{(p)} - {}^{r-1} J_{ij}^{(p)} \} J dV_n \end{aligned} \quad (55)$$

$$\text{INT3} : -\frac{h}{2} \int_{V_n} \left\{ \sum_m N^m (\delta^{r-1} u_i^m + \delta^r u_i^m) \right\}^T \{ {}^r \hat{f}_i^m \} J dV_n \quad (56)$$

$$\text{INT4} : -\frac{h}{2} \int_{\Gamma_n} \left\{ \sum_f \sum_x F^x (\delta^{r-1} u_i^x + \delta^r u_i^x) \right\}^T \{ {}^r \hat{t}_i^x \} J_f d\Gamma_n \quad (57)$$

$$\text{INT5} : \rho \int_{V_n} \left[\left\{ \sum_m N^m (\delta^r u_i^m) \right\}^T \{ {}^r \dot{v}_i^p \} - \left\{ \sum_m N^m (\delta^{r-1} u_i^m) \right\}^T \{ {}^{r-1} \dot{v}_i^p \} \right] J dV_n \quad (58)$$

Table 1
Integrations for elastodynamics.

Integrations	Description
INT1: $-\int_{t_{r-1}}^{t_r} \int_{V_n} \rho \{\delta \dot{u}_i\}^T \{\dot{u}_i\} J dV_n d\tau$	Kinetic energy
INT2: $\int_{t_{r-1}}^{t_r} \int_{V_n} \{\delta \varepsilon_{ij}\}^T \{J_{ij}\} J dV_n d\tau$	Work conjugate variation
INT3: $-\int_{t_{r-1}}^{t_r} \int_{V_n} \{\delta u_i\}^T \{f_i\} J dV_n d\tau$	Body force
INT4: $-\int_{t_{r-1}}^{t_r} \int_{\Gamma_i} (\sum_f \{\delta u_i\}^T \{\hat{t}_i\} J_f) d\Gamma_n d\tau$	Traction: the Jacobian is defined for each face
INT5: $\int_{V_n} [\{\delta \dot{u}_i\}^T \{\rho \dot{v}_i\}]_{t_{r-1}}^{t_r} J dV_n$	Initial/final momentum density
INT6: $-\int_{t_{r-1}}^{t_r} \int_{V_n} \{\delta j_{kl}\}^T [A_{ijkl}] \{J_{ij}\} J dV_n d\tau$	Constitutive relation
INT7: $\int_{t_{r-1}}^{t_r} \int_{V_n} \{\delta j_{ij}\}^T \{\varepsilon_{ij}\} J dV_n d\tau$	Work conjugate variation

With Table 1, the additional integrations that account for J_2 -viscoplasticity in (44) are given.

$$\text{INT6: } -\frac{1}{h} \left\{ \left(\delta^r J_{kl}^{(m)} - \delta^{r-1} J_{kl}^{(m)} \right) \right\}^T [A_{ijkl}] \left\{ \left(J_{ij}^{(p)} - r^{-1} J_{ij}^{(p)} \right) \right\} \int_{V_n} J dV_n \quad (59)$$

$$\text{INT7: } \frac{1}{2} \int_{V_n} \left\{ \delta^r J_{ij}^{(m)} - \delta^{r-1} J_{ij}^{(m)} \right\}^T \left\{ \sum_p B^p \{r u_i^p + r^{-1} u_i^p\} \right\} J dV_n \quad (60)$$

$$\text{INT8: } \left\{ \delta^r J_{kl}^{(m)} + \delta^{r-1} J_{kl}^{(m)} \right\}^T \left\{ {}_D \varphi \left(r D_{kl}^{(m)}, r^{-1} D_{kl}^{(m)} \right) \right\} \quad (61)$$

$$\text{INT9: } -\left[\left\{ \delta^r J_{kl}^{(m)} \right\}^T \left\{ r \hat{\varepsilon}_{kl}^{vp(p)} \right\} - \left\{ \delta^{r-1} J_{kl}^{(m)} \right\}^T \left\{ r^{-1} \hat{\varepsilon}_{kl}^{vp(p)} \right\} \right] \int_{V_n} J dV_n \quad (62)$$

In (55)–(62), B^m and F^α represent the strain–displacement matrix and the shape functions at each face of an element, respectively. Also, ${}_D \varphi \left(r D_{kl}^{(m)}, r^{-1} D_{kl}^{(m)} \right)$ is defined as

$${}_D \varphi \left(r D_{kl}^{(m)}, r^{-1} D_{kl}^{(m)} \right) = \frac{V}{2} \frac{1}{2\eta} \left\langle 1 - \frac{\sigma_Y}{\sqrt{r} J_2 \sqrt{3}} \right\rangle \left\{ r D_{kl}^{(m)} - r^{-1} D_{kl}^{(m)} \right\} \quad (63)$$

Afterwards, the numerical integration for spatial integral can be used as for the usual finite-element methods. That is, the coefficients of the discrete virtual fields such as $(\delta^r u_i^m, \delta^{r-1} u_i^m)$ in (54) and $(\delta^r J_{kl}^{(m)}, \delta^{r-1} J_{kl}^{(m)})$ in (59) are obtained by various numerical integration methods, such as Newton–Cotes and Gaussian cubature.

So far, it has been shown how each integration in $\delta_r A$ could be discretized into $\delta^r A$ by applying Galerkin’s method to space–time. That is, $\delta A = 0$ for the time duration $[0, T]$ is written

$$\delta A = 0 \Rightarrow \sum_{r=1}^N \delta_r A = 0 \xrightarrow[\text{Numerical integration for space}]{\text{Time integration, first}} \sum_{r=1}^N \delta^r A = 0 \Rightarrow \delta^r A = 0 \quad (64)$$

where the entire time duration $[0, T]$ is divided equally into N durations ($t_n = nh$), and $\delta^r A$ (the discrete version of $\delta_r A$) consist of all the discrete variables $(\delta^{r-1} u_i^m, \delta^r u_i^m, \delta^{r-1} J_{kl}^{(m)}, \delta^r J_{kl}^{(m)})$ and $(r^{-1} u_i^p, r u_i^p, r^{-1} \hat{v}_i^p, r \hat{v}_i^p, r^{-1} J_{ij}^{(p)}, r J_{ij}^{(p)}, r \hat{f}_i^p, r \hat{t}_i^p)$.

Table 2
Additional integrations for viscoplasticity.

Integrations	Description
INT8: $\int_{t_{r-1}}^{t_r} \int_{V_n} \{\delta j_{kl}\}^T \{\hat{\varepsilon}_{kl}^{vp}\} J dV_n d\tau$	Rate-compatibility relation
INT9: $-\int_{V_n} [\{\delta J_{kl}\}^T \{\hat{\varepsilon}_{kl}^{vp}\}]_{t_{r-1}}^{t_r} J dV_n$	Viscoplastic strain came from Rayleigh’s dissipation

In Tables 1 and 2, an isoparametric formulation for space is used, and J represents the Jacobian determinant given.

By making each coefficient of virtual fields $(\delta^{r-1} u_i^m, \delta^r u_i^m, \delta^{r-1} J_{kl}^{(m)}, \delta^r J_{kl}^{(m)})$ zero in $\delta^r A$, we have one time-step method as

$$[C] \{x_{unknowns}\} = \{b\} \quad (65)$$

where, $\{x_{unknowns}\} = [{}^r U, {}^r \hat{V}, {}^r J]^T$ and $\{b\}$ consists of the known values $(r^{-1} u_i^p, r^{-1} \hat{v}_i^p, r^{-1} J_{ij}^{(p)}, r \hat{f}_i^p, r \hat{t}_i^p)$. Here, block row vectors, ${}^r U = \{r u_i^p\}^T$, ${}^r \hat{V} = \{r \hat{v}_i^p\}^T$, and ${}^r J = \{r J_{ij}^{(p)}\}^T$ are used.

However, we propose a mixed-step algorithm with the consideration of numerical efficiency. The critical point is how to deal with the unknown $\{r \hat{v}_i^p\}$. In the mixed-step method, $\{r \hat{v}_i^p\}$ appears only in the last time step. This is obtained by collecting the coefficients of the virtual fields separately as $(\delta^0 u_i^m, \delta^0 J_{kl}^{(m)})$, $(\delta^k u_i^m, \delta^k J_{kl}^{(m)})$, and $(\delta^N u_i^m, \delta^N J_{kl}^{(m)})$, where k is the integer running from 1 to $N - 1$. That is, the stationarity of the action $\delta A = 0$ is viewed as

$$\delta A = 0 \Rightarrow \sum_{r=1}^N \delta^r A = 0 \Rightarrow \delta^0 \bar{A} + \sum_{k=1}^{N-1} \delta^k \bar{A} + \delta^N \bar{A} = 0 \Rightarrow \delta^0 \bar{A} = 0; \delta^k \bar{A} = 0; \delta^N \bar{A} = 0 \quad (66)$$

where $\delta^r \bar{A}$ is only composed of the relevant virtual fields $(\delta^r u_i^m, \delta^r J_{kl}^{(m)})$.

Then, a matrix equation for each space–time element is written

$$[D] \{\bar{x}_{unknowns}\} = \{c\} \quad (67)$$

where $\{\bar{x}_{unknowns}\} = [{}^r U, {}^r J]^T$.

Note that in (67), $\{c\}$ differs from the first time element, and the other time elements. That is, $\{c\}$ in the first time element consists of the known values $({}^0 u_i^p, {}^0 \hat{v}_i^p, {}^0 J_{ij}^{(p)}, {}^1 \hat{f}_i^p, {}^1 \hat{t}_i^p)$, and $\{c\}$ in the other time element (r th-element) consists of the known values $(r^{-2} u_i^p, r^{-2} J_{ij}^{(p)}, r^{-1} \hat{f}_i^p, r^{-1} \hat{t}_i^p, r^{-1} u_i^p, r^{-1} J_{ij}^{(p)}, r \hat{f}_i^p, r \hat{t}_i^p)$.

With this mixed-step method, we have an additional matrix equation for $\{N \hat{v}_i^p\}$ at the last time step N as

$$[L] \{N \hat{v}_i^p\} = \{q\} \quad (68)$$

where $\{q\}$ consists of the known values $(N^{-1} u_i^p, N^{-1} J_{ij}^{(p)}, N u_i^p, N J_{ij}^{(p)}, N+1 \hat{f}_i^p, N+1 \hat{t}_i^p)$.

Such a mixed-step method also makes it easier to zone the matrix $[D]$, and provides the displacement-based space-time finite element method, as in Fig. 5.

In Fig. 5, the block matrices $[D_{UJ}]$ and $[D_{JU}]$ have the relation

$$[D_{UJ}] = -[D_{JU}]^T \tag{69}$$

which came from the integration by parts property in the temporal domain (compare (55)–(60)).

Also, the block matrices $[D_{UU}]$ and $[D_{JJ}]$ are given by

$$[D_{UU}] = \frac{1}{h} [M] \tag{70}$$

and

$$[D_{JJ}] = \frac{V}{h} [A_{ijkl}] \tag{71}$$

where $[M]$ and V represent the consistent mass matrix and the volume of an element, respectively.

4.2. Numerical algorithm for elasticity

By identifying the stiffness-like matrix $[\hat{D}^i]$ for each element, the global matrix $[\hat{D}]$ for elasticity in Fig. 5 can be established as following a conventional finite element method (see Bathe, 1996; Cook et al., 1989; Hughes (2000); Strang and Fix (1973)). That is, the usual ID array for defining the equation numbers, the IEN array for relating the local node numbers to the global node numbers, and the LM array for connectivity in a conventional finite element method are still valid.

The algorithm for elasticity in the new method is given by

- Step 1. Identify ID, IEN, LM arrays.
- Step 2. Identify $[\hat{D}^i]$ and $\{\hat{c}^i\}$ for each element as in Fig. 5.
- Step 3. Establish the global matrix equation by using the LM array as $[\hat{D}]^n [U]^T = \{\hat{c}\}^n$.
- Step 4. Solve global $[U]^T$.
- Step 5. Recover each element's impulses $\{J^i\}$ by the relevant $\{u^i\}$, as

$$\{J^i\} = [D_{JJ}^i]^{-1} \{c_J\} - [D_{JU}^i]^{-1} [D_{JU}^i] \{u^i\}.$$

- Step 6. Update $\{\hat{c}^{n+1}\}$, and return to step 2 until the final step.

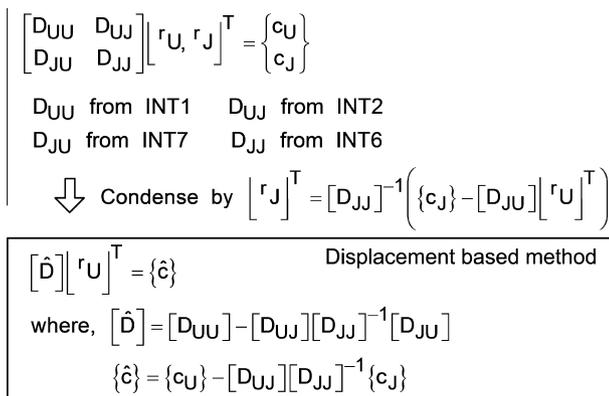


Fig. 5. Displacement-based space-time finite element method.

4.3. Numerical algorithm for viscoplasticity

4.3.1. Block matrix equations for each time-step

To have the mixed-step algorithm for viscoplasticity, the coefficients of ${}_D\varphi({}^1D_{kl}^{(m)}, {}^0D_{kl}^{(m)})$ for the first time step, and those of ${}_D\varphi({}^kD_{kl}^{(m)}, {}^{k-1}D_{kl}^{(m)}) + {}_D\varphi({}^{k+1}D_{kl}^{(m)}, {}^kD_{kl}^{(m)})$ for the k th time step, must be added to the block matrix $[D_{JJ}]$ in Fig. 5.

By substituting (52) into (63), ${}_D\varphi({}^kD_{kl}^{(m)}, {}^{k-1}D_{kl}^{(m)})$ can be expressed as ${}_D\varphi({}^kJ_{kl}^{(m)}, {}^{k-1}J_{kl}^{(m)})$:

$${}_D\varphi({}^kJ_{kl}^{(m)}, {}^{k-1}J_{kl}^{(m)}) = \frac{V}{2} \times \frac{1}{2\eta} \left\langle 1 - \frac{\sigma_Y}{\sqrt{k}J_2\sqrt{3}} \right\rangle \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \begin{Bmatrix} kJ_{xx}^{(m)} - {}^{k-1}J_{xx}^{(m)} \\ kJ_{yy}^{(m)} - {}^{k-1}J_{yy}^{(m)} \\ kJ_{zz}^{(m)} - {}^{k-1}J_{zz}^{(m)} \\ kJ_{yz}^{(m)} - {}^{k-1}J_{yz}^{(m)} \\ kJ_{xz}^{(m)} - {}^{k-1}J_{xz}^{(m)} \\ kJ_{xy}^{(m)} - {}^{k-1}J_{xy}^{(m)} \end{Bmatrix} \tag{72}$$

Define the matrix ${}^k[S]$ as

$${}^k[S] = ({}^kC)[S] \tag{73}$$

where, kC and $[S]$ are given by

$${}^kC = \frac{V}{2} \frac{1}{2\eta} \left\langle 1 - \frac{\sigma_Y}{\sqrt{k}J_2\sqrt{3}} \right\rangle \tag{74}$$

and

$$[S] = \begin{bmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} & 0 & 0 & 0 \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \end{bmatrix} \tag{75}$$

Then, a matrix equation for the r th time-steps is given by

$$\begin{bmatrix} D_{UU} & D_{UJ} \\ D_{JU} & D_{JJ} + {}^rS \end{bmatrix} \begin{bmatrix} r_U \\ r_J \end{bmatrix}^T = \begin{Bmatrix} r_{c_U} \\ r_{c_J} + {}^rS[r_{-1}J]^T \end{Bmatrix} \tag{76}$$

In (76), note that the known vector components c_U and c_J at the first time-step and the other time-steps are different from each other, as $\{c\}$ in (67).

4.3.2. Non-iterative algorithm

In (76), the block matrix rS remains unknown due to the unspecified coefficient rC . Here, these are specified.

Consider a viscoplastic element, where σ_Y and η in (74) are specified. Suppose the element does not experience any viscoplastic behavior at the r th time-step, then, every time-step solution is obtained by

$$\begin{bmatrix} D_{UU} & D_{UJ} \\ D_{JU} & D_{JJ} \end{bmatrix} \begin{bmatrix} r_U \\ r_J \end{bmatrix}^T = \begin{Bmatrix} r_{c_U} \\ r_{c_J} \end{Bmatrix} \tag{77}$$

Now, turn to (76) and (77). This time, consider the matrix condensation for impulses. Then, the elastic assumed solution $[r_J^E]^T$ in (77) is written

$$[D_E][r_J^E]^T = \{r_b\} \tag{78}$$

where, $[D_E]$ and $\{r_b\}$ are given by

$$[D_E] = [D_{JJ}] - [D_{JU}][D_{UU}]^{-1}[D_{UJ}] \tag{79}$$

and

$$\{r_b\} = \{r_{c_J}\} - [D_{JU}][D_{UU}]^{-1}\{r_{c_U}\} \tag{80}$$

Similarly, the viscoplastic solution $[rJ^{vp}]^T$ in (76) is written

$$[D_P][rJ^{vp}]^T = \{r b + (rC)[S][r^{-1}J]^T\} \tag{81}$$

where $[D_P]$ is

$$[D_P] = [D_E] + (rC)[S] \tag{82}$$

Substituting the relations (78) and (82) into (81) gives

$$[rJ^{vp}]^T = [rJ^E]^T - (rC)[D_E]^{-1}[S][rJ^{vp} - r^{-1}J]^T \tag{83}$$

Subtracting $[r^{-1}J]^T$ from both sides in (83), and pre-multiplying $\frac{1}{h}[S]$, yields

$$[I + (rC)SD_E^{-1}]\{rS^{vp}\} = \{rS^E\} \tag{84}$$

where $\{rS^{vp}\}$ and $\{rS^E\}$ represent the viscoplastic deviatoric stress, and the elastic assumed deviatoric stress at the r th discrete time, respectively. Also, $[I]$ is an identity matrix.

In (84), let us take the general solution form of $\{rS^{vp}\}$ in terms of the unknown parameter α :

$$\{rS^{vp}\} = \alpha\{rS^E\} \tag{85}$$

Then, rJ_2 in (74) is now written in terms of the elastic assumed J_2 invariant rJ_2^E as

$$rJ_2 = \alpha^2 rJ_2^E \tag{86}$$

By substituting (85) into (84), we have

$$[(1 - \alpha)I - \alpha(rC)SD_E^{-1}]\{rS^E\} = \{0\} \tag{87}$$

By introducing the rank 1 matrix R_1 as

$$R_1 = [1 \ 1 \ 1 \ 1 \ 1 \ 1] \tag{88}$$

and pre-multiplying R_1 with (87), the unknown parameter α is evaluated by

$$\alpha = \frac{C_1 + \beta X C_2}{C_1 + X C_2} \tag{89}$$

where C_1 , C_2 , X , and β are

$$C_1 = [R_1]\{rS^E\}; \quad C_2 = [R_1][S][D_E]^{-1}\{rS^E\}; \quad X = \frac{V}{4\eta}; \quad \beta = \frac{\sigma_Y}{\sqrt{3}\sqrt{rJ_2^E}} \tag{90}$$

After finding α , the coefficient $rC = \frac{V}{2} \frac{1}{2\eta} \left\langle 1 - \frac{\sigma_Y}{\alpha\sqrt{rJ_2^E}\sqrt{3}} \right\rangle$ is identified explicitly so that Eq. (76) can be specified.

Thus, the displacement-based finite element algorithm for viscoplasticity could be obtained as follows:

Step 1. Identify ID, IEN, LM arrays.

Step 2. Identify the assumed elastic matrix $[\hat{D}^i]$ and $\{r\hat{c}^i\}$ for each element.

Step 3. Establish the global matrix equation by using the LM array as $[\hat{D}][rU]^T = \{r\hat{c}\}$.

Step 4. Solve global $[rU]^T$.

Step 5. Recover each element's impulses $\{rJ^i\}$ by using the relevant $\{r u^i\}$, as $\{rJ^i\} = [D_{ij}^i]^{-1}\{r c_j\} - [D_{ij}^i]^{-1}[D_{ju}^i]\{r u^i\}$.

Step 6. Find the assumed elastic deviatoric stress $\{rS^i\}$ and the assumed elastic J_2 invariant, rJ_2^i by $\{rS^i\} = \frac{1}{h}[S]\{rJ^i - r^{-1}J^i\}$ and $rJ_2^i = \{rS^i\}^T\{rS^i\}$.

Step 7. Check the criterion.

(a) If all the elements have $rJ_2^i < \frac{1}{3}\sigma_Y^2$: $[rU]^T$ and $\{rJ^i\}$ are solutions.

(b) If one of the elements (suppose, the k th element) has $rJ_2^k > \frac{1}{3}\sigma_Y^2$:

(i) Find α from (89) for the k th element

(ii) Find kC from (74) for the k th element

(iii) Modify $[D_{ij}^k] = [D_{ij}^k] + ({}^kC)[S]$

(iv) Establish $[\hat{D}^k]\{r u^k\} = \{r\hat{c}^k\}$, where

$$[\hat{D}^k] = [D_{uu}^k] - [D_{uj}^k][D_{jj}^k]^{-1}[D_{ju}^k] \quad \text{and}$$

$$\{r\hat{c}^k\} = \{r c_{ij}^k\} - [D_{ij}^k][D_{jj}^k]^{-1}\{r c_j^k + ({}^kC)[S]\{r^{-1}J^k\}\}$$

(v) Establish the global matrix equation $[\hat{D}_P][rU]^T = \{r\hat{c}_P\}$ with the LM array and solve it.

Step 8. Update $\{r^{+1}\hat{c}\}$, and return to step 2 until the final time step.

While deriving the algorithm for viscoplasticity, the most critical point is to take the deviatoric viscoplastic stress form as Eq. (85). This comes from the notion that (1) the method implicitly deals with a stress field and (2) the elastic assumed deviatoric stress ${}^nS^E$ gives the direction of the viscoplastic deviatoric stress. For example, the direction of the viscoplastic stress in the Bingham-Norton model could be decided by the elastic assumed stress, as in Fig. 6.

Then, considering that the stress solution (84) in the new method is implicitly associated with the unknown invariant nJ_2 , the general solution form (85) can be adopted for the viscoplastic deviatoric stress.

4.4. Numerical properties of the new method

4.4.1. Dependent initial condition

In the new method, the initial value, ${}^0J_{ij}^{(p)}$ in each element, must be identified as in (67). This can only be carried out at a global level, where the true model is dynamically analyzed before the initial time.

The momentum balance equation in a region of a body at the initial time is written

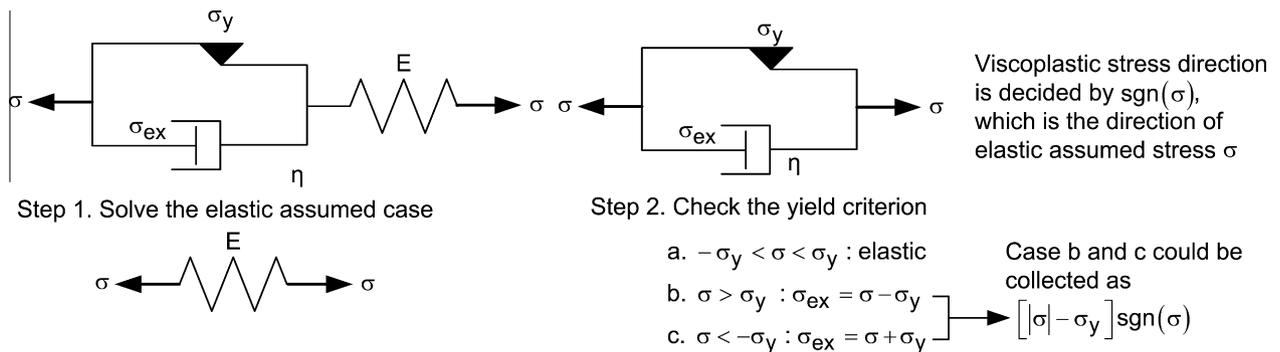


Fig. 6. The Bingham-Norton model.

$$\rho \hat{v}_i(0) - J_{ij,j}(0) - \hat{j}_i(0) = 0 \quad (91)$$

where $\hat{j}_i(0)$ is the impulse of the body force density \hat{f}_i evaluated at time zero by

$$\hat{j}_i(0) = \int_{-\infty}^0 \hat{f}_i(\tau) d\tau \quad (92)$$

while $\rho \hat{v}_i(0)$ and $J_{ij,j}(0)$ are the given initial momentum density, and the initial internal impulse of the body. In (92), $(-\infty, 0)$ is used to represent that this is the time interval before the initial time we are considering.

Then, by integrating (91) over the volume of a body, we have

$$\int_{\Omega} [\rho \hat{v}_i(0) - J_{ij,j}(0) - \hat{j}_i(0)] d\Omega = 0$$

$$\xrightarrow[\text{Theorem}]{\text{Divergence}} \int_{\Gamma} J_{ij}(0) n_j d\Gamma = \int_{\Omega} [\rho \hat{v}_i(0) - \hat{j}_i(0)] d\Omega \quad (93)$$

$$\xrightarrow[n_i]{\text{Multiply}} \int_{\Gamma} J_{ij}(0) n_j n_i d\Gamma = \int_{\Omega} [\rho \hat{v}_i(0) - \hat{j}_i(0)] n_i d\Omega$$

where n_i and n_j represent the tangential vector and normal vector to a boundary of a given body.

At the last step in (93), the initial condition $J_{ij}(0)$ of a body could be analytically identified by the given initial momentum, and the impulse of the body force density. That is, $J_{ij}(0)$ is dependent, and can be found by dynamically analyzing the true model (a body) before the initial time. Spatially distributing $J_{ij}(0)$ to ${}^0J_{ij}^{(p)}$ in each element completes the initial condition issues in the new method.

As far as dealing with the initially static continuum, the initial impulse in each element is zero (${}^0J_{ij}^{(p)} = 0$), because we have $\hat{j}_i(0) = 0$ without an inertia effect.

It should be noted that to identify ${}^0J_{ij}^{(p)}$ analytically, we need to allow C^0 spatial continuity for J_{ij} , as in (91). Thus, we may need shape functions N^p to discretize J_{ij} , and this is another reason to use the curly bracket in (50).

4.4.2. Unique solutions

The new method for both elastic and viscoplastic continuum yields a unique solution for every time step. For elastic continuum, the solution for every time step is

$$[[D_{UU}] + [D_{JU}]^T [D_{JJ}]^{-1} [D_{JU}]] [{}^nU^E]^T = \{{}^n\hat{c}\} \quad (94)$$

While deriving (94), we use the relation (69).

As in (47) and (71), the matrix $[D_{JJ}]$ is positive definite if $\nu \neq \frac{1}{2}$. Thus, $[D_{JJ}]^{-1}$ is always positive definite. Also, the matrix $[D_{UU}]$ is symmetric and positive definite by (70).

Thus, the left-side matrix in (94) is also symmetric and positive definite so the elastic solution $[{}^nU^E]^T$ is unique for every time-step.

For viscoplasticity, the solution for every time step is

$$[[D_{UU}] + [D_{JU}]^T [D_{JJ} + {}^nS]^{-1} [D_{JU}]] [{}^nU^{vp}]^T = \{{}^n\hat{c}\} \quad (95)$$

In (95), the matrix $[D_{JJ} + {}^nS]$ is symmetric positive definite since $[D_{JJ}]$ is symmetric positive definite, and $[{}^nS]$ is symmetric positive semi-definite. Subsequently, the left-side matrix in (95) is symmetric and positive definite, so the viscoplastic solution $[{}^nU^{vp}]^T$ in (95) is unique.

5. Conclusions

By using the extended framework, Hamilton's principle can account for compatible initial conditions to the strong form properly. As its canonical applications, we show how the new formulation recovers all the governing differential equations along with the pertinent initial and boundary conditions for an elastic and a viscoplastic continuum. The framework is quite simple: the action variation is newly defined by adding the counterparts to the terms

without the end-point constraints in Hamilton's principle, which confines a dynamical system to evolve uniquely from start to end. Interpreting these additional terms as sequentially assigning the known initial values completes this formulation.

It is not a complete variational method, since it still requires the Rayleigh's dissipation for a non-conservative process and it cannot define the functional action explicitly. However, it achieves a theoretical unification of a finite element method in space–time with the proper use of the initial conditions.

Based on the extended framework, we also present the numerical algorithms for an elastic and a viscoplastic continuum. The method is developed sequentially by (i) applying Galerkin's method to space–time with the new notations, (ii) directly integrating on a temporal domain, (iii) then, numerically integrating on a spatial domain, (iv) adopting the mixed-step algorithm for numerical efficiency, and (v) using the matrix condensation for the displacement-based finite element method. For both elasticity and viscoplasticity, the developed numerical method can (i) use the given initial/boundary conditions properly, and (ii) have a non-iterative algorithm that yields unique solutions.

We consider here the development of an extension framework of Hamilton's principle for continuum dynamics. Clearly, however, the extension framework is quite simple and general, and can be readily applied to different kinds of problems. We anticipate that the extension framework developed here will provide an interesting foundation for them. In addition, it is expected that the method presented here will provide insights into the development of various space–time elements.

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