RIGOROUS DERIVATION OF HAMILTONIAN FROM LAGRANGIAN FOR SOLID CONTINUUM

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This paper provides rigorous derivation of a Hamiltonian from a given Lagrangian of solid continuum, for a possible improvement of dynamic analysis. The derived Hamiltonian, unlike an ordinary one, has momentum and strain as argument, and the associated canonical equation includes spatial derivative in it. Characteristics of the Hamiltonian of this form are studied. The appearance of strain rate in the canonical equation, which has been overlooked in the past researches, is pointed out. For numerical computation, a Hamiltonian for discretized functions is derived. It is shown that discretized strain rate appears in the canonical equation when suitable discretization scheme is applied.

Key Words : Hamiltonian, Lagrangian, canonical equation, Lagrange’s equation, time integration

1. INTRODUCTION

Verification and validation of numerical analysis for the quality assurance has been a popular research topic recently in many fields of engineering; see, for instance, Oberkampf and Trucano¹ and Szabo and Babuska². Theoretical investigation is needed to improve the quality of numerical analysis from the viewpoint of verification. A good example of such investigation is time integration that is used for dynamic analysis. Algorithms of time integration³ are well established in solid continuum and structural mechanics, but are considered old-fashioned. There is plenty of room for improving their efficiency and accuracy by employing new algorithms that are developed in computational science and making necessary modification; see, for instance, symplectic time integration⁴,⁵,⁶.

There is a distance from dynamic analysis of solid continuum and structural mechanics and dynamic analysis to that of computational science. In our views, Hamiltonian represents that distance; see Binney⁷ and Tong⁸ for an easy reference of Hamiltonian; see also Riewe⁹. The utilization of Hamiltonian is efficient for time integration because it provides an explicit expression of the time derivative of physical quantities. Hamiltonian has been used in a quite limited manner in the field of solid continuum and structural mechanics in contrast to Lagrangian. As will be explained later, Hamiltonian’s disadvantage of doubling a number of unknowns is more significant than its advantage of providing the explicit expression of the time derivative.

Moreover, in our views, a proper Hamiltonian is not used in solid continuum and structural mechanics. A Hamiltonian used currently is of the form that has momentum and velocity as argument, just like an ordinary Hamiltonian. When a Hamiltonian is derived from a Lagrangian whose arguments are velocity and strain, the form of the resulting Hamiltonian will be different, because strain (not displacement) is used in the Lagrangian. We point out that the Hamiltonian for momentum and displacement ignores the fact that energy is induced by strain and not by displacement; as a more intuitive and clear evidence, rigid body motion produces no energy for deformation, but the Hamilton-
nian for displacement does not meet this condition.

Continuous improvement is needed for the quality assurance of numerical analysis, and the use of Hamiltonian in solid continuum and structural mechanics might open a new gateway for better algorithms of time integration. Based on this idea, we studied rigorous derivation of a Hamiltonian from a given Lagrangian for solid continuum mechanics.

The contents of the present paper are as follows: First, we present literature survey for the use of Hamiltonian in solid continuum and structural mechanics in Section 2. Next, following established procedures, we rigorously derive a Hamiltonian for momentum and strain from a Lagrangian of solid continuum in Section 3. The case of linear elasticity is studied as the simplest example. Characteristics of the derived Hamiltonian are studied in Section 4. A key characteristic is the appearance of strain rate, which, as far as our survey shows, has been overlooked in the past researches. Finally, a Hamiltonian is studied for numerical computation in Section 5. It shows that a Hamiltonian for momentum and displacement is derived when displacement function is discretized in an ordinary manner, but that a Hamiltonian for momentum and strain can be derived when a special discretization scheme is used.

2. LITERATURE SURVEY

Continuum mechanics often takes advantage of tools that are developed in analytical mechanics, and a typical tool is Lagrangian, a functional of velocity and strain that are computed by displacement functions. A variational problem of this Lagrangian is equivalent to an initial/boundary value problem of displacement function that is derived from the equation of motion. Structural mechanics adopts Lagrangian which is often reduced to a simpler form, by assuming a quasi-static state or spatially one- or two-dimensional. The use of Lagrangian is standard in computational mechanics. For instance, the use of two equations, namely, Lagrange’s equation for a Lagrangian of two variables, is derived from the stationarity condition, and the consistency condition is assigned for the two arguments of the Lagrangian, as one argument is actually the time derivative of the other; see Fig. 1. In this section, paying attention to the two equations, we seek to derive

1. connecting continuum mechanics and molecule dynamics,
2. solving bifurcation problems using dynamic analysis,
3. solving fracture mechanics problems considering energy, and
4. solving coupling (or multi-physics) problems, such as piezo-elasticity;

see also the recent work of Maugin. Fluid mechanics has a larger collection of references related to Hamiltonian, which employ advanced numerical analysis techniques. As for computational mechanics, we can find some relatively old works. In structural mechanics, a Hamiltonian is used to introduce a phase space that consists of location and velocity used in structural dynamics.

Aside from the limited use of Hamiltonian, we point out that Hamiltonian of solid continuum and structural mechanics is of an ordinary form; at least, all the above references, including those of fluid mechanics, use the Hamiltonian of this form. This seems odd, because the form of a Lagrangian of solid continuum, or a continuum Lagrangian for simplicity, is different from that of an ordinary Lagrangian. The continuum Lagrangian has both spatial and temporal derivatives as arguments while the ordinary one has temporal derivative only. A Hamiltonian that is derived from the continuum Lagrangian will be of a different form from that of the ordinary one. It is worth examining what form the Hamiltonian takes when it is derived from the continuum Lagrangian.

3. LAGRANGIAN AND HAMILTONIAN OF SOLID CONTINUUM

The procedures for deriving a Hamiltonian from a Lagrangian are well established; in Fig. 1, we provide a schematic view of the procedures for the case when a Lagrangian of two variables, \( \mathcal{L}(v, u) \) with \( v = \dot{u} \), is given. A key issue in deriving a Hamiltonian is the use of two equations, namely, Lagrange’s equation and consistency condition. Lagrange’s equation is derived from the stationarity condition, and the consistency condition is assigned for the two arguments of the Lagrangian, as one argument is actually the time derivative of the other; see Fig. 1. In this section, paying attention to the two equations, we seek to derive
a Hamiltonian of continuum or a continuum Hamiltonian.

(1) General case of solid continuum

We start from the case when a density of a continuum Lagrangian, denoted by $\ell$, is given for a continuum $V$. It is assumed that $\ell$ is a function of velocity vector and strain tensor, denoted by $v$ and $\epsilon$, respectively. In terms of displacement vector, $u(x,t)$ with $x$ and $t$ being point and time, respectively, they are expressed as

$$v(x,t) = u(x,t) \quad \text{and} \quad \epsilon(x,t) = \text{sym}[\nabla u](x,t),$$

where $\cdot$ and $\nabla (\cdot)$ are the temporal and spatial derivatives of $(\cdot)$, and sym stands for the symmetric part of the second order tensor; infinitesimally small deformation is assumed throughout this paper. A continuum Lagrangian is defined as the volume integral of $\ell$,

$$\mathcal{L}[v, \epsilon] = \int_V \ell(v, \epsilon) \, dv.$$  \hspace{1cm} (1)

Here, a square bracket means that $\mathcal{L}$ is a functional of a vector function and a tensor function, while a parenthesis (or a round bracket) means that $\ell$ is a function of a vector and a tensor; the same symbol $v$ and $\epsilon$ are used in $\mathcal{L}$ and $\ell$ for simplicity.

According to the Hamiltonian principle$^{[12,13]}$, we seek a displacement function that stationaries the time integration of the Lagrangian, i.e.,

$$\delta \left( \int_T \mathcal{L}[\dot{u}, \text{sym}[\nabla u]] \, dt \right) = 0,$$

where $T$ is a time domain. Note that $\dot{u}$ and $\text{sym}[\nabla u]$ are substituted into $v$ and $\epsilon$ of $\mathcal{L}$. The resulting Lagrange’s equation is

$$\frac{\partial}{\partial t} \frac{\partial \ell}{\partial \dot{v}} + \nabla \cdot \frac{\partial \ell}{\partial \epsilon} = 0, \hspace{1cm} (2)$$

where $\frac{\partial \ell}{\partial \dot{v}}$ and $\frac{\partial \ell}{\partial \epsilon}$ are the derivatives of $\ell$ with respect to $v$ and $\epsilon$, respectively, and $\nabla \cdot (\cdot)$ is the divergence of $(\cdot)$ with $\cdot$ standing for inner product; see Appendix A for the detailed manipulation.

It should be recalled that the arguments of the continuum Lagrangian, $v$ and $\epsilon$, are generated by $u$. Since they are given as $v = \dot{u}$ and $\epsilon = \text{sym}[\nabla u]$, they ought to satisfy

$$\dot{\epsilon} = \text{sym}[\nabla \dot{v}]. \hspace{1cm} (3)$$

This is the consistency condition of the continuum Lagrangian arguments.

In deriving a Hamiltonian of solid continuum, or a continuum Hamiltonian for simplicity, we define a new variable, $p$, as $p = \frac{\partial \ell}{\partial \dot{v}}$. According to the Legendre transform, we have $v = \frac{\partial h}{\partial p}$ by defining a new function, $h$, as

$$h(p, \epsilon) = v(p) \cdot p - \ell(v(p), \epsilon), \hspace{1cm} (4)$$

where the expression of $v(p)$ in the right side emphasizes that $v$ is an implicit function of $p$ and that $\ell$ is an implicit function of $p$ and $\epsilon$. We express Lagrange’s equation and the consistency condition, Eqs. (2) and (3), in terms of $h$ of Eq. (4). In view of $\frac{\partial h}{\partial \epsilon} = -\frac{\partial \ell}{\partial \epsilon}$, we obtain

$$\begin{bmatrix} \dot{p} \\ \dot{\epsilon} \end{bmatrix} = \begin{bmatrix} \nabla \cdot \frac{\partial h}{\partial \epsilon}(p, \epsilon) \\ \text{sym} \left\{ \nabla \frac{\partial h}{\partial \epsilon}(p, \epsilon) \right\} \end{bmatrix}. \hspace{1cm} (5)$$

As shown, the temporal derivative of $p$ and $\epsilon$ equal the spatial derivative of $h$; more precisely speaking, $\dot{p}$ equals the divergence of $\frac{\partial h}{\partial \epsilon}$ and $\dot{\epsilon}$ the symmetric part of its spatial derivative.
of the gradient of $\frac{\partial h}{\partial p}$. This is the canonical equation or Hamilton’s equation. A continuum Hamilton is defined as the volume integral of $h$ (which is now called a continuum Hamiltonian density), as follows:

$$\mathcal{H}[p, e] = \int_V h(p, e) \, dv. \quad (6)$$

Note that $\mathcal{H}$ is a functional of a vector function and a tensor function, just like $\mathcal{L}$. We present a schematic view of the procedures of deriving $h$ and $\mathcal{H}$ from $\mathcal{L}$ and $\mathcal{H}$ in Fig. 2, which is drawn in the same manner as Fig. 1. Also, we present the comparison of the key elements of deriving the ordinary Hamiltonian and the continuum Hamiltonian in Table 1.

(2) Simplest case of linearly elastic continuum

The derivation of $h$ and $\mathcal{H}$ shown in the preceding subsection is general but abstract. We consider the simplest case when $V$ is linearly elastic, to clarify the meaning of $h$ and $\mathcal{H}$. Furthermore, we employ index notation, introducing a Cartesian coordinate system, $\{x_1, x_2, x_3\}$ and denoting vector or tensor components by putting subscripts. In terms of the density and elasticity tensor, $\rho$ and $e$, the continuum Lagrangian density is now explicitly expressed as

$$\ell(v, e) = \frac{1}{2} \rho u_i u_i - \frac{1}{2} c_{ijkl} \varepsilon_{ij} \varepsilon_{kl}. \quad (7)$$

Here, summation convention is employed. Recall that the components of $v$ and $e$ are computed in terms of $u$, as

$$v_i = u_i \quad \text{and} \quad e_{ij} = \frac{1}{2}(u_{ij} + u_{ji}),$$

with $(.)_j = \frac{\partial (.)}{\partial x_j}$. A continuum Lagrangian is given as the volume integral of the continuum Lagrangian density, i.e.,

$$\mathcal{L}[v, e] = \int_V \frac{1}{2} \rho v_i v_i - \frac{1}{2} c_{ijkl} \varepsilon_{ij} \varepsilon_{kl} \, dv; \quad (8)$$

a square bracket is used for $\mathcal{L}$, since it is a functional. The following Lagrange’s equation is derived from

$$\delta \left( \int_T \mathcal{L}[\dot{u}, \text{sym}(\nabla u)] \, dt \right) = 0 \quad \text{for} \quad \mathcal{L} \quad \text{of Eq. (8)}:$$

$$\rho \ddot{u}_i - (c_{ijkl} u_{kl})_j = 0, \quad (9)$$

for $i = 1, 2, 3$. This is the wave equation; see Appendix B for the detailed derivation. Also, the consistency condition of the two arguments of $\mathcal{L}$ is

$$\dot{e}_{ij} = \frac{1}{2} ((\dot{v}_{ij} + \dot{v}_{ji}). \quad (10)$$

Equations (9) and (10) correspond to Eqs. (2) and (3), respectively.

Now, we derive a continuum Hamiltonian from the continuum Lagrangian of Eq. (8). We first define a new variable $p_i = \frac{\partial h}{\partial v_i}$ or $p_i = \rho v_i$, which is momentum. Applying the Legendre transform, we define

$$h(p, e) = \frac{1}{2} \rho p_i p_i + \frac{1}{2} c_{ijkl} \varepsilon_{ij} \varepsilon_{kl}, \quad (11)$$

so that $v_i = \frac{\partial h}{\partial p_i}$. Lagrange’s equation and the consistency condition, Eqs. (9) and (10), are now expressed in terms of this $h$. Since

$$\frac{\partial h}{\partial \varepsilon_{ij}} = c_{ijkl} \varepsilon_{kl} \quad \text{and} \quad \frac{\partial h}{\partial p_i} = \frac{1}{\rho} p_i,$$

we have

$$\left\{ \dot{p}_i, \dot{e}_{ij} \right\} = \left\{ \frac{1}{\rho} (p_{ij} + p_{ji}) \right\}. \quad (12)$$

This is the canonical equation of linearly elastic continuum. Note that Eq. (12) is rewritten in terms of stress ($\sigma_{ij} = c_{ijkl} \varepsilon_{kl}$) and velocity ($v_i = \frac{p_i}{\rho}$) as $\dot{p}_i = \sigma_{ij}$ and $\dot{e}_{ij} = \frac{1}{2} ((\varepsilon_{ij} + \varepsilon_{ji})$.

4. CHARACTERISTICS OF CONTINUUM HAMILTONIAN

We rigorously derive a continuum Hamiltonian from a given continuum Lagrangian, and show the form of the continuum Hamiltonian is different from that of an ordinary one. This is because the continuum Lagrangian has velocity and strain as argument, which are given as temporal and spatial derivatives of displacement. In this section, we study the characteristics of the continuum Hamiltonian of this particular form.

(1) Canonical equations

While the canonical equation of Eq. (5) is given in an abstract form, it has a clear physical meaning. The first equation,

$$\dot{p} = \nabla \cdot \frac{\partial h}{\partial \varepsilon}$$

corresponds to the equation of motion, since $\frac{\partial h}{\partial \varepsilon} = \sigma$. In the simplest case of linear elasticity, this equation coincides with the wave equation of Eq. (9).

The second equation of the canonical equation, which is derived from the consistency condition, is

$$\dot{\varepsilon} = \text{sym} \left\{ \nabla \frac{\partial h}{\partial p} \right\}.$$

This equation means that the strain rate, $\dot{\varepsilon}$, is the symmetric part of the velocity gradient, $\nabla v$, since, by definition, $h$ produces $v = \frac{\partial h}{\partial p}$. The physical meaning of the second equation could be regarded as the compatibility of the strain rate.

A canonical equation generally provides the temporal derivative of all the variables of a Hamiltonian. In the case of solid continuum, the temporal derivative or rate of momentum and strain is given in terms of the derivative of the continuum Hamiltonian density. Unlike the ordinary Hamiltonian, the spatial derivative is additionally taken to the continuum Hamiltonian den-
(2) Consistency condition

As has been pointed out, this is inevitable since the continuum Lagrangian density is given in terms of strain and the continuum Hamiltonian density is converted from the continuum Lagrangian density. The involvement of the spatial derivative is a key characteristic of the continuum Hamiltonian density.

(2) Conservation of energy

An advantage of using a Hamiltonian is the ease of guaranteeing the conservation of energy. For the continuum Hamiltonian that corresponds to the volume integral of the kinematic and strain energy densities, the conservation of energy is easily proved as well, just by using the canonical equation.

Indeed, it is straightforward to prove the conservation of the continuum Hamiltonian, which is expressed as the vanishing of the time derivative, i.e.,

\[ \mathcal{H}[p, \epsilon] = 0. \]  

In terms of the continuum Hamiltonian density, \( h \), the time derivative of \( \mathcal{H} \) is computed as

\[ \int_V \frac{\partial h}{\partial p} \cdot p + \frac{\partial h}{\partial \epsilon} \cdot \dot{\epsilon} \, dv. \]
where \( \varepsilon \) is the second-order contraction. Substituting the canonical equation, Eq. (5), into \( \rho \) and \( \dot{\varepsilon} \), the integrand becomes

\[
\frac{\partial h}{\partial p} \cdot \left( \nabla \cdot \frac{\partial h}{\partial \varepsilon} \right) + \frac{\partial h}{\partial \varepsilon} : \left( \nabla \frac{\partial h}{\partial p} \right) = \nabla \cdot \left( \frac{\partial h}{\partial \varepsilon} \cdot \frac{\partial h}{\partial p} \right).
\]

Here, symmetry of \( \frac{\partial h}{\partial \varepsilon} \) is used. The volume integral of the above integrand is converted to the surface integral, which identically vanishes when boundary conditions are suitably posed. Therefore, Eq. (13) holds for the continuum Hamiltonian; see Appendix C for more detailed proof of Eq. (13), which uses index notation.

### 3. Strain rate in canonical equation

The second equation of the canonical equation is for the strain rate. It should be noted that the strain rate appears naturally during the procedures of deriving the continuum Hamiltonian. The natural appearance of the strain rate could be an advantage in solving an elasto-plasticity problem that is based on flow rule. In flow rule, strain rate is decomposed into elastic and plastic parts, and plastic strain rate is given as the gradient of a yield function, i.e.,

\[
\dot{\varepsilon} = \dot{\varepsilon}^e \lambda \nabla f(\sigma).
\]

Here, \( \dot{\varepsilon}^e \) is elastic strain rate, and \( \lambda \nabla f \) is plastic strain rate with \( \lambda \) and \( f \) being plastic loading parameter and yield function of stress \( (\nabla f)_{ij} = \frac{\partial f}{\partial \sigma_{ij}} \). If the second equation of Eq. (5) is evaluated in view of the flow rule, it becomes possible to solve the canonical equation just by applying a suitable algorithm of time integration.

Solving the canonical equation by applying time integration will make a clear difference from the ordinary analysis of the elasto-plasticity problem, which is usually formulated in terms of displacement increment, \( du \), as

\[
\rho \, du - \nabla \cdot (c^{ep} : \nabla du) = 0,
\]

where \( c^{ep} \) is an elasto-plasticity tensor that is determined by the elasto-plasticity based on the flow rule, i.e.,

\[
c^{ep} = c - \frac{(c : \nabla f) \otimes (c : \nabla f)}{\nabla f : c : \nabla f},
\]

where \( \otimes \) stands for tensor product; \( c \) is elasticity tensor that determines strain rate in terms of elastic strain rate, i.e., \( \sigma = c : \dot{\varepsilon}^e \). The displacement increment is expressed in terms of time increment \( dr \) and velocity \( \nu = du \), hence, the above equation is regarded as the time derivative of the equation of motion, or the third-order differential equation with respect to time.

It is certain that a solution of the equation of motion (the original second-order differential equation) satisfies Eq. (14). However, the opposite does not have to be true; there is a possibility that Eq. (14) has a solution that does not satisfy the second-order equation when a solution of the non-linear elasto-plasticity problem is not unique. The investigation of the uniqueness of Eq. (14) is beyond the scope of the present study, as well as the development of an algorithm of the time integration of Eq. (5) for the non-linear elasto-plasticity based on the flow rule. Future research is needed to address these issues.

### 5. CONTINUUM HAMILTONIAN FOR MODAL ANALYSIS

As explained in Section 2, a Hamiltonian similar in form to an ordinary one has been used for continuum. This is well understood because a Lagrangian that has velocity and displacement as arguments has been used. A continuum Hamiltonian that is derived from a Lagrangian of velocity and strain is new in this sense.

Numerically solving a canonical equation of the continuum Hamiltonian is worth being studied. In this section, we derive a continuum Hamiltonian and a canonical equation for discretized functions. It should be emphasized that the canonical equation is equivalent with the equation of motion. However, different algorithms could be applied to solve it, since the canonical equation is in the rate form or a differential equation of the first order while the equation of motion is a differential equation of the second order.

### (1) Modal analysis

It is of importance to note that a continuum Hamiltonian becomes similar in form to an ordinary one, if we assume a specific form for a displacement function. In the simplest case, we consider modal analysis which approximates the displacement function of the following form:

\[
\mathbf{u}^v(x,t) = \sum_{\alpha=1}^{N} \mathbf{u}^\alpha(t) \phi(x) ,
\]

where \( \mathbf{u}^\alpha \) and \( \phi^\alpha \) are an amplitude and a mode function (or a mode shape) of the \( \alpha \)-th mode, respectively, and \( N \) is the number of the modes. Note that the superscript \( \ast \) above \( \alpha \) is meant to emphasize that it is a discretized function. Substitution of Eq. (15) into a given continuum Lagrangian density \( \ell \) leads to another Lagrangian density, as

\[
\ell^\ast([\mathbf{u}^\alpha],[\dot{\mathbf{u}}^\alpha]) = \ell^\ast(\mathbf{u}^\alpha, \text{sym}(\nabla \mathbf{u}^\alpha)),
\]

with \( v^\alpha = u^\alpha \). The Lagrangian density for the discretized displacement, \( \ell^\ast \), is a function of \( 2N \) variables; the spatial derivative is applied to \( \phi^\alpha \)'s only, and hence the second \( N \) variables of \( \ell \) are \( \{u^\alpha\} \). A continuum Lagrangian that is associated with this \( \ell^\ast \)
The following procedures: 1) obtain Lagrange’s equation as

\[ \frac{d}{dt} \frac{\partial L}{\partial v} - \frac{\partial L}{\partial u} = 0 \]

Note that this \( L \) is given as

\[ \dot{v} = \frac{\partial L}{\partial u} \]

is then given as

\[ \mathcal{L}^*([v^a], [u^a]) = \int \mathcal{L}([v^a], [u^a]) \, dv. \]

Note that this \( \mathcal{L}^* \) is a functional of the \( 2N \) functions, just like \( L \) of Eq. (1).

A continuum Hamiltonian that is associated with the above \( \mathcal{L}^* \) is readily obtained by taking the following procedures: 1) obtain Lagrange’s equation as \( \frac{\partial \mathcal{L}^*}{\partial v} - \frac{\partial \mathcal{L}^*}{\partial u} = 0 \); 2) obtain a consistency condition as \( v^a = \dot{u}^a \); 3) define a new variable as \( p^a = \frac{\partial \mathcal{L}^*}{\partial v} \); 4) derive a Hamiltonian as \( \mathcal{H}^* = \sum_{\alpha=1}^{N} v^a p^a - \mathcal{L}^* \) according to the Legendre transform; and 5) derive a canonical equation from Lagrange’s equation and the consistency condition using \( \mathcal{H}^* \). The resulting Hamiltonian is

\[ \mathcal{H}^*([p^a], [u^a]) = \sum_{\alpha=1}^{N} v^a p^a - \mathcal{L}^*([v^a], [u^a]), \quad (16) \]

and the resulting canonical equation is

\[ \begin{bmatrix} \dot{p}^a \\ \dot{u}^a \end{bmatrix} = \begin{bmatrix} \frac{\partial \mathcal{H}^*}{\partial u} \\ -\frac{\partial \mathcal{H}^*}{\partial p} \end{bmatrix} \quad (17) \]

for \( \alpha = 1, \ldots, N \). As shown, \( \mathcal{H}^* \) of Eq. (16) and the canonical equation of Eq. (17) of the same form as an ordinary Hamiltonian and its canonical equation. As for a linearly elastic continuum studied in Subsection 3.2, a continuum Hamiltonian of Eq. (16) takes the following simple form:

\[ \mathcal{H}^* = \sum_{\alpha=1}^{N} \frac{1}{2m^a} (p^a)^2 + \frac{1}{2} k^a (u^a)^2. \]

where

\[ m^a = \int_V \phi^a \cdot \phi^a \, dv \quad \text{and} \quad k^a = \int_V \nabla \phi^a : c : \nabla \phi^a \, dv, \]

the orthogonality of the mode functions,

\[ \int \phi^a \cdot \phi^\beta \, dv = 0 \quad \text{and} \quad \int \nabla \phi^a : c : \nabla \phi^\beta \, dv = 0, \]

for \( \alpha \neq \beta \) is used. A canonical equation of Eq. (17) becomes

\[ \begin{bmatrix} \dot{p}^a \\ \dot{u}^a \end{bmatrix} = \begin{bmatrix} -k^a u^a \\ \frac{1}{m^a} p^a \end{bmatrix}. \]

Recall that the first equation is for the equation of motion and that the second equation corresponds to the consistency condition, \( p^a = m^a \dot{u}^a \) with \( p^a \) being a discretized momentum.

(2) Finite element method

Lagrangian has been used to formulate the finite element method (FEM), and it is expected that Hamiltonian can be used as well. Like the modal analysis shown in the preceding subsection, we start from a discretized displacement function of the following form:

\[ u^a(x, t) = \sum u^a(t) \xi^a(x), \quad (18) \]

where \( u^a \) is a displacement vector of the \( \alpha \)-th node and \( \xi^a \) is an associated shape (or interpolation) function. For a given continuum Lagrangian density, we have

\[ \mathcal{L}^*([v^a], [u^a]) = \int \ell^*([v^a], [u^a]) \, dv, \]

with \( v^a = \dot{u}^a \) and \( \ell^* = (\sum v^a \xi^a, \sum \text{sym}(u^a \otimes \nabla \xi^a)). \)

This \( \mathcal{L}^* \) of FEM is essentially the same as \( \mathcal{L}^* \) of

Fig. 3 Schematic view of procedures of deriving continuum Hamiltonian from given continuum Lagrangian for FEM.
modal analysis, except for the fact that \( \mathbf{v}^\alpha \) and \( \mathbf{u}^\alpha \), nodal velocity and displacement, are vectors.

As shown in Fig. 3, a continuum Hamiltonian of FEM is readily derived from \( \mathcal{L}^* \) defined in the above equation as

\[
\mathcal{H}^*([p^\alpha],[u^\alpha]) = \sum \mathbf{v}^\alpha \cdot \mathbf{p}^\alpha - \mathcal{L}^*([u^\alpha],[u^\alpha]),
\]

(19)

where \( \mathbf{p}^\alpha \) is a momentum vector of the \( \alpha \)-th node. A canonical equation of this \( \mathcal{H}^* \) is

\[
\begin{bmatrix}
\dot{p}^\alpha \\
\dot{u}^\alpha
\end{bmatrix} = \begin{bmatrix}
-\frac{\partial \mathcal{H}^*}{\partial u^\alpha} \\
\frac{\partial \mathcal{H}^*}{\partial p^\alpha}
\end{bmatrix},
\]

(20)

which is of the same form as Eq. (17), except that Eq. (20) is a vector equation. As for linearly elastic continuum, we can derive mass and stiffness matrices that correspond to \( m^\alpha \) and \( k^\alpha \) of modal analysis, and the right side of Eq. (20) becomes the product of such matrices with \( \mathbf{u}^\alpha \) and \( \mathbf{p}^\alpha \); see Appendix D.

(3) Particle discretization scheme

The canonical equation of modal analysis or FEM is of the same form as a canonical equation of an ordinary Hamiltonian, since \( \mathcal{H}^* \) of Eq. (16) or (19) uses momentum and displacement as argument. As for FEM, however, there is an alternative derivation of a continuum Hamiltonian, which has momentum and strain as argument. To this end, we take advantage of particle discretization scheme (PDS)\(^{31,32,33} \). When a domain of continuum is decomposed into conjugate Voronoi and Delaunay tessellations, denoted by \([\Phi^\alpha]\) and \([\Psi^\beta]\), PDS uses a characteristic function of each \( \Phi^\alpha \) and \( \Psi^\beta \) as a basis function of discretization; see Fig. 4. That is,

\[
\begin{align*}
\mathbf{u}^*(x,t) &= \sum_\alpha \mathbf{u}^\alpha(t)\phi^\alpha(x), \\
\mathbf{e}^*(x,t) &= \sum_\beta \mathbf{e}^\beta(t)\psi^\beta(x),
\end{align*}
\]

(21)

where \( \mathbf{u}^\alpha \) and \( \phi^\alpha \) are displacement vector and a characteristic function of the \( \alpha \)-th Voronoi block (\( \Phi^\alpha \)), and \( \mathbf{e}^\beta \) and \( \psi^\beta \) are strain tensor and a characteristic function of the \( \beta \)-th Delaunay block (\( \Psi^\beta \)).

While \( \mathbf{u}^\alpha \) and \( \mathbf{e}^\beta \) of Eq. (21) are discretized differently, they must be consistent to each other. According to PDS, they are related by minimizing

\[
\int_V \left| \text{sym} [\nabla \mathbf{u}^*] - \mathbf{e}^* \right|^2 \, dv,
\]

where \( |.|^2 \) stands for the norm of a second-order tensor \( . \), i.e., \( |.|^2 = (.)(.) \). The following relation is readily derived from the minimization of the above integral:

\[
\mathbf{e}^\beta = \sum_\alpha \text{sym} [\mathbf{B}^{\alpha\beta} \otimes \mathbf{u}^\alpha],
\]

(22)

where \( \mathbf{B}^{\alpha\beta} = \frac{1}{V^{\Psi^\beta}} \int_{\Psi^\beta} \nabla \phi \, dv \) with \( \Psi^\beta \) standing for the volume. This vector is computable for a given set of conjugate Voronoi and Delaunay blocks.

For a given continuum Lagrangian density, \( \ell \), substitution of discretized displacement and strain of Eq. (21) leads to the following continuum Lagrangian:

\[
\mathcal{L}^*([\mathbf{v}^\alpha],[\mathbf{\dot{e}}^\beta]) = \int_V \ell^*([\mathbf{v}^\alpha],[\mathbf{\dot{e}}^\beta]) \, dv,
\]

with \( \mathbf{v}^\alpha = \dot{\mathbf{u}}^\alpha \) and \( \ell^* = \ell \sum v^\alpha \phi^\alpha : \sum \mathbf{e}^\beta \psi^\beta \). In view of Eq. (2), Lagrange’s equation of this \( \mathcal{L}^* \) is

\[
\frac{d}{dt} \frac{\partial \mathcal{L}^*}{\partial \mathbf{\dot{e}}^\beta} - \sum_\beta \mathbf{B}^{\alpha\beta} \cdot \mathbf{\dot{e}}^\beta = 0.
\]

(23)

As shown, \( \mathbf{B}^{\alpha\beta} \) plays a role of \( \nabla \) (spatial derivative) in Eq. (22) or (23).

Now, we readily derive a continuum Hamiltonian for functions discretized by PDS. Note that PDS is implementable to FEM since it is merely a discretization scheme; FEM that is implemented with PDS is called PDS-FEM. The resulting Hamiltonian is

\[
\mathcal{H}^*([\mathbf{p}^\alpha],[\mathbf{\dot{e}}^\beta]) = \sum \mathbf{v}^\alpha \cdot \mathbf{p}^\alpha - \mathcal{L}^*([\mathbf{v}^\alpha],[\mathbf{\dot{e}}^\beta]),
\]

(24)

and the associated canonical equation is

\[
\begin{align*}
\dot{\mathbf{p}}^\alpha &= \sum_\beta \mathbf{B}^{\alpha\beta} \frac{\partial \mathcal{H}^*}{\partial \mathbf{\dot{e}}^\beta} \\
\dot{\mathbf{\dot{e}}}^\beta &= \sum_\alpha \mathbf{B}^{\alpha\beta} \frac{\partial \mathcal{H}^*}{\partial \mathbf{p}^\alpha}
\end{align*}
\]

(25)

see Fig. 5 for the procedures of deriving Eqs. (24) and (25). The temporal derivative of \( \mathbf{p}^\alpha \) and \( \mathbf{\dot{e}}^\beta \) are com-
puted in terms of the derivative of \( \mathcal{H}^* \) multiplied by \( B^{\alpha\beta} \) that serves as a role of spatial derivative. Therefore, a continuum Hamiltonian of PDS-FEM requires only the time integration of \( \dot{p}^\alpha \) and \( \dot{\epsilon}^\beta \).

### 6. CONCLUDING REMARKS

In this paper, we rigorously derive a continuum Hamiltonian from a continuum Lagrangian that has velocity and strain as argument. The derived continuum Hamiltonian has momentum and strain as argument, and the associated canonical equation uses spatial derivative of the Hamiltonian for the temporal rate of its arguments. Since the form is different from that of an ordinary one, the derived continuum Hamiltonian has some interesting characteristics. In particular, the natural appearance of strain rate might be a clue to improve the numerical analysis of non-linear elasto-plasticity problems based on flow rule.

The present research is aimed at eventually improving the quality of numerical analysis, by adopting and modifying the achievements of computational science. The distance between continuum and structural mechanics to computational science might be shortened if a continuum Hamiltonian was used. Finite element method implemented with particle discretization scheme (PDS-FEM) is suitable for this treatment, since it can be reformulated for momentum and strain that are discretized by using Voronoi and Delaunay tessellations, respectively.

We have to point out that the present paper succeeded in rigorously deriving a continuum Hamiltonian from a continuum Lagrangian. However, we merely discussed the potential usefulness of the continuum Hamiltonian. Further investigation will be needed to realize the usefulness of the continuum Hamiltonian.

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### Appendix A DERIVATION OF EQ. (2)

The variation in \( \int_T \mathcal{L}[\dot{u}, \text{sym}\nabla u] \, dt \) is given as the following integral:

\[
\int_T \int_V \left( \frac{\partial \mathcal{L}}{\partial \dot{u}} \cdot \dot{\mathcal{L}} + \frac{\partial \mathcal{L}}{\partial \dot{\mathcal{L}}} \cdot \dot{\mathcal{L}} \right) \, dV \, dt.
\]

Here, \( \dot{\mathcal{L}} \) stands for a small perturbation of \( u \), and the symmetry of a second-order tensor \( \frac{\partial \mathcal{L}}{\partial \mathcal{L}} \) is used. Applying the integration by part, we obtain

\[- \int_T \int_V \dot{\mathcal{L}} \cdot \left( \frac{\partial \mathcal{L}}{\partial \dot{u}} + \nabla \cdot \frac{\partial \mathcal{L}}{\partial \dot{\mathcal{L}}} \right) \, dV \, dt.\]

We should note that the sign of the two terms in the integrand is changed.

The residual terms that are not shown in the above integral are

\[
\left[ \int_V \dot{\mathcal{L}} \cdot \frac{\partial \mathcal{L}}{\partial \dot{u}} \, dV \right] + \int_T \int_V \dot{\mathcal{L}} \cdot \left( n \cdot \frac{\partial \mathcal{L}}{\partial \dot{\mathcal{L}}} \right) \, ds \, dt,
\]

where \([\cdot]\) stands for the difference of \( \cdot \) at the initial
Appendix B  DERIVATION OF EQ. (9)

The variation in \( \int_T \mathcal{L} \left[ u, \text{sym} [\nabla u] \right] \, dt \) in the index notation is given as follows:

\[
\int_T \int_V \frac{\partial \mathcal{L}}{\partial \dot{u}_i} \dot{u}_i + \int_T \int_V \frac{\partial \mathcal{L}}{\partial \epsilon_{ij}} u_{ij} \, dv \, dt
\]
or
\[
\int_T \int_V \int_V \gamma v_i \delta \dot{u}_i - c_{ijkl} \epsilon_{ij} \epsilon_{kl} \, dv \, dt.
\]

Here, \( \frac{\partial \mathcal{L}}{\partial \epsilon_{ij}} = \frac{\partial \mathcal{L}}{\partial \epsilon_{ij}} \) is used. Applying the integration by part, we obtain

\[
- \int_T \int_V \delta u_i \left( \rho \dot{u}_i - (c_{ijkl} \epsilon_{ij} \epsilon_{kl}) \right) \, dv \, dt.
\]

As shown, the integrand gives the wave equation of linearly elasticity.

The residual terms that are not shown in the above integral are

\[
\int_V \delta u_i \left( \frac{\partial \mathcal{L}}{\partial \dot{u}_i} \right) \, dv + \int_T \int_V \delta u_i (n_i \frac{\partial \mathcal{L}}{\partial \epsilon_{ij}}) \, ds \, dt,
\]
or
\[
\left[ \int_V \delta u_i \frac{\partial \mathcal{L}}{\partial \dot{u}_i} \, dv \right] - \int_T \int_V \delta u_i (n_i \frac{\partial \mathcal{L}}{\partial \epsilon_{ij}}) \, ds \, dt.
\]

The integrand is used for boundary conditions; more precisely, the integrand of the first integral is for the initial condition, while the integrand of the second integral is for the boundary condition.

Appendix C  PROOF OF EQ. (13)

We write the rate of Hamiltonian in the following index form:

\[
\mathcal{H} [p, \epsilon] = \int_V \frac{\partial \mathcal{H}}{\partial p_i} \dot{p}_i + \frac{\partial \mathcal{H}}{\partial \epsilon_{ij}} \dot{\epsilon}_{ij} \, dv.
\]

In view of Eq. (5), the integrand is written as

\[
\frac{\partial \mathcal{H}}{\partial p_i} \left( \frac{\partial \mathcal{H}}{\partial \dot{p}_i} \right)_{,ij} + \frac{\partial \mathcal{H}}{\partial \epsilon_{ij}} \left( \frac{\partial \mathcal{H}}{\partial \dot{p}_i} \right)_{,ij}.
\]

This term is the form of \( A_i B_{ij} + B_{ij} A_{ij} \) with \( A_i = \frac{\partial \mathcal{H}}{\partial \dot{p}_i} \) and \( B_{ij} = \frac{\partial \mathcal{H}}{\partial \dot{\epsilon}_{ij}} \). Hence, it becomes

\[
\frac{\partial \mathcal{H}}{\partial p_i} \left( \frac{\partial \mathcal{H}}{\partial \dot{p}_i} \right)_{,ij} + \frac{\partial \mathcal{H}}{\partial \dot{p}_i} \left( \frac{\partial \mathcal{H}}{\partial \dot{\epsilon}_{ij}} \right)_{,ij} = \left( \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial \mathcal{H}}{\partial \dot{p}_i} \right)_{,ij}.
\]

The volume integral of the above equation is reduced to the surface integral,

\[
\int_{\partial V} n_i \frac{\partial \mathcal{H}}{\partial p_i} \frac{\partial \mathcal{H}}{\partial \dot{\epsilon}_{ij}} \, ds.
\]

The integrand of this surface integral identically vanishes when boundary conditions are suitably posed. Therefore, Eq. (13) is proved.

By definition, the derivative of \( \mathcal{H} \) produces velocity and stress, i.e., \( \mathcal{H} = \frac{\partial \mathcal{H}}{\partial p_i} \) and \( \sigma_{ij} = \frac{\partial \mathcal{H}}{\partial \dot{\epsilon}_{ij}} \). Therefore, the above surface integral becomes

\[
\int_{\partial V} v_i (n_i \sigma_{ij}) \, ds.
\]

It shows that \( v_i = 0 \) (zero velocity) or \( n_i \sigma_{ij} = 0 \) (traction free) is a suitable boundary condition.

Appendix D  HAMILTONIAN FOR FEM

Using index notation, we start from a continuum Lagrangian of \( \mathcal{L} [\{ u^a \}, \{ u^b \}] \). Defining a new variable as \( p^a = \frac{\partial \mathcal{L}}{\partial u^a} \), which is moment of the \( \alpha \)-th node, we derive a continuum Hamiltonian of Eq. (19) for this \( \mathcal{L}^* \) as

\[
\mathcal{H}^* [\{ u^a \}, \{ u^b \}] = \sum_{\alpha} u^a \frac{\partial \mathcal{L}^*}{p^a} - \mathcal{L}^* [\{ \dot{u}^a \}, \{ \dot{u}^b \}]
\]

A canonical equation of Eq. (20) for this \( \mathcal{H}^* \) is

\[
\dot{p}^a_i = \frac{\partial \mathcal{H}^*}{\partial u^a} \quad \text{and} \quad \dot{u}^a = \frac{\partial \mathcal{H}^*}{\partial p^a},
\]

see Fig. 3 for a schematic view of these procedures.

For simplicity, we assume that the derivatives of \( \mathcal{H}^* \) are given as a linear combination of its arguments, \( u^a \) and \( p^a \), i.e.,

\[
\frac{\partial \mathcal{H}^*}{\partial u^a} = \sum_{\beta} K_{ij}^{a\beta} u^b_j \quad \text{and} \quad \frac{\partial \mathcal{H}^*}{\partial p^a} = \sum_{\beta} R_{ij}^{a\beta} p^b_j,
\]

where \( R_{ij}^{a\beta} = \frac{\partial \mathcal{H}^*}{\partial u^a u^b} \) and \( K_{ij}^{a\beta} = \frac{\partial \mathcal{H}^*}{\partial p^a \epsilon_{ij}} \). We make two vectors, \( [u] \) and \( [p] \), by arranging \( u^a \) and \( p^a \), respectively, and make two matrices, \( [R] \) and \( [K] \), by arranging \( R_{ij}^{a\beta} \) and \( K_{ij}^{a\beta} \). In terms of these vectors and matrices, the continuum Hamiltonian of FEM is expressed as

\[
\mathcal{H}^* = \frac{1}{2} [p]^T [R][p] + \frac{1}{2} [u]^T [K][u],
\]

where superscript \( T \) stands for the transpose. The canonical equation becomes

\[
[p] = [K][u] \quad \text{and} \quad [u] = [M][p].
\]

It shows that \( [K] \) is a stiffness matrix and \( [R] \) is the inverse of a mass matrix.

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