Discrete Mechanics Based on Finite Element Methods

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Abstract
Discrete Mechanics based on finite element methods is presented in this paper. We also explore the relationship between this discrete mechanics and Veselov discrete mechanics. High order discretizations are constructed in terms of high order interpolations.

Keywords. Discrete mechanics, Finite element methods, Symplectic integrators

1 Introduction
We begin by recalling the variational principle for Lagrange mechanics. Suppose \( Q \) denotes the configuration space with coordinates \( q^i \) and \( TQ \) the tangent bundle with coordinates \( (q^i, \dot{q}^i) \), \( i = 1, 2, \cdots, n \). In the following, we will work with the extended configuration space \( R \times Q \) with coordinates \( (t, q^i) \) and the extended tangent bundle \( R \times TQ \) with coordinates \( (t, q^i, \dot{q}^i) \). Here \( t \) denotes the time \([1]\).

Consider a Lagrangian \( L : R \times TQ \rightarrow R \). The corresponding action functional is defined by

\[
S((t, q^i(t))) = \int_a^b L(t, q^i(t), \dot{q}^i(t)) \, dt, \tag{1.1}
\]

where \( q^i(t) \in C^2([a, b]) \), which is the set of all \( C^2 \) curves in \( Q \) defined on \([a, b]\).

The variational principle seeks the curves \( q^i(t) \) in \( C^2([a, b]) \), for which the action functional \( S \) is stationary under variations of \( q^i(t) \) with fixed endpoints.

Consider a vector field on \( R \times Q \)

\[
V = \xi(t, q^i) \frac{\partial}{\partial t} + \sum_{i=1}^n \phi^i(t, q^i) \frac{\partial}{\partial q^i}. \tag{1.2}
\]

Let \( F^e \) be the flow of \( V \). For \((t, q^i) \in R \times Q\), we have \( F^e(t, q^i) = (\tilde{t}, \tilde{q}^i)\).

\[
\tilde{t} = f(e, t, q^i), \tag{1.3}
\]

\[
\tilde{q}^i = g^i(e, t, q^i), \tag{1.4}
\]
where
\[
\frac{d}{d\epsilon} \bigg|_{\epsilon=0} f(\epsilon, t, q^i) = \xi(t, q^j),
\]
\[
\frac{d}{d\epsilon} \bigg|_{\epsilon=0} g^i(\epsilon, t, q^j) = \phi^i(t, q^j).
\]
(1.5)

The transformation (1.3-1.4) transforms a curve \(q^j(t)\) in \(Q\) into another curve \(\tilde{q}^i(\epsilon, \tilde{t})\) in \(Q\) determined by
\[
\tilde{t} = f(\epsilon, t, q^j(t)),
\]
\[
\tilde{q}^i = g^i(\epsilon, t, q^j(t)).
\]

Before calculating the variation of \(S\), we consider the first order prolongation of \(V\)
\[
pr^1V = \xi(t, q^j) \frac{\partial}{\partial t} + \sum_{i=1}^n \phi^i(t, q^j) \frac{\partial}{\partial q^i} + \sum_{i=1}^n \alpha^i(t, q^j, \dot{q}^j) \frac{\partial}{\partial \dot{q}^i},
\]
(1.6)

where \(pr^1V\) denote the first order prolongation of \(V\) and
\[
\alpha^i(t, q^j, \dot{q}^j) = D_t \phi^i(t, q^j) - \dot{q}^i D_t \xi(t, q^j),
\]
(1.7)

where \(D_t\) denotes the total derivative \([14]\).

Now we calculate the variation of \(S\) directly
\[
\delta S = \frac{d}{d\epsilon} \bigg|_{\epsilon=0} S(\tilde{t}, \tilde{q}^i(\epsilon, \tilde{t})))
\]
\[
= \frac{d}{d\epsilon} \bigg|_{\epsilon=0} \int_a^b \left( \frac{\partial L}{\partial t} + \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^j} \dot{q}^j - L \right) \right) \xi + \left( \frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} \phi^i \right) d\tilde{t}
\]
\[
+ \left[ \left( L - \frac{\partial L}{\partial \dot{q}^j} \dot{q}^j \right) \xi + \frac{\partial L}{\partial q^i} \phi^i \right]_{a}^{b}.
\]
(1.8)

If \(\xi(a, q^j(a)) = \xi(b, q^j(b)) = 0\) and \(\phi^i(a, q^j(a)) = \phi^i(b, q^j(b)) = 0\), the requirement of \(\delta S = 0\) yields the energy evolution equation
\[
\frac{\partial L}{\partial t} + \frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^j} \dot{q}^j - L \right) = 0
\]
(1.9)

from \(\xi\) and the Euler-Lagrange equation
\[
\frac{\partial L}{\partial q^i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}^i} = 0
\]
(1.10)

from \(\phi^i\)

If \(L\) does not depend on \(t\) explicitly, i.e., \(L\) is conservative and \(\frac{\partial L}{\partial t} = 0\), then (1.9) becomes the energy conservation law
\[
\frac{d}{dt} \left( \frac{\partial L}{\partial \dot{q}^j} \dot{q}^j - L \right) = 0.
\]
(1.11)

\[\text{Note that Hamilton's variational principle holds in fact for the vertical variation, while the horizontal variation gives rise to the conservation relation between the Euler-Lagrange equation and energy conservation, see, for example, [5]. Here, in order to transfer to discrete case more directly, this variational requirement is employed.}\]
If we drop the requirement
\[\xi(a, q^i(a)) = \xi(b, q^i(b)) = 0,\]
\[\phi^i(a, q^i(a)) = \phi^i(b, q^i(b)) = 0,\]
we can define from the second term in (1.8) the extended Lagrangian one form
\[\theta_L = \left(L - \frac{\partial L}{\partial \dot{q}^i}\right) dt + \frac{\partial L}{\partial \dot{q}^i} dq^i.\] (1.12)

We define the extended Lagrangian two form to be
\[\omega_L = d\theta_L.\]

Suppose \(g^i(t, v_q)\) is a solution of (1.10) depending on the initial condition \(v_q \in TQ\). Restricting \(\tilde{q}^i(\epsilon, \tilde{t})\) to the solution space of (1.10) and using the same method in [12], we can prove
\[\left(pr^1 g\right)^*\omega_L = \omega_L,\] (1.13)
where \(pr^1 g(s, v_q) = (s, g^i(s, v_q), \frac{d}{ds} g^i(s, v_q))\) denotes the first order prolongation of \(g^i(s, v_q)\).

By defining a discrete Lagrangian with fixed steps and constructing a discrete action, Veselov develops a kind of discrete mechanics [15, 16]. See also [13, 17]. The resulting discrete Euler-Lagrange equation (variational integrator) preserves a discrete Lagrange two form. However the discrete versions of (1.9) and (1.11) are not reflected in Veselov discrete mechanics. Using variable steps and a defined discrete energy, Kane, Marsden and Ortiz obtain symplectic-energy integrators [7]. Chen, Guo and Wu develop a discrete total variation and prove the symplectic-energy integrators preserve a discrete extended Lagrange two form [2]. Guo and Wu also present the difference variational approach with variable step-lengths [5].

The connection between Veselov discrete mechanics and finite element methods was first suggested in [12]. Symplectic and multisymplectic structures in simple finite element methods are explored in [4]. As is known, it is difficult to obtain high order discretizations in Veselov discrete mechanics. We find that the finite element methods provide a natural way to obtain a kind of discrete Lagrangian, including those of high order. The purpose of this paper is to develop such kind of discrete mechanics based on finite element methods.

This paper is organized as follows. In the next section, we will present the discrete mechanics based on finite element methods. Section 3 is devoted to discussing the role of time steps. We finish this paper by drawing some conclusions in Section 4.

2 Discrete mechanics based on finite element methods

2.1 Generalized Veselov discrete mechanics

We first present Veselov discrete mechanics in a more general formulation that allows for variable time steps. In this generalized Veselov discrete mechanics, \(M \times M\) is used for the discrete version of \(R \times TQ\). Here \(M = R \times Q\). A point \((t_k, q_k; t_{k+1}, q_{k+1}) \in M \times M\) corresponds to a tangent vector \(\frac{q_{k+1} - q_k}{t_{k+1} - t_k}\). Here for brevity of notations, we restrict ourselves to one-dimensional configuration space \(Q\). A discrete Lagrangian is defined to be \(L : M \times M \to R\) and the corresponding action to be
\[S = \sum_{k=0}^{N-1} L(t_k, q_k, t_{k+1}, q_{k+1})(t_{k+1} - t_k).\] (2.1)
The discrete variational principle is to extremize $S$ for variations of $q_k$ holding the endpoints $q_0$ and $q_N$ fixed. In this discrete variational principle, $t_k$ play the role of parameters (They can also play the role of variables, see next section). This discrete variational principle determines a discrete flow $\Phi : M \times M \rightarrow M \times M$ by

$$\Phi(t_{k-1}, q_{k-1}, t_k, q_k) = (t_k, q_k, t_{k+1}, q_{k+1}).$$ (2.2)

Here $q_{k+1}$ is found from the following discrete Euler-Lagrange equation (variational integrator)

$$(t_{k+1} - t_k)D_2\mathcal{L}(t_k, q_k, t_{k+1}, q_{k+1}) + (t_k - t_{k-1})D_4\mathcal{L}(t_{k-1}, q_{k-1}, t_k, q_k) = 0$$ (2.3)

for all $k \in \{1, 2, \ldots, N - 1\}$. Here $D_i$ denotes the partial derivative of $\mathcal{L}$ with respect to the $i$th argument. Notice that $t_k$ are parameters here. The reason we still call them arguments is that we want to keep the notations consistent since in next section they will play the role of variables.

Now we prove that the discrete flow $\Phi$ preserves a discrete version of the Lagrange two form

$$\omega^v_L = d\theta^v_L, \quad \theta^v_L = \frac{\partial L}{\partial q} dq.$$ (2.4)

We do this directly from the variational point of view, consistent with the continuous case [12].

As in continuous case, we calculate $dS$ for variations with varied endpoints.

$$dS(q_0, q_1, \ldots, q_N) \cdot (\delta q_0, \delta q_1, \ldots, \delta q_N)$$

$$= \left. \frac{d}{dt} \right|_{t=0} S(q_0 + \epsilon\delta q_0, q_1 + \epsilon\delta q_1, \ldots, q_N + \epsilon\delta q_N)$$

$$= \sum_{k=0}^{N-1} (\sum_{k=0}^{N-1} \sum_{k=1}^{N} D_2\mathcal{L}(t_k, q_k, t_{k+1}, q_{k+1}) \partial q_k + D_4\mathcal{L}(t_{k-1}, q_{k-1}, t_k, q_k)) (t_{k+1} - t_k)$$

$$= \sum_{k=0}^{N-1} (\sum_{k=1}^{N} D_2\mathcal{L}(t_k, q_k, t_{k+1}, q_{k+1}) (t_{k+1} - t_k) + D_4\mathcal{L}(t_{k-1}, q_{k-1}, t_k, q_k)) (t_{k-1} - t_k) \delta q_k$$

$$+ D_2\mathcal{L}(t_0, q_0, t_1, q_1) (t_1 - t_0) \delta q_0 + D_4\mathcal{L}(t_{N-1}, q_{N-1}, t_N, q_N) (t_N - t_{N-1}) \delta q_N.$$ (2.5)

We can see that the last two terms in (2.5) come from the boundary variations. Based on the boundary variations, we can define two one forms on $M \times M$

$$\theta^v_L^-(t_k, q_k, t_{k+1}, q_{k+1}) = D_2\mathcal{L}(t_k, q_k, t_{k+1}, q_{k+1}) (t_{k+1} - t_k) dq_k,$$ (2.6)

and

$$\theta^v_L^+(t_k, q_k, t_{k+1}, q_{k+1}) = D_4\mathcal{L}(t_k, q_k, t_{k+1}, q_{k+1}) (t_{k+1} - t_k) dq_{k+1}.$$ (2.7)

Here we have used the notation in [12]. We regard the pair $(\theta^v_L^-, \theta^v_L^+)$ as being the discrete version of the Lagrange one form $\theta^v_L$ in (2.4).

Now we parameterize the solutions of the discrete variational principle by the initial condition $(q_0, q_1)$, and restrict $\mathcal{S}$ to that solution space. Then Eq. (2.3) becomes

$$d\mathcal{S}(q_0, q_1, \ldots, q_N) \cdot (\delta q_0, \delta q_1, \ldots, \delta q_N)$$

$$= \theta^v_L^-(t_0, q_0, t_1, q_1) \cdot (\delta q_0, \delta q_1) + \theta^v_L^+(t_{N-1}, q_{N-1}, t_N, q_N) \cdot (\delta q_{N-1}, \delta q_N)$$

$$= \theta^v_L^-(t_0, q_0, t_1, q_1) \cdot (\delta q_0, \delta q_1) + (\Phi^{N-1})^* \theta^v_L^+(t_0, q_0, t_1, q_1) \cdot (\delta q_0, \delta q_1).$$ (2.8)
From (2.8), we can obtain
\[ dS = \theta_L^- + (\Phi^{N-1})^* \theta_L^+. \] (2.9)
The Eq. (2.8) holds for arbitrary \( N > 1 \). Taking \( N=2 \) leads to
\[ dS = \theta_L^- + \Phi^* \theta_L^+. \] (2.10)
By taking exterior differentiation of (2.10), we obtain
\[ \Phi^*(d\theta_L^+) = -d\theta_L^- . \] (2.11)
From the definition of \( \theta_L^- \) and \( \theta_L^+ \), we know that
\[ \theta_L^- + \theta_L^+ = d((t_{k+1} - t_k)L), \]
which means \( d\theta_L^+ = -d\theta_L^- . \)
Defining
\[ \omega_L^v =: d\theta_L^+ = -d\theta_L^- , \] (2.12)
we show from (2.11) that the discrete flow \( \Phi \) preserves the discrete Lagrange two form \( \omega_L^v : \)
\[ \Phi^*(\omega_L^v) = \omega_L^v . \] (2.13)

Let us consider an example. For the classical Lagrangian
\[ L(t, q, \dot{q}) = \frac{1}{2} \dot{q}^2 - V(q) , \] (2.14)
we choose the discrete Lagrangian \( \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) \) as
\[ \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) = \frac{1}{2} \left( \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right)^2 - V \left( \frac{q_{k+1} + q_k}{2} \right) . \] (2.15)
The discrete Euler-Lagrange equation (2.3) becomes
\[ \left( \frac{q_{k+1} - q_k}{t_{k+1} - t_k} - \frac{q_k - q_{k-1}}{t_k - t_{k-1}} \right) + \frac{V''(\bar{q}_k)(t_{k+1} - t_k) + V''(\bar{q}_{k-1})(t_k - t_{k-1})}{2} = 0 , \] (2.16)
which preserves the Lagrange two form
\[ \left( \frac{1}{t_{k+1} - t_k} + \frac{t_{k+1} - t_k}{4} V''(\bar{q}_k) \right) dq_{k+1} \wedge dq_k , \] (2.17)
where \( \bar{q}_k = \frac{q_k + q_{k+1}}{2} , \quad \bar{q}_{k-1} = \frac{q_{k-1} + q_k}{2} . \)
If we take fixed variables \( t_{k+1} - t_k = t_k - t_{k-1} = h \), then (2.14) becomes
\[ \frac{q_{k+1} - 2q_k + q_{k-1}}{h^2} + \frac{V''(\bar{q}_k) + V''(\bar{q}_{k-1})}{2} = 0 , \]
which preserves the Lagrange two form
\[ \left( \frac{1}{h} + \frac{h}{4} V''(\bar{q}_k) \right) dq_{k+1} \wedge dq_k . \]
2.2 Discrete mechanics based on finite element methods

Now we consider discrete mechanics based on finite element methods. Let us go back to the variation problem of the action functional (2.1). The finite element method is an approximate method for solving the variation problem. Instead of solving the variation problem in the space $C^2([a, b])$, the finite element method solves the problem in a subspace $V_h^m([a, b])$ of $C^2([a, b])$. $V_h^m([a, b])$ consists of piecewise $m$-degree polynomials interpolating the curves $q(t) \in C^2([a, b])$.

First, we consider the piecewise linear interpolation. Given a partition of $[a, b]$

$$a = t_0 < t_1 < \cdots < t_k < \cdots < t_{N-1} < t_N = b,$$

the intervals $I_k = [t_k, t_{k+1}]$ are called elements. $h_k = t_{k+1} - t_k$. $V_h([a, b])$ consists of piecewise linear function interpolating $q(t)$ at $(t_k, q_k)$, $k = 0, 1, \cdots, N$. Now we derive the expressions of $q_h(t) \in V_h([a, b])$. First we construct the basis functions $\varphi_h(t)$, which are piecewise linear function on $[a, b]$ satisfying $\varphi_h(t_i) = \delta_k^i$, $i = 0, 1, \cdots, N$.

$$\varphi_0(t) = \begin{cases} 1 - \frac{t-t_0}{h_0}, & t_0 \leq t \leq t_1; \\ 0, & \text{otherwise} \end{cases}; \quad \varphi_N(t) = \begin{cases} 1 + \frac{t-t_N}{h_{N-1}}, & t_{N-1} \leq t \leq t_N; \\ 0, & \text{otherwise} \end{cases} \quad (2.18)$$

and for $k = 1, 2, \cdots, N - 1$,

$$\varphi_k(t) = \begin{cases} 1 + \frac{t-t_k}{h_{k-1}}, & t_{k-1} \leq t \leq t_k; \\ 1 - \frac{t-t_k}{h_k}, & t_k \leq t \leq t_{k+1}; \\ 0, & \text{otherwise} \end{cases} \quad (2.19)$$

Using these basis functions, we obtain the expression $q_h(t) \in V_h([a, b])$:

$$q_h(t) = \sum_{k=0}^{N} q_k \varphi_h(t). \quad (2.20)$$

In the space $V_h([a, b])$, the action functional (2.1) becomes

$$S((t, q_h(t))) = \int_a^b L(t, q_h(t), \dot{q}_h(t)) \, dt$$

$$= \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} L \left( t, \sum_{i=0}^{N} (q_i \varphi_i(t)), \frac{d}{dt} \sum_{i=0}^{N} (q_i \varphi_i(t)) \right) \, dt$$

$$= \sum_{k=0}^{N-1} \mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) (t_{k+1} - t_k), \quad (2.21)$$

where

$$\mathbb{L}(t_k, q_k, t_{k+1}, q_{k+1}) = \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} L \left( t, \sum_{i=0}^{N} (q_i \varphi_i(t)), \frac{d}{dt} \sum_{i=0}^{N} (q_i \varphi_i(t)) \right) \, dt$$

$$= \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} L \left( t, \sum_{i=k}^{N} (q_i \varphi_i(t)), \frac{d}{dt} \sum_{i=k}^{N} (q_i \varphi_i(t)) \right) \, dt. \quad (2.22)$$

Therefore, restricting to the subspace $V_h([a, b])$ of $C^2([a, b])$, the original variational problem reduces to the extremum problem of the function $L$ in $q_k$, $k = 0, 1, \cdots, N$. Notice that (2.21) is just one of the discrete actions (2.1). Thus, what remains to be
done is just to perform the same calculations on (2.21) as on (2.1). We can then obtain the discrete Euler-Lagrange equation (2.3) that preserves the discrete Lagrange two form (2.13). Therefore, discrete mechanics based on finite element methods consists of two steps: first, use finite element methods to obtain a kind of discrete Lagrangian; second, use the method of Veselov mechanics to obtain the variational integrators.

Let us consider the previous example again. For the classical Lagrangian (2.14), we choose the discrete Lagrangian \( L(t, q_k, t_{k+1}, q_{k+1}) \) as

\[
L(t, q_k, t_{k+1}, q_{k+1}) = \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} \left( \frac{1}{2} \left( \frac{d}{dt} \sum_{i=0}^{N} (q_i \varphi_i(t)) \right)^2 - V \left( \sum_{i=0}^{N} (q_i \varphi_i(t)) \right) \right) dt
\]

\[
= \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} \left( \frac{1}{2} \left( \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right)^2 - V \left( \frac{t_{k+1} - t}{t_{k+1} - t_k} q_k + \frac{t - t_k}{t_{k+1} - t_k} q_{k+1} \right) \right) dt
\]

\[
= \frac{1}{2} \left( \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right)^2 - F(q_k, q_{k+1}),
\]

where

\[
F(q_k, q_{k+1}) = \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} V \left( \frac{t_{k+1} - t}{t_{k+1} - t_k} q_k + \frac{t - t_k}{t_{k+1} - t_k} q_{k+1} \right) dt.
\]

The discrete Euler-Lagrange equation (2.3) becomes

\[
\left( \frac{q_{k+1} - q_k}{t_{k+1} - t_k} - \frac{q_k - q_{k-1}}{t_k - t_{k-1}} \right) \frac{\partial F(q_k, q_{k+1})}{\partial q_k} + \frac{\partial F(q_{k-1}, q_k)}{\partial q_k} (t_{k-1} - t_k) = 0,
\]

which preserves the Lagrange two form

\[
\left( \frac{1}{t_{k+1} - t_k} + (t_{k+1} - t_k) \frac{\partial^2 F(q_k, q_{k+1})}{\partial q_k \partial q_{k+1}} \right) dq_{k+1} \wedge dq_k.
\]

Again, if we take fixed time steps \( t_{k+1} - t_k = t_k - t_{k-1} = h \), (2.25) becomes

\[
\frac{q_{k+1} - 2q_k + q_{k-1}}{h^2} + \frac{\partial F(q_k, q_{k+1})}{\partial q_k} + \frac{\partial F(q_{k-1}, q_k)}{\partial q_k} = 0,
\]

which preserves the Lagrange two form

\[
\left( \frac{1}{h} + h \frac{\partial^2 F(q_k, q_{k+1})}{\partial q_k \partial q_{k+1}} \right) dq_{k+1} \wedge dq_k.
\]

Suppose \( q_k \) is the solution of (2.23) and \( q(t) \) is the solution of

\[
\frac{d^2 q}{dt^2} + \frac{\partial V(q)}{\partial q} = 0,
\]

then from the convergence theory of finite element methods \( \| \cdot \| \) is the \( L^2 \) norm. \( q_h(t) = \sum_{k=0}^{N} q_k, h = \max_k \{ h_k \} \) and \( C \) is a constant independent of \( h \).
If we use mid-point numerical integration formula in (2.24), we obtain
\[
F(q_k, q_{k+1}) = \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} V \left( \frac{t_{k+1} - t}{t_{k+1} - t_k} q_k + \frac{t - t_k}{t_{k+1} - t_k} q_{k+1} \right) dt \\
\approx V \left( \frac{q_k + q_{k+1}}{2} \right).
\]
In this case, (2.23) is just (2.10). We can also use trapezoid formula or Simpson formula and so on to integrate (2.24) numerically and obtain another kind of discrete Lagrangian.

2.3 Discrete mechanics with Lagrangian of high order

Now we consider piecewise quadratic polynomial interpolation, which will result in a kind of discrete Lagrangian of high order. To this aim, we add an auxiliary node \( t_k + \frac{1}{2} \) to each element \( I_k = [t_k, t_{k+1}] \). There are two kinds of quadratic basis functions: \( \phi_k(t) \) for nodes \( t_k \) and \( \phi_{k+\frac{1}{2}}(t) \) for \( t_k + \frac{1}{2} \) that satisfy
\[
\phi_k(t_i) = \delta_i^k, \quad \phi_k(t_{i+\frac{1}{2}}) = 0, \\
\phi_{k+\frac{1}{2}}(t_{i+\frac{1}{2}}) = \delta_i^k, \quad \phi_{k+\frac{1}{2}}(t_i) = 0, \quad i, k = 0, 1, \ldots, N.
\]
We list the basis functions as follows:
\[
\phi_0(t) = \begin{cases} \frac{2(t-t_0)}{h_0} - 1 \left( \frac{t-t_0}{h_0} - 1 \right), & t_0 \leq t \leq t_1; \\ 0, & \text{otherwise}; \end{cases}
\]
(2.29)
\[
\phi_N(t) = \begin{cases} \frac{2(t_N-t)}{h_{N-1}} - 1 \left( \frac{t_N-t}{h_{N-1}} - 1 \right), & t_{N-1} \leq t \leq t_N; \\ 0, & \text{otherwise}; \end{cases}
\]
(2.30)
and for \( k = 1, 2, \ldots, N-1, \)
\[
\phi_k(t) = \begin{cases} \frac{2(t_k-t)}{h_k} - 1 \left( \frac{t_k-t}{h_k} - 1 \right), & t_{k-1} \leq t \leq t_k; \\ \frac{2(t_{k+1}-t)}{h_k} - 1 \left( \frac{t_{k+1}-t}{h_k} - 1 \right), & t_k \leq t \leq t_{k+1}; \\ 0, & \text{otherwise}; \end{cases}
\]
(2.31)
and for \( k = 0, 1, \ldots, N-1, \)
\[
\phi_{k+\frac{1}{2}}(t) = \begin{cases} \frac{4t-t_k}{h_k} \left( 1 - \frac{t-t_k}{h_k} \right), & t_k \leq t \leq t_{k+1}; \\ 0, & \text{otherwise}. \end{cases}
\]
(2.32)
Using these basis functions, we construct subspace \( V_{h^2}([a, b]) \) of \( C^2([a, b]) \):
\[
q_{h^2}(t) = \sum_{k=0}^N q_k \phi_k(t) + \sum_{k=0}^{N-1} q_{k+\frac{1}{2}} \phi_{k+\frac{1}{2}}(t), \quad q_{h^2}(t) \in V_{h^2}([a, b]).
\]
(2.33)
In the space \( V_{h^2}([a, b]) \), the action functional (1.1) becomes
\[
S((t, q_{h^2}(t))) = \int_a^b L(t, q_{h^2}(t), \dot{q}_{h^2}(t)) dt \\
= \sum_{k=0}^{N-1} \int_{t_k}^{t_{k+1}} L(t, q_{h^2}(t), \dot{q}_{h^2}(t)) dt \\
= \sum_{k=0}^{N-1} L(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+\frac{1}{2}}, q_{k+1}, (t_{k+1} - t_k)),
\]
(2.34)
where

\[
\mathcal{L}(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}) = \frac{1}{t_{k+1} - t_k} \int_{t_k}^{t_{k+1}} L(t, q_h z(t), \dot{q}_h z(t)) \, dt.
\]  

(2.35)

For the discrete action (2.34), we have

\[
dS(q_0, q_{\frac{1}{2}}, q_1, \ldots, q_{N-\frac{1}{2}}, q_N) \cdot (\delta q_0, \delta q_{\frac{1}{2}}, \delta q_1, \ldots, \delta q_{N-\frac{1}{2}}, \delta q_N) = \sum_{k=0}^{N-1} (D_2 \mathcal{L}(w_k) \delta q_k + D_3 \mathcal{L}(w_k) \delta q_{k+\frac{1}{2}} + D_3 \mathcal{L}(w_k) \delta q_{k+1})(t_{k+1} - t_k) 
\]

(2.36)

where \( w_k = (t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}), k = 0, 1, \ldots, N - 1 \). From (2.36), we obtain the discrete Euler-Lagrange equation

\[
D_2 \mathcal{L}(w_k)(t_{k+1} - t_k) + D_3 \mathcal{L}(w_{k-1})(t_k - t_{k-1}) = 0,
\]  

(2.37)

\[
D_3 \mathcal{L}(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}) = 0,
\]  

(2.38)

\[
D_3 \mathcal{L}(t_{k-1}, q_{k-1}, q_{k-\frac{1}{2}}, t_k, q_k) = 0.
\]  

(2.39)

We can from (2.38) and (2.39) solve for \( q_{k+\frac{1}{2}} \) and \( q_{k-\frac{1}{2}} \) respectively, then substitute them into (2.37) and finally solve for \( q_{k+1} \). Therefore, the discrete Euler-Lagrange equation (2.37-2.39) still determines a discrete flow

\[
\Psi : M \times M \rightarrow M \times M
\]

\[
\Psi(t_{k-1}, q_{k-1}, t_k, q_k) = (t_k, q_k, t_{k+1}, q_{k+1}).
\]

From (2.36), we can define two one forms

\[
\Theta_L^- (t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}) = D_2 \mathcal{L}(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1})(t_{k+1} - t_k) dq_k,
\]  

and

\[
\Theta_L^+ (t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}) = D_3 \mathcal{L}(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1})(t_{k+1} - t_k) dq_{k+\frac{1}{2}}.
\]  

Using the same method as before, we can prove that

\[
\Psi^*(d\Theta_L^+) = -d\Theta_L^-.
\]  

(2.40)

From the definition of \( \Theta_L^- \) and \( \Theta_L^+ \), we have

\[
\Theta_L^- + \Theta_L^+ = d((t_{k+1} - t_k)L) - D_3 \mathcal{L}(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}) dq_{k+\frac{1}{2}}.
\]  

(2.41)

From (2.38), we obtain \( D_3 \mathcal{L}(t_k, q_k, q_{k+\frac{1}{2}}, t_{k+1}, q_{k+1}) = 0 \). Thus,

\[
\Theta_L^- + \Theta_L^+ = d((t_{k+1} - t_k)L),
\]  

which means

\[
d\Theta_L^+ = -d\Theta_L^-.
\]  

(2.42)
From (2.40) and (2.42), we arrive at
\[ \Psi^*(\Omega^v_v) = \Omega^v_v, \] (2.43)
where \( \Omega^v_v = d\Theta^v_+ \).

For the classical Lagrangian (2.14), From (2.33) and (2.35), we obtain
\[
\mathbb{L}(t_k, q_k, q_k, q_k, t_k, q_k) = \frac{1}{t_k - t_{k+1}} \int_{t_k}^{t_{k+1}} \left( \frac{1}{2} (q_{k+1} - q_k)^2 - V(q_k (t)) \right) dt \\
= \frac{1}{2} \left( \frac{1}{3} a^2 (t_k^2 + t_k t_{k+1} + t_{k+1}^2) + ab(t_k + t_{k+1}) + b^2 \right) \\
- G(q_k, q_k, q_k, t_k, t_k) + 1, 
\]
where
\[
a = \frac{4}{h_k^2} \left( q_k + q_k - 2q_k \right), \\
b = \frac{1}{h_k} \left( 4(t_k + t_{k+1})q_k - (3t_k + t_{k+1})q_k - (t_k + 3t_{k+1})q_k \right), 
\]
and
\[
G(q_k, q_k, q_k, t_k, t_k) = \frac{1}{t_k - t_{k+1}} \int_{t_k}^{t_{k+1}} V \left( q_k f_k(t) + q_k f_{k+1}(t) + q_k f_{k+\frac{1}{2}}(t) \right) dt, 
\]
where
\[
f_k(t) = \left( \frac{2(t - t_k)}{h_k} - 1 \right) \left( \frac{t - t_k}{h_k} - 1 \right), \\
f_{k+1}(t) = \left( \frac{2(t_{k+1} - t)}{h_k} - 1 \right) \left( \frac{t_{k+1} - t}{h_k} - 1 \right), \\
f_{k+\frac{1}{2}}(t) = 4 \left( \frac{t - t_k}{h_k} \right) \left( \frac{1 - t_k}{h_k} \right). 
\]

For the discrete Lagrangian (2.44), the discrete Euler-Lagrange equation (2.37-2.39) becomes
\[
a_1 q_{k,-1} + a_2 q_k + a_3 q_{k+1} + a_4 q_{k-\frac{1}{2}} + a_5 q_{k+\frac{1}{2}} - d_1 h_k - d_2 h_{k-1} = 0, \] (2.45)
\[
- \frac{8}{3h_k^2} \left( q_k - q_k - 2q_k \right) - \frac{\partial G(q_k, q_k, q_k, t_k, t_k)}{\partial q_{k+\frac{1}{2}}} = 0, \] (2.46)
\[
- \frac{8}{3h_{k-1}^2} \left( q_{k-1} + q_h - 2q_{k-1+\frac{1}{2}} \right) - \frac{\partial G(q_{k-1}, q_{k-1+\frac{1}{2}}, q_k)}{\partial q_{k-1+\frac{1}{2}}} = 0, \] (2.47)
where
\[
a_1 = \frac{1}{3} h_{k-1}, \quad a_2 = \frac{7}{3} \left( \frac{1}{h_{k-1}} + \frac{1}{h_k} \right), \quad a_3 = \frac{1}{3} h_k, \quad a_4 = -\frac{8}{3} h_{k-1}, \quad a_5 = -\frac{8}{3} \frac{1}{h_k}, \\
d_1 = \frac{\partial G(q_k, q_k, q_k, t_k)}{\partial q_k}, \quad d_2 = \frac{\partial G(q_{k-1}, q_{k-1+\frac{1}{2}}, q_k)}{\partial q_k}. 
\]
The solution of (2.45-2.47) preserves the Lagrange two form
\[
\left( \frac{1}{3h_k} - h_k \frac{\partial^2 G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_k \partial q_{k+1}} - M \right) dq_k \wedge dq_{k+1},
\] (2.48)

where
\[
M = \left( \frac{16}{3h_k} + h_k \frac{\partial^2 G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_k \partial q_{k+1}} \right) \left( \frac{16}{3h_k} + h_k \frac{\partial^2 G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_k \partial q_{k+1}} \right).
\]

If we take the fixed time steps \( h_{k-1} = h_k = h \), then (2.45-2.47) become
\[
q_{k-1} - 8q_{k-\frac{1}{2}} + 14q_k - 8q_{k+\frac{1}{2}} + q_{k+1} = -d_1h_k - d_2h_{k-1} = 0,
\] (2.49)
\[
- \frac{8}{3h^2} \left( q_k + q_{k+1} - 2q_{k+\frac{1}{2}} \right) - \frac{\partial G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_{k+\frac{1}{2}}} = 0,
\] (2.50)
\[
- \frac{8}{3h^2} \left( q_{k-1} + q_k - 2q_{k-1+\frac{1}{2}} \right) - \frac{\partial G(q_{k-1}, q_{k-1+\frac{1}{2}}, q_k)}{\partial q_{k-1+\frac{1}{2}}} = 0,
\] (2.51)

which preserve
\[
\left( \frac{1}{3h} - h k \frac{\partial^2 G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_k \partial q_{k+1}} - M \right) dq_k \wedge dq_{k+1},
\] (2.52)

where
\[
M = \left( \frac{16}{3h_k} + h_k \frac{\partial^2 G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_k \partial q_{k+1}} \right) \left( \frac{16}{3h_k} + h_k \frac{\partial^2 G(q_k, q_{k+\frac{1}{2}}, q_{k+1})}{\partial q_k \partial q_{k+1}} \right).
\]

Suppose \( q_k \) is the solution of (2.45-2.47) and \( q(t) \) is the solution of (2.27), then from the convergence theory of finite element methods [3, 11], we have
\[
\| q(t) - q_h(t) \| \leq Ch^3,
\] (2.53)

where
\[
q_h(t) = \sum_{k=0}^{N} q_k \phi_k(t) + \sum_{k=0}^{N-1} q_{k+\frac{1}{2}} \phi_{k+\frac{1}{2}}(t);
\]
\[
h = \max_k \{ h_k \} \text{ and } C \text{ is a constant independent of } h.
\]

3  Time steps as variables

In §2, the time steps \( t_k \) play the role of parameters. They are determined beforehand according to some requirements. In fact, we can also regard \( t_k \) as variables and the variation of the discrete action with respect to \( t_k \) yields the discrete energy conservation law. This fact was first observed by Lee [3, 8, 9, 10]. The symplecticity of the resulting
integrators was investigated in [1, 2]. These results also apply to the discrete mechanics based on finite element methods.

We regard \( t_k \) as variables and calculate the variation of the discrete action \([2.1]\) as follows

\[
\delta \mathcal{S}(t_0, q_0, \cdots, t_N, q_N) \cdot (\delta t_0, \delta q_0, \cdots, \delta t_N, \delta q_N)
\]

\[
= \frac{d}{d\epsilon} \mathcal{S}(t_0 + \epsilon \delta t_0, q_0 + \epsilon \delta q_0, \cdots, t_N + \epsilon \delta t_N, q_N + \epsilon \delta q_N)
\]

\[
= \sum_{k=1}^{N-1} \left[ D_2 L(w_k)(t_{k+1} - t_k) + D_4 L(w_{k-1})(t_k - t_{k-1}) \right] \delta q_k
\]

\[
+ \sum_{k=1}^{N-1} \left[ D_1 L(w_k)(t_{k+1} - t_k) + D_3 L(w_{k-1})(t_k - t_{k-1}) + L(w_{k-1}) - L(w_k) \right] \delta t_k
\]

\[
+ D_2 L(w_0)(t_1 - t_0) \delta q_0 + D_4 L(w_{N-1})(t_N - t_{N-1}) \delta q_N
\]

\[
+ [D_1 L(w_0)](t_1 - t_0) \delta t_0
\]

\[
+ [D_3 L(w_{N-1})](t_N - t_{N-1}) + L(w_{N-1})] \delta t_N,
\]

(3.1)

where \( w_k = (t_k, q_k, t_{k+1}, q_{k+1}) \), \( k = 0, 1, \cdots, N - 1 \). From (3.1), we see that the variation \( \delta q_k \) yields the discrete Euler-Lagrange equation

\[
D_2 L(w_k)(t_{k+1} - t_k) + D_4 L(w_{k-1})(t_k - t_{k-1}) = 0
\]

(3.2)

and the variation \( \delta t_k \) yields the discrete energy evolution equation

\[
D_1 L(w_k)(t_{k+1} - t_k) + D_3 L(w_{k-1})(t_k - t_{k-1}) + L(w_{k-1}) - L(w_k) = 0,
\]

(3.3)

which is a discrete version of \([1.13]\). For a conservative \( L \), (3.3) becomes the discrete energy conservation law.

From the boundary terms in (3.1), we can define two one forms

\[
\theta^-_L(w_k) = (D_1 L(w_k)(t_{k+1} - t_k) - L(w_k)) dt_k + D_2 L(w_k)(t_{k+1} - t_k) dq_k,
\]

(3.4)

and

\[
\theta^+_L(w_k) = (D_3 L(w_k)(t_{k+1} - t_k) - L(w_k)) dt_{k+1} + D_4 L(w_k)(t_{k+1} - t_k) dq_{k+1}.
\]

(3.5)

These two one forms are the discrete version of the extended Lagrange form \([1.12]\).

Unlike the continuous case, the solution of (3.3) does not satisfy (3.3) in general. Therefore, we must solve (3.2) and (3.3) simultaneously. Using the same method in §2, we can show that the coupled integrator

\[
D_2 L(w_k)(t_{k+1} - t_k) + D_4 L(w_{k-1})(t_k - t_{k-1}) = 0,
\]

\[
D_1 L(w_k)(t_{k+1} - t_k) + D_3 L(w_{k-1})(t_k - t_{k-1}) + L(w_{k-1}) - L(w_k) = 0
\]

(3.6)

preserves the extended Lagrange two form \( \omega^-_L = d\theta^+_L \).

For the discrete Lagrangian \([2.23], [3.6]\) becomes

\[
\frac{q_{k+1} - q_k}{t_{k+1} - t_k} - \frac{q_k - q_{k-1}}{t_k - t_{k-1}} + \frac{\partial F(w_k)}{\partial q_k} h_k + \frac{\partial F(w_{k-1})}{\partial q_k} h_{k-1} = 0,
\]

\[
\frac{1}{2} \left( \frac{q_{k+1} - q_k}{t_{k+1} - t_k} \right)^2 + F(w_k) - \frac{\partial F(w_k)}{\partial t_k} h_k = \frac{1}{2} \left( \frac{q_k - q_{k-1}}{t_k - t_{k-1}} \right)^2 + F(w_{k-1}) + \frac{\partial F(w_{k-1})}{\partial t_k} h_{k-1}.
\]

For the kind of high order discrete Lagrangian, we can obtain similar formulas.
4 Conclusions

In this paper, we have presented the discrete mechanics based on finite element methods. The finite element methods provide a natural way to obtain a kind of discrete Lagrangian. Using piecewise quadratic functions, we have constructed a high order discrete Lagrangian and derived the corresponding variational integrator (the discrete Euler-Lagrange equation). The symplecticity of the high order variational integrator has also been proved.

The time steps can play the role of parameters or the role of variables. We can obtain discrete energy conservation law when the time steps are regarded as variables.

Finite element methods are well-established in numerical mathematics. Many results of finite element methods can be applied to the discrete mechanics presented in this paper such as convergence theory, error estimates as well as the solving method of the variational integrators.

Recently, it has been proved \cite{6} that the symplectic structure preserves not only on the phase flow but also on the flows with respect to symplectic vector fields as long as certain cohomological condition is satisfied in both continuous and discrete cases. This should be able to extend to the cases in this paper. We will study this issue elsewhere.

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