Total Variation in Hamiltonian Formalism and Symplectic-Energy integrators

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Abstract

We present a discrete total variation calculus in Hamiltonian formalism in this paper. Using this discrete variation calculus and generating functions for the flows of Hamiltonian systems, we derive two-step symplectic-energy integrators of any finite order for Hamiltonian systems from a variational perspective. The relationship between symplectic integrators derived directly from the Hamiltonian systems and the variationally derived symplectic-energy integrators is explored.

Keywords. Total variation, Hamiltonian formalism, Symplectic-energy integrators

1 Introduction

We begin by recalling the ordinary variational principle in Hamiltonian formalism. Suppose Q denotes the configuration space with coordinates q^i, and T^*Q the phase space with coordinates (q^i, p^i), $i = 1, 2, \cdots, n$. Consider a Hamiltonian $H: T^*Q \to \mathbb{R}$. The corresponding action functional is defined by

$$S((q^i(t), p^i(t))) = \int_a^b (p^i \dot{q}^i - H(q^i, p^i))\, dt, \tag{1.1}$$

where $(q^i(t), p^i(t))$ is a C^2 curve in phase space T^*Q.

The variational principle in Hamiltonian formalism seeks the curves $(q^i(t), p^i(t))$ for which the action functional S is stationary under variations of $(q^i(t), p^i(t))$ with fixed endpoints. We first define the variation of $(q^i(t), p^i(t))$.

Let

$$V = \sum_{i=1}^n \phi^i(\boldsymbol{q}, \boldsymbol{p}) \frac{\partial}{\partial q^i} + \sum_{i=1}^n \psi^i(\boldsymbol{q}, \boldsymbol{p}) \frac{\partial}{\partial p^i} \tag{1.2}$$

be a vector field on T^*Q. Here $\boldsymbol{q} = (q^1, \cdots, q^n)$, $\boldsymbol{p} = (p^1, \cdots, p^n)$. For simplicity, we will omit the summation notation $\sum$ in the following.

Denote the flow of V by F^ϵ: $F^\epsilon(\boldsymbol{q}, \boldsymbol{p}) = (\tilde{\boldsymbol{q}}, \tilde{\boldsymbol{p}})$, which is written in components as

$$\tilde{q}^i = f^i(\epsilon, \boldsymbol{q}, \boldsymbol{p}), \tag{1.3}$$
$$\tilde{p}^i = g^i(\epsilon, \boldsymbol{q}, \boldsymbol{p}), \tag{1.4}$$

where $(\boldsymbol{q}, \boldsymbol{p}) \in T^*Q$ and

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} f^i(\epsilon, \boldsymbol{q}, \boldsymbol{p}) = \phi^i(\boldsymbol{q}, \boldsymbol{p}).$$
$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} g^i(\epsilon, \boldsymbol{q}, \boldsymbol{p}) = \psi^i(\boldsymbol{q}, \boldsymbol{p}).$$

Let $(q^i(t), p^i(t))$ be a curve in T^*Q. The transformations (1.3-1.4) transform $(q^i(t), p^i(t))$ into a family of curves

$$(\tilde{q}^i(t), \tilde{p}^i(t)) = (f^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t)), g^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t))).$$

Now we are ready to define the variation of $(q(t), p(t))$:

$$\delta(q^i(t), p^i(t)) =: \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} (\tilde{q}^i(t), \tilde{p}^i(t)) = (\phi^i(\boldsymbol{q}, \boldsymbol{p}), \psi^i(\boldsymbol{q}, \boldsymbol{p})). \tag{1.5}$$

Next, we calculate the variation of S at $(q^i(t), p^i(t))$

$$\begin{aligned}
\delta S &= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} S((\tilde{q}^i(t), \tilde{p}^i(t))) \\
&= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} S((f^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t)), g^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t)))) \\
&= \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \int_a^b (g^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t)) \frac{d}{dt} f^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t)) - H(f^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t)), g^i(\epsilon, \boldsymbol{q}(t), \boldsymbol{p}(t))))dt \\
&= \int_a^b \left[\left(\dot{q}^i - \frac{\partial H}{\partial p^i} \right) \psi^i + \left(-\dot{p}^i - \frac{\partial H}{\partial q^i} \right) \phi^i \right] dt + p^i \phi^i \Big|_a^b.
\end{aligned} \tag{1.6}$$

If $\phi^i(\boldsymbol{q}(a), \boldsymbol{p}(a)) = \phi^i(\boldsymbol{q}(b), \boldsymbol{p}(b)) = 0$, the requirement of $\delta S = 0$ yields the Hamilton equation for $(q^i(t), p^i(t))$

$$\begin{aligned}
\dot{q}^i &= \frac{\partial H}{\partial p^i}, \\
\dot{p}^i &= -\frac{\partial H}{\partial q^i}.
\end{aligned} \tag{1.7}$$

If we drop the requirement of $\phi^i(\boldsymbol{q}(a), \boldsymbol{p}(a)) = \phi^i(\boldsymbol{q}(b), \boldsymbol{p}(b)) = 0$, we can naturally obtain the canonical one form on T^*Q from the second term in (1.6). $\theta = p^i dq^i$. Furthermore, restricting $(\tilde{q}^i(t), \tilde{p}^i(t))$ to the solution space of (1.7), we can prove the solution of (1.7) preserves the canonical two form $\omega = d\theta_L = dp^i \wedge dq^i$.

On the other hand, it is not necessary to restrict $(\tilde{q}^i(t), \tilde{p}^i(t))$ to the solution space of (1.7). Introducing the Euler-Lagrange one-form

$$E(q^i, p^i) = \left(\dot{q} - \frac{\partial H}{\partial p} \right) dp^i + \left(-\dot{p} - \frac{\partial H}{\partial q} \right) dq^i, \tag{1.8}$$

the nilpotency of d leads to

$$dE(q^i, p^i) + \frac{d}{dt}\omega = 0. \tag{1.9}$$

Namely, the necessary and sufficient condition for symplectic structure preserving is that the Euler-Lagrange one form (1.8) is closed [8, 9, 10].

Based on the above variational principle in Hamiltonian formalism and using the ideas of discrete Lagrange mechanics [15, 16, 19, 20, 21], we can develop a natural version of discrete Hamiltonian mechanics with fixed time steps and drive symplectic integrators for Hamilton canonical equations from a variational perspective [10].

However the symplectic integrators obtained in this way are not energy-preserving in general because of its fixed time steps [7, 18]. An energy-preserving symplectic integrator is a more preferable and natural candidate of approximations for conservative Hamilton equations since the solution of conservative Hamilton equations is not only symplectic but also energy-preserving. To attain this goal, we use variable time steps and a discrete total variation calculus developed in [11, 12, 13, 14, 4]. The basic idea is to construct a discrete action functional and then to apply a discrete total variation calculus. In this way, we can derive symplectic integrators and their associated energy conservation laws. These variationaly derived symplectic integrators are two-step integrators. If we take fixed time steps, the resulting integrators are equivalent to the symplectic integrators derived directly from the Hamiltonian systems in some special cases.

An outline of this paper is as follows. In Section 2, we present total variation for continuous variational principle in Hamiltonian formalism. Section 3 is devoted to deriving symplectic-energy integrators. In Section 4, using generating function methods, we obtain high order symplectic-energy integrators. We finish this paper by making some conclusions and comments in Section 5.

2 Total variation in Hamiltonian formalism

In order to discuss total variation in Hamiltonian formalism, we will work with extended phase space $\mathbb{R} \times T^*Q$ with coordinates (t, q^i, p^i) [1]. Here $t \in \mathbb{R}$ denotes time. By total variation, we refer to variations of both (q^i, p^i) and t. Consider a vector field on $\mathbb{R} \times T^*Q$

$$V = \xi(t, \boldsymbol{q}, \boldsymbol{p})\frac{\partial}{\partial t} + \phi^i(t, \boldsymbol{q}, \boldsymbol{p})\frac{\partial}{\partial q^i} + \psi^i(t, \boldsymbol{q}, \boldsymbol{p})\frac{\partial}{\partial p^i}. \tag{2.1}$$

Let F^ϵ be the flow of V. For $(t, q^i, p^i) \in \mathbb{R} \times T^*Q$, we have $F^\epsilon(t, q^i, p^i) = (\tilde{t}, \tilde{q}^i, \tilde{p}^i)$, which can be written as

$$\tilde{t} = h(\epsilon, t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.2}$$
$$\tilde{q}^i = f^i(\epsilon, t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.3}$$
$$\tilde{p}^i = g^i(\epsilon, t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.4}$$

where

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} h(\epsilon, t, \boldsymbol{q}, \boldsymbol{p}) = \xi(t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.5}$$
$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} f^i(\epsilon, t, \boldsymbol{q}, \boldsymbol{p}) = \phi^i(t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.6}$$
$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} g^i(\epsilon, t, \boldsymbol{q}, \boldsymbol{p}) = \psi^i(t, \boldsymbol{q}, \boldsymbol{p}). \tag{2.7}$$

The transformation (2.5-2.7) transforms a curve $(q^i(t), p^i(t))$ into a family of curves $(\tilde{q}^i(\epsilon, \tilde{t}), \tilde{p}^i(\epsilon, \tilde{t}))$ determined by

$$\tilde{t} = h(\epsilon, t, \boldsymbol{q}(t), \boldsymbol{p}(t)), \tag{2.8}$$
$$\tilde{q}^i = f^i(\epsilon, t, \boldsymbol{q}(t), \boldsymbol{p}(t)). \tag{2.9}$$
$$\tilde{p}^i = g^i(\epsilon, t, \boldsymbol{q}(t), \boldsymbol{p}(t)). \tag{2.10}$$

Suppose we can solve (2.8) for t: $t = h^{-1}(\epsilon, \tilde{t})$. Then we have

$$\tilde{q}^i(\epsilon, \tilde{t}) = f^i(\epsilon, h^{-1}(\epsilon, \tilde{t}), \boldsymbol{q}(h^{-1}(\epsilon, \tilde{t})), \boldsymbol{p}(h^{-1}(\epsilon, \tilde{t}))). \tag{2.11}$$

$$\tilde{p}^i(\epsilon, \tilde{t}) = g^i(\epsilon, h^{-1}(\epsilon, \tilde{t}), \boldsymbol{q}(h^{-1}(\epsilon, \tilde{t})), \boldsymbol{p}(h^{-1}(\epsilon, \tilde{t}))). \tag{2.12}$$

Before calculating the variation of S directly, we first consider the first order prolongation of V

$$\begin{aligned} \mathrm{pr}^1 V =& \xi(t, \boldsymbol{q}, \boldsymbol{p}) \frac{\partial}{\partial t} + \phi^i(t, \boldsymbol{q}, \boldsymbol{p}) \frac{\partial}{\partial q^i} + \psi^i(t, \boldsymbol{q}, \boldsymbol{p}) \frac{\partial}{\partial p^i} \\ &+ \alpha^i(t, \boldsymbol{q}, \dot{\boldsymbol{q}}, \dot{\boldsymbol{p}}) \frac{\partial}{\partial \dot{q}^i} + \beta^i(t, \boldsymbol{q}, \dot{\boldsymbol{q}}, \dot{\boldsymbol{p}}) \frac{\partial}{\partial \dot{p}^i}, \end{aligned} \tag{2.13}$$

where $\mathrm{pr}^1 V$ denote the first order prolongation of V and

$$\alpha^i(t, \boldsymbol{q}, \dot{\boldsymbol{q}}, \dot{\boldsymbol{p}}) = D_t \phi^i(t, \boldsymbol{q}, \boldsymbol{p}) - \dot{q}^i D_t \xi(t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.14}$$

$$\beta^i(t, \boldsymbol{q}, \dot{\boldsymbol{q}}, \dot{\boldsymbol{p}}) = D_t \psi^i(t, \boldsymbol{q}, \boldsymbol{p}) - \dot{p}^i D_t \xi(t, \boldsymbol{q}, \boldsymbol{p}), \tag{2.15}$$

where D_t denotes the total derivative. For example

$$D_t \phi^i(t, \boldsymbol{q}, \boldsymbol{p}) = \phi^i_t + \phi^i_{\boldsymbol{q}} \dot{\boldsymbol{q}} + \phi^i_{\boldsymbol{p}} \dot{\boldsymbol{p}}.$$

For prolongation of vector field and the formula (2.14-2.15), we refer the reader to [17].

Now we calculate the variation of S directly

$$\begin{aligned} \delta S =& \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} S((\tilde{q}^i(\epsilon, \tilde{t}), \tilde{p}^i(\epsilon, \tilde{t})) \\ =& \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \int_{\tilde{a}}^{\tilde{b}} \left(\tilde{p}^i(\epsilon, \tilde{t})) \frac{d}{d\tilde{t}} \tilde{q}^i(\epsilon, \tilde{t}) - H(\tilde{q}^i(\epsilon, \tilde{t}), \tilde{p}^i(\epsilon, \tilde{t})) \right) d\tilde{t} \\ =& \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \int_a^b \left(\tilde{p}^i(\epsilon, \tilde{t})) \frac{d}{d\tilde{t}} \tilde{q}^i(\epsilon, \tilde{t}) - H(\tilde{q}^i(\epsilon, \tilde{t}), \tilde{p}^i(\epsilon, \tilde{t})) \right) \frac{d\tilde{t}}{dt} dt \qquad (\tilde{t} = h(\epsilon, t, \boldsymbol{q}(t), \boldsymbol{p}(t))) \\ =& \int_a^b \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \left(\tilde{p}^i(\epsilon, \tilde{t})) \frac{d}{d\tilde{t}} \tilde{q}^i(\epsilon, \tilde{t}) - H(\tilde{q}^i(\epsilon, \tilde{t}), \tilde{p}^i(\epsilon, \tilde{t}) \right) dt \\ &+ \int_a^b \left(p^i(t) \dot{q}^i(t) - H(q^i(t), p^i(t)) \right) D_t \xi dt \qquad (2.16) \\ =& \int_a^b \left[\left(\frac{d}{dt} H(q^i(t), p^i(t)) \right) \xi + \left(-\dot{p}^i - \frac{\partial H}{\partial q^i} \right) \phi^i + \left(\dot{q}^i - \frac{\partial H}{\partial p^i} \right) \psi^i \right] dt \\ &+ \left[p^i \phi^i - H(q^i, p^i)) \xi \right] \Big|_a^b . \qquad (2.17) \end{aligned}$$

Here in (2.16), we used (2.5) and the fact

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \frac{d\tilde{t}}{dt} = \frac{d}{dt} \left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \tilde{t} = D_t \xi.$$

In (2.17), we used the prolongation formula (2.14).

If $\xi(a, \boldsymbol{q}(a), \boldsymbol{p}(a)) = \xi(b, \boldsymbol{q}(b), \boldsymbol{p}(a)) = 0$ and $\phi^i(a, \boldsymbol{q}(a), \boldsymbol{p}(a)) = \phi^i(b, \boldsymbol{q}(b), \boldsymbol{p}(b)) = 0$, the requirement of $\delta S = 0$ yields the Hamilton canonical equation

$$\begin{aligned} \dot{q}^i &= \frac{\partial H}{\partial p^i}, \\ \dot{p}^i &= -\frac{\partial H}{\partial q^i}, \end{aligned} \tag{2.18}$$

from the variation ϕ^i, ψ^i and the energy conservation law

$$\frac{d}{dt}H(q^i, p^i) = 0 \tag{2.19}$$

from the variation ξ.

Since

$$\frac{d}{dt}H(q^i, p^i) = \frac{\partial H}{\partial q^i}\dot{q}^i + \frac{\partial H}{\partial p^i}\dot{p}^i,$$

we can easily see that the energy conservation law (2.19) is a natural consequence of the Hamilton canonical equations (2.18).

If we drop the requirement

$$\begin{aligned}
&\xi(a, \boldsymbol{q}(a), \boldsymbol{p}(a)) = \xi(b, \boldsymbol{q}(b), \boldsymbol{p}(b)) = 0, \\
&\phi^i(a, \boldsymbol{q}(a), \boldsymbol{p}(a)) = \phi^i(b, \boldsymbol{q}(b), \boldsymbol{p}(b)) = 0,
\end{aligned}$$

we can define the extended canonical one form on $\mathbb{R} \times T^*Q$ from the second term in (2.17)

$$\theta = p^i dq^i - H(q^i, p^i)dt. \tag{2.20}$$

Furthermore, restricting $(\tilde{q}^i(t), \tilde{p}^i(t))$ to the solution space of (2.18), we can prove the solution of (2.18) preserves the extended canonical two form

$$\omega = d\theta = dp^i \wedge dq^i - dH(q^i, p^i) \wedge dt, \tag{2.21}$$

by using the same method in [15].

Remark: The vector field (2.1) can be decomposed along $(q^i(t), p^i(t))$ into vertical and horizontal components. The vertical component is

$$(\phi^i - \xi\dot{q}^i)\frac{\partial}{\partial q^i} + (\psi^i - \xi\dot{p}^i)\frac{\partial}{\partial p^i}$$

and the horizontal component is

$$\xi\frac{\partial}{\partial t} + \xi\dot{q}^i\frac{\partial}{\partial q^i} + \xi\dot{p}^i\frac{\partial}{\partial p^i}.$$

Then analogous to the Lagrangian formalism in [4], the total variation gives rise to the Hamilton equations along the vertical direction as well as a relation between the Hamilton equations and conservation law for the Hamiltonian along the horizontal direction (see also [15]).

3 A discrete total variation calculus in Hamiltonian formalism and symplectic-energy integrators

In this section, we develop a discrete version of total variation in Hamiltonian formalism. Using this discrete total variation calculus, we will derive symplectic-energy integrators.

Let

$$L(q^i, p^i, \dot{q}^i, \dot{p}^i) = p^i \dot{q}^i - H(q^i, p^i),$$

be a function from $\mathbb{R} \times T(T^*Q)$ to $\mathbb{R}$. Here L does not depend on t explicitly.

We use $P \times P$ for the discrete version of $\mathbb{R} \times T(T^*Q)$. Here P is the discrete version of $\mathbb{R} \times T^*Q$. A point $(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0; t_1, \boldsymbol{q}_1, \boldsymbol{p}_1) \in P \times P$ corresponds to a tangent vector $(\frac{\boldsymbol{q}_1 - \boldsymbol{q}_0}{t_1 - t_0}, \frac{\boldsymbol{p}_1 - \boldsymbol{p}_0}{t_1 - t_0})$. For simplicity, the vector symbols $\boldsymbol{q} = (q^1, \cdots, q^n)$ and $\boldsymbol{p} = (p^1, \cdots, p^n)$ are used throughout this section. A discrete L is defined to be $\mathbb{L} : P \times P \to \mathbb{R}$ and the corresponding action to be

$$\mathbb{S} = \sum_{k=0}^{N-1} \mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1})(t_{k+1} - t_k). \tag{3.1}$$

The discrete variational principle in total variation is to extremize $\mathbb{S}$ for variations of both $\boldsymbol{q}_k, \boldsymbol{p}_k$ and t_k holding the endpoints $(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0)$ and $(t_N, \boldsymbol{q}_N, \boldsymbol{p}_N)$ fixed. This discrete variational principle determines a discrete flow $\Phi : P \times P \to P \times P$ by

$$\Phi(t_{k-1}, \boldsymbol{q}_{k-1}, \boldsymbol{p}_{k-1}, t_k, \boldsymbol{q}_k, \boldsymbol{p}_k) = (t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}). \tag{3.2}$$

Here $(t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1})$ for all $k \in \{1, 2, \cdots, N-1\}$ are found from the following discrete Hamilton canonical equation and the discrete energy conservation law

$$\begin{aligned}
&(t_{k+1} - t_k) D_2 \mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) + (t_k - t_{k-1}) D_5 \mathbb{L}(t_{k-1}, \boldsymbol{q}_{k-1}, \boldsymbol{p}_{k-1}, t_k, \boldsymbol{q}_k, \boldsymbol{p}_k) = 0, \\
&(t_{k+1} - t_k) D_3 \mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) + (t_k - t_{k-1}) D_6 \mathbb{L}(t_{k-1}, \boldsymbol{q}_{k-1}, \boldsymbol{p}_{k-1}, t_k, \boldsymbol{q}_k, \boldsymbol{p}_k) = 0,
\end{aligned} \tag{3.3}$$

and

$$\begin{aligned}
&(t_{k+1} - t_k) D_1 \mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) + (t_k - t_{k-1}) D_4 \mathbb{L}(t_{k-1}, \boldsymbol{q}_{k-1}, \boldsymbol{p}_{k-1}, t_k, \boldsymbol{q}_k, \boldsymbol{p}_k) \\
&\quad - \mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) + \mathbb{L}(t_{k-1}, \boldsymbol{q}_{k-1}, \boldsymbol{p}_{k-1}, t_k, \boldsymbol{q}_k, \boldsymbol{p}_k) = 0.
\end{aligned} \tag{3.4}$$

Here D_i denotes the partial derivative of $\mathbb{L}$ with respect to the ith argument. The Eq. (3.3) is the discrete Hamilton canonical equation that is also called variational integrator. The Eq.(3.4) is the discrete energy conservation law associated to (3.3). Unlike the continuous case, the variational integrator (3.3) does not satisfy (3.4) in general. Therefore, we need to solve (3.3) and (3.4) simultaneously.

Now we prove that the discrete flow determined by (3.3) and (3.4) preserves a discrete version of the extended canonical two form $\boldsymbol{\omega}$ defined in (2.21). Therefore, we call (3.3)-(3.4) a symplectic-energy integrator. We do this directly from the variational point of view, consistent with the continuous case [15].

As in continuous case, we calculate $d\mathbb{S}$ for variations with varied endpoints.

$$
\begin{aligned}
&d\mathbb{S}(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0 \cdots, t_N, \boldsymbol{q}_N, \boldsymbol{p}_N) \cdot (\delta t_0, \delta\boldsymbol{q}_0, \delta\boldsymbol{p}_0 \cdots, \delta t_N, \delta\boldsymbol{q}_N, \delta\boldsymbol{p}_N) \\
&= \sum_{k=0}^{N-1} (D_2L(\boldsymbol{v}_k)\delta\boldsymbol{q}_k + D_5L(\boldsymbol{v}_k)\delta\boldsymbol{q}_{k+1} + D_3L(\boldsymbol{v}_k)\delta\boldsymbol{p}_k + D_6L(\boldsymbol{v}_k)\delta p_{k+1})(t_{k+1} - t_k) \\
&\quad + \sum_{k=0}^{N-1} (D_1L(\boldsymbol{v}_k)\delta t_k + D_4L(\boldsymbol{v}_k)\delta t_{k+1})(t_{k+1} - t_k) + \sum_{k=0}^{N-1} L(\boldsymbol{v}_k)(\delta t_{k+1} - \delta t_k) \\
&= \sum_{k=1}^{N-1} (D_2L(\boldsymbol{v}_k)(t_{k+1} - t_k) + D_5L(\boldsymbol{v}_{k-1})(t_k - t_{k-1}))\delta\boldsymbol{q}_k \\
&\quad + \sum_{k=1}^{N-1} (D_3L(\boldsymbol{v}_k)(t_{k+1} - t_k) + D_6L(\boldsymbol{v}_{k-1})(t_k - t_{k-1}))\delta\boldsymbol{p}_k \\
&\quad + \sum_{k=1}^{N-1} (D_1L(\boldsymbol{v}_k)(t_{k+1} - t_k) + D_4L(\boldsymbol{v}_{k-1})(t_k - t_{k-1}) + L(\boldsymbol{v}_{k-1}) - L(\boldsymbol{v}_k))\delta t_k \\
&\quad + D_2L(\boldsymbol{v}_0)(t_1 - t_0)\delta\boldsymbol{q}_0 + D_3L(\boldsymbol{v}_0)(t_1 - t_0)\delta\boldsymbol{p}_0 + (D_1L(\boldsymbol{v}_0)(t_1 - t_0) - L(\boldsymbol{v}_0))\delta t_0 \\
&\quad + D_5L(\boldsymbol{v}_{N-1})(t_N - t_{N-1})\delta\boldsymbol{q}_N + D_6L(\boldsymbol{v}_{N-1})(t_N - t_{N-1})\delta\boldsymbol{p}_N \\
&\quad + (D_4L(\boldsymbol{v}_{N-1})(t_N - t_{N-1}) - L(\boldsymbol{v}_{N-1}))\delta t_N,
\end{aligned} \tag{3.5}
$$

where $\boldsymbol{v}_k = (t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}), \quad k = 0, 1, \cdots, N-1$. We can see that the last six terms in (3.5) come from the boundary variations. Based on the boundary variations, we can define two one forms on $P \times P$

$$
\begin{aligned}
\theta_{\mathbb{L}}^-(\boldsymbol{v}_k) &= D_2\mathbb{L}(\boldsymbol{v}_k)(t_{k+1} - t_k)d\boldsymbol{q}_k + D_3\mathbb{L}(\boldsymbol{v}_k)(t_{k+1} - t_k)d\boldsymbol{p}_k \\
&\quad + (D_1\mathbb{L}(\boldsymbol{v}_k)(t_{k+1} - t_k) - \mathbb{L}(\boldsymbol{v}_k))dt_k
\end{aligned} \tag{3.6}
$$

and

$$
\begin{aligned}
\theta_{\mathbb{L}}^+(\boldsymbol{v}_k) &= D_5\mathbb{L}(\boldsymbol{v}_k)(t_{k+1} - t_k)d\boldsymbol{q}_{k+1} + D_6\mathbb{L}(\boldsymbol{v}_k)(t_{k+1} - t_k)d\boldsymbol{p}_{k+1} \\
&\quad + (D_4\mathbb{L}(\boldsymbol{v}_k)(t_{k+1} - t_k) - \mathbb{L}(\boldsymbol{v}_k))dt_{k+1}
\end{aligned} \tag{3.7}
$$

Here we have used the notation in [15]. We regard the pair $(\theta_{\mathbb{L}}^-, \theta_{\mathbb{L}}^+)$ as being the discrete version of the extended canonical one form $\boldsymbol{\theta}$ defined in (2.20).

Now we parameterize the solutions of the discrete variational principle by (t_0, q_0, t_1, q_1), and restrict $\mathbb{S}$ to that solution space. Then Eq. (3.5) becomes

$$
\begin{aligned}
&d\mathbb{S}(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0, \cdots, t_N, \boldsymbol{q}_N, \boldsymbol{p}_N) \cdot (\delta t_0, \delta\boldsymbol{q}_0, \delta\boldsymbol{p}_0 \cdots, \delta t_N, \delta q_N, \delta\boldsymbol{p}_N) \\
&= \theta_{\mathbb{L}}^-(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0, t_1, \boldsymbol{q}_1, \boldsymbol{p}_1) \cdot (\delta t_0, \delta\boldsymbol{q}_0, \delta\boldsymbol{p}_0, \delta t_1, \delta\boldsymbol{q}_1, \delta\boldsymbol{p}_1) \\
&\quad + \theta_{\mathbb{L}}^+(t_{N-1}, \boldsymbol{q}_{N-1}, \boldsymbol{p}_{N-1}, t_N, \boldsymbol{q}_N, \boldsymbol{p}_N) \cdot (\delta t_{N-1}, \delta\boldsymbol{q}_{N-1}, \delta\boldsymbol{p}_{N-1}, \delta t_N, \delta\boldsymbol{q}_N, \delta\boldsymbol{p}_N,) \\
&= \theta_{\mathbb{L}}^-(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0, t_1, \boldsymbol{q}_1, \boldsymbol{p}_1) \cdot (\delta t_0, \delta\boldsymbol{q}_0, \delta\boldsymbol{p}_0, \delta t_1, \delta\boldsymbol{q}_1, \delta\boldsymbol{p}_1) \\
&\quad + (\Phi^{N-1})^*\theta_{\mathbb{L}}^+(t_0, \boldsymbol{q}_0, \boldsymbol{p}_0, t_1, \boldsymbol{q}_1, \boldsymbol{p}_1) \cdot (\delta t_0, \delta\boldsymbol{q}_0, \delta\boldsymbol{p}_0, \delta t_1, \delta\boldsymbol{q}_1, \delta\boldsymbol{p}_1).
\end{aligned} \tag{3.8}
$$

From (3.8), we can obtain

$$
d\mathbb{S} = \theta_{\mathbb{L}}^- + (\Phi^{N-1})^*\theta_{\mathbb{L}}^+. \tag{3.9}
$$

The Eq. (3.9) holds for arbitrary $N > 1$. Taking N=2 leads to

$$
d\mathbb{S} = \theta_{\mathbb{L}}^- + \Phi^*\theta_{\mathbb{L}}^+. \tag{3.10}
$$

Taking exterior differentiation of (3.10) reveals that

$$\Phi^*(d\theta_{\mathbb{L}}^+) = -d\theta_{\mathbb{L}}^-. \tag{3.11}$$

From the definition of $\theta_{\mathbb{L}}^-$ and $\theta_{\mathbb{L}}^+$, we know that

$$\theta_{\mathbb{L}}^- + \theta_{\mathbb{L}}^+ = d\mathbb{L}. \tag{3.12}$$

Taking exterior differentiation of (3.12), we obtain $d\theta_{\mathbb{L}}^+ = -d\theta_{\mathbb{L}}^-$. Define

$$\omega_{\mathbb{L}} \equiv d\theta_{\mathbb{L}}^+ = \, - \, d\theta_{\mathbb{L}}^-. \tag{3.13}$$

Finally, we have shown that the discrete flow Φ preserves the discrete extended canonical two form $\omega_{\mathbb{L}}$.

$$\Phi^*(\omega_{\mathbb{L}}) = \omega_{\mathbb{L}}. \tag{3.14}$$

Thus we may call the coupled difference system (3.3)-(3.4) symplectic-energy integrator in the sense that it satisfies the discrete energy conservation law (3.4) and preserves the discrete extended canonical two form $\omega_{\mathbb{L}}$.

To illustrate the above discrete total variation calculus, we now present an example. We choose $\mathbb{L}$ in (3.1) as

$$\mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) = \boldsymbol{p}_{k+\frac{1}{2}} \frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_k}{t_{k+1} - t_k} - H(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}), \tag{3.15}$$

where $\boldsymbol{p}_{k+\frac{1}{2}} = \frac{\boldsymbol{p}_k + \boldsymbol{p}_{k+1}}{2}$, $\boldsymbol{q}_{k+\frac{1}{2}} = \frac{\boldsymbol{q}_k + \boldsymbol{q}_{k+1}}{2}$.

Using (3.3), we can obtain the corresponding discrete Hamilton equation

$$\begin{aligned}
&\frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_{k-1}}{2} - \frac{1}{2}\left((t_{k+1} - t_k) \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) + (t_k - t_{k-1}) \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}) \right) = 0, \\
&\frac{\boldsymbol{p}_{k+1} - \boldsymbol{p}_{k-1}}{2} + \frac{1}{2}\left((t_{k+1} - t_k) \frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) + (t_k - t_{k-1}) \frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}) \right) = 0,
\end{aligned} \tag{3.16}$$

where $\boldsymbol{p}_{k-\frac{1}{2}} = \frac{\boldsymbol{p}_k + \boldsymbol{p}_{k-1}}{2}$, $\boldsymbol{q}_{k-\frac{1}{2}} = \frac{\boldsymbol{q}_k + \boldsymbol{q}_{k-1}}{2}$. Using (3.4), we can obtain the corresponding discrete energy conservation law

$$H(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) = H(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}). \tag{3.17}$$

The symplectic-energy integrator (3.16)-(3.17) preserves the discrete two form $d\theta_{\mathbb{L}}^+ = -d\theta_{\mathbb{L}}^-$:

$$\frac{1}{2}(d\boldsymbol{p}_k \wedge d\boldsymbol{q}_{k+1} + d\boldsymbol{p}_{k+1} \wedge d\boldsymbol{q}_k) - H(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) \wedge \left(\frac{dt_k + dt_{k+1}}{2} \right). \tag{3.18}$$

If we take fixed time steps $t_{k+1} - t_k = h$ (h is a constant), then (3.16) becomes

$$\begin{aligned}
\frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_{k-1}}{2h} &= \frac{1}{2}\left(\frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) + \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}) \right), \\
\frac{\boldsymbol{p}_{k+1} - \boldsymbol{p}_{k-1}}{2h} &= -\frac{1}{2}\left(\frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) + \frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}) \right).
\end{aligned} \tag{3.19}$$

Now we explore the relationship between (3.19) and the mid-point integrator for the Hamiltonian system

$$\begin{aligned} \dot{\boldsymbol{q}} &= \frac{\partial H}{\partial \boldsymbol{p}}, \\ \dot{\boldsymbol{p}} &= -\frac{\partial H}{\partial \boldsymbol{q}}. \end{aligned} \tag{3.20}$$

The mid-point symplectic integrator for (3.20) is

$$\begin{aligned} \frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_k}{h} &= \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}), \\ \frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_k}{h} &= -\frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}). \end{aligned} \tag{3.21}$$

In (3.21), we replace k by $k-1$ and obtain

$$\begin{aligned} \frac{\boldsymbol{q}_k - \boldsymbol{q}_{k-1}}{h} &= \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}), \\ \frac{\boldsymbol{p}_k - \boldsymbol{p}_{k-1}}{h} &= -\frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}}). \end{aligned} \tag{3.22}$$

Adding (3.22) to (3.21) results in (3.19). Therefore, if we use (3.21) to obtain $\boldsymbol{p}_k, \boldsymbol{q}_k$, the two-step integrator (3.19) is equivalent to the mid-point integrator (3.21). However, the equivalence does not hold in general. For example, choose $\mathbb{L}$ in (3.1) as

$$\mathbb{L}(t_k, \boldsymbol{q}_k, \boldsymbol{p}_k, t_{k+1}, \boldsymbol{q}_{k+1}, \boldsymbol{p}_{k+1}) = \boldsymbol{p}_k \frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_k}{t_{k+1} - t_k} - H(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}), \tag{3.23}$$

and take fixed time steps $t_{k+1} - t_k = h$. Then (3.3) becomes

$$\begin{aligned} \frac{\boldsymbol{q}_{k+1} - \boldsymbol{q}_k}{h} &= \frac{1}{2}\left(\frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) + \frac{\partial H}{\partial \boldsymbol{p}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}})\right), \\ \frac{\boldsymbol{p}_k - \boldsymbol{p}_{k-1}}{h} &= -\frac{1}{2}\left(\frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k+\frac{1}{2}}, \boldsymbol{p}_{k+\frac{1}{2}}) + \frac{\partial H}{\partial \boldsymbol{q}}(\boldsymbol{q}_{k-\frac{1}{2}}, \boldsymbol{p}_{k-\frac{1}{2}})\right). \end{aligned} \tag{3.24}$$

The integrator (3.24) is a two-step integrator which preserves the two form $dp_k \wedge dq_{k+1}$. In this case, we cannot find one-step integrator that is equivalent to (3.24).

In conclusion, using discrete total variation calculus, we derive two-step symplectic-energy integrators. When taking fixed time steps, some of them are equivalent to one-step integrator derived directly from the Hamiltonian system while the others do not have this equivalence.

4 High order symplectic-energy integrators by generating functions

In this section, we develop high order symplectic-energy integrators by using the generating function of the flow of the Hamiltonian system

$$\dot{\boldsymbol{z}} = J \bigtriangledown H(\boldsymbol{z}), \tag{4.1}$$

where $\boldsymbol{z} = (\boldsymbol{p}, \boldsymbol{q})^T, J = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$.

We first recall the generating function with normal Darboux matrix of a symplectic transformation . For details, see [5, 6].

Suppose α is a $4n \times 4n$ nonsingular matrix with the form

$$\alpha = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

where A, B, C and D are both $2n \times 2n$ matrices.

We denote the inverse of α by

$$\alpha^{-1} = \begin{pmatrix} A_1 & B_1 \\ C_1 & D_1 \end{pmatrix},$$

where A_1, B_1, C_1 and D_1 are both $2n \times 2n$ matrices.

We call a $4n \times 4n$ matrix α *a Darboux matrix* if

$$\alpha^T J_{4n} \alpha = \tilde{J}_{4n}, \tag{4.2}$$

where

$$J_{4n} = \begin{pmatrix} 0 & -I_{2n} \\ I_{2n} & 0 \end{pmatrix}, \ \tilde{J}_{4n} = \begin{pmatrix} J_{2n} & 0 \\ 0 & -J_{2n} \end{pmatrix}, \ J_{2n} = \begin{pmatrix} 0 & -I_n \\ I_n & 0 \end{pmatrix},$$

where I_n is an $n \times n$ identity matrix and I_{2n} is a $2n \times 2n$ identity matrix.

Every Darboux matrix induces a *fractional transform* between symplectic and symmetric matrices

$$\begin{aligned} \sigma_\alpha : \quad & Sp(2n) \to Sm(2n), \\ & \sigma_\alpha(S) = (AS + B)(CS + D)^{-1} = M, \quad \text{for} \quad S \in Sp(2n), \ \det(CS + D) \neq 0 \end{aligned}$$

with the inverse transform $\sigma_\alpha^{-1} = \sigma_{\alpha^{-1}}$

$$\begin{aligned} \sigma_\alpha^{-1} : \quad & Sm(2n) \to Sp(2n), \\ & \sigma_\alpha^{-1}(M) = (A_1 M + B_1)(C_1 M + D_1)^{-1} = S, \end{aligned}$$

where $Sp(2n)$ is the group of symplectic matrices and $Sm(2n)$ the set of symmetric matrices.

We can generalize the above discussions to generally nonlinear transformations on $\mathbb{R}^{2n}$. Denote $Spnl(2n)$ the set of symplectic transformations on $\mathbb{R}^{2n}$ and $Smnl(2n)$ the set of symmetric transformations, i.e. transformations with symmetric Jacobian, on $\mathbb{R}^{2n}$. Every $f \in Smnl(2n)$ corresponds, at least locally, to a real function ϕ (unique to a constant) such that f is the gradient of ϕ:

$$f(\boldsymbol{w}) = \triangledown \phi(\boldsymbol{w}), \tag{4.3}$$

where $\triangledown \phi(\boldsymbol{w}) = (\phi_{w_1}(\boldsymbol{w}), \cdots, \phi_{w_{2n}}(\boldsymbol{w}))$.

Then we have

$$\begin{aligned} \sigma_\alpha : \quad & Spnl(2n) \to Smnl(2n), \\ & \sigma_\alpha(g) = (A \circ g + B) \circ (C \circ g + D)^{-1} = \triangledown \phi, \end{aligned}$$

for $g \in Spnl(2n), \ \det(Cg_{\boldsymbol{z}} + D) \neq 0$, or alternatively

$$Ag(\boldsymbol{z}) + B\boldsymbol{z} = (\triangledown \phi)(Cg(\boldsymbol{z}) + D\boldsymbol{z}),$$

where $\circ$ denotes the composition of transformation and the $2n \times 2n$ constant matrices A, B, C and D are regarded as linear transformations. $g_{\boldsymbol{z}}$ denotes the Jacobian of the symplectic transformation g.

We call ϕ the *generating function* of Darboux type α for the symplectic transformation g.

Conversely, we have

$$\begin{aligned}
&\sigma_\alpha^{-1}: \quad Smnl(2n) \to Spnl(2n), \\
&\sigma_\alpha^{-1}(\triangledown \phi) = (A_1 \circ \triangledown \phi + B_1) \circ (C_1 \circ \triangledown \phi + D_1)^{-1} = g,
\end{aligned}$$

for $\det(C_1 \phi_{\boldsymbol{ww}}$

$$A_1 \triangledown \phi(\boldsymbol{w}) + B_1 \boldsymbol{w} = g(C_1 \triangledown \phi(\boldsymbol{w}) + D_1 \boldsymbol{w}),$$

where g is called the symplectic transformation of Darboux type α for the generating function ϕ.

For the study of integrators, we may restrict ourselves to the *normal Darboux matrices*, i.e., those satisfying $A + B = 0, C + D = I_{2n}$. The normal Darboux matrices can be characterized as

$$\alpha = \begin{pmatrix} J_{2n} & -J_{2n} \\ E & I_{2n} - E \end{pmatrix}, \quad E = \frac{1}{2}(I_{2n} + J_{2n} F), \quad F^T = F, \tag{4.4}$$

and

$$\alpha^{-1} = \begin{pmatrix} (E - I_{2n}) J_{2n} & I_{2n} \\ E J_{2n} & I_{2n} \end{pmatrix}. \tag{4.5}$$

The fractional transform induced by a normal Darboux matrix establishes a one-one correspondence between symplectic transformations near *identity* and symmetric transformations near *nullity*.

For simplicity, we take $F = 0$, then $E = \frac{1}{2} I_{2n}$ and

$$\alpha = \begin{pmatrix} J_{2n} & -J_{2n} \\ \frac{1}{2} I_{2n} & \frac{1}{2} I_{2n} \end{pmatrix}. \tag{4.6}$$

Now we consider the generating function of the flow of (4.1). Denote the flow of (4.1) by e_H^t. The generating function $\phi(\boldsymbol{w}, t)$ for the flow e_H^t of Darboux type (4.6) is give by

$$\triangledown \phi = (J_{2n} \circ e_H^t - J_{2n}) \circ \left(\frac{1}{2} e_H^t + \frac{1}{2} I_{2n} \right)^{-1}, \quad \text{for small} \quad |t|. \tag{4.7}$$

$\phi(\boldsymbol{w}, t)$ satisfies the Hamilton-Jacobi equation

$$\frac{\partial}{\partial t} \phi(\boldsymbol{w}, t) = -H \left(\boldsymbol{w} + \frac{1}{2} J_{2n} \triangledown \phi(\boldsymbol{w}, t) \right) \tag{4.8}$$

and can be expressed by Taylor series in t

$$\phi(\boldsymbol{w}, t) = \sum_{k=1}^{\infty} \phi^k(w) t^k, \quad \text{for small} \quad |t|. \tag{4.9}$$

The coefficients $\phi^k(w)$ can be determined recursively

$$\begin{aligned}
&\phi^1(\boldsymbol{w}) = -H(w), \\
&\phi^{k+1}(\boldsymbol{w}) = \frac{-1}{k+1}\sum_{m=1}^{k}\frac{1}{m!}\sum_{\substack{j_1+\cdots+j_m=k \\ j_l\geqslant 1}} D^m H\left(\frac{1}{2}J_{2n}\bigtriangledown\phi^{j_1},\cdots,\frac{1}{2}J_{2n}\bigtriangledown\phi^{j_m}\right),
\end{aligned} \tag{4.10}$$

where $k \geqslant 1$, and we use the notation of the $\boldsymbol{m}$-linear form

$$\begin{aligned}
&D^m H\left(\frac{1}{2}J_{2n}\bigtriangledown\phi^{j_1},\cdots,\frac{1}{2}J_{2n}\bigtriangledown\phi^{j_m}\right) \\
&\quad := \sum_{i_1,\cdots,i_m=1}^{2n} H_{\boldsymbol{z}_{i_1}\cdots\boldsymbol{z}_{i_m}}(\boldsymbol{w})\left(\frac{1}{2}J_{2n}\bigtriangledown\phi^{j_1}(\boldsymbol{w})\right)_{i_1}\cdots\left(\frac{1}{2}J_{2n}\bigtriangledown\phi^{j_m}(\boldsymbol{w})\right)_{i_m}.
\end{aligned}$$

From (4.7), we can see that the phase flow $\hat{\boldsymbol{z}} := e_H^t\boldsymbol{z}$ satisfies

$$J_{2n}(\hat{\boldsymbol{z}}-\boldsymbol{z}) = \bigtriangledown\phi\left(\frac{\hat{\boldsymbol{z}}-\boldsymbol{z}}{2}\right) = \sum_{j=1}^{\infty} t^j\bigtriangledown\phi^j\left(\frac{\hat{\boldsymbol{z}}+\boldsymbol{z}}{2}\right). \tag{4.11}$$

Now we choose $\mathbb{L}$ in (3.1) as

$$\mathbb{L}(t_k,\boldsymbol{q}_k,\boldsymbol{p}_k,t_{k+1},\boldsymbol{q}_{k+1},\boldsymbol{p}_{k+1}) = \boldsymbol{p}_{k+\frac{1}{2}}\frac{\boldsymbol{q}_{k+1}-\boldsymbol{q}_k}{t_{k+1}-t_k} - \psi^m(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}}), \tag{4.12}$$

where

$$\psi^m(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}}) = \sum_{j=1}^{m} t^j\phi^j(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}}). \tag{4.13}$$

The corresponding symplectic-energy integrator is

$$\begin{aligned}
&\frac{\boldsymbol{q}_{k+1}-\boldsymbol{q}_{k-1}}{2} - \frac{1}{2}\left((t_{k+1}-t_k)\frac{\partial\psi^m}{\partial\boldsymbol{p}}(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}}) + (t_k-t_{k-1})\frac{\partial\psi^m}{\partial\boldsymbol{p}}(\boldsymbol{q}_{k-\frac{1}{2}},\boldsymbol{p}_{k-\frac{1}{2}})\right) = 0, \\
&\frac{\boldsymbol{p}_{k+1}-\boldsymbol{p}_{k-1}}{2} + \frac{1}{2}\left((t_{k+1}-t_k)\frac{\partial\psi^m}{\partial\boldsymbol{q}}(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}}) + (t_k-t_{k-1})\frac{\partial\psi^m}{\partial\boldsymbol{q}}(\boldsymbol{q}_{k-\frac{1}{2}},\boldsymbol{p}_{k-\frac{1}{2}})\right) = 0, \\
&\psi^m(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}}) = \psi^m(\boldsymbol{q}_{k-\frac{1}{2}},\boldsymbol{p}_{k-\frac{1}{2}}),
\end{aligned} \tag{4.14}$$

which preserves the discrete extended canonical two form

$$\frac{1}{2}(d\boldsymbol{p}_k\wedge d\boldsymbol{q}_{k+1} + d\boldsymbol{p}_{k+1}\wedge d\boldsymbol{q}_k) - \psi^m(\boldsymbol{q}_{k+\frac{1}{2}},\boldsymbol{p}_{k+\frac{1}{2}})\wedge\left(\frac{dt_k+dt_{k+1}}{2}\right). \tag{4.15}$$

The integrator (4.14) is a two-step symplectic-energy integrator with $2m$th order of accuracy.

5 Concluding remarks

We have developed a discrete total variation calculus in Hamiltonian formalism in this paper. This calculus provides a new method for constructing structure-preserving integrators for Hamiltonian systems from a variational view of point. Using this calculus, we have derived discrete energy conservation laws associated to the integrators with variable time-steps. The coupled integrators are two-step integrators and preserve a discrete version of the extended canonical two form. If we take fixed time-steps, the resulting integrators are equivalent to the symplectic integrators derived directly from the Hamiltonian systems only in special cases. Thus, some new two-step symplectic integrators have variationally been obtained. Using generating function method, we have also obtained high order symplectic-energy integrators.

In principle, our discussions can be generalized to multisymplectic Hamiltonian system

$$M\boldsymbol{z}_t + K\boldsymbol{z}_x = \bigtriangledown_{\boldsymbol{z}} H(\boldsymbol{z}), \quad \boldsymbol{z} \in \mathbf{R}^n, \tag{5.1}$$

where M and K are skew-symmetric matrices on $\mathbf{R}^n, n \geq 3$ and $S : \mathbf{R}^n \to \mathbf{R}$ is a smooth function [2, 3]. We call the above system multi-symplectic Hamiltonian system, since it has a multi-symplectic conservation law

$$\frac{\partial}{\partial t}\omega + \frac{\partial}{\partial x}\kappa = 0, \tag{5.2}$$

where $\boldsymbol{\omega}$ and $\boldsymbol{\kappa}$ are the pre-symplectic forms

$$\omega = \frac{1}{2} d\boldsymbol{z} \wedge M d\boldsymbol{z}, \qquad \kappa = \frac{1}{2} d\boldsymbol{z} \wedge K d\boldsymbol{z}.$$

Constructing action functional

$$S = \int \left(\frac{1}{2} \boldsymbol{z}^T (M\boldsymbol{z}_t + K\boldsymbol{z}_x) - H(\boldsymbol{z}) \right) dx \wedge dt \tag{5.3}$$

and performing total variation on (5.3), we obtain the multisymplectic Hamiltonian system (5.1) as well as the corresponding local energy conservation law

$$\frac{\partial}{\partial t} \left(S(z) - \frac{1}{2} z^T K z_x \right) + \frac{\partial}{\partial x} \left(\frac{1}{2} z^T K z_t \right) = 0, \tag{5.4}$$

and the corresponding local momentum conservation law

$$\frac{\partial}{\partial t} \left(\frac{1}{2} z^T M z_x \right) + \frac{\partial}{\partial x} \left(S(z) - \frac{1}{2} z^T M z_t \right) = 0. \tag{5.5}$$

In the same way, we can develop a discrete total variation in multisymplectic formulation and obtain multisymplectic-energy-momentum integrators. We shall explore this issue elsewhere.

On the other hand, we may also get symplectic/multisymplectic-energy-momentum integrators by means of the difference variational principle [8], [10] in view of regarding difference with variable steps as an entire object. In this approach, the difference Legendre transformation may be introduced so as to the discrete total variations in Lagrangian and Hamiltonian formalism may be transformed to each other. We shall also explore this issue elsewhere.

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