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VARIATIONAL INTEGRATORS FOR HIGHER ORDER DIFFERENTIAL EQUATIONS*[1)]

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Abstract

We analyze three one parameter families of approximations and show that they are symplectic in Lagrangian sence and can be related to symplectic schemes in Hamiltonian sense by different symplectic mappings. We also give a direct generalization of Veselov variational principle for construction of scheme of higher order differential equations. At last, we present numerical experiments.

Key words: Variational integrator, Symplectic mapping

1. Introduction

The two main formalisms of mechanics are Lagrangian mechanics based on variational principle and Hamiltonian mechanics based on symplectic structure of cotangent bundle. In many cases two formalisms are equivalent. For a mechanical system once a n-dimensional configuration space Q is chosen, then its Lagrangian flow F_t is defined on the tangent bundle TQ with its coordinates $(q_i, \dot{q}_i)$ and its Hamiltonian flow G_t is defined on cotangent bundle T^*Q with its coordinates (p_i, q_i). The equivalence between these two flows is realized by the well known Legendre transformation $FL : TQ \longrightarrow T^*Q$, which depends on the Lagrangian function $L : TQ \longrightarrow R$ and is a local diffeomorphism in general. Consequently, we have the following commutative diagram

$$\begin{tikzcd}
TQ \arrow[r, "F_t"] \arrow[d, "FL"'] & TQ \arrow[d, "FL"] \\
T^*Q \arrow[r, "G_t"'] & T^*Q
\end{tikzcd}$$

$FL^{-1} \circ G_t \circ FL = F_t$, F_t preserves the symplectic form $\omega_L = FL^*\omega$, i.e., $F_t^*\omega_L = \omega_L$, in canonical coordinates,

$$\omega_L = \frac{\partial^2 L}{\partial \dot{q}_i \partial q_j} dq_i \wedge dq_j + \frac{\partial^2 L}{\partial \dot{q}_i \partial \dot{q}_j} dq_i \wedge d\dot{q}_j.$$

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Note that $G_t^*\omega = \omega$, in canonical coordinates,

$$\omega = dq_i \wedge dp_i.$$

Taking $Q \times Q$ as the discrete version of TQ, we can define the specific discrete Legendre transformations $\mathbf{FL}: Q \times Q \longrightarrow T^*Q$, $\quad \mathbf{FL}(q^{n+1}, q^n) = (p^n, q^n)$ which are symplectic mappings between $Q \times Q$ and T^*Q, and have the following commutative diagram

$$\begin{array}{ccc} Q \times Q & \xrightarrow{\mathbf{F}} & Q \times Q \\ \mathbf{FL}\big\downarrow & & \big\downarrow\mathbf{FL} \\ T^*Q & \xrightarrow[\mathbf{G}]{} & T^*Q \end{array}$$

therefore, the discrete Lagrangian flow $\mathbf{F}$ preserves the symplectic form $\omega_{\mathbf{L}} = \mathbf{FL}^*\omega$, i.e., $\mathbf{F}^*\omega_{\mathbf{L}} = \omega_{\mathbf{L}}$, in canonical coordinates,

$$\omega_{\mathbf{L}} = \frac{\partial^2 \mathbf{L}(q^{n+1}, q^n)}{\partial q_i^{n+1} \partial q_j^n} dq_i^n \wedge dq_j^{n+1}.$$

Note that the discrete Hamiltonian flow $\mathbf{G}$ preserves the canonical symplectic form, i.e., $\mathbf{G}^*\omega = \omega$, in canonical coordinates,

$$\omega = dq_i^n \wedge dp_i^n.$$

In [1] Veselov developed a variational way to construct numerical integrators for Lagrangian mechanical systems based on a discretization of Hamilton's principle. Such an integrator is derived from the corresponding discrete Euler-Lagrange equations and preserves some symplectic forms on the discrete tangent space. The idea was highlighted by Marsden et al in [2] where the "variational integrators" of Veselov type were generalized to PDEs for field theory in the framework of multisymplectic geometry. Variational integrators often enjoy some amazing properties such as the preservation of the integrability of mechanical systems. In the case of Hamiltonian mechanics, however, symplectic integrators have been extensively studied and some nice results in both quantitative and qualitative aspects of numerical analysis are obtained. Therefore, it is interesting to bridge the gap between the variational integrators and symplectic ones, which should be an analogue to the continuous case as described above.

An outline of the paper is as follows. The variational descriptions of one parameter families of approximations studied in [3] for mechanical systems are presented in section 2. A direct generalization to higher order differential equations of Euler-Lagrange type is given in section 3. In section 4, we give some numerical results.

2. Variational descriptions of symplectic integrators

Consider the following system of ODEs

$$M \frac{\partial^2 q}{\partial t^2} = -\frac{\partial V(q)}{\partial q} = F(q), \tag{1}$$

where q is the collective position vector, M is a positive symmetric matrix and F is the collective force vector. (1) can be rewritten as following two equivalent forms

$$\dot{q} = M^{-1}p, \qquad \dot{p} = -\frac{\partial V(q)}{\partial q} \tag{2}$$

and

$$\frac{\partial L}{\partial q} = \frac{d}{dt}\frac{\partial L}{\partial \dot{q}}, \tag{3}$$

where $L(q, \dot{q}) = \frac{1}{2}\dot{q}^T M \dot{q} - V(q)$.

In [3], the following approximations of one parameter families for system (1) are studied:

$$\frac{1}{h^2}M(q^{n+1}-2q^n+q^{n-1})+(1-\alpha)\frac{\partial V}{\partial q}(\alpha q^{n+1}+(1-\alpha)q^n)+\alpha\frac{\partial V}{\partial q}(\alpha q^n+(1-\alpha)q^{n-1})=0, \tag{4}$$

$$\frac{1}{h^2}M(q^{n+1}-2q^n+q^{n-1})+\frac{\partial V}{\partial q}(\alpha q^{n+1}+(1-2\alpha)q^n+\alpha q^{n-1})=0, \tag{5}$$

when $\alpha=\frac{1}{12}$, the scheme is of fourth-order accuracy,

$$\frac{1}{h^2}M(\bar{q}^{n+1}-2\bar{q}^n+\bar{q}^{n-1})+\alpha\frac{\partial V}{\partial q}(\bar{q}^{n-1})+(1-2\alpha)\frac{\partial V}{\partial q}(\bar{q}^n)+\alpha\frac{\partial V}{\partial q}(\bar{q}^{n+1})=0. \tag{6}$$

In these formulas h is the step size, q^n is the numerical approximation to q at the time nh, $\bar{q}^n=q^n-\alpha h^2M^{-1}\frac{\partial V}{\partial q}(\bar{q}^n)$.

First, we show that (4), (5), (6) can be derived by discretizing the corresponding Lagrangian. Choose respectively

$$\mathbf{L}(q^{n+1},q^n)=\frac{1}{2}(\frac{q^{n+1}-q^n}{h})^TM(\frac{q^{n+1}-q^n}{h})-V(\alpha q^{n+1}+(1-\alpha)q^n), \tag{7}$$

$$\mathbf{L}(q^{n+1},q^n)=\frac{1}{2}(\frac{q^{n+1}-q^n}{h})^TM(\frac{q^{n+1}-q^n}{h})-\int_0^{q^n}F(\sigma-\alpha h^2M^{-1}F)d\sigma, \tag{8}$$

$$\mathbf{L}(\bar{q}^{n+1},\bar{q}^n)=\frac{1}{2}(\frac{q^{n+1}-q^n}{h})^TM(\frac{q^{n+1}-q^n}{h})-\int_0^{q^n}F(\sigma-\alpha h^2M^{-1}F)d\sigma \tag{9}$$

as the definition of the discrete Lagrangians, where $\bar{q}^n=q^n-\alpha h^2M^{-1}\frac{\partial V}{\partial q}(\bar{q}^n)$, $F=\frac{\partial V}{\partial q}(q^n-\alpha h^2M^{-1}F)$, we can derive (4), (5), (6) directly from the DEL equations

$$D_2\mathbf{L}(q^{n+1},q^n)+D_1\mathbf{L}(q^n,q^{n-1})=0. \tag{10}$$

We only give the proof of (8).

Let $F=\frac{\partial V}{\partial q}(q^n+\alpha(q^{n+1}-2q^n+q^{n-1}))$, then (5) turn into

$$\frac{1}{h^2}M(q^{n+1}-2q^n+q^{n-1})+F(q^n-\alpha h^2M^{-1}F)=0, \tag{11}$$

where the nonlinear term F is determined implicitly from the equations $F(q^n)=\frac{\partial V}{\partial q}(q^n-\alpha h^2M^{-1}F)$. Taking (8) as the definition of the discrete Lagrangian of (10), from (10), (11) can be derived.

Next, we show that by the specific symplectic mappings, the above three one parameter families of approximations can be related to the symplectic schemes in Hamiltonian sense.

Remark 2.1. By using the transformation

$$p^n=-hD_2\mathbf{L}(q^{n+1},q^n)=\frac{M}{h}(q^{n+1}-q^n)+h(1-\alpha)\frac{\partial V}{\partial q}(\alpha q^{n+1}+(1-\alpha)q^n)$$

(4) is equivalent to

$$\begin{aligned}&p^n-p^{n-1}=-h\tfrac{\partial V}{\partial q}(\alpha q^n+(1-\alpha)q^{n-1}),\\&(1-\alpha)p^n+\alpha p^{n-1}=\tfrac{M}{h}(q^n-q^{n-1}),\end{aligned} \tag{12}$$

which is the approximation of (2). It is clear that the discrete Lagrangian flow $\mathbf{F}:(q^n,q^{n-1})\longrightarrow(q^{n+1},q^n)$ defined by (4) preserves

$$\omega_{\mathbf{L}}=\frac{\partial^2\mathbf{L}(q^n,q^{n-1})}{\partial q_i^{n-1}\partial q_j^n}dq_i^{n-1}\wedge dq_j^n$$

and the discrete Hamiltonian flow $\mathbf{G}:(p^{n-1},q^{n-1})\longrightarrow(p^n,q^n)$, determined by (12) preserves the canonical symplectic form, i.e., $dp_i^n\wedge dq_i^n=dp_i^{n-1}\wedge dq_i^{n-1}$, when $\alpha=\frac{1}{2}$, (12) is the centered implicit Euler scheme.

Remark 2.2. By using the transformation

$$p^n = -hD_2\mathbf{L}(q^{n+1}, q^n) = \frac{M}{h}(q^{n+1} - q^n) + h\frac{\partial V}{\partial q}(\alpha(q^{n+1} - 2q^n + q^{n-1}) + q^n),$$

(5) is equivalent to

$$\begin{aligned} &p^n - p^{n-1} = -h\tfrac{\partial V}{\partial q}(\alpha(q^n - q^{n-1} - M^{-1}hp^{n-1}) + q^{n-1}),\\ &p^n = \tfrac{M}{h}(q^n - q^{n-1}). \end{aligned} \tag{13}$$

It is clear that the discrete Lagrangian flow determined by (5) $\mathbf{F} : (q^n, q^{n-1}) \longrightarrow (q^{n+1}, q^n)$ preserves

$$\omega_{\mathbf{L}} = \frac{\partial^2 \mathbf{L}(q^n, q^{n-1})}{\partial q_i^{n-1}\partial q_j^n} dq_i^{n-1} \wedge dq_j^n$$

and the Hamiltonian flow $\mathbf{G} : (p^{n-1}, q^{n-1}) \longrightarrow (p^n, q^n)$, determined by (13) preserves the canonical symplectic form, i.e., $dp_i^n \wedge dq_i^n = dp_i^{n-1} \wedge dq_i^{n-1}$.

Remark 2.3. By using the transformation

$$p^n = -hD_2\mathbf{L}(\bar{q}^{n+1}, \bar{q}^n) = (\frac{M}{h}(q^{n+1} - q^n) + h\frac{\partial V}{\partial q}(\bar{q}^n))(I + \alpha h^2 M^{-1}\frac{\partial^2 V}{\partial q^2}(\bar{q}^n)),$$

(6) is equivalent to

$$\begin{aligned} &p^n - p^{n-1} = -h\tfrac{\partial V}{\partial q}(\bar{q}^{n-1})(I + \alpha h^2 M^{-1}\tfrac{\partial^2 V}{\partial q^2}(\bar{q}^n)),\\ &p^n = \tfrac{M}{h}(\bar{q}^n + \alpha h^2 M^{-1}\tfrac{\partial V}{\partial q}(\bar{q}^n) - q^{n-1} - \alpha h^2 M^{-1}\tfrac{\partial V}{\partial q}(\bar{q}^{n-1}))(I + \alpha h^2 M^{-1}\tfrac{\partial^2 V}{\partial q^2}(\bar{q}^n)). \end{aligned} \tag{14}$$

It is clear that the discrete Lagrangian flow defined by (6) $\mathbf{F} : (\bar{q}^n, \bar{q}^{n-1}) \longrightarrow (\bar{q}^{n+1}, \bar{q}^n)$ preserves

$$\omega_{\mathbf{L}} = \frac{\partial^2 \mathbf{L}(\bar{q}^n, \bar{q}^{n-1})}{\partial \bar{q}_i^{n-1}\partial \bar{q}_j^n} d\bar{q}_i^{n-1} \wedge d\bar{q}_j^n.$$

and the Hamiltonian flow $\mathbf{G} : (p^{n-1}, \bar{q}^{n-1}) \longrightarrow (p^n, \bar{q}^n)$ determined by (14) preserves the canonical symplectic form, i.e., $dp_i^n \wedge d\bar{q}_i^n = dp_i^{n-1} \wedge d\bar{q}_i^{n-1}$.

Introducing the substitution $p^n = \frac{Mjkbm}{2h}(q^{n+1} - q^{n-1})$, (4), (5), (6) are equivalent respectively to

$$\begin{aligned} &p^{n+\frac{1}{2}} = p^{n-\frac{1}{2}} - h((1-\alpha)\tfrac{\partial V}{\partial q}(\alpha q^{n+1} + (1-\alpha)q^n)\\ &+\alpha\tfrac{\partial V}{\partial q}(\alpha q^n + (1-\alpha)(q^{n+1} - h(p^{n+\frac{1}{2}} + p^{n-\frac{1}{2}})),\\ &q^{n+1} = q^n + hM^{-1}p^{n+\frac{1}{2}}. \end{aligned} \tag{15}$$

$$\begin{aligned} &p^{n+\frac{1}{2}} = p^{n-\frac{1}{2}} - h\tfrac{\partial V}{\partial q}(2\alpha q^{n+1} + (1-2\alpha)q^n - \alpha h(p^{n+\frac{1}{2}} + p^{n-\frac{1}{2}})),\\ &q^{n+1} = q^n + hM^{-1}p^{n+\frac{1}{2}}, \end{aligned} \tag{16}$$

and

$$\begin{aligned} p^{n+\frac{1}{2}} &= p^{n-\frac{1}{2}} - h\tfrac{\partial V}{\partial q}(\bar{q}^n),\\ \tfrac{1}{h^2}(\bar{q}^{n+1} - \bar{q}^n - \tfrac{h}{2}M^{-1}(p^{n+\frac{1}{2}} + p^{n-\frac{1}{2}})) &= -M^{-1}\tfrac{1}{2}((1-2\alpha)\tfrac{\partial V}{\partial q}(\bar{q}^n) + 2\alpha\tfrac{\partial V}{\partial q}(\bar{q}^{n+1})). \end{aligned} \tag{17}$$

Remark 2.4. It is clear that the discrete Hamiltonian flows $\mathbf{G} : (p^{n-\frac{1}{2}}, q^n) \longrightarrow (p^{n+\frac{1}{2}}, q^{n+1})$, defined by (15), (16) preserve the canonical symplectic form i.e., $dp_i^{n+\frac{1}{2}} \wedge dq_i^{n+1} = dp_i^{n-\frac{1}{2}} \wedge dq_i^n$, the discrete Hamiltonian flow $\mathbf{G} : (p^{n-\frac{1}{2}}, \bar{q}^n) \longrightarrow (p^{n+\frac{1}{2}}, \bar{q}^{n+1})$ defined by (17) preserves the K-symplectic form, which is

$$K = \begin{pmatrix} 0 & I + h^2 M^{-1}\alpha\frac{\partial^2 V}{\partial q^2}(\bar{q}^n) \\ -I - h^2 M^{-1}\alpha\frac{\partial^2 V}{\partial q^2}(\bar{q}^n) & 0 \end{pmatrix},$$

i.e., $(1 + h^2 M^{-1}\alpha\frac{\partial^2 V}{\partial q^2}(\bar{q}^{n+1}))_{ij} dp_i^{n+\frac{1}{2}} \wedge d\bar{q}_j^{n+1} = (1 + h^2 M^{-1}\alpha\frac{\partial^2 V}{\partial q^2}(\bar{q}^n))_{ij} dp_i^{n-\frac{1}{2}} \wedge d\bar{q}_j^n$. Let $\psi = f^{-1} \circ \varphi \circ f$, where $f : (p^{n-\frac{1}{2}}, q^n) \to (p^{n-\frac{1}{2}}, \bar{q}^n)$, then the discrete flow $\psi : (p^{n-\frac{1}{2}}, q^n) \to (p^{n+\frac{1}{2}}, q^{n+1})$ preserves the canonical symplectic form, i.e., $dp_i^{n+\frac{1}{2}} \wedge dq_i^{n+1} = dp_i^{n-\frac{1}{2}} \wedge dq_i^n$.

3. Variational integrators for higher order differential equations of Euler-Lagrange type

In this section, we generalize the discrete Veselov variational principle to higher order differential equations.

Theorem 3.1 (The variational principle for k-order classical field theory).
Let L be a k-order Lagrangian on a given $T^kQ = T\cdots(TQ)$. A curve $q(t):[a,b]\longrightarrow Q$ joining $\delta q_i,\cdots,\delta q_i^{(k-1)}$ which vanish at the endpoints a,b, satisfies the higher order Euler-Lagrange equations

$$\frac{\partial L}{\partial q_i}+\sum_{s=1}^{k}(-1)^s\frac{d^s}{dt^s}\frac{\partial L}{\partial q_i^{(s)}}=0, \tag{18}$$

if and only if $dS=\delta\int\limits_a^b Ldt=\delta\int\limits_a^b L(q_i(t),\cdots,q_i^{(k)}(t))dt=0$, where $S=\int_a^b L(q_i(t),\cdots,q_i^{(k)}(t))dt$ is the action functional, q_i, $(q_i,\cdots,q_i^{(k-1)})$ denote the coordinates of Q and T^kQ respectively.

Proof. Using integration by parts, the variational equation becomes

$$\begin{aligned}\delta S(q(t))\delta q(t) &= \int\limits_a^b\Big(\frac{\partial L}{\partial q_i}\delta q_i+\frac{\partial L}{\partial \dot q_i}\delta\dot q_i+\cdots+\frac{\partial L}{\partial q_i^{(k)}}\delta q_i^{(k)}\Big)dt\\ &= \int\limits_a^b\Big(\frac{\partial L}{\partial q_i}+\sum_{s=1}^{k}(-1)^s\frac{d^s}{dt^s}\frac{\partial L}{\partial q_i^{(s)}}\Big)\delta q_i dt+\sum_{s=0}^{k-1}\Big[\sum_{r=s}^{k-1}(-1)^{r-s}\frac{d^{r-s}}{dt^{r-s}}\frac{\partial L}{\partial q_i^{(r+1)}}\Big]\delta q_i^{(s)}\ \Big|_a^b\ .\end{aligned}$$

Using the boundary conditions δq_i, $\cdots$, $\delta q_i^{(k-1)}$ which vanish at the endpoints a, b. Since δq_i is arbitrary (apart from being zero at the endpoints), we have the k-order Euler-Lagrange equations

$$\frac{\partial L}{\partial q_i}+\sum_{s=1}^{k}(-1)^s\frac{d^s}{dt^s}\frac{\partial L}{\partial q_i^{(s)}}=0.$$

When the boundary conditions are not considered, from the "boundary part" of the functional derivative of the action we can define the Lagrangian 1-form on $T^{2k-1}Q$

$$\theta_L=\sum_{s=0}^{k-1}\Big[\sum_{r=s}^{k-1}(-1)^{r-s}\frac{d^{r-s}}{dt^{r-s}}\frac{\partial L}{\partial q_i^{(r+1)}}\Big]dq_i^{(s)}. \tag{19}$$

Consequently, we have the following theorem.

Theorem 3.2. The solutions of k-order Euler-Lagrange equations (18) give rise to a symplectic map.

Proof. We denote the flow of the vector field on T^kQ by F_t, and restrict the actions S to the subspace C_L of solutions of the variational principle. The space C_L may be identified with the initial conditions, elements of T^kQ, for the flow: to $v_q\in T^kQ$, we associate the integral curve $s\mapsto F_s(v_q)$, $s\in[0,t]$. Thus, we have a well-defined map $S_t: T^kQ\to R$,

$$S_t(v_q)=\int\limits_0^t L\big(q(s),\dot q(s),\cdots,q^{(k)}(s)\big)\,ds,$$

where $F_s(v_q)=\big(q(s),\dot q(s),\cdots,q^{(k)}(s)\big)$. So the variational equation becomes

$$dS_t(v_q)w_{v_q}=\theta_L(F_t(v_q))\frac{d}{d\varepsilon}\Big|_{\varepsilon=0}F_t(v_q^\varepsilon)-\theta_L(v_q)w_{v_q},$$

where $\varepsilon\mapsto v_q^\varepsilon$ is an arbitrary curve on T^kQ such that $v_q^0=v_q$ and $\frac{d}{d\varepsilon}|_{\varepsilon=0}\,v_q^\varepsilon=w_{v_q}$. Therefore, we have

$$dS_t=F_t^*\theta_L-\theta_L,$$

taking the exterior derivative on both sides of the above equality, we have

$$0 = ddS_t = F_t^* d\theta_L - d\theta_L,$$

or $F_t^*\omega_L = \omega_L$, where

$$\begin{aligned}\omega_L &= d\Big(\sum_{s=0}^{k-1}\Big[\sum_{r=s}^{k-1}(-1)^{r-s}\frac{d^{r-s}}{dt^{r-s}}\frac{\partial L}{\partial q_i^{(r+1)}}\Big]\wedge dq_i^{(s)}\\ &= \sum_{l=0}^{k}\sum_{s=0}^{k-1}\sum_{r=s}^{k-1}(-1)^{r-s}\frac{d^{r-s}}{dt^{r-s}}\frac{\partial^2 L}{\partial q_j^{(l)}\partial q_i^{(r+1)}}dq_j^{(l)}\wedge dq_i^{(s)}.\end{aligned}$$

The Euler-Lagrange equation (18) can be reformulated as

$$\dot{p}_i^{s+1} = -\frac{\partial H}{\partial q_i^{s+1}} \qquad \dot{q}_i^{s+1} = \frac{\partial H}{\partial p_i^{s+1}}, \tag{20}$$

where $q_i^{s+1} = q_i^{(s)}, p_i^{s+1} = \sum\limits_{r=s}^{k-1}(-1)^{r-s}\frac{d^{r-s}}{dt^{r-s}}\frac{\partial L}{\partial q_i^{(r+1)}}, s = 0,\cdots,k-1, i = 1,\cdots,n,$

$$H(p,q) = -L + \sum_{i=1}^{n}\sum_{s=0}^{k-1} p_i^{s+1}\dot{q}_i^{s+1}.$$

It is clear that the Hamiltonian flow defined by (20) preserves the canonical symplectic form

$$\omega_J = \sum_{i=1}^{n}\sum_{s=0}^{k-1} dp_i^{s+1}\wedge dq_i^{s+1}.$$

Take $\underbrace{Q\times Q\times\cdots Q}_{k+1}$ as the discrete version of T^kQ and define a discrete Lagrangian

$$\mathbf{L} : \underbrace{Q\times Q\times\cdots Q}_{k+1} = \{q_k,\cdots,q_0\}\longrightarrow R,$$

and the corresponding action

$$\mathbf{S} = \sum_{m=0}^{n-k}\mathbf{L}(q_{k+m},\cdots,q_m).$$

The variational principle states that $\delta S = 0$ with the variation $\delta q_0,\cdots,\delta q_{k-1},\delta q_{n-k+1},\cdots,\delta q_n$ vanishing, which determines a "discrete flow"

$$F : \underbrace{Q\times Q\times\cdots Q}_{k+1}\longrightarrow\underbrace{Q\times Q\times\cdots Q}_{k+1}$$

by

$$F(q_0,\cdots,q_k) = (q_1,\cdots,q_{k+1}).$$

But

$$\begin{aligned}&d\mathbf{S}(q_0,\cdots,q_n)(\delta q_0,\cdots,\delta q_n)\\ &= \sum_{m=0}^{n-k}(D_1\mathbf{L}(q_{m+k},\cdots,q_m)\delta q_{m+k} + D_2\mathbf{L}(q_{m+k},\cdots,q_m)\delta q_{m+k-1}\\ &+\cdots + D_{k+1}\mathbf{L}(q_{m+k},\cdots,,q_m)\delta q_m)\\ &= \sum_{m=k}^{n} D_1\mathbf{L}(q_m,\cdots,q_{m-k})\delta q_m + \sum_{m=k-1}^{n-1} D_2\mathbf{L}(q_{m+1},\cdots,q_{m-k+1})\delta q_m\\ &+\cdots + \sum_{m=0}^{n-k} D_{k+1}\mathbf{L}(q_{m+k},\cdots,q_m)\delta q_m\\ &= \sum_{m=k}^{n-k}(D_1\mathbf{L}(q_m,\cdots,q_{m-k}) + D_2\mathbf{L}(q_{m+1},\cdots,q_{m-k+1}) + \cdots\\ &+D_{k+1}\mathbf{L}(q_{m+k},\cdots,q_m))\delta q_m + D_1\mathbf{L}(q_n,\cdots,q_{n-k})\delta q_n + \cdots\\ &+D_1\mathbf{L}(q_{n-k+1},\cdots,q_{n-2k+1})\delta q_{n-k+1} + D_2\mathbf{L}(q_n,\cdots,q_{n-k})\delta q_{n-1} + \cdots\\ &+D_2\mathbf{L}(q_{n-k+2},\cdots,q_{n-2k+2})\delta q_{n-k+1} + D_2\mathbf{L}(q_k,\cdots,q_0)\delta q_{k-1} + \cdots\\ &+D_{k+1}\mathbf{L}(q_{2k-1},\cdots,q_{k-1})\delta q_{k-1} + \cdots + D_{k+1}\mathbf{L}(q_k,\cdots,q_0)\delta q_0.\end{aligned} \tag{21}$$

So $\delta S(q_0,\cdots,q_n)=0$ if the following DEL equations hold:

$$D_1\mathbf{L}(q_k,q_{k-1},\cdots,q_0)+D_2\mathbf{L}(q_{k+1},q_k,\cdots,q_1)+\cdots+D_{k+1}\mathbf{L}(q_{2k},q_{k+1},\cdots,q_k)=0.$$

Define two 1-forms on $\underbrace{Q\times Q\times\cdots Q}$ by the boundary terms as follows

$$\begin{aligned}
&\theta^1_{\mathbf{L}}\\
&=D_{k+1}\mathbf{L}(q_{2k-1},\cdots,q_{k-1})dq_{k-1}+D_k\mathbf{L}(q_{2k-2},\cdots,q_{k-2})dq_{k-1}+\cdots+D_2\mathbf{L}(q_k,\cdots,q_0)dq_{k-1}\\
&+D_{k+1}\mathbf{L}(q_{2k-2},\cdots,q_{k-2})dq_{k-2}+D_k\mathbf{L}(q_{2k-3},\cdots,q_{k-3})dq_{k-2}+\cdots+D_3\mathbf{L}(q_k,\cdots,q_0)dq_{k-2}\\
&+\cdots+D_{k+1}\mathbf{L}(q_{k+1},\cdots,q_1)dq_1+D_k\mathbf{L}(q_k,\cdots,q_0)dq_1+D_{k+1}\mathbf{L}(q_k,\cdots,q_0)dq_0,
\end{aligned}$$

and

$$\begin{aligned}
\theta^2_{\mathbf{L}}&=D_k\mathbf{L}(q_{2k-1},\cdots,q_{k-1})dq_k+D_{k-1}\mathbf{L}(q_{2k-1},\cdots,q_{k-1})dq_{k+1}\\
&+D_{k-1}\mathbf{L}(q_{2k-2},\cdots,q_{k-2})dq_k\\
&+\cdots+D_2\mathbf{L}(q_{2k-1},\cdots,q_{k-1})dq_{2k-2}+\cdots+D_2\mathbf{L}(q_{k+1},\cdots,q_1)dq_k\\
&+D_1\mathbf{L}(q_{2k-1},\cdots,q_{k-1})dq_{2k-1}+\cdots+D_1\mathbf{L}(q_k,\cdots,q_0)dq_k.
\end{aligned}$$

The equation (21) becomes

$$d\mathbf{S}=\theta^1_{\mathbf{L}}+F^*\theta^2_{\mathbf{L}}.$$

Taking the exterior derivative on the both sides of the above equality, we have

$$0=dd\mathbf{S}=d\theta^1_{\mathbf{L}}+F^*d\theta^2_{\mathbf{L}}.$$

From the fact

$$\theta^1_{\mathbf{L}}+\theta^2_{\mathbf{L}}=d(\mathbf{L}(q_k,q_{k-1},\cdots,q_0)+\mathbf{L}(q_{k+1},q_k,\cdots,q_1)+\mathbf{L}(q_{2k-1},q_{2k-2},\cdots,q_{k-1})),$$

it follows that

$$d\theta^1_{\mathbf{L}}+d\theta^2_{\mathbf{L}}=0.$$

Let $-d\theta^2_{\mathbf{L}}=\omega_{\mathbf{L}}$, then

$$F^*\omega_{\mathbf{L}}=\omega_{\mathbf{L}}.$$

Further we define the discrete Legendre transformation

$$\begin{aligned}
p_{2k-1}&=D_1\mathbf{L}(q_{2k-1},q_{2k-2},\cdots,q_{k-1}),\\
&\cdots\cdots\\
p_{k+1}&=D_1\mathbf{L}(q_{k+1},q_k,\cdots,q_1)+D_2\mathbf{L}(q_{k+2},q_{k+1},\cdots,q_0)\\
&+\cdots+D_{k-1}\mathbf{L}(q_{2k-1},q_{2k-2},\cdots,q_{k-1}),\\
p_k&=D_1\mathbf{L}(q_k,q_{k-1},\cdots,q_0)+D_2\mathbf{L}(q_{k+1},q_k,\cdots,q_1)+\cdots+D_k\mathbf{L}(q_{2k-1},q_{2k-2},\cdots,q_{k-1}).
\end{aligned}$$

Under which the corresponding discrete Hamiltonian flow

$$\mathbf{G}:(q_{2k-2},\cdots,q_{k-1},p_{2k-2},\cdots,p_{k-1})\longrightarrow(q_{2k-1},\cdots,q_k,p_{2k-1},\cdots,p_k)$$

preserves the canonical symplectic form

$$\omega_J=-\sum_{r=0}^{k-1}dp_{k+r}\wedge dq_{k+r}.$$

We give a simple example, consider fourth-order differential equations

$$Mq^{(4)}-N\ddot{q}+\frac{\partial V(q)}{\partial q}=0, \tag{22}$$

where M and N are positive symmetric matrix. (22) can be reformulated as

$$\frac{\partial L}{\partial q}=\frac{d}{dt}\frac{\partial L}{\partial\dot{q}}-\frac{d^2}{dt^2}\frac{\partial L}{\partial\ddot{q}}$$

and

$$\dot{p^i}=-\frac{\partial H}{\partial q^i},\qquad \dot{q^i}=\frac{\partial H}{\partial p^i},$$

where $i=1,2$, $q_1=q$, $q_2=\dot{q}$, $p_1=N\dot{q}-M\dddot{q}$, $p_2=M\ddot{q}$, $L(q,\dot{q},\ddot{q})=\frac{1}{2}\ddot{q}^TM\ddot{q}+\frac{1}{2}\dot{q}^TN\dot{q}+V(q)$, $H=-L+p_1\dot{q}_1+p_2\dot{q}_2$.

We use the following definition for the discrete Lagrangian

$$\mathbf{L}(q_{k+2},q_{k+1},q_k)=L(\alpha_1q_{k+2}+\alpha_2q_{k+1}+\alpha_3q_k,\frac{q_{k+1}-q_k}{h},\frac{q_{k+2}-2q_{k+1}+q_k}{h^2}),$$

where $\alpha_1+\alpha_2+\alpha_3=1$, then the DEL equations are

$$\begin{aligned}&M\tfrac{q_{k+2}-2q_{k+1}+q_k}{h^4}-N\tfrac{q_{k+1}-q_k}{h^2}+\alpha_3\tfrac{\partial V}{\partial q}(\alpha_1q_{k+2}+\alpha_2q_{k+1}+\alpha_3q_k)-\\&2M\tfrac{q_{k+1}-2q_k+q_{k-1}}{h^4}+N\tfrac{q_k-q_{k-1}}{h^2}+\alpha_2\tfrac{\partial V}{\partial q}(\alpha_1q_{k+1}+\alpha_2q_k+\alpha_3q_{k-1})+\\&M\tfrac{q_k-2q_{k-1}+q_{k-2}}{h^4}+\alpha_1\tfrac{\partial V}{\partial q}(\alpha_1q_k+\alpha_2q_{k-1}+\alpha_3q_{k-2})=0,\end{aligned}\tag{23}$$

i.e.,

$$\begin{aligned}&M\tfrac{q_{k+2}-4q_{k+1}+6q_k-4q_{k-1}+q_{k-2}}{h^4}-N\tfrac{q_{k+1}-2q_k+q_{k-1}}{h^2}+\alpha_3\tfrac{\partial V}{\partial q}(\alpha_1q_{k+2}+\alpha_2q_{k+1}+\alpha_3q_k)\\&+\alpha_2\tfrac{\partial V}{\partial q}(\alpha_1q_{k+1}+\alpha_2q_k+\alpha_3q_{k-1})+\alpha_1\tfrac{\partial V}{\partial q}(\alpha_1q_k+\alpha_2q_{k-1}+\alpha_3q_{k-2})=0.\end{aligned}$$

The discrete Lagrangian flow $\mathbf{F}:(q_k,q_{k-1},q_{k-2})\longrightarrow(q_{k+1},q_k,q_{k-1})$, defined by (23) preserves the form

$$\omega_{\mathbf{L}}=-d(D_1\mathbf{L}(q_k,q_{k-1},q_{k-2})+D_2\mathbf{L}(q_{k+1},q_k,q_{k-1}))\wedge dq_k-d(D_1\mathbf{L}(q_{k+1},q_k,q_{k-1}))\wedge dq_{k+1}.$$

Define the discrete Legendre transformation

$$\begin{aligned}p_{k+1}&=D_1\mathbf{L}(q_{k+1},q_k,q_{k-1}),\\p_k&=D_1\mathbf{L}(q_k,q_{k-1},q_{k-2})+D_2\mathbf{L}(q_{k+1},q_k,q_{k-1}),\end{aligned}$$

then the corresponding discrete Hamiltonian flow $\mathbf{G}:(q_{k-1},q_k,p_{k-1},p_k)\longrightarrow(q_k,q_{k+1},p_k,p_{k+1})$ preserves

$$\omega_J=-\sum_{r=0}^{1}(dp_{k+r}\wedge dq_{k+r}).$$

4. Numerical experiments

In section, we present some numerical results and show the scheme given by us in this paper involves more computational efforts over long time. Consider the one dimensional mechanical equation with the double well potential

$$\ddot{q}=-2q^3+q,\tag{24}$$

(24) can be rewritten as

$$\dot{p}=-V'(q),\qquad \dot{q}=p.\tag{25}$$

Discretizing (25) by using the generating function method of first kind [9-11]

$$\begin{cases}p_{k+1}=t^{-1}(q_{k+1}-q_k)-t\sum\limits_{n=1}^{\infty}\frac{n(q_{k+1}-q_k)^{n-1}}{(n+1)!}\frac{\partial^nV(q_k)}{\partial q^n},\\-p_k=t^{-1}(q_k-q_{k+1})+t\sum\limits_{n=1}^{\infty}\frac{n(q_{k+1}-q_k)^{n-1}}{(n+1)!}\frac{\partial^nV(q_k)}{\partial q^n}-t\sum\limits_{n=0}^{\infty}\frac{(q_{k+1}-q_k)^n}{(n+1)!}\frac{\partial^{n+1}V(q_k)}{\partial q^{n+1}},\end{cases}\tag{26}$$

where $V(q)=\frac{1}{2}(q^4-q^2)$. Eliminating p_{k+1}, p_k from (26), we can derive

$$\frac{q_{k+1}-2q_k+q_{k-1}}{h^2}=(\frac{q_k^4-q_k^2}{2(q_{k+1}-q_k)}-\frac{3(q_{k+1}^5-q_k^5)-5(q_{k+1}^3-q_k^3)}{30(q_{k+1}-q_k)^2}-\frac{q_k^4-q_k^2}{2(q_k-q_{k-1})}+\frac{3(q_k^5-q_{k-1}^5)-5(q_k^3-q_{k-1}^3)}{30(q_k-q_{k-1})^2}).\tag{27}$$

The computation is done by using scheme (27) and the following initial conditions

$$q_0=q_1=0.74,\tag{28}$$

$$q_0=q_1=0.995,\tag{29}$$

$$q_0=q_1=1.0.\tag{30}$$

The discrete energy that we used is

$$E=\frac{1}{2}(\frac{q_{k+1}-q_k}{h})^2+\frac{3q_{k+1}^5-5q_{k+1}^3-3q_k^5+5q_k^3}{30(q_{k+1}-q_k)}.$$

In Fig. 1, the left top plot showes a periodic orbit that oscillates around the stable equilibrium position $q = \frac{1}{\sqrt{2}}$, $\dot{q} = 0$, the right top plot showes a periodic orbit with high period just inside the homoclinic orbit in the positive q half space, while that in bottom plot is a periodic orbit just outside the homoclinic orbit. Using the three initial conditions the energy errors over initial 800 timesteps and over 800 timesteps after 100000 timesteps is showed in Fig.2.

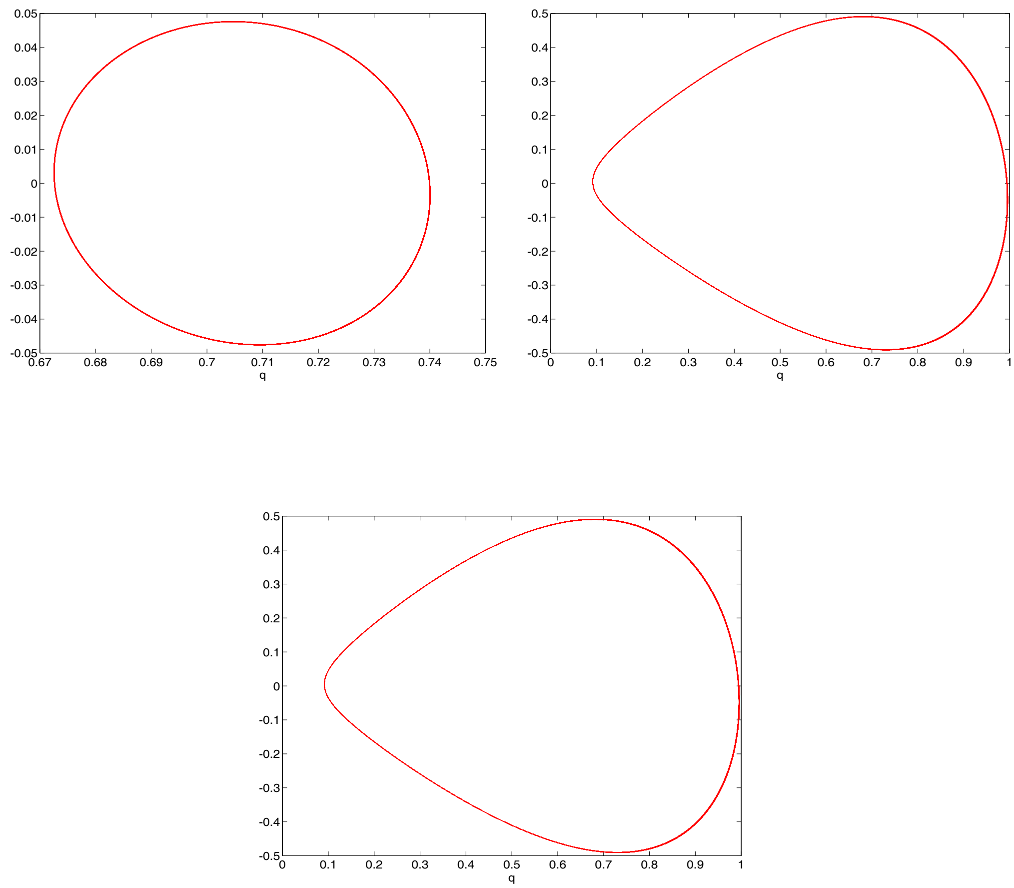
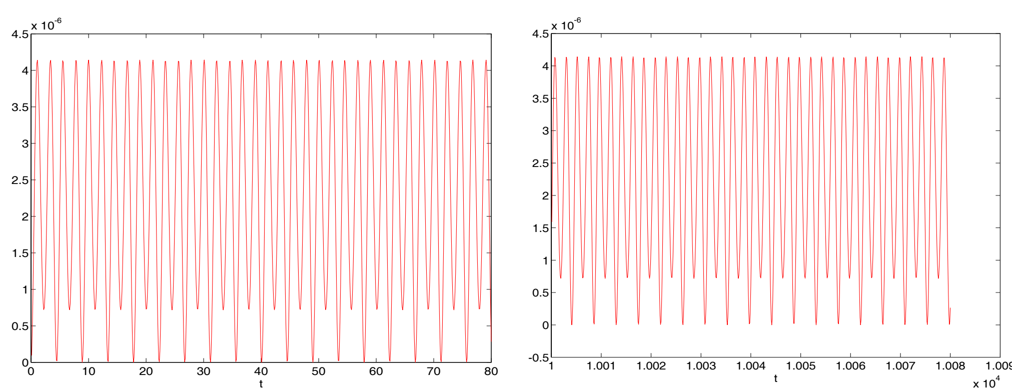


Figure 1. The three orbit plots are showed respectively by using initial conditions (28), (29), (30) with the time step h=0.1 after 100000 timestep.



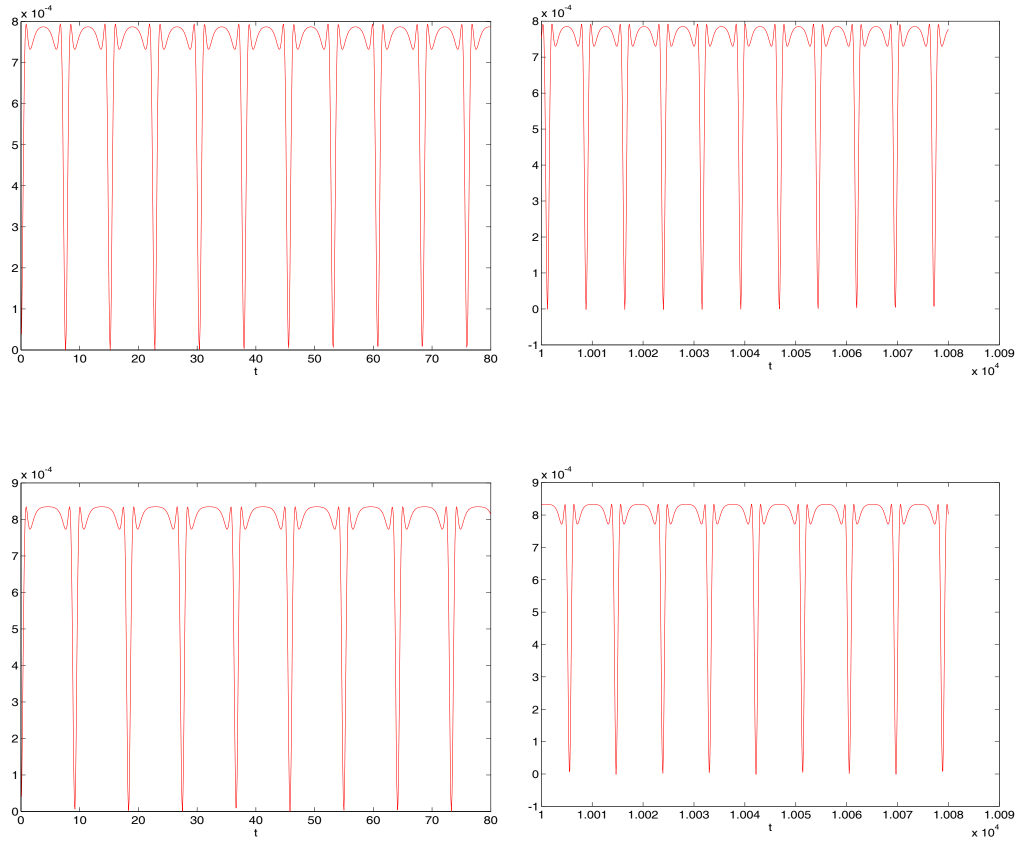


Figure 2. The energy errors are showed with the initial dates correspond to Fig. 1. Left: the energy errors at beginning; right: the energy errors after 100000 timestep.

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