

Energy-conserving numerical methods for multi-symplectic Hamiltonian PDEs *

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Abstract

In this paper, the discrete gradient methods are investigated for ODEs with first integral, and the recursive formula is presented for deriving the high-order numerical methods. We generalize the idea of discrete gradient methods to PDEs and construct the high-order energy-preserving numerical methods for multi-symplectic Hamiltonian PDEs. By integrating nonlinear Schrödinger equation, some numerical experiments are presented to demonstrate the conservative property of the proposed numerical methods.

1 Introduction

Recent years, there has been an increased emphasis on constructing numerical methods to preserve certain invariant quantities in the continuous dynamical systems. The idea of designing finite difference methods that possess the conserved quantities dates back to the late 1920s. Constructing the special numerical methods that are not only consistent with the differential equations, but also inherit some conserved quantities, is the basic idea of earlier attempts. Subsequently, this idea becomes a criterion to judge the success of the numerical simulation. By studying the internal structure of dynamical systems, it is natural to design schemes which can preserve as much as possible the intrinsic properties of the systems. The numerical method which can preserve at least some of structural properties of systems is called geometric integrator or structure-preserving numerical method. In the numerical analysis of differential equations which use the theoretical knowledge, geometric integrator plays an important role for the development and enhancement of practical discretization methods. As geometric integration has gained remarkable success in

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the numerical analysis of ODEs, not only in the integration of Hamiltonian equations by symplectic methods, but also in the recent theory of Lie-group solvers [8]. It is believable to extend the idea of geometric integration to significant PDEs arising in important application areas. The introduction of multi-symplectic formulation [12, 19] provides a new way for computing conservative PDEs based on multi-symplectic geometry. Some conservative PDEs, for instance KDV equation, Schrödinger equation, wave equation can be rewritten in this formulation, which has the properties of multi-symplectic structure, energy and momentum conservation laws. To inherit the multi-symplectic structure, by using the symplectic Runge-Kutta methods both in space and time the multi-symplectic Runge-Kutta methods are presented in [2, 19] and are applied successfully to many soliton equations [5, 6, 7, 20]. For more details in applications, please refer to review article [3] and references therein. Except the multi-symplectic conservation law, multi-symplectic Hamiltonian systems also have the energy and momentum conservation laws. It is well known that conservation law plays an important role in conservative PDEs, especially in the theory of solitons, and the conservation of energy is an essential property in an elastic collision of two solitons. Therefore, it is valuable to expect that the energy-preserving discretizations for conservative PDEs will produce richer information on the discrete systems. In several areas of mechanics, the design of energy-conserving numerical methods has been made, for instance, in the incompressible magnetohydrodynamics (MHD) systems [11], in the two-dimensional shallow water systems [24], in the derivative nonlinear Schrödinger (DNLS) equations [23] etc. In [10] authors present several finite difference methods that preserve certain algebraic invariants for nonlinear Klein-Gordon equations based on finite difference calculus. In [9], author developed the energy-preserving numerical methods for PDEs with variable coefficients by using the discrete variational derivative approach. To construct the conservative numerical methods for some PDEs, [14, 15] establish a unify spatial discretization approach for get the ODEs with integrals which is suitable for integration by discrete gradient methods [18]. Comparing with the traditional method of line [22], our purpose in this paper is to construct energy-preserving numerical methods based on multi-symplectic Hamiltonian systems in which PDEs are taken as the finite dimensional systems defined on the bundle coordinate space. Since it has been proved in [21], generally, multi-symplectic Runge-Kutta methods can only preserve the quadratic conservation laws of systems, it is meaningful to construct the integrators which can retain the energy or momentum conservation laws. We study the discrete gradient methods which are developed systematically for integral-preserving systems in [13, 18]. By generalizing the idea to PDEs, we establish the high-order energy-conserving numerical algorithms for multi-symplectic Hamiltonian systems and implement it to nonlinear Schrödinger equation.

We begin by reviewing the integral-preserving systems and the discrete gradient methods. Let us consider the following first-order ODEs

$$\dot{z} = f(z) \tag{1}$$

with a first integral $I(z)$, i.e., $\frac{d}{dt}I(z) = (\nabla I(z))^T f(z) = 0$, then there is a skew-symmetric matrix S such that

$$f(z) = S(z)\nabla I(z).$$

Clearly, the choice of S is not unique. For example, it can be chosen as [13]

$$S = \frac{1}{a^T \nabla I} (f a^T - a f^T) \quad (2)$$

with an arbitrary vector a . When $a = \nabla I$, S is reduced to

$$S = \frac{1}{|\nabla I|^2} (f(\nabla I)^T - (\nabla I) f^T). \quad (3)$$

The following is a simple example of ODEs with the first integral.

Example 1.1. We consider Lotka-Volterra equation [8]

$$\begin{aligned} \dot{u} &= u(v - 2), \\ \dot{v} &= v(1 - u). \end{aligned} \quad (4)$$

It is known, along the solution curves of (4)

$$I(u, v) = \ln u - u - v + 2 \ln v = \text{Const},$$

i.e., the smooth function $I(u, v)$ is a first integral of system (4). Therefore, we can calculate the skew-symmetric matrix S by (3)

$$S(u, v) = \begin{pmatrix} 0 & -uv \\ uv & 0 \end{pmatrix}.$$

And (4) is rewritten as

$$\begin{pmatrix} \dot{u} \\ \dot{v} \end{pmatrix} = S(u, v) \nabla I(u, v) = \begin{pmatrix} 0 & -uv \\ uv & 0 \end{pmatrix} \begin{pmatrix} (1-u)/u \\ (2-v)/v \end{pmatrix}.$$

There exist two main methods: projection methods and discrete gradient methods which can preserve the first integral of original systems [8]. Here, we are particularly interested in the discrete gradient methods.

For a differentiable function $I(z)$, the discrete gradient of I is defined as

$$\begin{aligned} (z' - z)^T \bar{\nabla} I(z', z) &= I(z') - I(z), \\ \bar{\nabla} I(z, z) &= \nabla I(z). \end{aligned}$$

As an example, $\bar{\nabla} I(z', z)$ can be taken as $\bar{\nabla} I(z', z) = \begin{pmatrix} \frac{I(z'_1, z_2, \dots, z_n) - I(z_1, z_2, \dots, z_n)}{z'_1 - z_1} \\ \frac{I(z'_1, z'_2, \dots, z_n) - I(z'_1, z_2, \dots, z_n)}{z'_2 - z_2} \\ \dots \\ \frac{I(z'_1, z'_2, \dots, z'_n) - I(z'_1, z'_2, \dots, z_n)}{z'_n - z_n} \end{pmatrix}$. By multiplying

$\bar{\nabla}I(z', z)$ with $(z' - z)^T$, it is easy to know

$$\begin{aligned}
(z' - z)^T \bar{\nabla}I(z', z) &= I(z'_1, z_2, \dots, z_n) - I(z_1, z_2, \dots, z_n) \\
&\quad + I(z'_1, z'_2, \dots, z_n) - I(z'_1, z_2, \dots, z_n) \\
&\quad + \dots \\
&\quad + I(z'_1, z'_2, \dots, z'_n) - I(z'_1, z'_2, \dots, z_n) \\
&= I(z'_1, z'_2, \dots, z'_n) - I(z_1, z_2, \dots, z_n) \\
&= I(z') - I(z).
\end{aligned}$$

With the use of the discrete gradient of I , the numerical methods for ODEs (1) with $f(z) = S(z)\nabla I(z)$ is presented in [13, 18]

$$z_{k+1} - z_k = \Delta t \tilde{S}(z_{k+1}, z_k, \Delta t) \bar{\nabla}I(z_{k+1}, z_k). \quad (5)$$

Here, \tilde{S} is a skew-symmetric matrix satisfying $\tilde{S}(z_{k+1}, z_k, \Delta t) = S(z_k) + O(\Delta t)$. As an approximation of $S(z)$, \tilde{S} can be chosen as

$$\tilde{S}(z', z, \Delta t) = S(z)$$

or

$$\tilde{S}(z', z, \Delta t) = S\left(\frac{z' + z}{2}\right).$$

Multiplying (5) with $(\bar{\nabla}I(z_{k+1}, z_k))^T$, it is easy to derive

$$I(z_{k+1}) = I(z_k).$$

This states that the first integral I is preserved exactly by integrator (5). Therefore, integrator (5) is called integral-preserving numerical method.

The rest of the paper is organized as follows. In the next section, we observe the high-order integral-preserving numerical methods presented by bootstrapping approach in [17] and provide the recursive formula for getting any-order numerical methods. In section 3, we introduce and investigate the multi-symplectic Hamiltonian systems. By combining the symplectic discretization in temporal direction with the discrete gradient discretization in spatial direction, the high-order energy-preserving numerical algorithms are constructed in the fourth section. In this paper, we concentrate on the preservation of geometric properties of numerical methods, therefore our interests are focused on the conservative properties when we present the numerical experiments. Some numerical results are shown in the last section.

2 High-order integral-preserving integrators

In the above introduction, we review the differential equations with first integral and the numerical algorithms which can inherit the first integral. Generally, the integral-preserving integrators given by using the discrete gradient are low-order of accuracy, the high-order integrators can be constructed by composition approach or by the use of bootstrapping approach [16, 17]. In this section,

we observe the bootstrapping approach and provide the recursive formula for the construction of the high-order integrators. Let us start this section with an arbitrary ODEs

$$\dot{z} = f(z). \quad (6)$$

The idea of bootstrapping approach can be explained as follows. Discretizing (6) by using a p -order numerical method $z_{n+1} = \varphi_{\Delta t}(z_n)$, the error between exact solution and numerical solution is denoted by $\hat{z} - z_{n+1} = \Delta t^{p+1}R_p$. Absorbing $\Delta t^p R_p$ into original equations (6), we derive the modification equations of (6)

$$\dot{z} = f(z) + \Delta t^p R_p(z). \quad (7)$$

Applying the p -order numerical method $z_{n+1} = \varphi_{\Delta t}(z_n)$ again to (7), we obtain the numerical solution \bar{z}_{n+1} which satisfies

$$\begin{aligned} \bar{z}_{n+1} &= z_{n+1} + \Delta t^{p+1}R_p(z_n) + O(\Delta t^{p+2}) \\ &= \hat{z} - \Delta t^{p+1}R_p(z_n) + \Delta t^{p+1}R_p(z_n) + O(\Delta t^{p+2}) \\ &= \hat{z} + O(\Delta t^{p+2}). \end{aligned}$$

This implies that the new obtained numerical method $\bar{z}_{n+1} = \psi_{\Delta t}(z_n)$ is at least $p + 1$ -order. By continuing the above procedure, the integrators of any order of accuracy can be gained in this way. We also can illustrate the idea of bootstrapping approach with the following diagram

$$\begin{array}{c} \dot{z} = f(z) \\ \text{first-order method} \quad \Downarrow \quad \text{error} = z_{ex} - z_{nm} \\ \dot{z} = f(z) + \text{error}/\Delta t = f(z) + \Delta t R_1(z) \\ \text{first-order method} \\ \Downarrow \\ \text{second-order method} \quad \text{error1} = z_{ex} - z_{nm1} \\ \Downarrow \\ \dot{z} = f(z) + \text{error}/\Delta t + \text{error1}/\Delta t = f(z) + \Delta t R_1(z) + \Delta t^2 R_2(z) \\ \Downarrow \\ \text{first-order method} \\ \Downarrow \\ \text{third-order method} \quad \text{error2} = z_{ex} - z_{nm2} \\ \dots\dots \end{array}$$

As above, we have shown that by taking the error R_p of low-order integrator as the corrector of continue systems, we can get the high-order numerical methods. What follows, based on backward error analysis we will reveal that the error R_p is closely related to the term f_p of modified equation. According to backward error analysis, the numerical solution z_{n+1} can be taken as the exact solution of the following formal differential equations

$$\dot{\tilde{z}} = \tilde{f}(\tilde{z}),$$

where $\tilde{f}(z)$ is a formal vector field which is written as a infinite series $\tilde{f}(z) = f(z) + \Delta t^p f_p(z) + \dots = f(z) + \Delta t^p f_p(z) + O(\Delta t^{p+1})$. This implies that $z_{n+1} = \tilde{z}(t_{n+1})$. Denote $\mathcal{D} = f^l \frac{\partial}{\partial z^l}$, it reads by Taylor expansion

$$\hat{z} = z(t_{n+1}) = z_n + \Delta t f(z_n) + \sum_{i=2}^p \frac{\Delta t^i}{i!} \mathcal{D}^{i-1} f(z_n) + \frac{\Delta t^{p+1}}{(p+1)!} \mathcal{D}^p f(z_n) + O(\Delta t^{p+2}),$$

$$\begin{aligned} z_{n+1} = \tilde{z}(t_{n+1}) &= z_n + \Delta t (f(z_n) + \Delta t^p f_p(z_n)) + \sum_{i=2}^{p+1} \frac{\Delta t^i}{i!} \mathcal{D}^{i-1} f(z_n) + O(\Delta t^{p+2}) \\ &= z_n + \Delta t f(z_n) + \sum_{i=2}^p \frac{\Delta t^i}{i!} \mathcal{D}^{i-1} f(z_n) + \Delta t^{p+1} (f_p(z_n) + \frac{\mathcal{D}^p f(z_n)}{(p+1)!}) + O(\Delta t^{p+2}), \end{aligned}$$

then $R_p(z) = (\hat{z} - z_{n+1})/\Delta t^{p+1} = -f_p(z)$. Specially, for the integral-preserving system, we have the following theorem.

Theorem 2.1. *Applying a discrete gradient method $z_{n+1} = \varphi_{\Delta t}(z_n)$ to integral-preserving system (1), then the resulting discretization can be taken as the exact solution of the following modified equations*

$$\dot{\tilde{z}} = f(\tilde{z}) + \sum_{i=1}^{\infty} \Delta t^i f_i(\tilde{z}) = S(\tilde{z}) \nabla I(\tilde{z}) + \sum_{i=1}^{\infty} \Delta t^i S_i(\tilde{z}) \nabla I(\tilde{z}). \quad (8)$$

Proof. Assume the first r -terms $f_i(z), 1 \leq i \leq r$ can be written in the form $f_i(z) = S_i(z) \nabla I(z)$. Consider the r -order truncation of modified equations (8), it is written in the following formulation by the assumption

$$\dot{\tilde{z}} = f(\tilde{z}) + \Delta t f_1(\tilde{z}) + \dots + \Delta t^r f_r(\tilde{z}) = S(\tilde{z}) \nabla I(\tilde{z}) + \sum_{i=1}^r \Delta t^i S_i(\tilde{z}) \nabla I(\tilde{z}). \quad (9)$$

Suppose $\tilde{z} = \psi_{r,t}(z)$ is the solution of (9), then

$$\varphi_{\Delta t}(z) = \psi_{r,\Delta t}(z) + \Delta t^{r+2} f_{r+1}(z) + O(\Delta t^{r+3}).$$

Further,

$$\begin{aligned} I(z) = I(\varphi_{\Delta t}(z)) &= I(\psi_{r,\Delta t}(z) + \Delta t^{r+2} f_{r+1} + O(\Delta t^{r+3})) \\ &= I(\psi_{r,\Delta t}(z)) + \Delta t^{r+2} (\nabla I)^T f_{r+1} + O(\Delta t^{r+3}) \\ &= I(z) + \Delta t^{r+2} (\nabla I)^T f_{r+1} + O(\Delta t^{r+3}). \end{aligned}$$

By comparing both sides of the above equality, we derive

$$(\nabla I)^T f_{r+1} = 0$$

which implies that $f_{r+1} = S_{r+1} \nabla I$ with S_{r+1} being a skew-symmetric matrix. \square

For constructing the high-order integral-preserving integrators, from the above analysis we know that the calculation of modification terms R_i is important. From Theorem 2.1, it is clear that the modification terms R_i can be expressed in the form of $R_i(z) = \mathcal{S}_i(z) \nabla I(z)$. Therefore, we suppose that the modification equations of (1) derived by absorbing \mathbf{N} error terms is written as

$$\dot{z} = \sum_{i=0}^{\mathbf{N}} \Delta t^i \mathcal{S}_i(z) \nabla I(z), \quad (10)$$

where $\mathcal{S}_0(z) \nabla I(z) = f(z)$. The modification terms $\mathcal{S}_i(z)$ are calculated from the following theorem.

Theorem 2.2. $\mathcal{S}_i(z), 1 \leq i \leq \mathbf{N}$ can be derived by the following recursive formula

$$(\mathcal{S}_i)_{jp} I_0^p = \frac{1}{(i+1)!} \mathcal{D}^i f^j - (\mathcal{S}_0)_{jp} I_i^p - \sum_{l=1}^{i-1} (\mathcal{S}_l)_{jp} I_{i-l}^p, \quad (11)$$

$$\begin{aligned} (\mathcal{S}_0)_{jl} I_{N-1}^l = & - \sum_{i=1}^{N-2} (\mathcal{S}_i)_{jl} I_{N-i-1}^l + \sum_{i=0}^{N-2} \sum_{n=2}^{N-i} \sum_{\substack{p_1 + \dots + p_{n-1} \\ = N-i-1}} (\mathcal{S}_i)_{jl} A_{li_2 \dots i_n} \left(\sum_{i=0}^{p_1-1} (\mathcal{S}_i)_{i_2 m_1} I_{p_1-i-1}^{m_1} \right) \cdots \\ & \left(\sum_{i=0}^{p_n-1} (\mathcal{S}_i)_{i_n m_{n-1}} I_{p_n-1-i-1}^{m_{n-1}} \right), \end{aligned} \quad (12)$$

where $I_0 = I, \mathcal{S}_0 = \mathcal{S}$, \mathcal{D} is the derivative operator $\mathcal{D} = f^l \frac{\partial}{\partial z^l}$, $A_{li_2 \dots i_n}, l, i_2, \dots, i_n \geq 1$ are the coefficients of discrete gradient $\bar{\nabla} I(z_{k+1}, z_k)$ by Taylor expansion

$$\begin{aligned} (\bar{\nabla} I(z', z))_l = & I_0^l + B_{lp} (z'^p - z^p) + M_{lpj} (z'^p - z^p) (z'^j - z^j) + \cdots \\ = & I_0^l + \sum_{n=2}^{\infty} \sum_{i_2, \dots, i_n \geq 1} A_{li_2 \dots i_n} (z'^{i_2} - z^{i_2}) \cdots (z'^{i_n} - z^{i_n}). \end{aligned} \quad (13)$$

Proof. According to the definition of discrete gradient, $\bar{\nabla} I(z_{k+1}, z_k)$ can be expanded in the form of (13). Applying a discrete gradient method $z_{k+1} = \varphi_{\Delta t}(z_k)$ to \mathbf{N} -modification equations (10), then it is clear that $\bar{\nabla} I(z_{k+1}, z_k)$ can also be expanded in a series with respect to Δt

$$\bar{\nabla} I(z_{k+1}, z_k) = I_0 + \Delta t I_1 + \Delta t^2 I_2 + \cdots. \quad (14)$$

Therefore, we have

$$\begin{aligned}
z_{k+1}^j - z_k^j &= \sum_{i=0}^{\mathbf{N}} \Delta t^{i+1} (\mathcal{S}_i(z_k))_{jp} (\bar{\nabla} I(z_{k+1}, z_k))_p \\
&= \sum_{i=0}^{\mathbf{N}} \Delta t^{i+1} (\mathcal{S}_i(z_k))_{jp} (I_0^p + \Delta t I_1^p + \Delta t^2 I_2^p + \dots) \\
&= \sum_{i=0}^{\mathbf{N}} \Delta t^{i+1} (\mathcal{S}_i(z_k))_{jp} \left(\sum_{l=0}^{\infty} \Delta t^l I_l^p \right) \\
&= \sum_{l=1}^{\mathbf{N}+1} \Delta t^l \sum_{i=0}^{l-1} (\mathcal{S}_i(z_k))_{jp} I_{l-i-1}^p + \sum_{l=\mathbf{N}+2}^{\infty} \Delta t^l \sum_{i=0}^{\mathbf{N}} (\mathcal{S}_i(z_k))_{jp} I_{l-i-1}^p.
\end{aligned} \tag{15}$$

With the use of notation $\mathcal{D} = f^l \frac{\partial}{\partial z^l}$, we can expand the exact solution of (1) as

$$\begin{aligned}
z^j(t_{k+1}) - z^j(t_k) &= \Delta t f^j(z_k) + \frac{\Delta t^2}{2} \mathcal{D} f^j(z_k) + \dots \\
&= \sum_{l=1}^{\infty} \frac{\Delta t^l}{l!} \mathcal{D}^{l-1} f^j(z_k).
\end{aligned} \tag{16}$$

Let $z_k^j = z^j(t_k)$ and noticing $z^j(t_{k+1}) - z_{k+1}^j = O(\Delta t^{\mathbf{N}+2})$, we obtain the following equality by comparing (15) with (16),

$$\frac{1}{(i+1)!} \mathcal{D}^i f^j - (\mathcal{S}_0)_{jp} I_i^p - \sum_{l=1}^{i-1} (\mathcal{S}_l)_{jp} I_{i-l}^p = (\mathcal{S}_i)_{jp} I_0^p, i = 1, \dots, \mathbf{N} + 1. \tag{17}$$

For getting the value of I_l , $l \geq 1$, we expand (15) by using (13)

$$z_{k+1}^j - z_k^j = \Delta t \left(\sum_{i=0}^{\mathbf{N}} \Delta t^i (\mathcal{S}_i(z_k))_{jl} (I_0^l + B_{lp} (z_{k+1}^p - z_k^p) + M_{lpj} (z_{k+1}^p - z_k^p) (z_{k+1}^j - z_k^j) + \dots) \right). \tag{18}$$

It follows by substituting (15) into (18)

$$\begin{aligned}
z_{k+1}^j - z_k^j &= \sum_{i=0}^{\mathbf{N}} \Delta t^{i+1} (\mathcal{S}_i(z_k))_{jl} I_0^l + \sum_{N=2}^{\infty} \Delta t^N \sum_{i=0}^{N-2} \sum_{n=2}^{N-i} \sum_{\substack{p_1 + \dots + p_{n-1} \\ = N-i-1}} (\mathcal{S}_i)_{jl} A_{li_2 \dots i_n} \left(\sum_{i=0}^{p_1-1} (\mathcal{S}_i)_{i_2 m_1} I_{p_1-i-1}^{m_1} \right) \dots \\
&\quad \left(\sum_{i=0}^{p_n-1} (\mathcal{S}_i)_{i_n m_{n-1}} I_{p_n-1-i-1}^{m_{n-1}} \right),
\end{aligned} \tag{19}$$

where $\mathcal{S}_i(z) = 0$, when $i \geq \mathbf{N} + 1$. The combination of (15) and (19) provides us

$$(\mathcal{S}_0)_{jl} I_{N-1}^l = - \sum_{i=1}^{N-2} (\mathcal{S}_i)_{jl} I_{N-i-1}^l + \sum_{i=0}^{N-2} \sum_{n=2}^{N-i} \sum_{\substack{p_1 + \dots + p_{n-1} \\ = N-i-1}} (\mathcal{S}_i)_{jl} A_{li_2 \dots i_n} \left(\sum_{i=0}^{p_1-1} (\mathcal{S}_i)_{i_2 m_1} I_{p_1-i-1}^{m_1} \right) \dots \left(\sum_{i=0}^{p_{n-1}-1} (\mathcal{S}_i)_{i_n m_{n-1}} I_{p_{n-1}-i-1}^{m_{n-1}} \right)$$

with $\mathcal{S}_i = 0, i \geq \mathbf{N} + 1$. □

Remark 2.3. From (11), we know \mathcal{S}_i depends on $\mathcal{S}_l (0 \leq l \leq i-1)$ and $I_l (0 \leq l \leq i)$. And from (12), it is known that I_{N-1} depends on $\mathcal{S}_l (0 \leq l \leq N-2)$ and $I_l (0 \leq l \leq N-2)$. Therefore, the procedure for getting the modification terms $\mathcal{S}_i (i \geq 1)$ can be illustrated as follows

$$(\mathcal{S}_0, I_0) \implies I_1 \implies \mathcal{S}_1 \implies I_2 \implies \mathcal{S}_2 \dots$$

With $\mathcal{S}_i (0 \leq i \leq p)$, the $p+1$ -order integral-preserving numerical methods can be constructed by

$$z_{k+1} - z_k = \Delta t \left(\sum_{i=0}^p \Delta t^i \mathcal{S}_i(z_k) \right) \bar{\nabla} I(z_{k+1}, z_k).$$

3 Multi-symplectic Hamiltonian systems

Multi-symplectic geometry is introduced in two different ways [12] and [19] for dealing with Hamiltonian PDEs. Based on this geometry, Hamiltonian PDEs are treated as the finite-dimensional multi-symplectic Hamiltonian systems defined on bundle coordinate space. This provides us a new way to study Hamiltonian PDEs. By the inverse variational principle [1], some conservative PDEs, for instance, KDV equation, Schrödinger equation, wave equation etc. allow for the multi-symplectic formulation. In this section, first we give a brief introduction of multi-symplectic Hamiltonian systems based on [19].

Consider the following first-order PDEs

$$Mz_t + Kz_x = \nabla S(z), z \in \mathbf{R}^d \tag{20}$$

with two skew-symmetric matrices M and K . Multi-symplectic reformulation (20) of conservative PDEs is interesting for several reasons. One of them is the existence of the following properties:

The multi-symplectic conservation law is

$$\frac{\partial}{\partial t} dz \wedge M dz + \frac{\partial}{\partial x} dz \wedge K dz = 0. \tag{21}$$

The local energy conservation law is

$$\frac{\partial}{\partial t} \left(S(z) - \frac{1}{2} z^T K z_x \right) + \frac{1}{2} \frac{\partial}{\partial x} z^T K z_t = 0. \tag{22}$$

And the local momentum conservation law is

$$\frac{1}{2} \frac{\partial}{\partial t} (z^T M z_x) + \frac{\partial}{\partial x} (S(z) - \frac{1}{2} z^T M z_t) = 0. \quad (23)$$

We demonstrate the above introduction with nonlinear Schrödinger equation.

Example 3.1. Nonlinear Schrödinger equation

$$i\psi_t + \psi_{xx} + |\psi|^2\psi = 0. \quad (24)$$

Let $\psi = p + qi$ and by introducing two new variables $q_x = v$, $p_x = w$, (24) can be rewritten as

$$p_t + v_x = -(p^2 + q^2)q, \quad (25)$$

$$-q_t + w_x = -(q^2 + p^2)p, \quad (26)$$

$$q_x = v, \quad p_x = w. \quad (27)$$

Denote $E(z) = \frac{1}{2}(\frac{1}{2}(p^2 + q^2)^2 - v^2 - w^2)$ and $F(z) = vp_t + wq_t$, (25) has the local energy conservation law

$$\frac{\partial E(z)}{\partial t} + \frac{\partial F(z)}{\partial x} = 0. \quad (28)$$

And the local momentum conservation law is also formulated as

$$\frac{\partial I(z)}{\partial t} + \frac{\partial G(z)}{\partial x} = 0, \quad (29)$$

where $I(z) = \frac{1}{2}(pw - qv)$ and $G(z) = \frac{1}{2}(v^2 + w^2 + \frac{1}{2}(p^2 + q^2)^2) - \frac{1}{2}(pq_t - qp_t)$. By adding the appropriate boundary conditions, for example, periodic boundary condition, the global conservation laws for (24) are stated as follows

$$\begin{aligned} 0 &= \frac{d}{dt} \int E(z) dx = \frac{d}{dt} \int \frac{1}{2} (\frac{1}{2}(p^2 + q^2)^2 - v^2 - w^2) dx \\ &= \frac{d}{dt} \int \frac{1}{2} (\frac{1}{2}(p^2 + q^2)^2 - (q_x)^2 - (p_x)^2) dx \\ &= \frac{d}{dt} \int (\frac{1}{4} |\psi|^4 - \frac{1}{2} |\psi_x|^2) dx, \end{aligned}$$

$$\begin{aligned} 0 &= \frac{d}{dt} \int I(z) dx = \frac{d}{dt} \int \frac{1}{2} (pw - qv) dx \\ &= \frac{d}{dt} \int \frac{1}{2} (pp_x - qq_x) dx \\ &= \frac{d}{dt} \int \frac{1}{2} \text{Re}(\psi \bar{\psi}_x) dx. \end{aligned}$$

We discretize (20) by applying s -stage and r -stage Runge-Kutta (R-K) method both in temporal direction and spatial direction [19], respectively. It follows

$$z_m^1 - z_m^0 = \Delta t \sum_{i=1}^s b_i \partial_t Z_{i,m}, \quad (30)$$

$$Z_{i,m} - z_m^0 = \Delta t \sum_{j=1}^s a_{ij} \partial_t Z_{j,m}, \quad (31)$$

$$z_1^i - z_0^i = \Delta x \sum_{m=1}^r \tilde{b}_m \partial_x Z_{i,m}, \quad (32)$$

$$Z_{i,m} - z_0^i = \Delta x \sum_{n=1}^r \tilde{a}_{mn} \partial_x Z_{i,n}, \quad (33)$$

$$M \partial_t Z_{i,m} + K \partial_x Z_{i,m} = \nabla S(Z_{i,m}). \quad (34)$$

When the coefficients $a_{ij}, \tilde{a}_{mn}, b_i, \tilde{b}_m, i, j = 1, \dots, s, m, n = 1, \dots, r$ of (30)-(34) satisfy

$$b_i a_{ij} + b_j a_{ji} - b_i b_j = 0, \quad i, j = 1, \dots, s \quad (35)$$

$$\tilde{b}_m \tilde{a}_{mn} + \tilde{b}_n \tilde{a}_{nm} - \tilde{b}_n \tilde{b}_m = 0, \quad m, n = 1, \dots, r, \quad (36)$$

it has been proved that the integrator (30-34) is multi-symplectic, and preserves the discrete multi-symplectic conservation law [4]

$$\Delta x \sum_{m=1}^r (dz_m^1 \wedge M dz_m^1 - dz_m^0 \wedge M dz_m^0) + \Delta t \sum_{i=1}^s (dz_1^i \wedge K dz_1^i - dz_0^i \wedge K dz_0^i) = 0.$$

In [21], it is also shown, the multi-symplecticity of numerical methods implies the preservation of quadratic conservation laws of systems

$$\Delta x \sum_{m=1}^r \tilde{b}_m (z_m^1 - z_m^0)^T \bar{L}_1 (z_m^1 + z_m^0) + \Delta t \sum_{i=1}^s b_i (z_1^i - z_0^i)^T \bar{L}_2 (z_0^i + z_1^i) = 0,$$

where \bar{L}_1 and \bar{L}_2 are two symmetric matrices. Since the local energy and momentum conservation laws are not always in the quadratic formulation, generally, the multi-symplecticity of integrators can not naturally bring us the preservation of energy and momentum. It is our interest to construct the new numerical methods which can preserve the local energy and momentum exactly.

Rewrite (20) as

$$K z_x = \nabla S(z) - M z_t. \quad (37)$$

Applying r -stage symplectic R-K methods to (37) in space, it is obtained

$$\begin{aligned} z_1 &= z_0 + \Delta x \sum_{m=1}^r \tilde{b}_m \partial_x Z_m, \\ Z_m &= z_0 + \Delta x \sum_{n=1}^r \tilde{a}_{mn} \partial_x Z_n, \\ K \partial_x Z_m &= \nabla S(Z_m) - M(Z_m)_t. \end{aligned} \quad (38)$$

By denoting $Z_{dr \times 1} = (Z_1^T, \dots, Z_r^T)^T$, (38) is expressed in a compact form

$$\begin{aligned}\bar{K}Z - \bar{K}z_0 &= \Delta x \bar{\bar{A}}(\nabla \bar{S}(Z) - \bar{M}Z_t), \\ Kz_1 - Kz_0 &= \Delta x \tilde{b}(\nabla \bar{S}(Z) - \bar{M}Z_t),\end{aligned}\tag{39}$$

where $\bar{K}_{dr \times dr} = \text{diag}(K, \dots, K)$, $(\nabla \bar{S}(Z))_{dr \times 1} = ((\nabla S(Z_1))^T, \dots, (\nabla S(Z_r))^T)^T$, $\tilde{b}_{d \times dr} = (\tilde{b}_1 I_{d \times d}, \dots, \tilde{b}_r I_{d \times d})$, $\bar{\bar{A}}_{dr \times dr} = \begin{pmatrix} \tilde{a}_{11} I_{d \times d} & \cdots & \tilde{a}_{1r} I_{d \times d} \\ \cdots & \cdots & \cdots \\ \tilde{a}_{r1} I_{d \times d} & \cdots & \tilde{a}_{rr} I_{d \times d} \end{pmatrix}$. Suppose $\bar{\bar{A}}$ is reversible, it follows from (39) that

$$\begin{aligned}\bar{M}Z_t &= \nabla \bar{S}(Z) - \frac{1}{\Delta x} \bar{\bar{A}}^{-1}(\bar{K}Z - \bar{K}z_0), \\ Kz_1 - Kz_0 &= \tilde{b} \bar{\bar{A}}^{-1}(\bar{K}Z - \bar{K}z_0).\end{aligned}\tag{40}$$

Choosing N as the number of spatial grid points. With the periodic boundary condition $z_0 = z_N$, (40) is rewritten over all spatial grid points

$$\mathbb{K}z = \mathbb{K}Ez + \bar{\bar{b}}D\bar{\mathbb{K}}Z - \bar{\bar{b}}D\bar{\mathbb{K}}\bar{E}z,\tag{41}$$

$$\bar{\mathbb{M}}Z_t = \nabla \bar{S}(Z) - \frac{1}{\Delta x} D(\bar{\mathbb{K}}Z - \bar{\mathbb{K}}\bar{E}z),\tag{42}$$

where $z_{dN \times 1} = (z_1^T, \dots, z_N^T)^T$, $Z_{drN \times 1} = ((Z^1)^T, \dots, (Z^N)^T)^T$, $\bar{\bar{b}}_{dN \times drN} = \begin{pmatrix} \tilde{b} & \cdots & \cdots & \tilde{b} \\ \cdots & \cdots & \cdots & \cdots \\ \tilde{b} & \cdots & \cdots & \tilde{b} \end{pmatrix}$,

$D_{drN \times drN} = \text{diag}(\bar{\bar{A}}^{-1}, \dots, \bar{\bar{A}}^{-1})$, $\mathbb{K}_{dN \times dN} = \text{diag}(K, \dots, K)$, $\bar{\mathbb{K}}_{drN \times drN} = \text{diag}(\bar{K}, \dots, \bar{K})$. Denote the identity matrix by I , $E_{dN \times dN}$ and $\bar{E}_{drN \times drN}$ are, respectively, expressed as $E_{dN \times dN} = \begin{pmatrix} 0 & \cdots & \cdots & I_{d \times d} \\ I_{d \times d} & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & I_{d \times d} & \cdots & \cdots \end{pmatrix}$, $\bar{E}_{drN \times drN} = \begin{pmatrix} 0 & \cdots & \cdots & I_{dr \times dr} \\ I_{dr \times dr} & \cdots & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots \\ 0 & I_{dr \times dr} & \cdots & \cdots \end{pmatrix}$, $(\nabla \bar{S}(Z))_{drN \times 1} = (\nabla \bar{S}(Z^1)^T, \dots, \nabla \bar{S}(Z^N)^T)^T$.

The notations $\bar{\bar{B}}_{drN \times drN} = \text{diag}(\bar{\bar{B}}_{dr \times dr}, \dots, \bar{\bar{B}}_{dr \times dr})$, $\bar{\bar{B}}_{dr \times dr} = \text{diag}(\tilde{b}_1 I_{d \times d}, \dots, \tilde{b}_r I_{d \times d})$ are used here and the geometric property of systems (41-42) is revealed by the following theorem.

Theorem 3.2. *The solution flow of systems (41) and (42) can preserve the following geometric structure*

$$\frac{d}{dt}(dZ \wedge \bar{\bar{B}}\bar{\mathbb{M}}dZ) = 0.\tag{43}$$

Proof. Taking the exterior differential and the wedge product $\bar{\bar{B}}dZ$ on both sides of equality (42), we proceed with

$$\bar{\bar{B}}dZ \wedge \bar{\mathbb{M}}dZ_t = -\frac{1}{\Delta x} \bar{\bar{B}}dZ \wedge (D\bar{\mathbb{K}}dZ - D\bar{\mathbb{K}}\bar{E}dz),\tag{44}$$

where $(\frac{\partial^2 \bar{S}(\mathcal{Z})}{\partial \bar{Z}^2})^T = \frac{\partial^2 \bar{S}(\mathcal{Z})}{\partial \bar{Z}^2}$ has been used. With $E^T \mathbb{K} E = \mathbb{K}$ and $\bar{\mathbb{K}} D = D \bar{\mathbb{K}}$, it follows from (41)

$$\begin{aligned}
dz \wedge \mathbb{K} dz &= (Edz + \bar{b} D d\mathcal{Z} - \bar{b} D \bar{E} dz) \wedge (\mathbb{K} Edz + \bar{b} D \bar{\mathbb{K}}(d\mathcal{Z} - \bar{E} dz)) \\
&= dz \wedge E^T \mathbb{K} E dz + \bar{B} D (d\mathcal{Z} - \bar{E} dz) \wedge \bar{\mathbb{K}} \bar{E} dz + \bar{E} dz \wedge \bar{B} D \bar{\mathbb{K}}(d\mathcal{Z} - \bar{E} dz) \\
&\quad + \bar{b} D (d\mathcal{Z} - \bar{E} dz) \wedge \bar{b} D \bar{\mathbb{K}}(d\mathcal{Z} - \bar{E} dz) \\
&= dz \wedge \mathbb{K} dz + (-\bar{B} D - D^T \bar{B} + D^T \bar{b}^T \bar{b} D)(d\mathcal{Z} - \bar{E} dz) \wedge \bar{\mathbb{K}}(d\mathcal{Z} - \bar{E} dz) \\
&\quad + \bar{B} D (d\mathcal{Z} - \bar{E} dz) \wedge \bar{\mathbb{K}} d\mathcal{Z} + d\mathcal{Z} \wedge \bar{B} D \bar{\mathbb{K}}(d\mathcal{Z} - \bar{E} dz) \\
&= dz \wedge \mathbb{K} dz + 2d\mathcal{Z} \wedge \bar{B} D \bar{\mathbb{K}}(d\mathcal{Z} - \bar{E} dz).
\end{aligned} \tag{45}$$

By substituting (44) into (45), this is further transformed to

$$dz \wedge \mathbb{K} dz = dz \wedge \mathbb{K} dz - 2\Delta x d\mathcal{Z} \wedge \bar{B} \bar{\mathbb{M}} d\mathcal{Z}_t.$$

(43) can be derived from the above equality. This completes the proof of this theorem. \square

Remark 3.3. If a differential equation can be determined by (41) and (42)

$$\bar{\mathbb{M}} \mathcal{Z}_t = F(\mathcal{Z}), \tag{46}$$

it reads from the above theorem that

$$0 = d\mathcal{Z} \wedge \bar{B} \bar{\mathbb{M}} d\mathcal{Z}_t = d\mathcal{Z} \wedge \bar{B} F'(\mathcal{Z}) d\mathcal{Z}. \tag{47}$$

This implies that $\bar{B} F'(\mathcal{Z})$ is a symmetric matrix, i.e., there is a function $G(\mathcal{Z})$ such that $\bar{B} F(\mathcal{Z}) = \nabla G(\mathcal{Z})$. Therefore, (46) can be rewritten as

$$\bar{B} \bar{\mathbb{M}} \mathcal{Z}_t = \nabla G(\mathcal{Z}), \tag{48}$$

By using $(\bar{B} \bar{\mathbb{M}})^T = \bar{B} \bar{\mathbb{M}}$, it leads to

$$0 = \mathcal{Z}_t^T \bar{B} \bar{\mathbb{M}} \mathcal{Z}_t = \mathcal{Z}_t^T \nabla G(\mathcal{Z}) = \frac{d}{dt} G(\mathcal{Z}),$$

i.e., $G(\mathcal{Z})$ is a first integral of (46).

4 High-order energy-conserving numerical methods

In the above section, we observe the multi-symplectic system and analyze the semi-discrete system obtained by using the symplectic R-K methods in space. Our new numerical methods constructed

in the section are based on the analysis. Using the symplectic R-K method in space and the higher-order discrete gradient method in time, we derive the following numerical methods

$$z_1^{1/2} = z_0^{1/2} + \Delta x \sum_{m=1}^r \tilde{b}_m \partial_x Z_{m1}, \quad (49)$$

$$Z_{m1} = z_0^{1/2} + \Delta x \sum_{n=1}^r \tilde{a}_{mn} \partial_x Z_{n1}, \quad (50)$$

$$z_m^1 = z_m^0 + \Delta t \partial_t Z_{m1}, \quad (51)$$

$$Z_{m1} = z_m^0 + \frac{\Delta t}{2} \partial_t Z_{m1}, \quad (52)$$

$$\tilde{M}(z_m^1, z_m^0, \Delta t, \Delta x) \partial_t Z_{m1} + K \partial_x Z_{m1} = \bar{\nabla} S(z_m^1, z_m^0), \quad (53)$$

where $\tilde{M}(z_m^1, z_m^0, \Delta t, \Delta x)$ is a skew-symmetric matrix and p -order approximation of M which satisfying

$$\tilde{M}(z_m^1, z_m^0, \Delta t, \Delta x) = M + O(\Delta t^p),$$

$\bar{\nabla}$ is the discrete gradient operator, which satisfies

$$(x - y)^T \bar{\nabla} S(x, y) = S(x) - S(y).$$

Here, we have used the notations

$$z_1^{1/2} = \frac{1}{2}(z_1^1 + z_1^0), z_1^1 \approx z(\Delta x, \Delta t), Z_{m1} \approx z(c_m \Delta x, \Delta t/2), z_m^1 \approx z(c_m \Delta x, \Delta t), \partial_t Z_{m1} \approx z_t(c_m \Delta x, \Delta t/2)$$

Theorem 4.1. *Applying the new numerical methods (49-53) to multi-symplectic Hamiltonian systems (20), the resulting discretization conserves exactly the following discrete energy conservation law*

$$\Delta x \sum_{m=1}^r \tilde{b}_m (E(z_m^1) - E(z_m^0)) + \Delta t (F(z_1^{1/2}) - F(z_0^{1/2})) = 0, \quad (54)$$

where

$$E(z_m^0) = S(z_m^0) + \frac{1}{2} (\partial_x z_m^0)^T K z_m^0,$$

$$F(z_0^{1/2}) = -\frac{1}{2} (\partial_t z_0^{1/2})^T K z_0^{1/2}$$

with $\partial_x z_m^0$ and $\partial_t z_0^{1/2}$ satisfying $z_m^0 = z_0^0 + \Delta x \sum_{n=1}^r \tilde{a}_{mn} (\partial_x z)_n^0$, $z_0^{1/2} = z_0^0 + \frac{\Delta t}{2} (\partial_t z)_0^{1/2}$.

Proof. To evaluate the discrete energy conservation law, it is natural to introduce four auxiliary

equations

$$\partial_t z_1^{1/2} = \partial_t z_0^{1/2} + \Delta x \sum_{m=1}^r \tilde{b}_m \partial_x (\partial_t Z_{m1}), \quad (55)$$

$$\partial_t Z_{m1} = \partial_t z_0^{1/2} + \Delta x \sum_{n=1}^r \tilde{a}_{mn} \partial_x (\partial_t Z_{n1}), \quad (56)$$

$$\partial_x z_m^1 = \partial_x z_m^0 + \Delta t \partial_t (\partial_x Z_{m1}), \quad (57)$$

$$\partial_x Z_{m1} = \partial_x z_m^0 + \frac{\Delta t}{2} \partial_t (\partial_x Z_{m1}) \quad (58)$$

with

$$z_m^0 = z_0^0 + \Delta x \sum_{n=1}^r \tilde{a}_{mn} (\partial_x z)_n^0, \quad z_0^{1/2} = z_0^0 + \frac{\Delta t}{2} (\partial_t z)_0^{1/2}. \quad (59)$$

Let us check the preservation of conservation law (54), it reads

$$\begin{aligned} E(z_m^1) - E(z_m^0) &= S(z_m^1) + \frac{1}{2} (\partial_x z_m^1)^T K z_m^1 - S(z_m^0) - \frac{1}{2} (\partial_x z_m^0)^T K z_m^0 \\ &= S(z_m^1) - S(z_m^0) + \frac{\Delta t}{2} (\partial_x Z_{m1})^T K \partial_t Z_{m1} + \frac{\Delta t}{2} (\partial_t (\partial_x Z_{m1}))^T K Z_{m1} \\ &= (z_m^1 - z_m^0)^T \bar{\nabla} S(z_m^1, z_m^0) + \frac{\Delta t}{2} (\partial_x Z_{m1})^T K \partial_t Z_{m1} + \frac{\Delta t}{2} (\partial_t (\partial_x Z_{m1}))^T K Z_{m1}. \end{aligned} \quad (60)$$

From (53), we get

$$(z_m^1 - z_m^0)^T \bar{\nabla} S(z_m^1, z_m^0) = \Delta t (\partial_t Z_{m1})^T K \partial_x Z_{m1}. \quad (61)$$

By applying (61) to (60), we gain

$$E(z_m^1) - E(z_m^0) = -\frac{\Delta t}{2} (\partial_x Z_{m1})^T K \partial_t Z_{m1} + \frac{\Delta t}{2} (\partial_t (\partial_x Z_{m1}))^T K Z_{m1}. \quad (62)$$

Similarly, we get

$$\begin{aligned} F(z_1^{1/2}) - F(z_0^{1/2}) &= -\frac{1}{2} (\partial_t z)_1^{1/2} K z_1^{1/2} + \frac{1}{2} (\partial_t z)_0^{1/2} K z_0^{1/2} \\ &= -\frac{\Delta x}{2} \sum_{m=1}^r \tilde{b}_m (\partial_t Z_{m1})^T K \partial_x Z_{m1} - \frac{\Delta x}{2} \sum_{m=1}^r \tilde{b}_m (\partial_x (\partial_t Z_{m1}))^T K Z_{m1}. \end{aligned} \quad (63)$$

It is noticed from (50), (57) and (59) that

$$Z_{m1} = z_0^{1/2} + \Delta x \sum_{n=1}^r \tilde{a}_{mn} \partial_x Z_{n1} = z_0^{1/2} + z_m^0 - z_0^0 + \frac{\Delta t \Delta x}{2} \sum_{n=1}^r \tilde{a}_{mn} \partial_t (\partial_x Z_{n1}), \quad (64)$$

$$Z_{m1} = z_m^0 + \frac{\Delta t}{2} \partial_t Z_{m1} = z_m^0 + z_0^{1/2} - z_0^0 + \frac{\Delta t \Delta x}{2} \sum_{n=1}^r \tilde{a}_{mn} \partial_x (\partial_t Z_{n1}). \quad (65)$$

When matrix $A = (\tilde{a}_{mn})$ is reversible, it implies that

$$\partial_t(\partial_x Z_{n1}) = \partial_x(\partial_t Z_{n1}), \quad n = 1, \dots, r. \quad (66)$$

By using (62), (63) and (66), we conclude that (54) holds. \square

Remark 4.2. Similarly, we can construct the following momentum-conserving numerical methods

$$z_{1/2}^1 = z_{1/2}^0 + \Delta t \sum_{i=1}^s b_i \partial_t Z_{1i}, \quad (67)$$

$$Z_{1i} = z_{1/2}^0 + \Delta t \sum_{j=1}^s a_{ij} \partial_t Z_{1j}, \quad (68)$$

$$z_1^i = z_0^i + \Delta x \partial_x Z_{1i}, \quad (69)$$

$$Z_{1i} = z_0^i + \frac{\Delta x}{2} \partial_x Z_{1i}, \quad (70)$$

$$M \partial_t Z_{1i} + \tilde{K}(z_1^i, z_0^i, \Delta t, \Delta x) \partial_x Z_{1i} = \bar{\nabla} S(z_1^i, z_0^i). \quad (71)$$

It is easy to prove that the numerical methods (67-71) preserve the discrete momentum conservation law

$$\Delta x \sum_{i=1}^s b_i (I(z_1^i) - I(z_0^i)) + \Delta t (G(z_{1/2}^1) - G(z_{1/2}^0)) = 0, \quad (72)$$

where

$$I(z_0^i) = -\frac{1}{2} (\partial_x z_0^i)^T M z_0^i,$$

$$G(z_{1/2}^0) = S(z_{1/2}^0) + \frac{1}{2} (\partial_t z_{1/2}^0)^T M z_{1/2}^0.$$

Remark 4.3. When $r = 1$, the energy-preserving numerical method (49-53) is reduced to

$$M \frac{z_1^{1/2} - z_0^{1/2}}{\Delta t} + K \frac{z_{1/2}^1 - z_{1/2}^0}{\Delta x} = \bar{\nabla} S(z_1^{1/2}, z_0^{1/2}). \quad (73)$$

And when $s = 1$, the momentum-preserving numerical method (67-71) is reduced to

$$M \frac{z_1^{1/2} - z_0^{1/2}}{\Delta t} + K \frac{z_{1/2}^1 - z_{1/2}^0}{\Delta x} = \bar{\nabla} S(z_{1/2}^1, z_{1/2}^0).$$

What follows, let us consider the more general formulation of (20)

$$M(x, z) z_t + K(t, z) z_x = F(x, t, z), \quad (74)$$

where $M(x, z)$ and $K(t, z)$ are two matrices. When $M(x, z)$ and $K(t, z)$ are skew-symmetric and satisfy the following Jacobi identity, respectively,

$$\begin{aligned}\frac{\partial M_{ij}}{\partial z_k} + \frac{\partial M_{ki}}{\partial z_j} + \frac{\partial M_{jk}}{\partial z_i} &= 0, \\ \frac{\partial K_{ij}}{\partial z_k} + \frac{\partial K_{ki}}{\partial z_j} + \frac{\partial K_{jk}}{\partial z_i} &= 0, \\ \frac{\partial F_i(x, t, z)}{\partial z_j} &= \frac{\partial F_j(x, t, z)}{\partial z_i}, \quad i, j = 1, \dots, d,\end{aligned}\tag{75}$$

system (74) is multi-symplectic and satisfies the multi-symplectic conservation law

$$\frac{\partial}{\partial t} dz \wedge M(x, z) dz + \frac{\partial}{\partial x} dz \wedge K(t, z) dz = 0.$$

Remark 4.4. With the coefficients of (74) M_{ij} , K_{ij} and F_i , $i, j = 1, \dots, d$, we define a 3-form on the extended space \mathbf{R}^{2d+2}

$$\omega = \frac{1}{2} \sum_{i,j=1}^d M_{ij}(x, z) dz_i \wedge dz_j \wedge dx + \frac{1}{2} \sum_{i,j=1}^d K_{ij}(t, z) dz_i \wedge dz_j \wedge dt + \sum_{i=1}^d F_i(x, t, z) dz_i \wedge dt \wedge dx.$$

(74) is multi-symplectic if and only if the three form ω is closed. The Poincare Lemma implies that there is a 2-form

$$\theta = \sum_{i=1}^d A_i(x, t, z) dz_i \wedge dx + \sum_{i=1}^d B_i(x, t, z) dz_i \wedge dt + S(x, t, z) dx \wedge dt$$

such that $\omega = d\theta$. And the coefficients $S(x, t, z)$, $A_i(x, t, z)$ and $B_i(x, t, z)$ can be calculated by the following formulae

$$\begin{aligned}S(x, t, z) &= - \sum_{i=1}^d \int_0^1 F_i(\tau x, \tau t, \tau z) \tau^2 z_i d\tau, \quad A_i = - \sum_{j=1}^d \int_0^1 M_{ij}(\tau x, \tau z) \tau z_j d\tau - \int_0^1 F_i(\tau x, \tau t, \tau z) \tau^2 t d\tau, \\ B_i &= - \sum_{j=1}^d \int_0^1 K_{ij}(\tau t, \tau z) \tau z_j d\tau + \int_0^1 F_i(\tau x, \tau t, \tau z) \tau^2 x d\tau, \quad i = 1, 2, \dots, d.\end{aligned}$$

Remark 4.5. If the two matrices $M(x, z)$ and $K(t, z)$ are only skew-symmetric, in general, system (74) will not be multi-symplectic. But it is easy to know that the energy conservation law (22) and the momentum conservation law (23) still hold. And the idea of constructing the energy and momentum conserving numerical methods can be generalized to this kind of systems, when one of $M(x, z)$ and $K(t, z)$ is a constant matrix.

5 Numerical experiments

In this section, with nonlinear Schrödinger equations (24), we present the numerical experiments. We use the new energy-preserving numerical method (73) presented in the last section. Specifically,

for (24), it is written as

$$\begin{aligned}
\frac{q_{i+1/2}^{j+1} - q_{i+1/2}^j}{\Delta t} - \frac{v_{i+1}^{j+1/2} - v_i^{j+1/2}}{\Delta x} &= \frac{((p_{i+1/2}^{j+1})^2 + (q_{i+1/2}^j)^2)^2 - ((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)^2}{4(p_{i+1/2}^{j+1} - p_{i+1/2}^j)}, \\
\frac{p_{i+1/2}^{j+1} - p_{i+1/2}^j}{\Delta t} + \frac{w_{i+1}^{j+1/2} - w_i^{j+1/2}}{\Delta x} &= -\frac{((p_{i+1/2}^{j+1})^2 + (q_{i+1/2}^j)^2)^2 - ((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)^2}{4(q_{i+1/2}^{j+1} - q_{i+1/2}^j)}, \\
\frac{p_{i+1}^{j+1/2} - p_i^{j+1/2}}{\Delta x} &= v_{i+1/2}^{j+1/2}, \\
\frac{q_{i+1}^{j+1/2} - q_i^{j+1/2}}{\Delta x} &= w_{i+1/2}^{j+1/2},
\end{aligned} \tag{76}$$

where $z_{i+1/2}^{j+1/2} = \frac{1}{4}(z_i^{j+1} + z_{i+1}^j + z_{i+1}^{j+1} + z_i^j)$, $z_i^{j+1/2} = z_i^j + z_i^{j+1}$, $z_{i+1/2}^j = z_i^j + z_{i+1}^j$.

After eliminating the medium variables, (76) is equivalent to

$$\begin{aligned}
D_t q_i^j - D_{xx} p_i^j &= \frac{((p_{i+1/2}^{j+1})^2 + (q_{i+1/2}^j)^2)^2 - ((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)^2}{8(p_{i+1/2}^{j+1} - p_{i+1/2}^j)} \\
&\quad + \frac{((p_{i-1/2}^{j+1})^2 + (q_{i-1/2}^j)^2)^2 - ((p_{i-1/2}^j)^2 + (q_{i-1/2}^j)^2)^2}{8(p_{i-1/2}^{j+1} - p_{i-1/2}^j)}, \\
-D_t p_i^j - D_{xx} q_i^j &= \frac{((p_{i+1/2}^{j+1})^2 + (q_{i+1/2}^j)^2)^2 - ((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)^2}{8(q_{i+1/2}^{j+1} - q_{i+1/2}^j)} \\
&\quad + \frac{((p_{i-1/2}^{j+1})^2 + (q_{i-1/2}^j)^2)^2 - ((p_{i-1/2}^j)^2 + (q_{i-1/2}^j)^2)^2}{8(q_{i-1/2}^{j+1} - q_{i-1/2}^j)},
\end{aligned} \tag{77}$$

where $D_t q_i^j = \frac{q_{i+1/2}^{j+1} - q_{i+1/2}^j + q_{i-1/2}^{j+1} - q_{i-1/2}^j}{2\Delta t}$, $D_{xx} q_i^j = \frac{p_{i+1}^{j+1/2} - 2p_i^{j+1/2} + p_{i-1}^{j+1/2}}{\Delta x^2}$. According to Theorem 4.1, we know that (76) can preserve the discrete energy conservation law

$$\frac{E_{i+1/2}^{j+1} - E_{i+1/2}^j}{\Delta t} + \frac{F_{i+1}^{j+1/2} - F_i^{j+1/2}}{\Delta x} = 0 \tag{78}$$

with

$$E_{i+1/2}^j = \frac{1}{4}((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)^2 - \frac{1}{2}((v_{i+1/2}^j)^2 + (w_{i+1/2}^j)^2)$$

and

$$F_i^{j+1/2} = v_i^{j+1/2} \frac{p_i^{j+1} - p_i^j}{\Delta t} + w_i^{j+1/2} \frac{q_i^{j+1} - q_i^j}{\Delta t}.$$

We compute this problem over $[-50, 50]$ till time 100 with the following initial and periodic boundary conditions

$$\psi(x, 0) = \text{sech}(\sqrt{2}x/2) \exp(ix/2) \tag{79}$$

$$\psi(-50, t) = \psi(50, t). \tag{80}$$

To investigate the conservative property of method (77), we define the discrete conservative quantities as follows.

The discrete norm is given by

$$NE_i^j = \frac{P_{i+1/2}^{j+1} - P_{i+1/2}^j}{\Delta t} + \frac{Q_{i+1}^{j+1/2} - Q_i^{j+1/2}}{\Delta x}, \quad (81)$$

where

$$P_{i+1/2}^j = \frac{1}{2}((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)$$

and

$$Q_i^{j+1/2} = w_i^{j+1/2} p_i^{j+1/2} - v_i^{j+1/2} q_i^{j+1/2}.$$

The discrete local energy is defined as

$$LE_i^j = \frac{E_{i+1/2}^{j+1} - E_{i+1/2}^j}{\Delta t} + \frac{F_{i+1}^{j+1/2} - F_i^{j+1/2}}{\Delta x}, \quad (82)$$

where

$$E_{i+1/2}^j = \frac{1}{4}((p_{i+1/2}^j)^2 + (q_{i+1/2}^j)^2)^2 - \frac{1}{2}((v_{i+1/2}^j)^2 + (w_{i+1/2}^j)^2)$$

and

$$F_i^{j+1/2} = v_i^{j+1/2} \frac{p_i^{j+1} - p_i^j}{\Delta t} + w_i^{j+1/2} \frac{q_i^{j+1} - q_i^j}{\Delta t}.$$

And the discrete local momentum is

$$LG_{i+1/2}^{j+1/2} = \frac{I_{i+1/2}^{j+1} - I_{i+1/2}^j}{\Delta t} + \frac{G_{i+1}^{j+1/2} - G_i^{j+1/2}}{\Delta x}, \quad (83)$$

where

$$G_i^{j+1/2} = \frac{1}{2}((v_i^{j+1/2})^2 + (w_i^{j+1/2})^2) + \frac{1}{2}((p_i^{j+1/2})^2 + (q_i^{j+1/2})^2) - \frac{1}{2\Delta t}(p_i^{j+1/2}(q_i^{j+1} - q_i^j) - q_i^{j+1/2}(p_i^{j+1} - p_i^j))$$

and

$$I_{i+1/2}^j = \frac{1}{2}(p_{i+1/2}^j w_{i+1/2}^j - q_{i+1/2}^j v_{i+1/2}^j).$$

The global norm, energy and momentum are derived by taking the sum over the spatial grid points and using the periodic boundary conditions. In the computation, the value of medium variables v, w is calculated by $v_{i+1/2}^j = \frac{1}{\Delta x}(p_{i+1}^j - p_i^j)$, $w_{i+1/2}^j = \frac{1}{\Delta x}(q_{i+1}^j - q_i^j)$, $V^{j+1/2} = \frac{2}{\Delta x}B^{-1}AP^{j+1/2}$

and $W^{j+1/2} = \frac{2}{\Delta x}B^{-1}AQ^{j+1/2}$, where $V^{j+1/2} = (v_1^{j+1/2}, \dots, v_N^{j+1/2})$, $A = \begin{pmatrix} 1 & \dots & \dots & -1 \\ -1 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & -1 & 1 \end{pmatrix}$

and $B = \begin{pmatrix} 1 & \dots & \dots & 1 \\ 1 & 1 & \dots & 0 \\ \dots & \dots & \dots & \dots \\ 0 & \dots & 1 & 1 \end{pmatrix}$. With the time step $\Delta t = 0.05$ and space step $\Delta x = 100/301$, we

compare the error propagation of the conservation of local and global norm, energy and momentum obtained by algorithm (ME) (76) and multi-symplectic numerical algorithm (MS) [21]. The numerical results are shown in the Fig.1-7.

Fig.1 exhibits the global numerical error of global norm conservation by $\sum_i (P_{i+1/2}^j - P_{i+1/2}^1)$. It is shown that the global norm is preserved by MS within roundoff errors of the computer when ME can only preserve the norm in the scale of $O(10^{-2})$. The tolerance 10^{-14} is chosen for solving the nonlinear algebraic systems by the fixed-point iteration methods.

Fig.2 shows the variation of global numerical error for the global energy conservation. ME can conserve the global energy exactly comparing with that MS can only preserve the global energy in the scale of $O(10^{-6})$, but the error as a function of time is decreasing.

We also test the error propagation for the global momentum by using two numerical methods MS and ME in Fig.3. From the figure, we know that MS has the less error than ME and the error is decreasing. ME can preserve the global momentum in the scale of $O(10^{-2})$ and it is bounded.

Furthermore, we demonstrate the preservation of local conservative quantities computed by MS and ME in Fig.4-6.

It is known that with the initial condition (79), (24) has the exact solution

$$\psi = \operatorname{sech}\left(\frac{\sqrt{2}}{2}(x-t)\right) \exp\left(\sqrt{-1}\left(\frac{x-t}{2} + \frac{3t}{4}\right)\right).$$

Taking $\Delta t = 0.006$ and $\Delta x = 100/501$, we exhibit the match between numerical solution and the exact solution by

$$\max_i |u(x_i, t_j) - u(i\Delta x, j\Delta t)|$$

in the last figure. Fig.7 shows the linear growth with a minor difference of maximum error 0.08136271098751 for ME and 0.08004417804602 for MS.

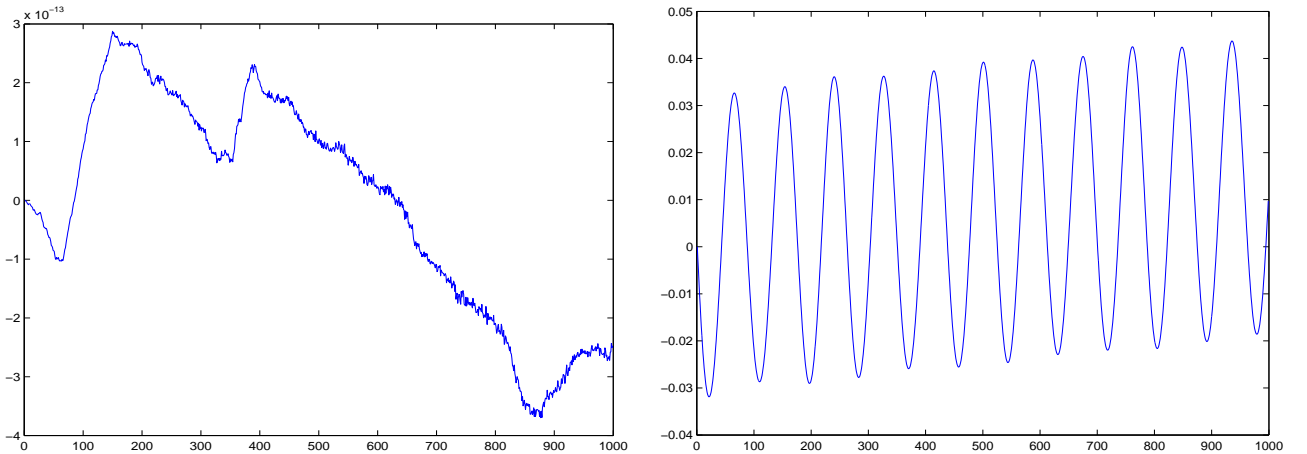


Figure 1. The error of global norm conservation. Left is calculated by MS and right is calculated by ME.

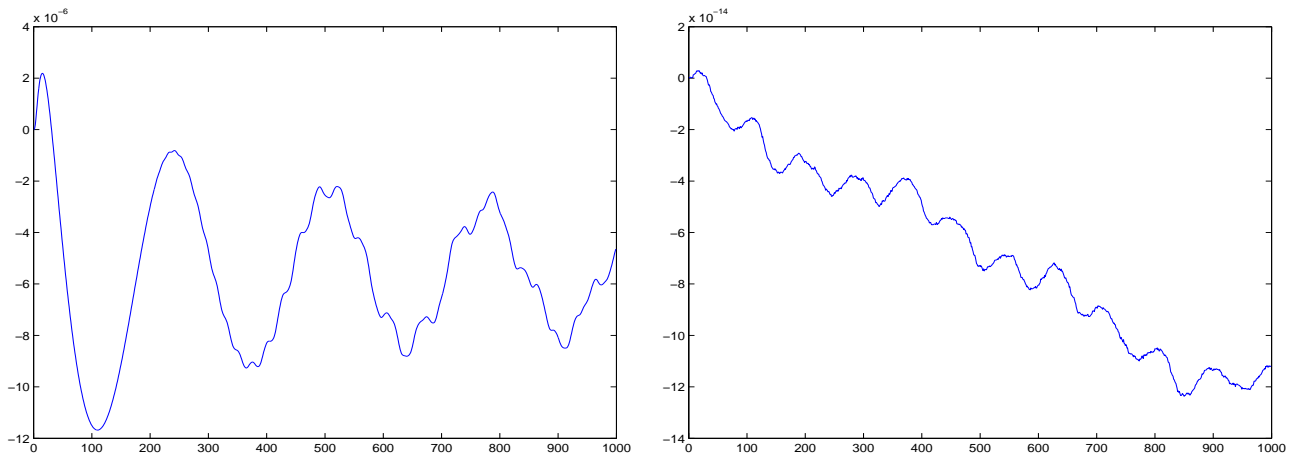


Figure 2. The error of global energy conservation. Left is calculated by MS and right is calculated by ME.

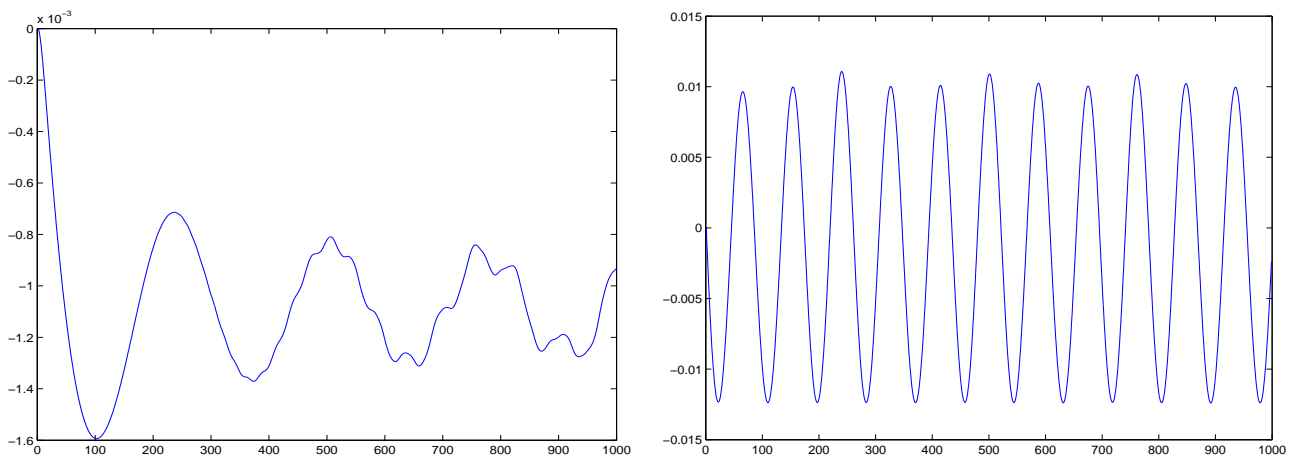


Figure 3. The error of global momentum conservation. Left is calculated by MS and right is calculated by ME.

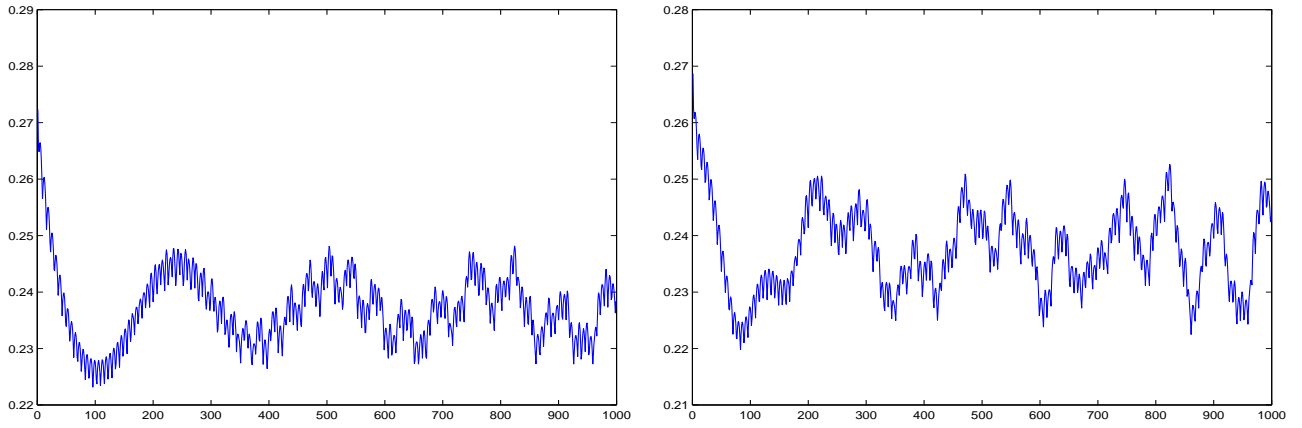


Figure 4. The error of local norm conservation. Left is calculated by MS and right is calculated by ME.

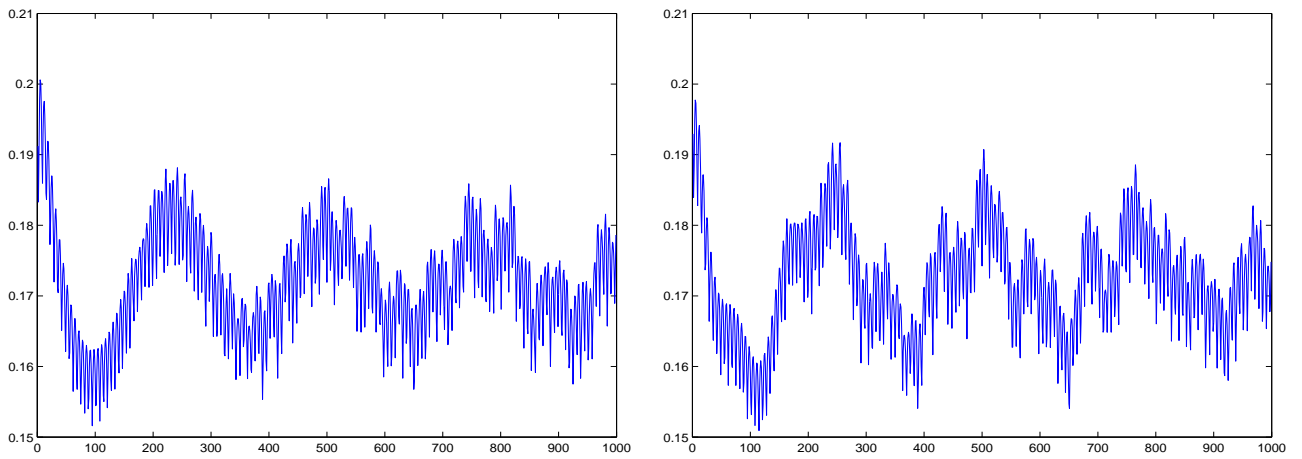


Figure 5. The error of local energy conservation. Left is calculated by MS and right is calculated by ME.

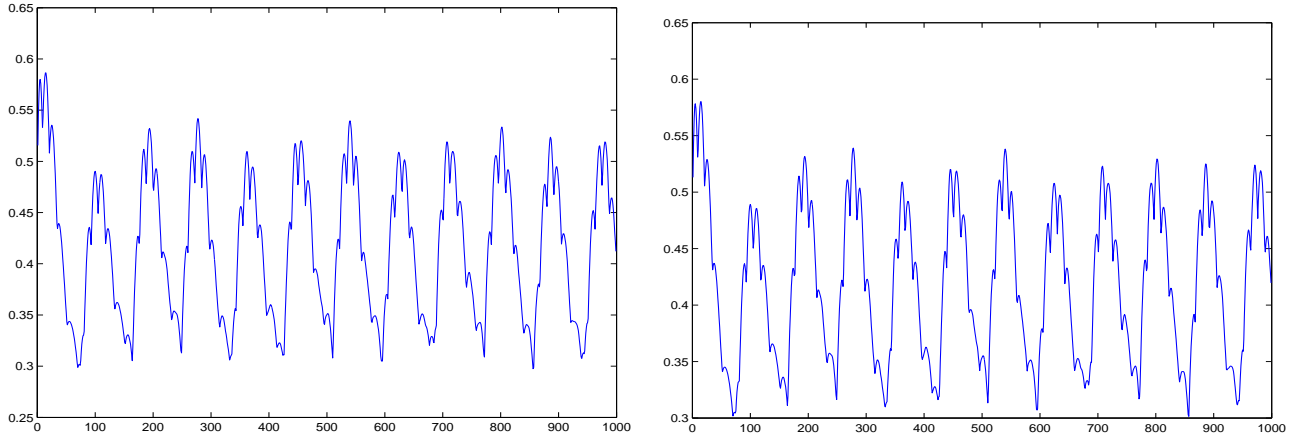


Figure 6. The error of local momentum conservation. Left is calculated by MS and right is calculated by ME.

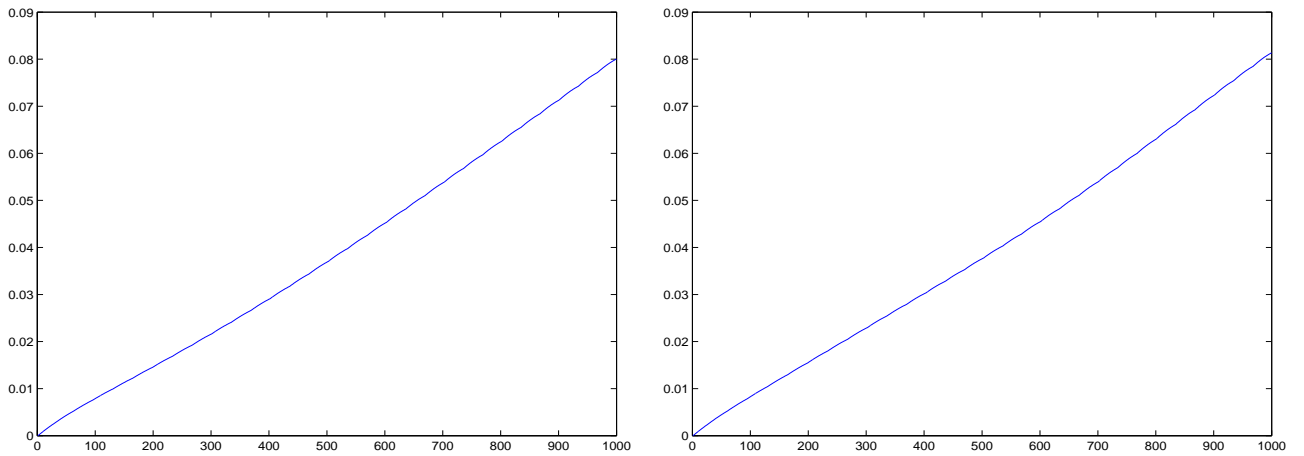


Figure 7. The error of exact solution and numerical solution. Left is calculated by MS and right is calculated by ME.

6 Conclusion

In this paper, we study the discrete gradient methods and present the recursive formula for constructing high-order integral-preserving numerical algorithms. By the use of discrete gradient methods, we have tried to construct the high-order energy-conserving and momentum-conserving numerical algorithms for multi-symplectic Hamiltonian systems. It remains still interesting in the further application of the new numerical algorithms and the implementation of the high-order integrators constructed in this paper.

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