Available online at www.sciencedirect.com
ScienceDirect
Applied Mathematics and Computation 186 (2007) 670–684
APPLIED MATHEMATICS AND COMPUTATION
www.elsevier.com/locate/amc

A survey on symplectic and multi-symplectic algorithms

Linghua Kong [a], Ruxun Liu [a], Xiaohong Zheng [b,*]

[a] Department of Mathematics, University of Science and Technology of China, Hefei, Anhui 230026, PR China
[b] School of Mathematics and Information, Jiaxing Institute, Jiaxing, Zhejiang 314001, PR China

Abstract

We simply review symplectic and multi-symplectic algorithms in the paper. These algorithms have many superiorities to general non-symplectic algorithms, such as: they have long time behavior; they can preserve the symplectic geometry structure of the Hamiltonian system exactly; and they can simulate original physical phenomena well. Some commonly used methods to construct symplectic and multi-symplectic schemes are simply surveyed. Numerical examples are also enumerated to illustrate their performances.

Keywords: Symplectic; Multi-symplectic; Hamiltonian system; Conservation law

1. Introduction

Classical mechanics has three equivalent expressions: *Newton mechanics, Lagrange mechanics and Hamiltonian mechanics* [1,5]. They are different mathematical formulations for the same physical problem, which supply different approaches in solving practical problems. Symplectic geometry (its preliminary knowledge is introduced in appendix) is the foundation of Hamiltonian system. Let H be a differentiable function of $z = (p^1, p^2, \ldots, p^n, q^1, q^2, \ldots, q^n)^{\mathrm{T}} \in R^{2n}$, then the general formulation of Hamiltonian system is

$$\begin{cases} p_t^i = -\frac{\delta H}{\delta q^i} \\ q_t^i = \frac{\delta H}{\delta p^i} \end{cases} \quad \text{for } i = 1, 2, \ldots, n, \tag{1}$$

where $H(z)$ is called *Hamiltonian function*.

That is,

$$z_t = J^{-1}\nabla_z H(z), \quad \text{where } J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}. \tag{2}$$

* Corresponding author.
E-mail addresses: konglh@mail.ustc.edu.cn (L. Kong), liurx@ustc.edu.cn (R. Liu), zhxh0795@sohu.com (X. Zheng).

0096-3003/$ - see front matter
doi:10.1016/j.amc.2006.08.012

The Hamiltonian system (2) has area invariant of phase flow in the phase space, energy invariant and momentum invariant, etc. Its advantages over the other two formations are its symmetric formation and wide applications, etc. Any real physical process with negligible dissipative effect, can be rewritten into the Hamiltonian formulation.

General numerical techniques neglect the intrinsical symplectic geometry structure of the Hamiltonian system. As a result, they are powerful in simulation of short-time physical phenomena, however, may be stringent limitation to those of long time. Is it possible to devise a numerical method that approximates the symplecticity exactly? Such a method is called *symplectic method*.

Definition 1. Any numerical scheme can be regarded as a mapping from this moment to the next. If the mapping is symplectic, i.e., $A^{\mathrm{T}}JA = J$, where J is any skew-symmetric matrix and A is the matrix corresponding to the mapping, we call it *symplectic scheme*.

The symplectic algorithm was first introduced by De Vogelaere [2] in 1956 in a series of unpublished reports. Ruth [3] devised some low order symplectic rules for the separable Hamiltonian system in 1983. Feng [4] put forward the symplectic geometry algorithm firstly and formally for the general Hamiltonian system on the Beijing international "D.D." symposium in 1984. It conserves the property of symplectic transformation character of Hamiltonian system. Its superiorities to general non-symplectic numerical methods are its globality, structure and long-term tracking ability. Thereafter, many researchers have studied in the field (see [6–20,23,24] and references therein).

Furthermore, the symplectic algorithm has been generalized from the finite-dimensional Hamiltonian system to the infinite-dimensional one. The basic technique to design symplectic integrators for an infinite-dimensional Hamiltonian system is dimensional reduction, in other words, the system is discretized in space firstly, and reduces to a system of ODEs, which ought to be a finite-dimensional Hamiltonian system. Then the system is discretized with symplectic integrators in time.

A natural generalization of Hamiltonian ODEs is Hamiltonian PDEs, which possesses symplectic structures both in time and space. Symplectic numerical methods for Hamiltonian ODEs have been well established, notwithstanding, numerical integrator for multi-symplectic Hamiltonian system is a beardless subject. The multi-symplectic numerical integrator was explored by Reichs and Bridges and Marsden in the late 1990s from distinct aspects.

We survey numerical integrators for Hamiltonian mechanics—symplectic algorithm and multi-symplectic algorithm in the paper.

The outline of this paper is as follows: We firstly survey some methods to construct symplectic schemes in Section 2, and introduce the general multi-symplectic formulation and its conservation laws in Section 3. Then, Section 4 reviews some multi-symplectic schemes constructed by combining method. Numerical experiments are enumerated in Section 5 to illustrate the performance of multi-symplectic schemes. Conclusions are set forth in the end.

2. Methods to construct symplectic algorithms

In the following, we review some methods adopted to construct symplectic schemes.

2.1. Generating function methods

During the initial developing stage of the symplectic algorithm, a general technique, applied by most researchers to design symplectic schemes, is the generating function method. This method makes use of the fact that *any transformation derives from a generating function is symplectic*. We give some concrete symplectic schemes designed by the generating function method. Readers who are interested in this method refer to [7–9] for details.

For a function $W = W(q,p')$, the mapping $(q,p) \mapsto (q',p')$ can be determined by

$$p = W_q, \quad q' = W_{p'}.$$

This is a symplectic mapping since W is a *generating function* [10].

If we take $W = qp' + \tau H(q,p')$, then we have

$$q' = q + \tau H_{p'}, \quad p' = p - \tau H_q.$$

This is a first-order symplectic scheme.

If we take $W = qp' + \tau H(q,p') + \frac{1}{2}\tau^2 H_{p'}H_q$, then we have

$$\begin{cases} q' = q + \tau H_{p'} + \frac{1}{2}\tau^2(H_{p'p'}H_q + H_{p'}H_{p'q}), \\ p' = p - \tau H_q - \frac{1}{2}\tau^2(H_{p'q}H_q + H_{p'}H_{qq}), \end{cases}$$

which is a second-order symplectic scheme.

2.2. Runge–Kutta methods

Runge–Kutta method is the most widely used method to numerically simulate the solution of ODEs, which was initiated by Runge and Kutta.

For a given initial value problem of ODE

$$y' = f(t,y), \quad y(0) = y_0, \tag{3}$$

the general formation of an s-stage Runge–Kutta method is

$$\begin{aligned} k_i &= y_n + \tau \sum_{j=1}^{s} a_{ij} f(t_n + c_i\tau, k_j), \quad \text{for } i = 1,2,\ldots,s, \\ y_{n+1} &= y_n + \tau \sum_{j=1}^{s} b_j f(t_n + c_j\tau, k_j), \end{aligned} \tag{4}$$

whose coefficients a_{ij}, b_j, c_j satisfy

$$c_j \geqslant 0, \quad \sum_{j=1}^{s} c_j = 1, \quad \sum_{j=1}^{s} a_{ij} = c_i, \quad \sum_{j=1}^{s} b_j = 1, \quad \text{for } i,j = 1,2,\ldots,s.$$

Theorem 1 [18–20]. *If $b_ib_j - a_{ij}b_i - a_{ji}b_j = 0$ are all satisfied, for $i, j = 1,2,\ldots,s$, then the corresponding Runge–Kutta scheme is symplectic.*

The ordinarily used symplectic Runge–Kutta methods are

$$Z_{n+1} = Z_n + \tau f\left(\frac{Z_{n+1} + Z_n}{2}\right). \tag{5}$$

$$A = \begin{bmatrix} \frac{1}{4} & \frac{1}{4} - \frac{\sqrt{3}}{6} \\ \frac{1}{4} + \frac{\sqrt{3}}{6} & \frac{1}{4} \end{bmatrix}, \quad b = \begin{bmatrix} \frac{1}{2} & \frac{1}{2} \end{bmatrix}, \quad c = \begin{bmatrix} \frac{1}{2} - \frac{\sqrt{3}}{6} & \frac{1}{2} + \frac{\sqrt{3}}{6} \end{bmatrix}. \tag{6}$$

Scheme (5) is the most usually used Euler centered rule, which is an 1-stage second-order scheme. And scheme (6) is a 2-stage fourth-order one.

2.3. Explicit symplectic schemes for the separable Hamiltonian system

For a separable Hamiltonian system, i.e., $H(p,q) = U(p) + V(q)$, we have the m-stage explicit symplectic scheme [13]

$$\begin{cases} (p_0, q_0) = (p_n, q_n), \\ p_{i+1} = p_i + \tau c_{i+1} V_q(q_i), \\ q_{i+1} = q_i + \tau d_{i+1} U_p(p_{i+1}), \\ (p_m, q_m) = (p_{n+1}, q_{n+1}), \end{cases} \quad \text{for } i = 0,1,2,\ldots,m-1, \tag{7}$$

where c_i and d_i are undetermined coefficients.

When $m = 1$, we have $c_1 = d_1 = 1$, that is

$$p_{n+1} = p_n + \tau V_q(q_n), \quad q_{n+1} = q_n + \tau U_p(p_{n+1}).$$

When $m = 2$, we have

$$c_1 = c_2 = \frac{1}{2}, \quad d_1 = 1, \quad d_2 = 0 \quad \text{or} \quad c_1 = 0, \quad c_2 = 1, \quad d_1 = d_2 = \frac{1}{2}.$$

When $m = 3$, we have

$$c_1 = \frac{7}{24}, \quad c_2 = \frac{3}{4}, \quad c_3 = -\frac{1}{24}, \quad d_1 = \frac{2}{3}, \quad d_2 = -\frac{2}{3}, \quad d_3 = 1;$$

or

$$c_1 = 1, \quad c_2 = -\frac{2}{3}, \quad c_3 = \frac{2}{3}, \quad d_1 = -\frac{1}{24}, \quad d_2 = \frac{3}{4}, \quad d_3 = \frac{7}{24}.$$

When $m = 4$, we have

$$c_1 = 0, \quad c_2 = c_4 = \frac{1}{3}(1+\alpha), \quad c_3 = -\frac{1}{3}(2+\alpha), \quad d_1 = d_4 = \frac{1}{6}(2+\alpha), \quad d_2 = d_3 = \frac{1}{6}(1-\alpha);$$

or

$$c_1 = c_4 = \frac{1}{6}(2+\alpha), \quad c_2 = c_3 = \frac{1}{6}(1-\alpha), \quad d_1 = d_3 = \frac{1}{3}(2+\alpha), \quad d_2 = -\frac{1}{3}(2+\alpha), \quad d_4 = 0,$$

where $\alpha = \sqrt[3]{2} + \frac{1}{\sqrt[3]{2}}$.

Above symplectic schemes can be implemented easily, as well as less memory in that they are all explicit integrators.

2.4. Composition methods

Higher order symplectic schemes can be constructed by lower ones through the composition method.

Definition 2. Suppose there exist n integrators whose corresponding operators are $s_1(\tau), s_2(\tau), \ldots, s_n(\tau)$, respectively, and their corresponding orders are $p_1, p_2, \ldots, p_n$, respectively. If there exist constants $c_1, c_2, \ldots, c_n$ such that the order of the integrator, whose operator is the composition $S(\tau) = s_1(c_1\tau)s_2(c_2\tau)\ldots s_n(c_n\tau)$, is m, $m > \max\{p_1, p_2, \ldots, p_n\}$, then the new integrator is called a *composition integrator of the original n integrators*. Such a method which is used to construct higher order integrators from lower ones is called the *composition method*.

Interested readers see [11,14,15] and references therein for details of this method. The following scheme is a 3-stage fourth-order symplectic scheme used in common by the composition method,

$$\begin{aligned} Z_{\frac{1}{3}} &= Z_n + \frac{1}{2 - \sqrt[3]{2}}\tau f\left(\frac{Z_n + Z_{\frac{1}{3}}}{2}\right), \\ Z_{\frac{2}{3}} &= Z_{\frac{1}{3}} - \frac{\sqrt[3]{2}}{2 - \sqrt[3]{2}}\tau f\left(\frac{Z_{\frac{1}{3}} + Z_{\frac{2}{3}}}{2}\right), \\ Z_{n+1} &= Z_{\frac{2}{3}} + \frac{1}{2 - \sqrt[3]{2}}\tau f\left(\frac{Z_{n+1} + Z_{\frac{2}{3}}}{2}\right). \end{aligned} \tag{8}$$

It can be regarded as a composition scheme via 3 Euler centered rules (5) with different steps.

There are some other methods, such as Partition Runge–Kutta methods, Runge–Kutta–Nyström methods and so on, which lead to symplectic schemes for finite-dimensional Hamiltonian system. We do not enumerate them any more, for detail, see [11,21,22] and references therein.

As mentioned in Section 1, symplectic algorithms can be generalized from finite-dimensional Hamiltonian systems to infinite-dimensional ones. The basic technique to design symplectic algorithms for them is dimen-

sional reduction. In other words, we discretize them in space firstly which result in finite-dimensional ones. We introduce a spatially discrete method (Fourier spectral method), which leads an infinite-dimensional Hamiltonian system to a finite-dimensional one in the following.

2.5. Spectral methods

In the last two decades, spectral methods have been developed rapidly. They have been applied successfully to numerical simulations in many fields, such as heat conduction, fluid dynamics, quantum mechanics and so on. The basic idea of them derives from Fourier analysis; and the main feature of them is to take various orthogonal systems of infinitely differentiable global functions as trial functions. One of their fascinating merits is the high accuracy, the so-called convergence of "infinite order". We explore the Fourier spectral method via wave equation

$$u_{tt} - u_{xx} + C'(u) = 0, \tag{9}$$

whose Hamiltonian formulation is

$$\begin{cases} u_t = v, \\ v_t = u_{xx} - C'(u), \end{cases} \tag{10}$$

with

$$H(u,v) = \frac{1}{2}\int (v^2 + u_x^2 - 2C(u)).$$

Functions u, v in the infinite-dimensional Hamiltonian system (10) which includes spatial partial derivatives of u, v, are functions about independent variables x and t. We can get exponential convergent rate symplectic schemes if we discretize it with the Fourier spectral method in space properly. We review it in this section simply. For details, readers may refer to [24,31,35,41].

The Fourier spectral method includes the following two steps: Firstly, the discrete expression of the solution is constructed by trigonometric polynomials; Secondly, approximate equations are attained at collocation points through original equations. The second step is the crucial one.

The spatial domain we consider here is $[a,b]$. The function $u(x,t)$ satisfies periodic boundary conditions $u(a,t) = u(b,t)$. The interpolation of $u(x,t)$ at collocation points $x_j = \frac{b-a}{N} j$, for $j = 0,1,\ldots,N-1$, is denoted by $I_N u(x,t)$, where N is an even number, then we have

$$I_N u(x,t) = \sum_{j=0}^{N-1} u_j g_j(x), \quad \text{where } g_j(x) = \frac{1}{N}\sum_{l=-N/2}^{N/2} \frac{1}{c_l} \mathrm{e}^{\mathrm{i}l\mu(x-x_j)}, \tag{11}$$

where

$$u_j = u(x_j,t), \quad \mu = \frac{2\pi}{b-a}, \quad c_l = \begin{cases} 2, & |l| = N/2, \\ 1, & \text{otherwise.} \end{cases}$$

We can draw $g_j(x_k) = \delta_j^k$ obviously, thus

$$I_N u(x,t) = \sum_{l=-N/2}^{N/2} \frac{1}{c_l} \mathrm{e}^{\mathrm{i}l\mu x} \frac{1}{N} \sum_{j=0}^{N-1} u_j \mathrm{e}^{-\mathrm{i}l\mu x_j}.$$

The interpolation of the function $v(x,t)$ is similar to $u(x,t)$.

Let $\widehat{u_l} = \frac{1}{Nc_l}\sum_{j=0}^{N-1} u_j \mathrm{e}^{-\mathrm{i}l\mu x_j}$, then we have

$$u_j = I_N u(x_j,t) = \sum_{l=-N/2}^{N/2} \widehat{u_l} \mathrm{e}^{\mathrm{i}l\mu x_j}. \tag{12}$$

The collocation method needs that (10) is exactly held at collocation points after u, v are replaced by u_j, v_j, that is,

$$\begin{cases} ((I_N u(x,t))_t = (I_N v(x,t)))|_{x=x_j}, \\ ((I_N v(x,t))_t = (I_N u(x,t))_{xx} - C'(u))|_{x=x_j}, \end{cases} \quad \text{for } j = 0,1,2,\ldots,N-1. \tag{13}$$

This is a coupled system about u_j, v_j, for $j = 0,1,\ldots,N-1$, which contains kth-order spatial partial derivatives $\frac{\partial^k I_N u(x,t)}{\partial x^k}$ and $\frac{\partial^k I_N v(x,t)}{\partial x^k}$ at collocation points. The key is to express them by u_j, v_j at collocation points. Taking differential with (11) k times continuously at collocation points, we have

$$\frac{\partial^k I_N u(x_j,t)}{\partial x^k} = \sum_{l=0}^{N-1} u_l \frac{\mathrm{d}^k g_l(x_j)}{\mathrm{d}x^k} = (D_k U)_j \quad \text{for } j = 0,1,2,\ldots,N-1, \tag{14}$$

where D_k is an $N \times N$ matrix with elements $(D_k)_{j,l} = \frac{\mathrm{d}^k g_l(x_j)}{\mathrm{d}x^k}$, $U = (u_0, u_1, \ldots, u_{N-1})^{\mathrm{T}}$. After some calculations, we get

$$(D_1)_{j,l} = \begin{cases} \frac{1}{2}(-1)^{j+l}\mu \cot\left(\mu\frac{x_j - x_l}{2}\right), & j \neq l, \\ 0, & j = l, \end{cases} \quad \text{for } j,l = 0,1,2,\ldots,N-1; \tag{15}$$

$$(D_2)_{j,l} = \begin{cases} \frac{1}{2}(-1)^{j+l+1}\mu^2 csc^2(\mu\frac{x_j - x_l}{2}), & j \neq l, \\ -\mu^2\frac{N^2+2}{12}, & j = l, \end{cases} \quad \text{for } j,l = 0,1,2,\ldots,N-1; \tag{16}$$

$$(D_3)_{j,l} = \begin{cases} (-1)^{j+l}\mu^3 \frac{\cos\left(\mu\frac{x_j - x_l}{2}\right)}{\sin^3\left(\mu\frac{x_j - x_l}{2}\right)} + (-1)^{j+l+1}\frac{\mu^3 N^2}{8}\cot\left(\mu\frac{x_j - x_l}{2}\right), & j \neq l, \\ 0, & j = l. \end{cases} \tag{17}$$

From (15)–(17) we can see that D_1, D_3 are skew-symmetric, and D_2 is symmetric. D_k ($k \geqslant 4$) also can be calculated, and we do not enumerate them here. Partial derivatives can be calculated by fast Fourier transformation (FFT) other than D_k, either.

Acting differential matrix D_2 on (10), we amount to the standard Fourier spectral semi-discretization of the wave equation

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}u_j = v_j, \\ \frac{\mathrm{d}}{\mathrm{d}t}v_j = (D_2 U)_j - C'(u_j). \end{cases} \tag{18}$$

This is a Hamiltonian system since D_2 is symmetric, whose Hamiltonian function is

$$H(U,V) = \frac{1}{2}[V^2 + U^{\mathrm{T}} D_2 U - 2C(U)].$$

We can discrete it by symplectic method in time, such as Euler centered scheme.

There are some other methods to reduce a finite-dimensional Hamiltonian system to an infinite-dimensional one, such as finite element method (FEM) [23], etc. Due to the limitation of the length of the summary, we will not expatiate them any more. Interested readers may consult literatures in point for details.

3. Multi-symplectic formulation and its conservation laws

A natural generalization of Hamiltonian ODEs is Hamiltonian PDEs. Therefore, a natural generalization of symplectic integrators is multi-symplectic integrators which preserve symplectic structures in each directions. Multi-symplectic integrator was first introduced by Bridges, Reich and Marsden from different aspects independently in the late 1990s. For Marsden's multi-symplectic integrator, we refer to [25] and references therein. We present multi-symplectic integrators from Bridges and Reich's aspect [26–29]. The central idea for multi-symplectic numerical integrators is that symplecticity is directional: symplectic structures of PDEs are decomposed into distinct components showing space and time independently. In this setting, numerical integrators of Hamiltonian PDEs can be structured by concatenating uni-directional symplectic integrators of ODEs.

The general multi-symplectic formulation with m-dimensional spatial variables is

$$M(x,t)\partial_t z + \sum_{i=1}^{m} K_i(x,t)\partial_{x_i} z = \nabla_z S(z,x,t), \quad x \in R^m, \ z \in R^n, \tag{19}$$

where $M(x,t)$, $K_i(x,t)$ are $n \times n (n \geqslant 3)$ skew-symmetric matrixes, and $S: R^n \mapsto R$ is some smooth function, and ∇_z is the gradient with respect to z. For more details, we refer to literatures [32,33,38]. For simplicity, we discuss the multi-symplectic formulation with one-dimensional spatial variable and constant coefficients for autonomic system, that is,

$$M\partial_t z + K\partial_x z = \nabla_z S(z), \quad z \in R^n. \tag{20}$$

The variational formulation associated with (20) is

$$M\mathrm{d}(\partial_t z) + K\mathrm{d}(\partial_x z) = D_{zz}S(z)\mathrm{d}z. \tag{21}$$

A large class of PDEs can be reformulated into (20), such as [26–29,39,41–43]: water waves, Dirac, generalized KdV, non-linear Schrödinger, SRLW, and Klein–Gordon–Schrödinger equations, etc. Moreover, the multi-symplectic formulation (20) satisfies the following conservation laws:

Taking inner product with (21) by $\mathrm{d}z$ and using the skew-symmetry of M, K as well as the symmetry of $D_{zz}S(z)$, we amount to the *multi-symplectic conservation law* (MCL),

$$\partial_t \omega + \partial_x \kappa = 0, \tag{22}$$

where 2-forms $\omega(U,V) = \langle MU, V\rangle$, $\kappa(U,V) = \langle KU, V\rangle$, and U, V are any two solutions of (21).

This conservation law implies that changes in time can be exactly compensated for by those in space. It is a strictly local conservation concept, in other words, it does not depend on the specific boundary conditions.

Taking inner product with (20) by z_t, we get the *local energy conservation law* (LECL),

$$\partial_t E(z) + \partial_x F(z) = 0, \tag{23}$$

where $E(z) = S(z) - \frac{1}{2}\kappa(z_x, z)$, $F(z) = \frac{1}{2}\kappa(z_t, z)$.

Taking inner product with (20) by z_x, it leads to the *local momentum conservation law* (LMCL),

$$\partial_t I(z) + \partial_x G(z) = 0, \tag{24}$$

where $G(z) = S(z) - \frac{1}{2}\omega(z_t, z)$, $I(z) = \frac{1}{2}\omega(z_x, z)$.

We give some examples of PDEs accompanied their multi-symplectic formulations:

(i) For the wave equation (9), we have the multi-symplectic formulation [26]

$$\begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_t \\ v_t \\ w_t \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} u_x \\ v_x \\ w_x \end{bmatrix} = \begin{bmatrix} C'(u) \\ v \\ -w \end{bmatrix} \tag{25}$$

and

$$S(z) = \frac{1}{2}(v^2 - w^2) + C(u).$$

This is a separable system which satisfies conservation laws with

$$\omega(z) = \mathrm{d}u \wedge \mathrm{d}v, \quad \kappa(z) = \mathrm{d}u \wedge \mathrm{d}w;$$

$$E(z) = \frac{1}{2}(v^2 + w^2) + C(u), \quad F(z) = -vw;$$

$$G(z) = \frac{1}{2}(v^2 + w^2) - C(u), \quad I(z) = -vw.$$

(ii) For the symmetry regular long wave equation (SRLWE) [40]

$$u_{tt} - u_{xx} - u_{xxtt} + \frac{1}{2}(u^2)_{xt} = 0, \tag{26}$$

which describes weakly non-linear ion acoustic waves, we have the multi-symplectic formulation

$$\begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -2 & 0 \\ -1 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \varphi_t \\ \phi_t \\ u_t \\ p_t \\ q_t \\ v_t \\ w_t \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 & 2 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ -2 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} \varphi_x \\ \phi_x \\ u_x \\ p_x \\ q_x \\ v_x \\ w_x \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \frac{2}{n}u^n - 2v - 2w \\ -q \\ -p \\ -2u \\ -2u \end{bmatrix}, \tag{27}$$

as well as

$$S(z) = \frac{1}{3}u^3 - pq - 2uv - 2uw.$$

For more details, we refer to [41,42].

The corresponding conservation laws (22)–(24) hold with

$$\omega(z) = \mathrm{d}\varphi \wedge \mathrm{d}u - \mathrm{d}p \wedge \mathrm{d}u - 2\mathrm{d}\phi \wedge \mathrm{d}v, \quad \kappa(z) = \mathrm{d}u \wedge \mathrm{d}q - \mathrm{d}u \wedge \mathrm{d}\phi + 2\mathrm{d}\varphi \wedge \mathrm{d}w;$$

$$E(z) = \frac{1}{6}u^3 + \frac{1}{4}(q\varphi - p\varphi - 4uv - pq - 2uw - uq_x + u\phi_x),$$

$$F(z) = \frac{1}{4}(u^2 - q^2 + \phi q + 2\varphi w_t - 2w\varphi_t + uq_t);$$

$$G(z) = \frac{1}{4}(\varphi p - 2\phi v_x + up_x - u^2 - p^2 + 2v\phi_x),$$

$$I(z) = \frac{1}{6}u^3 + \frac{1}{4}(p\phi - pq - 4uw - 2uv - q\varphi - u\varphi_t - up_t).$$

(iii) The coupled Klein–Gordon–Schrödinger (KGS) system [34]

$$\begin{cases} \mathrm{i}\psi_t + \frac{1}{2}\psi_{xx} + \psi\varphi = 0, \quad \mathrm{i} = \sqrt{-1}, \\ \varphi_{tt} - \varphi_{xx} + \varphi - |\psi|^2 = 0 \end{cases} \tag{28}$$

is a classical model which describes the interaction between conservative complex neutron field and neutral meson Yukawa in quantum field theory. Here $\psi(x,t)$ and $\varphi(x,t)$ are complex and real functions, respectively.

Letting $\psi = p + \mathrm{i}q$, $\psi_x = p_x + \mathrm{i}q_x = f + \mathrm{i}g$, $\varphi_t = v$, $\varphi_x = w$, $z = (p,q,f,g,\varphi,v,w)^{\mathrm{T}}$, where $p(x,t)$, $q(x,t)$ are real functions, we have the multi-symplectic formation of the KGS system (28) [43]

$$\begin{bmatrix} 0 & -2 & 0 & 0 & 0 & 0 & 0 \\ 2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} p_t \\ q_t \\ f_t \\ g_t \\ \varphi_t \\ v_t \\ w_t \end{bmatrix} + \begin{bmatrix} 0 & 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -1 & 0 & 0 \end{bmatrix} \begin{bmatrix} p_x \\ q_x \\ f_x \\ g_x \\ \varphi_x \\ v_x \\ w_x \end{bmatrix} = \begin{bmatrix} -2\varphi p \\ -2\varphi q \\ -f \\ -g \\ \varphi - (p^2 + q^2) \\ v \\ -w \end{bmatrix} \tag{29}$$

and the Hamiltonian function is

$$S(z) = -\varphi(p^2 + q^2) + \frac{1}{2}(\varphi^2 + v^2 - w^2 - f^2 - g^2).$$

As for the three local conservation laws corresponding to (22)–(24), we have

$$\omega(z) = -2\mathrm{d}p \wedge \mathrm{d}q - \mathrm{d}\varphi \wedge \mathrm{d}v,$$
$$\kappa(z) = \mathrm{d}p \wedge \mathrm{d}f + \mathrm{d}q \wedge \mathrm{d}g + \mathrm{d}\varphi \wedge \mathrm{d}w;$$
$$E(z) = -\frac{1}{2}\varphi(p^2+q^2) + \frac{1}{4}(\varphi^2 + v^2 - pf_x - qg_x - \varphi w_x),$$
$$F(z) = \frac{1}{4}(pf_t + qg_t + \varphi w_t - fp_t - gq_t - vw);$$
$$I(z) = -\frac{1}{2}\varphi(p^2+q^2) + \frac{1}{4}(\varphi^2 - w^2 - f^2 - g^2 + \varphi v_t) + \frac{1}{2}(pq_t - qp_t),$$
$$G(z) = \frac{1}{4}(-2pg + 2qf - \varphi v_x + vw).$$

4. Some multi-symplectic algorithms

The basic idea to construct a numerical scheme for (20) is to preserve the discrete multi-symplectic conservation law for the sake of its importance to Hamiltonian PDEs.

Definition 3. If a scheme satisfies the discretization multi-symplectic conservation law

$$\partial_t^{i,j}\omega_i^j + \partial_x^{i,j}\kappa_i^j = 0, \tag{30}$$

then we call it a *multi-symplectic scheme*.

The multi-symplectic formulation is a system with symplectic structures both in time and space, namely, we can rewrite it as Hamiltonian ODEs in each directions. Hence, we can construct multi-symplectic schemes by combining method. That is, symplectic schemes are constructed first for each Hamiltonian ODEs, then combine them altogether. We review this method via SRLWE (26).

If we adopt l-stage and s-stage symplectic Runge–Kutta methods in time and space, respectively, we can get a multi-symplectic scheme for the multi-symplectic formulation (20). Its accuracy is $O(h^{2s} + \tau^{2l})$. For example, taking $l = s = 1$, we get the multi-symplectic Euler centered scheme

$$M\delta_t z_{i+1/2}^{j+1/2} + K\delta_x z_{i+1/2}^{j+1/2} = \nabla_z S(z_{i+1/2}^{j+1/2}), \tag{31}$$

where

$$z_i^j = z(x_i,\ t_j), \quad \delta_t z_{i+1/2}^{j+1/2} = \frac{z_{i+1/2}^{j+1} - z_{i+1/2}^{j}}{\tau}, \quad \delta_x z_{i+1/2}^{j+1/2} = \frac{z_{i+1}^{j+1/2} - z_i^{j+1/2}}{h}, \quad z_{i+1/2}^{j+1/2} = \frac{1}{4}(z_{i+1}^{j+1} + z_{i+1}^{j} + z_i^{j+1} + z_i^j),$$

and h, τ are spatial and time step lengths, respectively.

When scheme (31) is applied to the multi-symplectic formulation (26) [42], we have

$$\begin{cases} \delta_t u_{i+1/2}^{j+1/2} + 2\delta_x w_{i+1/2}^{j+1/2} = 0, \quad 2\delta_t v_{i+1/2}^{j+1/2} - \delta_x u_{i+1/2}^{j+1/2} = 0, \\ -\delta_t \varphi_{i+1/2}^{j+1/2} + \delta_t p_{i+1/2}^{j+1/2} - \delta_x \phi_{i+1/2}^{j+1/2} + \delta_x q_{i+1/2}^{j+1/2} = (u_{i+1/2}^{j+1/2})^2 - 2v_{i+1/2}^{j+1/2} - 2w_{i+1/2}^{j+1/2}, \\ \delta_t u_{i+1/2}^{j+1/2} = q_{i+1/2}^{j+1/2}, \quad \delta_x u_{i+1/2}^{j+1/2} = p_{i+1/2}^{j+1/2}, \\ \delta_t \phi_{i+1/2}^{j+1/2} = -u_{i+1/2}^{j+1/2}, \quad \delta_x \varphi_{i+1/2}^{j+1/2} = u_{i+1/2}^{j+1/2}. \end{cases} \tag{32}$$

Eliminating transition variables from (32), we obtain a single variable multi-symplectic scheme

$$\frac{1}{\tau^2}(\delta_t^2 u_{i+1}^j + 2\delta_t^2 u_i^j + \delta_t^2 u_{i-1}^j) - \frac{1}{h^2}\left(1 + \frac{4}{\tau^2}\right)(\delta_x^2 u_i^{j+1} + \delta_x^2 u_i^{j-1}) - \frac{2}{h^2}\left(1 - \frac{4}{\tau^2}\right)\delta_x^2 u_i^j$$
$$= -\frac{1}{2}\frac{1}{h\tau}\{(u_{i+1/2}^{j+1/2})^2 + (u_{i-1/2}^{j+1/2})^2 + (u_{i+1/2}^{j-1/2})^2 + (u_{i-1/2}^{j-1/2})^2\}_{xt}, \tag{33}$$

where $\delta_t^2 u_i^j = u_i^{j+1} - 2u_i^j + u_i^{j-1}$, $\delta_x^2 u_i^j = u_{i+1}^j - 2u_i^j + u_{i-1}^j$, etc.

When space is discretized with the Fourier pseudo-spectral method while time with the Euler centered rule, we get multi-symplectic Fourier spectral method for (26) [41]

$$\begin{cases} \delta_t u_i^{j+1/2} + 2(D_1 W^{j+1/2})_i = 0, \quad 2\delta_t v_i^{j+1/2} - (D_1 U^{j+1/2})_i = 0, \\ -\delta_t \varphi_i^{j+1/2} + \delta_t p_i^{j+1/2} - (D_1(\Phi^{j+1/2} - Q^{j+1/2}))_i = (u_i^{j+1/2})^2 - 2v_i^{j+1/2} - 2w_i^{j+1/2}, \\ \delta_t u_i^{j+1/2} = q_i^{j+1/2}, \quad (D_1 U^{j+1/2})_i = p_i^{j+1/2}, \quad \delta_t \phi_i^{j+1/2} = -u_i^{j+1/2}, \quad (D_1 \Psi^{j+1/2})_i = u_i^{j+1/2}. \end{cases} \tag{34}$$

where the differential matrix D_1 is defined by (15), and $W = (w_0, w_1, \ldots, w_{N-1})^{\mathrm{T}}$, etc.

We can also eliminate transition variables from (34) and have

$$\begin{aligned} &(4I_N - (\tau^2+4)D_1^2)U^{j+1} - 2(4I_N + (\tau^2-4)D_1^2)U^j + (4I_N - (\tau^2+4)D_1^2)U^{j-1} \\ &\quad = -\tau[D_1((U^{j+1/2})^2 + (U^{j-1/2})^2)_t]. \end{aligned} \tag{35}$$

If the multi-symplectic Hamiltonian system (20) is separable, explicit multi-symplectic schemes can be constructed by combing method. We introduce it by non-linear wave equation (9). Applying 1-stage explicit symplectic scheme (7) to time and 1-stage explicit symplectic Runge–Kutta method to space, we have explicit multi-symplectic scheme for the wave equation (9)

$$\begin{cases} \frac{u_i^{j+1} - u_i^j}{\tau} = v_i^{j+1}, \quad \frac{u_{i+1}^j - u_i^j}{h} = w_{i+1}^j, \\ \frac{v_i^{j+1} - v_i^j}{\tau} - \frac{w_{i+1}^j - w_i^j}{h} + C'(u_i^j) = 0. \end{cases} \tag{36}$$

Eliminating mid-variables v, w, we amount to

$$\frac{u_i^{j-1} - 2u_i^j + u_i^{j+1}}{\tau^2} - \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2} + C'(u_i^j) = 0. \tag{37}$$

This is the classical leap-frog rule which is explicit. Some other explicit multi-symplectic schemes can be obtained similarly, for more details, see [36].

There are some other methods to construct multi-symplectic schemes, such as: finite volume method [30], composition method [37], etc. We do not set forth any more here. For more details, we refer to references and references therein. As for the error analysis of the discrete conservation laws for multi-symplectic schemes, we refer to [38,39] for details.

5. Numerical experiments

We have said in the previous section that symplectic and multi-symplectic methods have advantages over general non-symplectic numerical methods. We carry out some experiments to illustrate these superiorities by SRLWE (26).

Two signs are to be used in experiments:

(i) Errors in sense of maximum norm,

$$\mathrm{Error}^j = \max_{0 \leqslant i \leqslant N} |u_i^j - u(x_0 + ih, j\tau)|, \tag{38}$$

where N is the mesh number, and $u(x_0 + ih, j\tau)$ is the theoretical solution.

(ii) Residual of the discrete energy conservation law,

$$\mathrm{Res}^j = \sum_{i=0}^{N-1} \left(\frac{E_{i+1/2}^{j+1} - E_{i+1/2}^j}{\tau} + \frac{F_{i+1}^{j+1/2} - F_i^{j+1/2}}{h} \right). \tag{39}$$

SRLWE (26) has the theoretical solitary wave solution

$$u(x,t,v,x_0) = 3\frac{v^2-1}{v} \operatorname{sech}^2 \frac{\sqrt{v^2-1}}{2v}(x - vt + x_0), \tag{40}$$

where v, x_0 are the velocity and initial phase of the wave, respectively.

Table 1
Errors in sense of infinity and energy residual

Scheme	t	0	20	40	60	80	100
(33)	Error	–	1.1139E−2	1.8079E−2	2.4982E−2	3.1967E−2	3.8951E−2
(35)	Error	–	5.79189E−4	7.63637E−4	9.54526E−4	1.14578E−3	1.33902E−3
(33)	Res	–	4.8638E−8	1.2424E−9	3.3171E−11	8.7530E−013	−2.1522E−14
(35)	Res	–	−9.8267E−10	−2.3374E−11	−9.1703E−13	−8.1722E−10	−2.8845E−9

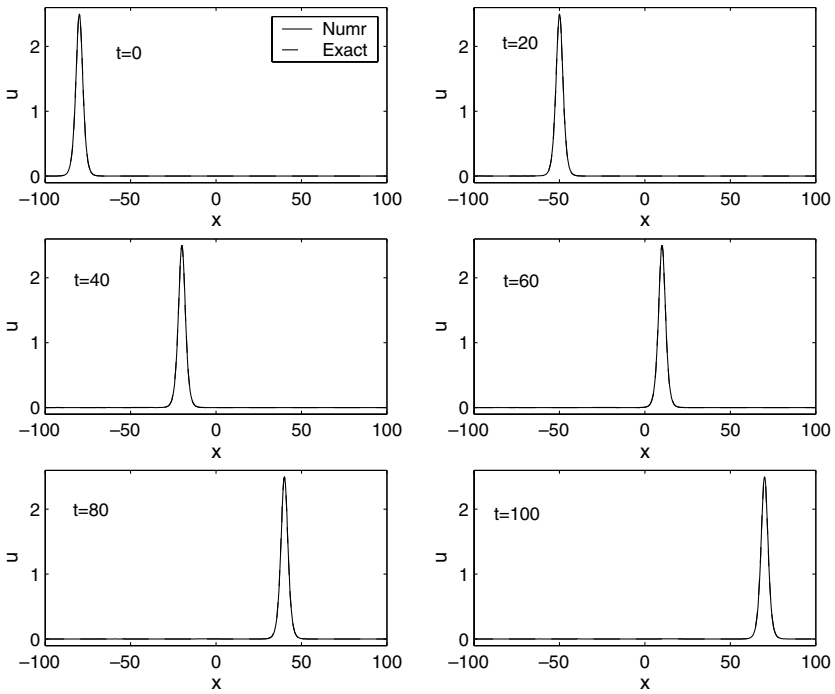

Fig. 1. Comparisons between numerical solution and exact solution at various times.

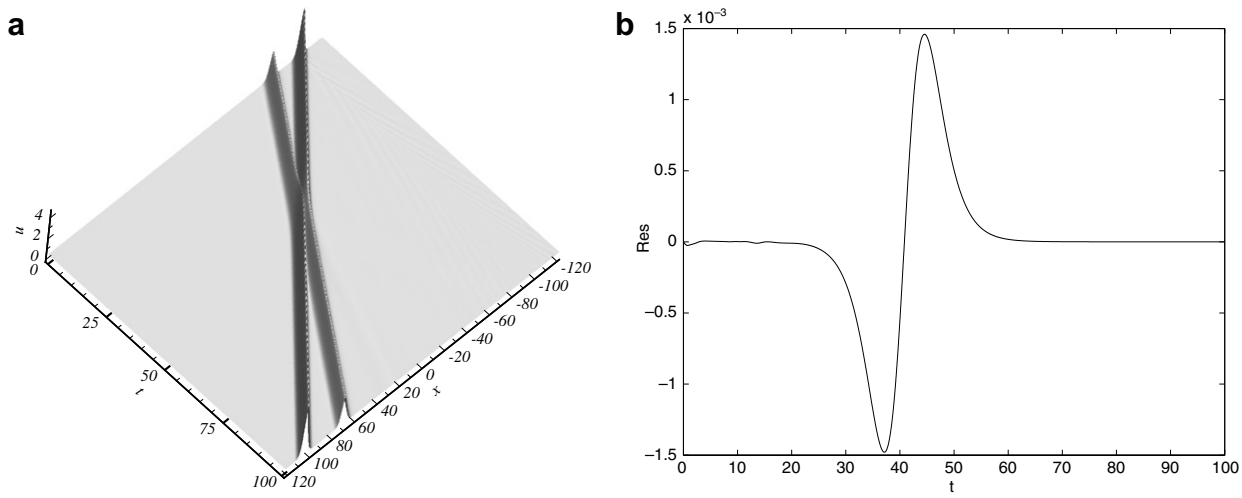

Fig. 2. (a) Same directional solitons and (b) energy residual.

In all of the following experiments, we take boundary conditions $u(a,t) = u(b,t) = 0$.

Taking $h = 0.25$, $\tau = 0.02$, $v = 1.5$, $x_0 = 80$ and the computational domain $[-100, 100]$, we simulate the solitary wave with scheme (33) and (35) as far as $t = 100$. Errors in sense of maximum norm and energy residual are listed in Table 1, and comparisons between the numerical solution (solid '–') and the theoretical solution (dashed '–') of scheme (33) are shown in Fig. 1.

From Table 1 and Fig. 1, we can find the following: exact solution and numerical solution are almost superposition in that errors are small; errors of the pseudo-spectral method are smaller than those of the centered scheme; energy residual is small even though it cannot preserve it exactly.

Taken initial conditions $u(x,0) = u_1(x,0,2,100) + u_2(x,0,1.5,75)$, $u_t(x,0) = u_1t(x,0,2,100) + u_2t(x,0,1.5,75)$, this is two solitons with distinct both amplitudes and initial phases, and velocities $v_1 = 2$, $v_2 = 1.5$, propagating to the right. Chosen $h = 0.2$, $\tau = 0.025$, and the spatial computational domain $[-120, 120]$, waves are simulated by scheme (33) while $t = 100$. Solitary waves with time evolution are presented in Fig. 2(a), and the energy residual is shown in Fig. 2(b).

We choose initial conditions $u(x,0) = u_1(x,0,1.5,100) + u_2(x,0,-1.5,-100)$, and $u_t(x,0) = u_1t(x,0,1.5,100) + u_2t(x,0,-1.5,-100)$. Two solitons with distinct amplitudes and different initial phases propagate to opposite directions with speeds $v_1 = 1.5$, $v_2 = -1.5$, respectively. Time step and spatial mesh number are $\tau = 0.05$, $N = 1024$, respectively. We calculate with multi-symplectic pseudo-spectral scheme (35) in interval

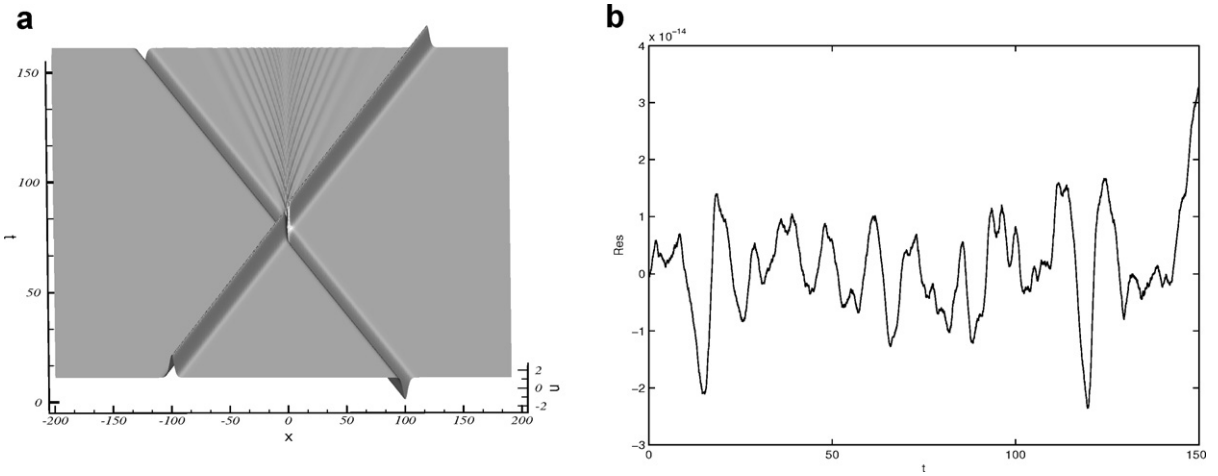

Fig. 3. (a) Opposite directional solitons and (b) energy residual.

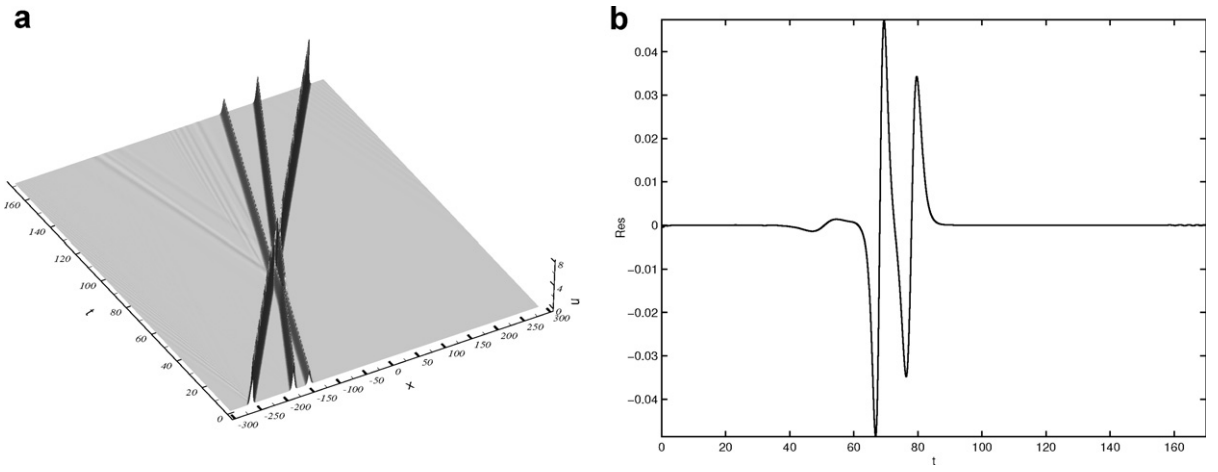

Fig. 4. (a) Same directional solitary waves with three solitons and (b) energy residual.

$[-200, 200]$ till $t = 150$. Fig. 3(a) shows solitary waves with time evolution, and Fig. 3(b) shows the energy residual.

Chosen initial conditions $u(x,0) = u_1(x,0,3,260) + u_2(x,0,2,180) + u_3(x,0,1.5,150)$ and $u_t(x,0) = u_1t(x, 0,3,260) + u_2t\ (x,0,2,180) + u_3t(x,0,1.5,150)$, this is three solitons with distinct both amplitudes and phases, and velocities $v_1 = 3$, $v_2 = 2$, $v_3 = 1.5$, all propagating to the right. Time step and spatial mesh number are $\tau = 0.0425$, $N = 1024$, respectively. We calculate with multi-symplectic pseudo-spectral scheme (35) in interval $[-300, 300]$ till $t = 170$. Solitary waves with time evolution are shown in Fig. 4(a), and energy residual is figured in Fig. 4(b).

6. Conclusions

Symplectic and multi-symplectic algorithms for Hamiltonian system are reviewed. We review some methods to construct these algorithms. Some numerical experiments are shown to demonstrate the validity and superiorities of them to general non-symplectic algorithms. These algorithms have long time behavior; they also can preserve original physical phenomena well; they can simulate all kind of solitary waves in a long time. They cannot preserve the energy and momentum exactly, whereas their residual is relatively small and takes on quasi-periodic changes.

Acknowledgements

This work is supported by the 2005 postgraduate innovational fund of USTC, NNSFC under Grant Nos. 10371118, 90411009 and the Computational Physical Laboratory of the Institute of Beijing Applied Physics and Computational Mathematics. The first author thanks Zhenli Xu Ph.D. candidate for his useful suggestions.

Appendix. Preliminary knowledge of symplectic geometry

Since Hamiltonian system is based on symplectic geometry, we review the basic knowledge of symplectic geometry simply in this section. For more details, we refer to [12] and references therein. Vectors are defined on R^{2n}.

Inner product:

$$[x, y] = \sum_{i=1}^{n} (x_i y_{n+i} - x_{n+i} y_i) = x^{\mathrm{T}} J_{2n} y,$$

where $x, y \in R^{2n}$, $J = \begin{bmatrix} 0 & I_n \\ -I_n & 0 \end{bmatrix}$.

The above defined inner product has the following properties:

(1) *Bilinear*: $[x + y, v + w] = [x, v] + [x, w] + [y, v] + [y, w]$.
(2) *Skew-symmetry*: $[x, y] = -[y, x]$.
(3) *Non-degenerate*: $\forall y \neq 0$, $\exists x$, $[x, y] = 0 \Rightarrow x = 0$.
(4) $[x, x] = 0$, $\forall x$.

Definition 1. Let V be a vector space defined on R^{2n}, the bilinear mapping ω on $V \times V$ is *symplectic*, if it satisfies (i) $\forall x \in V$, s.t. $\omega(x, y) = 0$, $\forall y \in V$, $\Rightarrow x = 0$; (ii) $\forall x, y \in V, \omega(x, y) = -\omega(y, x)$. (V, ω) is called *symplectic space*, and ω is called *symplectic structure*.

Definition 2. A linear transformation S on (V, ω) is a called *symplectic transformation* if it meets $[Sx, Sy] = [x, y]$, $\forall x, y$.

Definition 3. The matrix $S \in R^{2n \times 2n}$ is called *symplectic matrix* if $S^{\mathrm{T}} J S = J$. The group which is consisted of all symplectic matrixes is called *symplectic group*. We sign it as $Sp(2n)$.

Definition 4. $B \in R^{2n\times 2n}$ is an *infinitesimally symplectic matrix* if $B^{\mathrm{T}}J + JB = 0$.

Theorem. *S is symplectic iff* $S^{\mathrm{T}}JS = J$.

All of infinitesimally symplectic matrixes are composed of *Lie algebra* via anti-commutable Lie Poisson bracket $[A, B] = AB - BA$.

The following conclusions are correct:

(1) $S \in Sp(2n) \Rightarrow$ (i) $\det S = 1$; (ii) $S^{-1} = -JS^{\mathrm{T}}J = J^{-1}S^{\mathrm{T}}J$; (iii) $SJS^{\mathrm{T}} = J$.

(2) Assuming $S = \begin{bmatrix} A & B \\ C & D \end{bmatrix}, A, B, C, D \in R^{n\times n}$, then $S \in Sp(2n) \iff AB^{\mathrm{T}} = BA, CD^{\mathrm{T}} = DC^{\mathrm{T}}, AD^{\mathrm{T}} - BC^{\mathrm{T}} = I$, $A^{\mathrm{T}}D - C^{\mathrm{T}}B = I, A^{\mathrm{T}}C = C^{\mathrm{T}}A, B^{\mathrm{T}}D = D^{\mathrm{T}}B$.

(3) $\begin{bmatrix} I & B \\ 0 & I \end{bmatrix}, \begin{bmatrix} I & 0 \\ D & I \end{bmatrix}$ is symplectic $\iff B^{\mathrm{T}} = B, D^{\mathrm{T}} = D$.

(4) $\begin{bmatrix} A & 0 \\ 0 & B \end{bmatrix} \in Sp(2n) \Longleftrightarrow A = (B^{\mathrm{T}})^{-1}$.

(5) $S = M^{-1}N \in Sp(2n) \iff M^{\mathrm{T}}JM = N^{\mathrm{T}}JN$.

(6) $B \in Sp(2n) \Rightarrow \exp(B) \in Sp(2n)$.

(7) $B \in Sp(2n)$, $\det(I + B) \neq 0 \Rightarrow F = (I + B)^{-1}(I - B) \in Sp(2n)$, which is called the *Cayley transformation* of B.

References

[1] K. Feng, M. Qin, Symplectic Geometric Algorithm for Hamiltonian System, Zhejiang Science and Technology Press, Hangzhou, 2002.

[2] De Vogelaere, Methods of integration which preserve the contact transformation property of the Hamiltonian equations, Report 4, Department of Mathematics, University of Notre Dame, 1956.

[3] R. Ruth, A canonical integration technique, IEEE Trans. Nucl. Sci. 30 (1983) 2669–2671.

[4] K. Feng, On difference schemes and symplectic geometry, in: K. Feng (Ed.), Proceeding of the 1984 Beijing Symposium on D.D., Science Press, Beijing, 1985, pp. 42–58.

[5] V.I. Arnold, Mathematical Methods of Classical Mechanics, Springer, Berlin, 1999.

[6] K. Feng, Feng Kang's Collected Work (II), Defense Industry Press, Beijing, 1995.

[7] K. Feng, Difference schemes for Hamiltonian formalism and symplectic geometry, J. Comput. Math. 4 (1986) 279–289.

[8] K. Feng, H. Wu, M. Qin, D. Wang, Construct of canonical difference schemes for Hamiltonian formalism via generating functions, J. Comput. Math. 7 (1989) 71–96.

[9] C. Li, M. Qin, A symplectic difference scheme for the infinite-dimensional Hamiltonian system, J. Comput. Math. 6 (1988) 164–174.

[10] H. Yoshida, Recent progress in the theory and application of symplectic integrators, Celest. Mech. Dynam. Astronom. 56 (1993) 27–43.

[11] E. Hairer, Ch. Lubich, G. Wanner, Geometric Numerical Integration, Springer, Berlin, 2002.

[12] M. Qin, Symplectic geometry and computational Hamilton mechanics, Mech. Practice (6) (1990) 1–20.

[13] M. Qin, Multi-stage symplectic schemes of two kinds of Hamiltonian systems of wave equations, Comput. Math. Appl. 19 (1990) 51–62.

[14] M. Qin, W. Zhu, Construction of higher order symplectic schemes by composition, Computing 47 (1991) 309–321.

[15] H. Yoshida, Construction of higher order symplectic integrators, Phys. Lett. A 150 (1990) 262–268.

[16] W. Zeng, L. Kong, History and present state of symplectic algorithm, J. Huaqiao Univ. 25 (2004) 113–117.

[17] P.J. Channell, C. Scovel, Symplectic integration of Hamiltonian system, Nonlinearity 3 (1990) 231–259.

[18] F.M. Lasagni, Canonical Runge–Kutta methods, Z. Angew. Math. Phys. 39 (1988) 952–953.

[19] J.M. Sanz-Serna, Runge–Kutta schemes for Hamiltonian systems, BIT 28 (1988) 877–883.

[20] Yu.B. Suris, On the canonicity of mappings that can be generated by methods of Runge–Kutta type for integrating systems $x'' = -\partial U/\partial x$, Zh. Vychisl. Mat. i Mat. Fiz. 29 (1989) 202–211.

[21] G. Sun, Symplectic partitioned Runge–Kutta methods, J. Comput. Math. 11 (1993) 365–372.

[22] D. Okunbor, R.D. Skeel, Explicit canonical methods for Hamiltonian systems, Math. Comput. 59 (1992) 439–455.

[23] Z. Liu, Y. Bai, Q. Li, K. Wu, Symplectic and multi-symplectic schemes with the simple finite element method, Phys. Lett. A 314 (2003) 443–455.

[24] M. Huang, Q. Ru, C. Gong, A structure preserving discretization of nonlinear Schrödinger equation, J. Comput. Math. 17 (1999) 553–560.

[25] J. Marsden, G.W. Patrick, S. Shkoller, Multi-symplectic geometry, variational integrators, and nonlinear PDEs, Commun. Math. Phys. 199 (1998) 351–395.
[26] T.J. Bridges, Multi-symplectic structures and wave propagation, Math. Proc. Camb. Phil. Soc. 121 (1997) 147–190.
[27] T.J. Bridges, A geometric formulation of the conservation of wave action and its implications for signature and the classification of instabilities, Proc. R. Soc. Lond. A 453 (1997) 1365–1395.
[28] T.J. Bridges, S. Recih, Multi-symplectic integrators: numerical schemes for Hamiltonian PDEs that conserve symplecticity, Phys. Lett. A 284 (2001) 184–193.
[29] S. Reich, Multi-symplectic Runge–Kutta method for Hamiltonian wave equations, J. Comput. Phys. 157 (2001) 473–499.
[30] S. Reich, Finite volume method for multi-symplectic PDEs, BIT 40 (2000) 559–582.
[31] T.J. Bridges, S. Reich, Multi-symplectic spectral discretizations for the Zakharov–Kuznetsov and shallow water equations, Physica D 152–153 (2001) 491–504.
[32] J. Hong, Y. Liu, A novel numerical approach to simulating nonlinear Schrödinger equation with variable coefficients, Appl. Math. Lett. 16 (2002) 759–765.
[33] J. Hong, M. Qin, Multisymplecticity of centered box discretizations for Hamiltonian PDEs with $m \geqslant 2$ space dimensions, Appl. Math. Lett. 15 (2002) 1005–1011.
[34] F. Tsutsumim, On coupled Klein–Gordon–Schrödinger equations, J. Math. Anal. Appl. 66 (1978) 358–378.
[35] J. Chen, M. Qin, Multi-symplectic Fourier pseudo-spectral method for the nonlinear Schrödinger equation, Electron. Trans. Numer. Anal. 12 (2001) 193–204.
[36] Y. Wang, B. Wang, High-order multi-symplectic schemes for the nonlinear Klein–Gordon equation, Appl. Math. Comput. 166 (2005) 608–632.
[37] J. Chen, M. Qin, multi-symplectic composition integrator of high order, J. Comput. Math. 21 (2003) 647–656.
[38] J. Hong, Y. Liu, Hans Munthe-Kaas, Antonella Zanna, Globally conservative properties and error estimation of a multi-symplectic scheme for Schrödinger equations with variable coefficients, Appl. Numer. Math. 56 (2006) 814–843.
[39] J. Hong, C. Li, Multi-symplectic Runge–Kutta methods for nonlinear Dirac equations, J. Comput. Phys. 211 (2006) 448–472.
[40] C.E. Seyler, D.C. Fenstermmacler, A symmetry regularized long wave equation, Phys. Fluid. 27 (1984) 4–7.
[41] L.H. Kong, W. Zeng, R. Liu, L.J. Kong, Multi-symplectic quasi-spectral method and its conservation laws for SRLW equation, Chin. J. Comput. Phys. 23 (2006) 29–35.
[42] L.H. Kong, W. Zeng, R. Liu, L.J. Kong, Multi-symplectic scheme of SRLW equation and its conservation laws, J. Univ. Sci. Tech. China 35 (2005) 770–776.
[43] L. Kong, R. Liu, Z. Xu, Numerical simulation of interaction between Schrödinger field and Klein–Gordon field by multi-symplectic method, Appl. Math. Comput., in press, doi:10.1016/j.amc.2006.01.044.