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Generalized multi-symplectic integrators for a class of Hamiltonian nonlinear wave PDEs

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ABSTRACT

Nonlinear wave equations, such as Burgers equation and compound KdV–Burgers equation, are a class of partial differential equations (PDEs) with dissipation in Hamiltonian space, the numerical method of which plays an important role in complex fluid analysis. Based on the multi-symplectic idea, a new theoretical framework named generalized multi-symplectic integrator for a class of nonlinear wave PDEs with small damping is proposed in this paper. The generalized multi-symplectic formulation is introduced, and a twelve-point generalized multi-symplectic scheme, which satisfies two discrete modified conservation laws approximately as well as the local momentum conservation law accurately, is constructed to solve the first-order PDEs that derived from the compound KdV–Burgers equation. To test the generalized multi-symplectic scheme, several numerical experiments on the travelling front solution are carried out, the results of which imply that the generalized multi-symplectic scheme can simulate the travelling front solution accurately and satisfy the modified conservation laws well when step sizes and the damping parameter satisfy the inequality (41). It is more remarkable that the scheme (36) can be used to capture the shock wave structure of the compound KdV–Burgers equation within one data point, which can further illustrate the good structure-preserving property of the generalized multi-symplectic scheme (36). From the results of this paper, we can conclude that, similar to the multi-symplectic scheme, the generalized multi-symplectic scheme also has two remarkable advantages: the excellent long-time numerical behavior and the good conservation property. For the existing of the excellent numerical properties, the generalized multi-symplectic method can be used to exposit some specific phenomena in the complex fluid.

1. Introduction

The concept of a multi-symplectic integrator, proven to be a very robust framework for the accurate, efficient and long-time integration of infinite-dimensional Hamiltonian systems, has been widely investigated during the last decade [1–10]. Bridges, Reich and Moore presented the concept of the multi-symplectic integrator and applied it to solving several nonlinear wave equations [1–4] and the nonlinear Schrödinger equation [2]. Subsequently, focusing on the excellent long-time numerical behavior and the good conservation property of the multi-symplectic integrator, the multi-symplectic schemes of several conservative partial differential equations (PDEs), such as the membrane free vibration equation [5], the KdV

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equation [8], the coupled 1D nonlinear Schrödinger equation [9] and so on, were constructed to obtain their solutions numerically.

The basic idea of a multi-symplectic integrator is that the numerical scheme is designed to preserve the multi-symplectic form at each time step [1–5]. For example, let $\mathbf{M}, \mathbf{K}_i \in \mathbf{R}^{d\times d}$ $(i = 1, 2, \ldots, n)$ be skew-symmetric matrices, $S:\mathbf{R}^d \to R$ be a smooth function and $\mathbf{z} = \mathbf{z}(t, x_1, x_2, \ldots, x_n)$ be a state variable, the infinite-dimensional multi-symplectic PDEs system

$$\mathbf{M}\partial_t \mathbf{z} + \sum_{i=1}^{n} \mathbf{K}_i \partial_{x_i} \mathbf{z} = \nabla_{\mathbf{z}} S(\mathbf{z}), \quad \mathbf{z} \in \mathbf{R}^d \tag{1}$$

satisfies multi-symplectic conservation law exactly [1–4]

$$\partial_t(\omega) + \sum_{i=1}^{n} \partial_{x_i}(\kappa_i) = 0 \tag{2}$$

where $\omega = (\mathbf{M}U, V)$, $\kappa_i = ((\mathbf{K}_i)U, V)$ $(i = 1, 2, \ldots, n)$, U, V are any solutions of the variational equation associated with Eq. (1) [1].

For systems in the abstract form (1) there is a natural geometric form for local energy and local momentum conservation [1–4]. Using the time invariance of the multi-symplectic PDEs (1), a local energy conservation law can be derived by taking the inner product of (1) with $\partial_t \mathbf{z}$

$$\partial_t e + \sum_{i=1}^{n} \partial_{x_i} f_i = 0 \tag{3}$$

with energy density $e = S(\mathbf{z}) - \frac{1}{2}\sum_{i=1}^{n} \mathbf{z}^{\mathrm{T}} \mathbf{K}_i \partial_{x_i} \mathbf{z}$ and energy fluxes $f_i = \frac{1}{2}\mathbf{z}^{\mathrm{T}} \mathbf{K}_i \partial_t \mathbf{z}$ $(i = 1, 2, \ldots, n)$

Similarly, a local momentum conservation law in the x_m $(m = 1, 2, \ldots, n)$ direction can be derived by taking the inner product of Eq. (1) with $\partial_{x_m}\mathbf{z}$

$$\partial_t(h_m) + \sum_{i=1}^{n} \partial_{x_i} g_{mi} = 0 \tag{4}$$

where $h_m = \frac{1}{2}\mathbf{z}^{\mathrm{T}}\mathbf{M}\partial_{x_m}\mathbf{z}$, $g_{mm} = S(\mathbf{z}) - \frac{1}{2}\mathbf{z}^{\mathrm{T}}\mathbf{M}\partial_t\mathbf{z} - \frac{1}{2}\sum_{i=1}^{m-1}\mathbf{z}^{\mathrm{T}}\mathbf{K}_i\partial_{x_i}\mathbf{z} - \frac{1}{2}\sum_{i=m+1}^{n}\mathbf{z}^{\mathrm{T}}\mathbf{K}_i\partial_{x_i}\mathbf{z}$ and $g_{mi} = \frac{1}{2}\mathbf{z}^{\mathrm{T}}\mathbf{K}_i\partial_{x_m}\mathbf{z}$ $(i = 1, \ldots, m-1, m+1, \ldots, n)$

A multi-symplectic integrator is a numerical approximation for Eq. (1), which can be expressed schematically as

$$\mathbf{M}(\partial_t)^k_{j_1 j_2 \cdots j_n} \mathbf{z}^k_{j_1, j_2 \cdots j_n} + \sum_{i=1}^{n} \mathbf{K}_i (\partial_{x_i})^k_{j_1 j_2, \cdots j_n} \mathbf{z}^k_{j_1, j_2, \cdots j_n} = (\nabla_{\mathbf{z}} S(\mathbf{z}^k_{j_1 j_2, \cdots j_n}))^k_{j_1, j_2, \cdots j_n} \tag{5}$$

where $\mathbf{z}^k_{j_1, j_2 \cdots j_n} = \mathbf{z}(t_k, (x_1)_{j_1}, (x_2)_{j_2}, \ldots, (x_n)_{j_n})$, $(\partial_t)^k_{j_1 j_2 \cdots j_n}$ and $(\partial_{x_i})^k_{j_1 j_2, \cdots j_n}$ $(i = 1, 2, \ldots, n)$ are discrete schemes of the derivatives ∂_t and ∂_{x_i} $(i = 1, 2, \ldots, n)$ respectively. The multi-symplectic integrator (5) respects a discrete approximation of multi-symplectic conservation:

$$(\partial_t)^k_{j_1 j_2 \cdots j_n} \omega^k_{j_1 j_2 \cdots j_n} + \sum_{i=1}^{n} (\partial_{x_i})^k_{j_1 j_2 \cdots j_n} (\kappa_i)^k_{j_1 j_2 \cdots j_n} = 0 \tag{6}$$

where $\omega^k_{j_1 j_2 \cdots j_n} = (\mathbf{M}U^k_{j_1 j_2 \cdots j_n}, V^k_{j_1 j_2 \cdots j_n})$,$(\kappa_i)^k_{j_1 j_2 \cdots j_n} = ((\mathbf{K}_i)U^k_{j_1 j_2 \cdots j_n}, V^k_{j_1 j_2 \cdots j_n})$ $(i = 1, 2, \ldots, n)$, $\{U^k_{j_1 j_2 \cdots j_n}\}^k_{j_1 j_2 \cdots j_n} \in Z \times Z$ and $\{V^k_{j_1 j_2 \cdots j_n}\}^k_{j_1 j_2 \cdots j_n} \in Z \times Z$ satisfy the corresponding discrete variational equations

$$\mathbf{M}(\partial_t)^k_{j_1 j_2 \cdots j_n} Z^k_{j_1, j_2 \cdots j_n} + \sum_{i=1}^{n} \mathbf{K}_i (\partial_{x_i})^k_{j_1 j_2, \cdots j_n} Z^k_{j_1 j_2, \cdots j_n} = \nabla_{\mathbf{z}} S''(\mathbf{z}^k_{j_1 j_2, \cdots j_n}) Z^k_{j_1 j_2, \cdots j_n} \tag{7}$$

where $S''(\mathbf{z}^k_{j_1 j_2, \cdots j_n})$ denotes the discrete form of the (symplectic) Hessian matrix of Hamiltonian function $S(\mathbf{z})$. It has been recognized widely that this conservation property gives rise to the excellent long-time behavior of the multi-symplectic integrator [1–10].

The common characteristic of the PDEs investigated by the multi-symplectic method in all previous works is that the multi-symplectic form (1) can be constructed by introducing appropriate intermediate variables, which serves as a prerequisite of the multi-symplectic integrator. This prerequisite suggests that the multi-symplectic integrator can only be used in minority Hamiltonian PDEs systems which can be written into the form (1), such as the Sine–Gordon equation, KdV equation, nonlinear Schrödinger equation and so on [5,7–10]. For majority Hamiltonian PDEs systems, especially for the Hamiltonian systems with damping, so far, we must recur to other numerical methods, which maybe can obtain solutions with high accuracy. But these methods cannot preserve the local geometrical properties of the systems exactly, which play an important role in analyzing the dynamic property of the systems. Thus, it is significant to present a new numerical method that pays more attention to the local geometrical properties of the generalized Hamiltonian PDEs systems in light of the multi-symplectic integrator idea.

This paper presents the generalized multi-symplectic integrator concept and approach to analyze a class of Hamiltonian nonlinear wave PDEs with small damping that cannot be written into the strict multi-symplectic form (1) focusing on the local geometrical properties of the systems. To illustrate the generalized multi-symplectic integrator approach, the generalized multi-symplectic method of compound KdV–Burgers equation is introduced subsequently. Finally, the results of the numerical experiments show that the generalized multi-symplectic method owns some excellent numerical properties as well as the potential applications in complex fluid analysis.

2. The generalized multi-symplectic integrators

In this section, a brief overview of the multi-symplectic theory needed is reviewed with emphasis on the multi-symplectic PDEs form as well as the conservation laws, and then the generalized multi-symplectic integrator concept is presented in detail.

According to the multi-symplectic integrator theory of Bridges [1,3], the skew-symmetry of the coefficient matrices $\mathbf{M}$, $\mathbf{K}_i$, the Hamiltonian function S and the appropriate canonical transformation are three vital prerequisites for getting the conservation laws (including the multi-symplectic conservation law (2), the local energy conservation law (3) and the local momentum conservation law (4)) associated with the multi-symplectic PDEs system (1). In many cases, the Hamiltonian PDEs systems can be written into the form that is very similar to the multi-symplectic form (1) except for the skew-symmetry of the coefficient matrices, such as compound KdV–Burgers equation and Burgers equation, which represent a class of Hamiltonian nonlinear wave PDEs systems that can be written into the form

$$\mathbf{M}^*\partial_t\mathbf{z} + \sum_{i=1}^{n}\mathbf{K}_i^*\partial_{x_i}\mathbf{z} = \nabla_{\mathbf{z}}S(\mathbf{z}), \quad \mathbf{z}\in\mathbf{R}^d \tag{8}$$

where $\mathbf{M}^*, \mathbf{K}_i^* \in \mathbf{R}^{d\times d}$ $(i = 1, 2, \ldots, n)$ (they can be any square matrices), $S{:}\mathbf{R}^d \to R$ is the Hamiltonian function. To ensure that the system (8) is well-posed, we assume that there is only a finite number of eigenvalues λ_m, which have positive real part, of the eigenvalue problem with characteristic polynomial

$$\det(\lambda_m\mathbf{M}^* + \sum_{m=1}^{n} i\mathbf{K}_m^* - \mathbf{H}) = 0 \tag{9}$$

for all real $\mathbf{K}_m^*$, where $\mathbf{H}$ is the Hessian of S($\mathbf{z}$) ,and $\mathbf{K}_m^* \in R^n$ $(m = 1, 2, \ldots, n)$, here $i = \sqrt{-1}$ (not to be confused with the later usage of subscript i).

According to the matrix theory, a generalized square matrix $\mathbf{A}$ can be split into the form $\frac{1}{2}(\mathbf{A} - \mathbf{A}^{\mathrm{T}}) + \frac{1}{2}(\mathbf{A} + \mathbf{A}^{\mathrm{T}})$, where $\frac{1}{2}(\mathbf{A} - \mathbf{A}^{\mathrm{T}})$ is a skew-symmetric matrix and $\frac{1}{2}(\mathbf{A} + \mathbf{A}^{\mathrm{T}})$ is a symmetric matrix obviously, thus the square matrices $\mathbf{M}^*, \mathbf{K}_i^*$ can be expressed in the form

$$\mathbf{M}^* = \frac{1}{2}[\mathbf{M}^* - (\mathbf{M}^*)^{\mathrm{T}}] + \frac{1}{2}[\mathbf{M}^* + (\mathbf{M}^*)^{\mathrm{T}}], \quad \mathbf{K}_i^* = \frac{1}{2}[\mathbf{K}_i^* - (\mathbf{K}_i^*)^{\mathrm{T}}] + \frac{1}{2}[\mathbf{K}_i^* + (\mathbf{K}_i^*)^{\mathrm{T}}] \tag{10}$$

Defining the skew-symmetric matrices $\mathbf{M}$, $\mathbf{K}_i$

$$\mathbf{M} = \frac{1}{2}[\mathbf{M}^* - (\mathbf{M}^*)^{\mathrm{T}}], \quad \mathbf{K}_i = \frac{1}{2}[\mathbf{K}_i^* - (\mathbf{K}_i^*)^{\mathrm{T}}]$$

and the symmetric matrices $\widehat{\mathbf{M}}$, $\widehat{\mathbf{K}}_i$ $\widehat{\mathbf{M}} = \frac{1}{2}[\mathbf{M}^* + (\mathbf{M}^*)^{\mathrm{T}}]$, $\widehat{\mathbf{K}}_i = \frac{1}{2}[\mathbf{K}_i^* + (\mathbf{K}_i^*)^{\mathrm{T}}]$ then the form (8) can be rewritten as

$$(\mathbf{M} + \widehat{\mathbf{M}})\partial_t\mathbf{z} + \sum_{i=1}^{n}(\mathbf{K}_i + \widehat{\mathbf{K}}_i)\partial_{x_i}\mathbf{z} = \nabla_{\mathbf{z}}S(\mathbf{z}), \quad \mathbf{z}\in\mathbf{R}^d \tag{11}$$

which is named as approximate multi-symplectic system provisionally.

Note that if the symmetric matrices $\widehat{\mathbf{M}} = \widehat{\mathbf{K}}_i = 0$, Eq. (11) degenerates to the strict multi-symplectic form (1), which satisfies conservation laws (2)–(4) exactly. Actually, if the symmetric matrices $\widehat{\mathbf{M}}$ and $\widehat{\mathbf{K}}_i$ are small enough, then Eq. (11) is an approximate multi-symplectic form, which satisfies the approximate multi-symplectic conservation law

$$\partial_t(\omega) + \sum_{i=1}^{n}\partial_{x_i}(\kappa_i) = -\partial_t(\widehat{\omega}) - \sum_{i=1}^{n}\partial_{x_i}(\widehat{\kappa}_i) \tag{12}$$

The discrete form of the approximate multi-symplectic system (11) can be written schematically as

$$(\mathbf{M} + \widehat{\mathbf{M}})(\partial_t)^k_{j_1 j_2\cdots j_n}\mathbf{z}^k_{j_1,j_2\cdots j_n} + \sum_{i=1}^{n}(\mathbf{K}_i + \widehat{\mathbf{K}}_i)(\partial_{x_i})^k_{j_1 j_2,\ldots,j_n}\mathbf{z}^k_{j_1 j_2,\ldots,j_n} = (\nabla_{\mathbf{z}}S(\mathbf{z}^k_{j_1 j_2,\ldots,j_n}))^k_{j_1 j_2,\ldots,j_n} \tag{13}$$

and the discrete form of the approximate multi-symplectic conservation law (12) is

$$(\partial_t)^k_{j_1 j_2\cdots j_n}\omega^k_{j_1 j_2\cdots j_n} + \sum_{i=1}^{n}(\partial_{x_i})^k_{j_1 j_2\cdots j_n}(\kappa_i)^k_{j_1 j_2\cdots j_n} = -(\partial_t)^k_{j_1 j_2\cdots j_n}\widehat{\omega}^k_{j_1 j_2\cdots j_n} - \sum_{i=1}^{n}(\partial_{x_i})^k_{j_1 j_2\cdots j_n}(\widehat{\kappa}_i)^k_{j_1 j_2\cdots j_n} \tag{14}$$

where $\omega^k_{j_1 j_2\cdots j_n} = ((\mathbf{M} + \widehat{\mathbf{M}})\mathbf{U}^k_{j_1 j_2\cdots j_n}, \mathbf{V}^k_{j_1 j_2\cdots j_n})$,$(\kappa_i)^k_{j_1 j_2\cdots j_n} = ((\mathbf{K}_i + \widehat{\mathbf{K}}_i)\mathbf{U}^k_{j_1 j_2\cdots j_n}, \mathbf{V}^k_{j_1 j_2\cdots j_n})$, $\{\mathbf{U}^k_{j_1 j_2\cdots j_n}\}^k_{j_1 j_2\cdots j_n} \in \mathbf{Z}\times\mathbf{Z}$ and $\{\mathbf{V}^k_{j_1 j_2\cdots j_n}\}^k_{j_1 j_2\cdots j_n} \in \mathbf{Z}\times\mathbf{Z}$ satisfy the corresponding discrete variational equations

$$(\mathbf{M}+\widehat{\mathbf{M}})(\partial_t)^k_{j_1,j_2\cdots j_n}\mathbf{Z}^k_{j_1,j_2\cdots j_n}+\sum_{i=1}^{n}(\mathbf{K}_i+\widehat{\mathbf{K}}_i)(\partial_{x_i})^k_{j_1,j_2,\cdots j_n}\mathbf{Z}^k_{j_1,j_2,\cdots j_n}=\nabla_{\mathbf{z}}S''(\mathbf{z}^k_{j_1,j_2,\cdots j_n})\mathbf{Z}^k_{j_1,j_2,\cdots j_n} \tag{15}$$

while $\widehat{\omega}^k_{j_1,j_2\cdots j_n}=\widehat{\mathbf{M}}\,\widehat{\mathbf{U}}^k_{j_1,j_2\cdots j_n},\widehat{\mathbf{V}}^k_{j_1,j_2\cdots j_n})$, $(\widehat{\kappa}_i)^k_{j_1,j_2\cdots j_n}=((\widehat{\mathbf{K}}_i)\widehat{\mathbf{U}}^k_{j_1,j_2\cdots j_n},\widehat{\mathbf{V}}^k_{j_1,j_2\cdots j_n}),\{\widehat{\mathbf{U}}^k_{j_1,j_2\cdots j_n}\}^k_{j_1,j_2\cdots j_n}\in\mathbf{Z}\times\mathbf{Z}$ and $\{\widehat{\mathbf{V}}^k_{j_1,j_2\cdots j_n}\}^k_{j_1,j_2\cdots j_n}\in\mathbf{Z}\times\mathbf{Z}$ satisfy the corresponding discrete variational equations

$$\widehat{\mathbf{M}}(\partial_t)^k_{j_1,j_2\cdots j_n}\mathbf{Z}^k_{j_1,j_2\cdots j_n}+\sum_{i=1}^{n}\widehat{\mathbf{K}}_i(\partial_{x_i})^k_{j_1,j_2,\cdots j_n}\mathbf{Z}^k_{j_1,j_2,\cdots j_n}=\nabla_{\mathbf{z}}S''(\mathbf{z}^k_{j_1,j_2,\cdots j_n})\mathbf{Z}^k_{j_1,j_2,\cdots j_n} \tag{16}$$

Similar to other difference numerical methods, the multi-symplectic scheme (5) has definite difference truncation error inevitably. Thus, in the following section, we try to present a new algorithm for the systems (11) with definite conservation law errors which are limited in the range of the difference truncation error.

Let $o(\Delta t,\Delta t^2,\ldots,\Delta x_1,\Delta x_1^2,\ldots,\ldots,\Delta x_n,\Delta x_n^2,\ldots,)$ denote the difference truncation error of the discrete form of the system (11) with the time step size Δt and the space step sizes Δx_1, Δx_2, ..., Δx_n, and $\Delta_k$denote the error of the discrete approximate multi-symplectic conservation law in step k. If we deem that the discrete multi-symplectic conservation law (6) is exact, Δ_k can be expressed schematically as

$$|\Delta_k|=\max\left\{\left|-(\partial_t)^k_{j_1,j_2\cdots j_n}\widehat{\omega}^k_{j_1,j_2\cdots j_n}-\sum_{i=1}^{n}(\partial_{x_i})^k_{j_1,j_2\cdots j_n}(\widehat{\kappa}_i)^k_{j_1,j_2\cdots j_n}\right|\right\} \tag{17}$$

the specific formulation of which will be presented in Section 3.

Actually, $\Delta_k$is the error value of the discrete approximate multi-symplectic conservation law whose absolute value is maximum among the spatial points of the kth time layer. If the absolute values of Δ_k $(k=1,2,\ldots,T/\Delta t)$ (where T is the total time interval) are less than or equal to the difference truncation error of the discrete form (13), we can think that the approximate multi-symplectic scheme (13) has the same numerical performance of the multi-symplectic scheme (5) because the error of the approximate multi-symplectic conservation law is too small to affect the numerical performance. Based on this idea, we propose the concept of the generalized multi-symplectic integrator as follows.

Definition. The discrete system (13) is called a generalized multi-symplectic integrator while the corresponding approximate multi-symplectic conservation law (14) a generalized discrete multi-symplectic conservation law associated with the generalized PDEs system (11) if and only if the scheme satisfies the following inequality at each step.

$$|\Delta_k|\leqslant o(\Delta t,\Delta t^2,\ldots,\Delta x_1,\Delta x_1^2,\ldots,\ldots,\Delta x_n,\Delta x_n^2,\ldots,) \tag{18}$$

that is,

$$\max\{|\Delta_k|\}\leqslant o(\Delta t,\Delta t^2,\ldots,\Delta x_1,\Delta x_1^2,\ldots,\ldots,\Delta x_n,\Delta x_n^2,\ldots,) \tag{19}$$

where $|\Delta_k|$is the absolute value of Δ_k.

Superficially, there are no difference between the inequalities (18) and (19); actually, the inequality (19) is more convenient to be operated by computer because it only needs one memory variable and $\left(\frac{L_1}{\Delta x_1}-1\right)\left(\frac{L_2}{\Delta x_2}-1\right)\cdots\left(\frac{L_n}{\Delta x_n}-1\right)$ times comparison while the inequality (18) needs $T/\Delta t$ memory variables and $\frac{T}{\Delta t}\left(\frac{L_1}{\Delta x_1}-1\right)\left(\frac{L_2}{\Delta x_2}-1\right)\cdots\left(\frac{L_n}{\Delta x_n}-1\right)$ times comparison, where L_i $(i=1,2,\ldots,n)$ is the computational length of the ith dimension space. The definition implies that the generalized multi-symplectic integrator should have the perfect numerical performance similar to the multi-symplectic integrator although there is definite error in the discrete form of the generalized multi-symplectic conservation law, which extends the multi-symplectic integrator idea to generalized Hamiltonian nonlinear wave PDEs.

In addition, according to the multi-symplectic integrator theory of Bridges [1,3], the multi-symplectic integrator can preserve the local properties of the system (1) exactly, which suggests us to investigate the local conservation laws of the system (11). Thus we will present the modified local energy conservation law and the modified local momentum conservation law of the system (11) in the following section.

We first show that the generalized Hamiltonian nonlinear wave PDEs system (11) satisfies modified local energy conservation law. Following the process of getting the local energy conservation law of the multi-symplectic system (1), we take the inner product of (11) with $\partial_t\mathbf{z}$ and define the modified energy density $\hat{e}=S(\mathbf{z})-\frac{1}{2}\sum_{i=1}^{n}\mathbf{z}^{\mathrm{T}}(\mathbf{K}_i+\widehat{\mathbf{K}}_i)\partial_{x_i}\mathbf{z}$ as well as the modified energy fluxes $\hat{f}_i=\frac{1}{2}\mathbf{z}^{\mathrm{T}}(\mathbf{K}_i+\widehat{\mathbf{K}}_i)\partial_t\mathbf{z}$ $(i=1,2,\ldots,n)$ for system (11). Then we can get

$$\begin{aligned}\partial_t\hat{e}+\sum_{i=1}^{n}\partial_{x_i}\hat{f}_i&=\partial_t[S(\mathbf{z})-\frac{1}{2}\sum_{i=1}^{n}\mathbf{z}^{\mathrm{T}}(\mathbf{K}_i+\widehat{\mathbf{K}}_i)\partial_{x_i}\mathbf{z}]+\frac{1}{2}\sum_{i=1}^{n}\partial_{x_i}\mathbf{z}^{\mathrm{T}}(\mathbf{K}_i+\widehat{\mathbf{K}}_i)\partial_t\mathbf{z}\\&=\partial_t[S(\mathbf{z})-\frac{1}{2}\sum_{i=1}^{n}\mathbf{z}^{\mathrm{T}}\mathbf{K}_i\partial_{x_i}\mathbf{z}]+\frac{1}{2}\sum_{i=1}^{n}\partial_{x_i}\mathbf{z}^{\mathrm{T}}\mathbf{K}_i\partial_t\mathbf{z}+\frac{1}{2}\sum_{i=1}^{n}\partial_{x_i}\mathbf{z}^{\mathrm{T}}\widehat{\mathbf{K}}_i\partial_t\mathbf{z}-\frac{1}{2}\partial_t\sum_{i=1}^{n}\mathbf{z}^{\mathrm{T}}\widehat{\mathbf{K}}_i\partial_{x_i}\mathbf{z}\end{aligned} \tag{20}$$

Substituting (3) into (20), we can obtain the modified local energy conservation law

$$\partial_t \hat{e} + \sum_{i=1}^{n} \partial_{x_i} \hat{f}_i = \frac{1}{2} \sum_{i=1}^{n} \partial_{x_i} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_t \mathbf{z} - \frac{1}{2} \partial_t \sum_{i=1}^{n} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_i} \mathbf{z} \tag{21}$$

Proceeding as outlined above, we can obtain the modified local momentum conservation law in the x_m $(m = 1, 2, \ldots, n)$ direction

$$\begin{aligned} \partial_t(\hat{h}_m) + \sum_{i=1}^{n} \partial_{x_i} \hat{g}_{mi} = {} & \frac{1}{2} \partial_t (\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{M}} \partial_{x_m} \mathbf{z}) + \frac{1}{2} \partial_{x_m} \left(-\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{M}} \partial_t \mathbf{z} - \sum_{i=1}^{m-1} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_i} \mathbf{z} - \sum_{i=m+1}^{n} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_i} \mathbf{z} \right) \\ & + \frac{1}{2} \left[\sum_{i=1}^{m-1} \partial_{x_i} \left(\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_m} \mathbf{z} \right) + \sum_{i=m+1}^{n} \partial_{x_i} (\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_m} \mathbf{z}) \right] \end{aligned} \tag{22}$$

where $\hat{h}_m = \frac{1}{2} \mathbf{z}^{\mathrm{T}} (\mathbf{M} + \widehat{\mathbf{M}}) \partial_{x_m} \mathbf{z}$, $\hat{g}_{mm} = S(\mathbf{z}) - \frac{1}{2} \mathbf{z}^{\mathrm{T}} (\mathbf{M} + \widehat{\mathbf{M}}) \partial_t \mathbf{z} - \frac{1}{2} \sum_{i=1}^{m-1} \mathbf{z}^{\mathrm{T}} (\mathbf{K}_i + \widehat{\mathbf{K}}_i) \partial_{x_i} \mathbf{z} - \frac{1}{2}$

$\sum_{i=m+1}^{n} \mathbf{z}^{\mathrm{T}} (\mathbf{K}_i + \widehat{\mathbf{K}}_i) \partial_{x_i} \mathbf{z}$ and $\hat{g}_{mi} = \frac{1}{2} \mathbf{z}^{\mathrm{T}} (\mathbf{K}_i + \widehat{\mathbf{K}}_i) \partial_{x_i} \mathbf{z}$ $(i = 1, \ldots, m-1, m+1, \ldots, n)$

Let $\Delta_e = \frac{1}{2} \sum_{i=1}^{n} \partial_{x_i} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_t \mathbf{z} - \frac{1}{2} \partial_t \sum_{i=1}^{n} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_i} \mathbf{z}$ denote the error of the modified local energy while $\Delta_p = \frac{1}{2} \partial_t (\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{M}} \partial_{x_m} \mathbf{z}) + \frac{1}{2} \partial_{x_m} (-\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{M}} \partial_t \mathbf{z} - \sum_{i=1}^{m-1} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_i} \mathbf{z} - \sum_{i=m+1}^{n} \mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_i} \mathbf{z}) + \frac{1}{2} [\sum_{i=1}^{m-1} \partial_{x_i} (\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_m} \mathbf{z}) \sum_{i=m+1}^{n} \partial_{x_i} (\mathbf{z}^{\mathrm{T}} \widehat{\mathbf{K}}_i \partial_{x_m} \mathbf{z})]$ the error of the modified local momentum in the x_m direction.

Referring to the results obtained by Sebastian Reich and Thomas J. Bridges about errors of the discrete local energy and the discrete local momentum [4,11], we can deem that the discrete forms of the local energy conservation law (3) and the local momentum conservation law (4) are exact, then the error of the discrete modified local energy conservation law can be expressed schematically as:

$$\{\Delta_e\}^k_{j_1 j_2 \ldots j_n} = \frac{1}{2} \sum_{i=1}^{n} (\partial_{x_i})^k_{j_1 j_2, \ldots j_n} (\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{K}}_i (\partial_t)^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n} - \frac{1}{2} (\partial_t)^k_{j_1 j_2, \ldots j_n} \sum_{i=1}^{n} (\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{K}}_i (\partial_{x_i})^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n} \tag{23}$$

and the error of the modified local momentum conservation law in the x_m direction can be expressed schematically as:

$$\begin{aligned} \{\Delta_p\}^k_{j_1 j_2 \ldots j_n} = {} & \frac{1}{2} (\partial_t)^k_{j_1 j_2, \ldots j_n} ((\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{M}} (\partial_{x_m})^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n}) + \frac{1}{2} \\ & \times (\partial_{x_m})^k_{j_1 j_2, \ldots j_n} \left[-(\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{M}} (\partial_t)^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n} - \sum_{i=1}^{m-1} (\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{K}}_i (\partial_{x_i})^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n} - \sum_{i=m+1}^{n} (\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{K}}_i (\partial_{x_i})^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n} \right] \\ & + \frac{1}{2} \sum_{i=1}^{m-1} (\partial_{x_i})^k_{j_1 j_2, \ldots j_n} [(\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{K}}_i (\partial_{x_m})^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n}] + \frac{1}{2} \sum_{i=m+1}^{n} (\partial_{x_i})^k_{j_1 j_2, \ldots j_n} [(\mathbf{z}^{\mathrm{T}})^k_{j_1 j_2, \ldots j_n} \widehat{\mathbf{K}}_i (\partial_{x_m})^k_{j_1 j_2, \ldots j_n} \mathbf{z}^k_{j_1 j_2, \ldots j_n}] \end{aligned} \tag{24}$$

3. The generalized multi-symplectic discretization for the compound KdV–Burgers equation

To illustrate the numerical performance of the generalized multi-symplectic integrator, we consider the compound KdV–Burgers equation [12,13]

$$\partial_t u + \alpha u \partial_x u + \beta u^2 \partial_x u + \gamma \partial_{xx} u + \varepsilon \partial_{xxx} u = 0 \tag{25}$$

where α, β and ε are real parameters, γ is a damping parameter, which can be considered as a composition of the KdV, mKdV and Burgers equations describing a model for long-wave propagation in nonlinear media with dispersion and dissipation effects [12,13]. Eq. (25) has general physical background and contains the following particular important cases

(1) $\alpha \neq 0$, $\beta = \gamma = 0$, $\varepsilon \neq 0$; Eq. (25) becomes the KdV equation

$$\partial_t u + \alpha u \partial_x u + \varepsilon \partial_{xxx} u = 0 \tag{26}$$

(2) $\beta \neq 0$, $\alpha = \gamma = 0$, $\varepsilon \neq 0$; Eq. (25) becomes the mKdV equation

$$\partial_t u + \beta u^2 \partial_x u + \varepsilon \partial_{xxx} u = 0 \tag{27}$$

(3) $\alpha = 0$, $\beta \neq 0$, $\gamma \neq 0$, $\varepsilon \neq 0$; Eq. (25) becomes the mKdV–Burgers equation

$$\partial_t u + \beta u^2 \partial_x u + \gamma \partial_{xx} u + \varepsilon \partial_{xxx} u = 0 \tag{28}$$

(4) $\alpha \neq 0$, $\beta = 0$, $\gamma \neq 0$, $\varepsilon \neq 0$; Eq. (25) becomes the KdV–Burgers equation

$$\partial_t u + \alpha u \partial_x u + \gamma \partial_{xx} u + \varepsilon \partial_{xxx} u = 0 \tag{29}$$

(5) $\alpha \neq 0$, $\beta \neq 0$, $\gamma = 0$, $\varepsilon \neq 0$; Eq. (25) becomes the KdV- mKdV equation

$$\partial_t u + \alpha u \partial_x u + \beta u^2 \partial_x u + \varepsilon \partial_{xxx} u = 0 \tag{30}$$

Each of the KdV, mKdV and Burgers equations is exactly solvable and many studies on these equations have already been reported. However, detailed studies on the compound KdV–Burgers equation are only beginning, and the numerical methods of the compound KdV–Burgers equation haven't been reported formally up to now. So choosing this equation as an example to illustrate the merits of the generalized multi-symplectic integrator is more challenging and significative.

According to the generalized multi-symplectic theory mentioned in Section 2, if we introduce canonical momenta $\partial_x v = u,\ w = \partial_x u,\ \partial_x p = -\frac{1}{2}\partial_t u$, we can get the generalized multi-symplectic PDEs of the compound KdV–Burgers equation

$$\begin{cases} \frac{1}{2}\partial_t u + \partial_x p = 0 \\ -\frac{1}{2}\partial_t v - \varepsilon\partial_x w - \gamma\partial_x u = -p + \frac{\alpha}{2}u^2 + \frac{\beta}{3}u^3 \\ \varepsilon\partial_x u = \varepsilon w \\ -\partial_x v = -u \end{cases} \tag{31}$$

if and only if the discrete form of which satisfies the inequality (41) at each time step.

Defining the state variable $\mathbf{z} = (v, u, w, p)^{\mathrm{T}}$, Eq. (31) can be rewritten as the matrix form

$$\begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}\partial_t\mathbf{z} + \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & -\gamma & -\varepsilon & 0 \\ 0 & \varepsilon & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}\partial_x\mathbf{z} = \nabla_{\mathbf{z}}S(\mathbf{z}) \tag{32}$$

where $S(\mathbf{z}) = \frac{\varepsilon}{2}w^2 - up + \frac{\alpha}{6}u^3 + \frac{\beta}{12}u^4$ is the Hamiltonian function.

From Eq. (32), we can get the matrices

$$\mathbf{M} = \begin{bmatrix} 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}, \quad \mathbf{K} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -\varepsilon & 0 \\ 0 & \varepsilon & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}; \quad \widehat{\mathbf{M}} = 0, \quad \widehat{\mathbf{K}} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & -\gamma & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

According to the generalized multi-symplectic integrator theory mentioned above, the generalized multi-symplectic conservation law of generalized multi-symplectic PDEs (32) is

$$\frac{1}{2}\partial_t(dv\Lambda du) + \partial_x(dv\Lambda dp + \varepsilon dw\Lambda du) = -\gamma d(\partial_x u)\Lambda du \tag{33}$$

The error of the modified local energy is

$$\Delta_e = \frac{\gamma}{2}\partial_t(u\partial_x u) - \frac{\gamma}{2}\partial_x u\partial_t u \tag{34}$$

and for $\widehat{\mathbf{M}} = \mathbf{0}$, the error of the modified local momentum is $\Delta_p = 0$, that is, the generalized multi-symplectic PDEs (32) satisfy the local momentum conservation law (4) exactly.

To investigate the good numerical properties of the generalized multi-symplectic method, we must discretize the generalized multi-symplectic PDEs (31) firstly. Obviously, all of the discretize rules leading to multi-symplectic schemes also lead to generalized multi-symplectic schemes.

It is well known that the midpoint rule is the simplest implicit discretization that leads to a symplectic scheme for Hamiltonian ordinary differential equations, and it is one of the lowest order schemes in the Gauss–Legendre class of discretization. Thus, in this paper, using a typical box scheme—Preissman scheme [10] derived from the midpoint rule to illustrate the merit of the generalized multi-symplectic method is well-grounded. The Preissman scheme of (31) is

$$\begin{cases} \frac{u_{i+1}^{j+1/2} - u_i^{j+1/2}}{2\Delta t} + \frac{p_{i+1/2}^{j+1} - p_{i+1/2}^{j}}{\Delta x} = 0 \\ \frac{v_{i+1}^{j+1/2} - v_i^{j+1/2}}{-2\Delta t} - \varepsilon\frac{w_{i+1/2}^{j+1} - w_{i+1/2}^{j}}{\Delta x} - \gamma\frac{u_{i+1/2}^{j+1} - u_{i+1/2}^{j}}{\Delta x} = -p_{i+1/2}^{j+1/2} + \frac{\alpha}{2}(u_{i+1/2}^{j+1/2})^2 + \frac{\beta}{3}(u_{i+1/2}^{j+1/2})^3 \\ \varepsilon\frac{u_{i+1/2}^{j+1} - u_{i+1/2}^{j}}{\Delta x} = \varepsilon w_{i+1/2}^{j+1/2} \\ -\frac{v_{i+1/2}^{j+1} - v_{i+1/2}^{j}}{\Delta x} = -u_{i+1/2}^{j+1/2} \end{cases} \tag{35}$$

Eliminating v, w and p from the scheme (35), we get a twelve-point implicit scheme that is equivalent to the Preissman scheme

$$\begin{aligned} &\frac{1}{16\Delta t}(\delta_t u_{i+1}^j + 3\delta_t u_i^j + 3\delta_t u_{i-1}^j + \delta_t u_{i-2}^j) + \frac{\alpha}{8\Delta x}[(\bar{u}_i^{j-1})^2 - (\bar{u}_{i-2}^{j-1})^2 + (\bar{u}_i^j)^2 - (\bar{u}_{i-2}^j)^2] + \frac{\beta}{8\Delta x}[(\bar{u}_i^{j-1})^3 - (\bar{u}_{i-2}^{j-1})^3 + (\bar{u}_i^j)^3 \\ &\quad - (\bar{u}_{i-2}^j)^3] + \frac{\gamma}{8(\Delta x)^2}(\delta_x^2 u_i^{j-1} + 2\delta_x^2 u_i^j + \delta_x^2 u_i^{j+1}) + \frac{\varepsilon}{4(\Delta x)^3}(\delta_x^3 u_i^{j-1} + 2\delta_x^3 u_i^j + \delta_x^3 u_i^{j+1}) \\ &\quad = 0 \end{aligned} \tag{36}$$

where Δt and Δx denote the time step size and the space step size respectively, $\bar{u}_i^j \approx \frac{1}{4}(u_i^j + u_i^{j+1} + u_{i+1}^j + u_{i+1}^{j+1})$, $\delta_t u_i^j = u_{i+1}^j - u_{i-1}^j, \delta_x^3 u_i^j = u_i^{j+1} - 3u_i^j + 3u_i^{j-1} - u_i^{j-2}$ and $\delta_x^2 u_i^j = u_i^{j+1} - 2u_i^j + u_i^{j-1}$ etc.

The discrete form of the generalized multi-symplectic conservation law is

$$\begin{aligned}&(dv_{i+1}^{j+1/2}\Lambda du_{i+1}^{j+1/2} - dv_i^{j+1/2}\Lambda du_i^{j+1/2})/2\Delta t + (dv_{i+1/2}^{j+1}\Lambda dp_{i+1/2}^{j+1} - dv_{i+1/2}^{j}\Lambda dp_{i+1/2}^{j})/\Delta x + \varepsilon(dw_{i+1/2}^{j+1}\Lambda du_{i+1/2}^{j+1}\\ &- dw_{i+1/2}^{j}\Lambda du_{i+1/2}^{j})/\Delta x\\ &= -\gamma[d(u_{i+1/2}^{j+1} - u_{i+1/2}^{j})/\Delta x]\Lambda du_{i+1/2}^{j+1/2}\end{aligned} \tag{37}$$

so the absolute value of the discrete generalized multi-symplectic conservation law error in step i is

$$|\Delta_i| = \max_j\left\{\left|-\gamma[d(u_{i+1/2}^{j+1} - u_{i+1/2}^{j})/\Delta x]\Lambda du_{i+1/2}^{j+1/2}\right|\right\} \tag{38}$$

and the difference truncation error (ignoring the high order items) of the form (35) is

$$o(\Delta t, \Delta t^2, \ldots, \Delta x, \Delta x^2, \ldots,) = o(\Delta t + \Delta x + \Delta x^2 + \Delta x^3) \approx \Delta t^2 + \Delta x^2 + \Delta x^3 + \Delta x^4 \tag{39}$$

Thus, for the compound KdV–Burgers equation (25), the specific formulation of the inequality (19) can be expressed as

$$\max_{i,j}\left\{\left|-\gamma[d(u_{i+1/2}^{j+1} - u_{i+1/2}^{j})/\Delta x]\Lambda du_{i+1/2}^{j+1/2}\right|\right\} \leqslant \Delta t^2 + \Delta x^2 + \Delta x^3 + \Delta x^4 \tag{40}$$

Assuming the damping parameter γ is time-invariant, the inequality (40) can be rearranged as

$$|\gamma| \leqslant (\Delta t^2 + \Delta x^2 + \Delta x^3 + \Delta x^4)/\max_{i,j}\left\{\left|[d(u_{i+1/2}^{j+1} - u_{i+1/2}^{j})/\Delta x]\Lambda du_{i+1/2}^{j+1/2}\right|\right\} \tag{41}$$

where

$$\begin{aligned}&\left[d(u_{i+1/2}^{j+1} - u_{i+1/2}^{j})/\Delta x\right]\Lambda du_{i+1/2}^{j+1/2} = (1/\Delta x)\left[\left(u_{i+1/2}^{j+3/2} - u_{i+1/2}^{j+1/2}\right)dx/\Delta x + \left(u_{i+1}^{j+1} - u_i^{j+1}\right)dt/\Delta t - \left(u_{i+1/2}^{j+1/2} - u_{i+1/2}^{j-1/2}\right)dx/\Delta x\right.\\ &\left.-\left(u_{i+1}^{j} - u_i^{j}\right)dt/\Delta t\right]\Lambda\left[\left(u_{i+1/2}^{j+1} - u_{i+1/2}^{j}\right)dx/\Delta x + \left(u_{i+1}^{j+1/2} - u_i^{j+1/2}\right)dt/\Delta t\right] = (1/\Delta x)\left[\delta_x^2 u_{i+1/2}^{j+1/2}dx/\Delta x\right.\\ &\left.+\left(u_{i+1}^{j+1} - u_i^{j+1} - u_{i+1}^{j} + u_i^{j}\right)dt/\Delta t\right]\Lambda\left[\left(u_{i+1/2}^{j+1} - u_{i+1/2}^{j}\right)dx/\Delta x + \left(u_{i+1}^{j+1/2} - u_i^{j+1/2}\right)dt/\Delta t\right]\\ &= \delta_x^2 u_{i+1/2}^{j+1/2}\left(u_{i+1}^{j+1/2} - u_i^{j+1/2}\right)dx\Lambda dt/\Delta x^2\Delta t + \left(u_{i+1}^{j+1} - u_i^{j+1} - u_{i+1}^{j} + u_i^{j}\right)\left(u_{i+1/2}^{j+1} - u_{i+1/2}^{j}\right)dt\Lambda dx/\Delta x^2\Delta t\\ &= \left[\delta_x^2 u_{i+1/2}^{j+1/2}\left(u_{i+1}^{j+1/2} - u_i^{j+1/2}\right) - \left(u_{i+1}^{j+1} - u_i^{j+1} - u_{i+1}^{j} + u_i^{j}\right)\left(u_{i+1/2}^{j+1} - u_{i+1/2}^{j}\right)\right]dx\Lambda dt/\Delta x^2\Delta t\end{aligned}$$

The inequality (41) implies that we can adjust the damping parameter γ as well as step sizes Δt, Δx to ensure that the scheme (36) is generalized multi-symplectic.

The discrete form of modified local energy error is

$$(\Delta_e)_{i,j} = \frac{\gamma}{2}\left[\frac{1}{\Delta t}\left(u_{i+3/2}^{j+1/2}\frac{u_{i+3/2}^{j+1} - u_{i+3/2}^{j}}{\Delta x} - u_{i+1/2}^{j+1/2}\frac{u_{i+1/2}^{j+1} - u_{i+1/2}^{j}}{\Delta x}\right) - \frac{u_{i+1/2}^{j+1} - u_{i+1/2}^{j}}{\Delta x}\frac{u_{i+1}^{j+1/2} - u_i^{j+1/2}}{\Delta t}\right] \tag{42}$$

thus the absolute value of the discrete modified local energy error in step i is

$$|(\Delta_e)_i| = \max_j\left\{\left|\frac{\gamma}{2}\left[\frac{1}{\Delta t}\left(u_{i+3/2}^{j+1/2}\frac{u_{i+3/2}^{j+1} - u_{i+3/2}^{j}}{\Delta x} - u_{i+1/2}^{j+1/2}\frac{u_{i+1/2}^{j+1} - u_{i+1/2}^{j}}{\Delta x}\right) - \frac{u_{i+1/2}^{j+1} - u_{i+1/2}^{j}}{\Delta x}\frac{u_{i+1}^{j+1/2} - u_i^{j+1/2}}{\Delta t}\right]\right|\right\} \tag{43}$$

Actually, $(\Delta_e)_i$is the error value of the discrete modified local energy whose absolute value is maximum among the spatial points of ith time layer. It has been mentioned that the generalized multi-symplectic PDEs (32) satisfy the local momentum conservation law (4) exactly, thus the implicit scheme (36) satisfies the discrete local momentum conservation law naturally, the detail of which can be found in the literature [1,3].

4. Testing the generalized multi-symplectic scheme

In this section, we will test the generalized multi-symplectic scheme (36) via simulating the travelling front solution of the compound KdV–Burgers equation. According to the literatures [12,13], the compound KdV–Burgers equation (25) has the travelling front solution

$$u(t,x) = \sqrt{\xi/2\beta}\tanh[\sqrt{-\xi/12\varepsilon}(x - \omega t)] - \alpha 2\beta - \gamma/\sqrt{-6\beta\varepsilon} \tag{44}$$

where $\xi = \gamma^2/\beta + 3\alpha^2/2\beta + 6\omega$ and ω is an arbitrary real constant. In the following experiments, we let $\alpha = \beta = 6$ and $\omega = -\varepsilon = 1$.Obviously, the scheme (36) is a nonlinear discrete equation, so we solve it with Gauss–Seidel iterative method [14] in the following numerical experiments, which has been proved to be an efficient algorithm for nonlinear discrete equation.

Experiment 1. In this experiment, we let step sizes $\Delta t = 0.001, \Delta x = 0.025$ as fixed values, which implies $o \approx 6.420156 \times 10^{-4}$, and then obtain the maximum permissible value of γ according to the scheme (36) and the inequality (41).

Case 1 Firstly, we let $\gamma = 0.01$ tentatively, then we can get $\xi = 15.000017$. We simulate the travelling front solution in the domain $D:(t, x) \in [0, 30] \times [-30, 30]$ according to the scheme (36). Fig.1 shows the evolution of the travelling front solution (44) over the time interval $[0, 30]$. To verify the scheme (36) is generalized multi-symplectic with $\gamma = 0.01$, we record the discrete generalized multi-symplectic conservation law error according to Eq. (38) and the discrete modified local energy error according to Eq. (43) over the time interval $[0, 30]$, the results of which can be found in Fig.2 and Fig.3.

From the results above, we can conclude that the scheme (36) can simulate the travelling front solution well with minute modified local energy error when we let $\gamma = 0.01$. In addition, it is found that the absolute value of the generalized multi-symplectic conservation law error is far less than the difference truncation error $o \approx 6.420156 \times 10^{-4}$ in each step, which suggests that if we increase the parameter γ or increase the time step Δt and space step Δx, the scheme (36) will still satisfy the inequality (41) probably. So in the further experiment, we increase the parameter γ with fixed step sizes ($\Delta t = 0.001, \Delta x = 0.025$), and then find that the scheme (36) still satisfies the inequality (41) narrowly when we take the damping parameter $\gamma = 0.533$. The corresponding results are presented in case 2.

Case 2 let $\gamma = 0.533$, then we can get $\xi = 15.047348$. We simulate the travelling front solution in the domain $D:(t, x) \in [0, 30] \times [-30, 30]$ according to the generalized multi-symplectic scheme (36) again. The wave forms $u(t, x)$ for travelling front solution (44) over the time interval $[0, 30]$ is very similar to that of case 1, thus we just present the generalized multi-symplectic conservation law error over the time interval $[0, 30]$in Fig.4 to illustrate that the generalized multi-symplectic scheme (36) satisfies the inequality (41) narrowly with $\gamma = 0.533$ ($\Delta t = 0.001$, $\Delta x = 0.025$). In addition, the modified local energy error can be found in Fig.5. To illustrate the high accuracy of the generalized multi-symplectic method, the supremum norm of error between the exact solution and the numerical solution derived from the scheme (36) with $\gamma = 0.533$ as $\|u\|_s = \sup|u_i^j - u(x_i, t_j)|$ for different nodes at $t = 0, t = 10, t = 20$ and $t = 30$ is presented in Table 1, the first column of which reports the supremum norm of error between the exact solutions and the numerical solutions for $x_i = -20$ and $t_j = 0$, and so on for other columns. The notation $*.********-**$ represents $*.******** \times 10^{-**}$in the Table 1.

From the results of Experiment 1, we can find that the wave forms with $\gamma = 0.533$ is almost as same as that with $\gamma = 0.01$, but the absolute value of the generalized multi-symplectic conservation law error and the modified local energy error with $\gamma = 0.533$ are larger than those with $\gamma = 0.01$. According to the generalized multi-symplectic integrator concept presented in Section 2, we can conclude that the scheme (36) is generalized multi-symplectic if $\gamma \leqslant 0.533$ when we let $\Delta t = 0.001$ and $\Delta x = 0.025$.

Experiment 2. In this experiment, we let the step sizes be variables and simulate the travelling front solution (44) with $\gamma = 0.2$, $\gamma = 0.4$, $\gamma = 0.6$, $\gamma = 0.8$ and $\gamma = 1$ respectively to obtain the relationships between the critical step sizes according to the scheme (36) with the corresponding inequality (41). The relationship curves between the critical step sizes with different

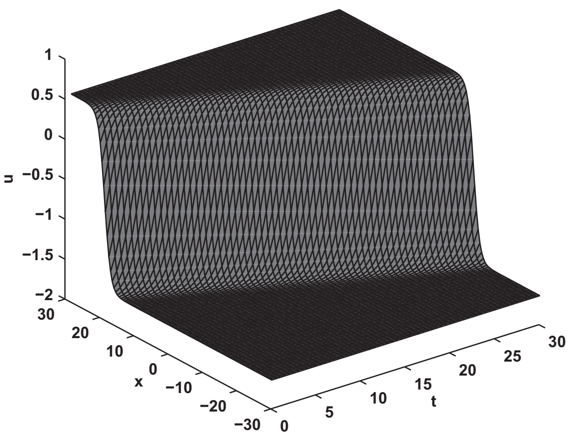

Fig. 1. The evolution of the travelling front solution $t \in [0, 30]$.

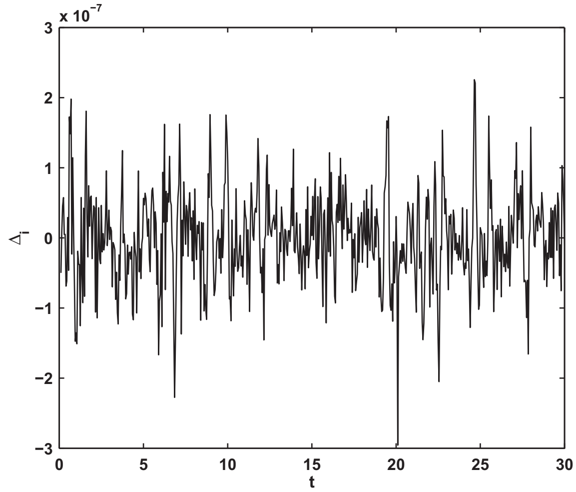

Fig. 2. Numerical error in the generalized multi-symplectic conservation law with $\gamma = 0.01$.

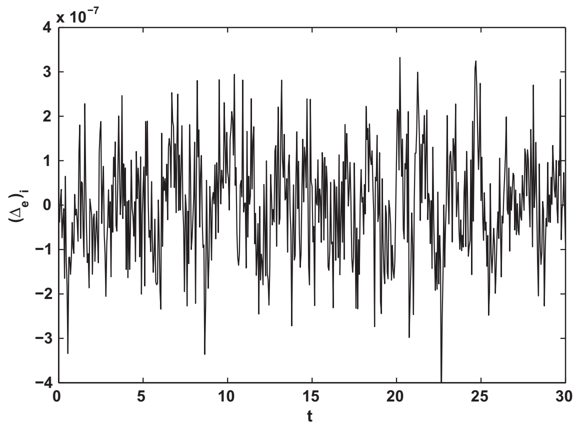

Fig. 3. Numerical error in the modified local energy with $\gamma = 0.01$.

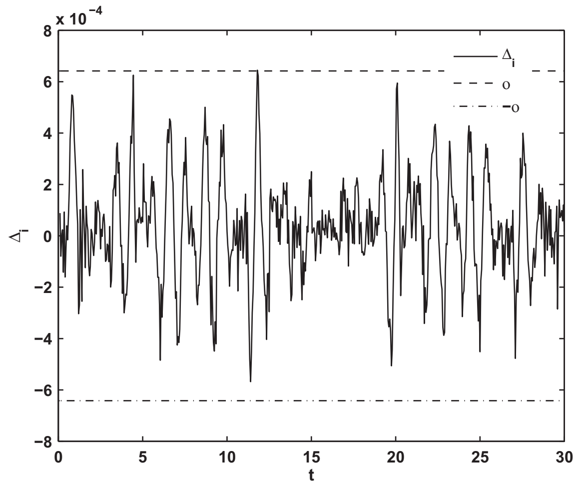

Fig. 4. Numerical error in the generalized multi-symplectic conservation law with $\gamma = 0.533$.

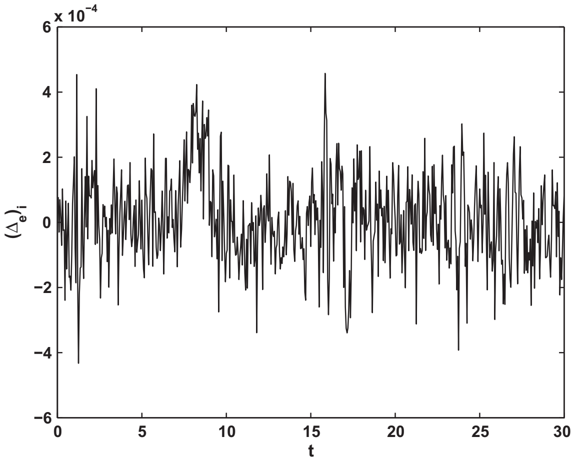

Fig. 5. Numerical error in the modified local energy with $\gamma = 0.533$.

Table 1
The supremum norm of error between the numerical solution and exact solution with $\gamma = 0.533$.

$x_i \setminus t_j$	0	10	20	30
-20	0.00000000–00	0.00000000–00	0.00000000–00	0.00000000–00
-16	0.00000000–00	0.00000000–00	0.00000000–00	6.00986130–20
-12	0.00000000–00	0.00000000–00	0.00000000–00	3.27218792–18
-8	0.00000000–00	0.00000000–00	1.75286813–20	5.19872174–18
-4	0.00000000–00	0.00000000–00	4.08112169–19	1.01963951–19
0	0.00000000–00	8.03113851–21	1.05789135–17	8.20264735–21
4	0.00000000–00	1.76209683–19	1.79193703–18	0.00000000–00
8	0.00000000–00	7.61543348–18	6.01527391–21	0.00000000–00
12	1.29085519–20	5.40570621–18	0.00000000–00	0.00000000–00
16	1.85036431–19	6.93546960–19	0.00000000–00	0.00000000–00
20	5.76209683–17	0.00000000–00	0.00000000–00	0.00000000–00

damping parameter values are shown in Fig. 6, which suggest that the scheme (36) is generalized multi-symplectic if the point $(\Delta\tau, \Delta\xi)$ belongs to the region that enclosed by the Δt axis, the Δx axis and the corresponding relationship curve with a certain parameter γ.

From the relationship curve with a certain parameter value, we can find that the critical space step size Δx decreases rapidly with the increasing of the critical time step size Δt. Comparing the relationship curves with different parameter values, we can conclude that the area of the region enclosed by the Δt axis, the Δx axis and the corresponding relationship curve with a certain parameter value reduces rapidly with the increasing of the parameter γ.

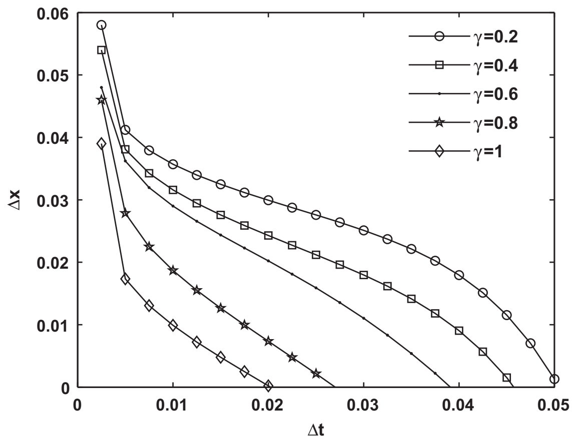

Fig. 6. The relationship curves between the critical step sizes.

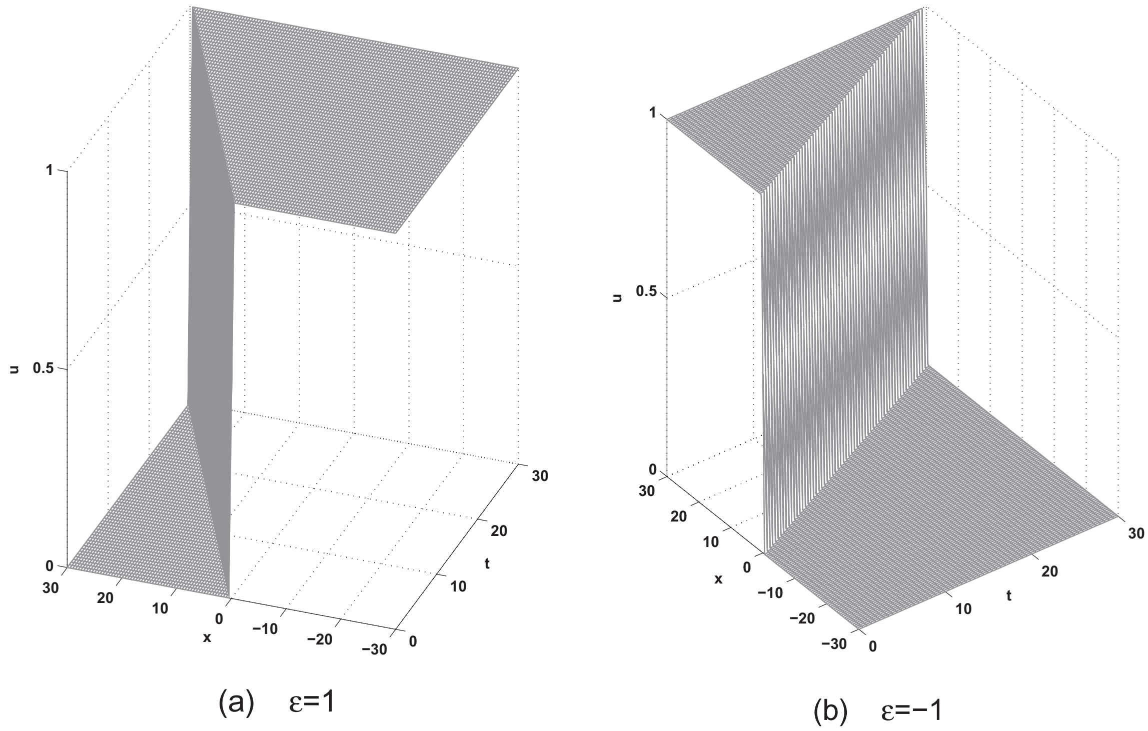

Fig. 7. The wave form of the shocks with $\varepsilon = \pm 1$.

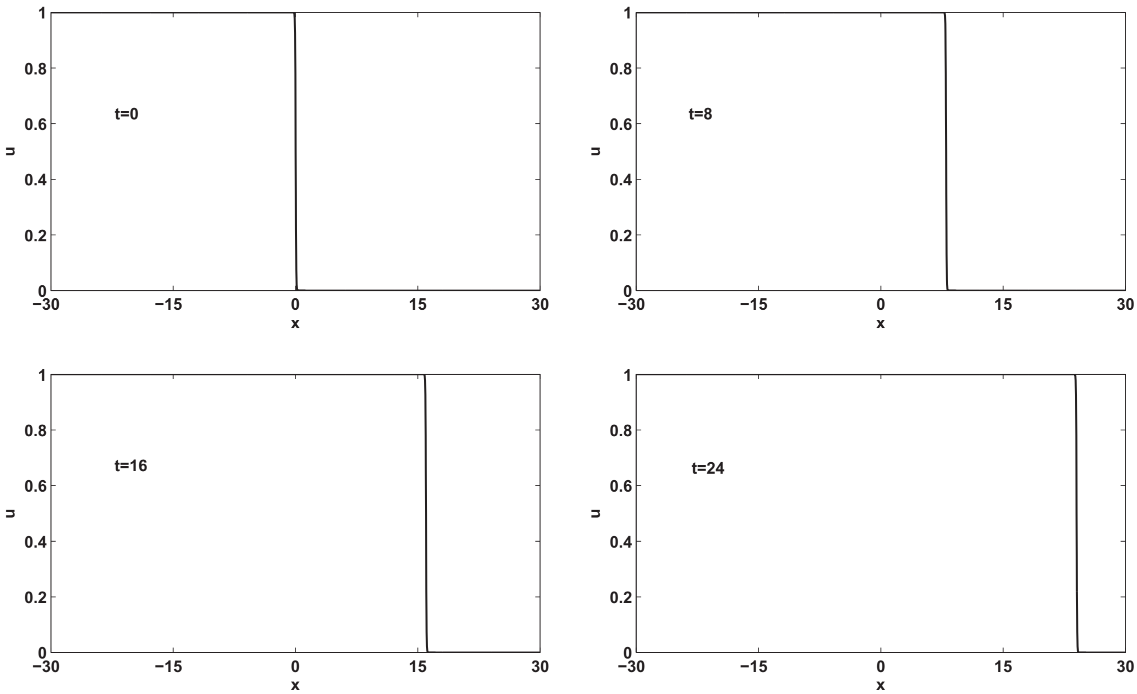

Fig. 8. The wave form of the shocks with $\varepsilon = 1$ at different time.

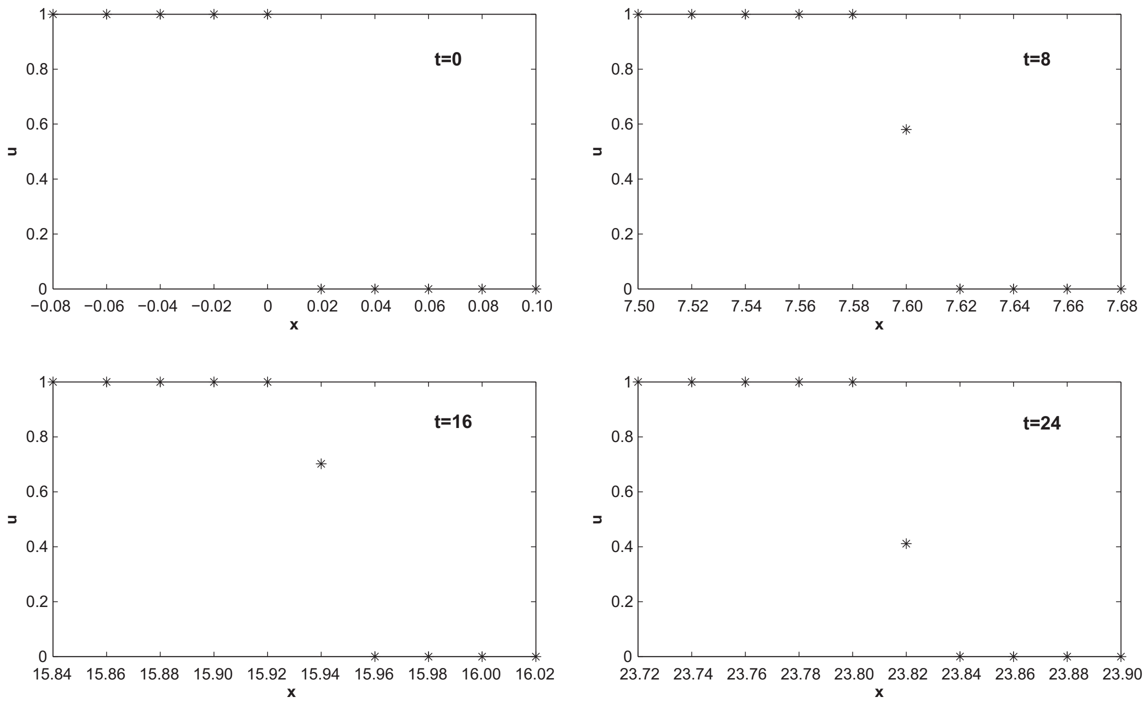

Fig. 9. The data points close to the shocks with $\varepsilon = 1$ at different time.

5. Capturing the shock wave in the compound KdV–Burgers equation by the generalized multi-symplectic method

It is well known that the shock wave exists in the Burgers-type equation, and capturing shock accurately by numerical method is a very difficult work although there are several shock-capturing methods reported. In this section, we study the compound KdV–Burgers equation by the scheme (36) to capture the shocks in the compound KdV–Burgers equation.

After a great deal of numerical experiments, we find that the shock may occur when we let $\alpha = \beta = 6$, $\gamma = 0.1$ and $\varepsilon = \pm 1$ in the compound KdV–Burgers equation with the following initial conditions:

$$\begin{aligned} u(0,x) &= \begin{cases} 0 & \text{for } x \leqslant 0 \\ 1 & \text{for } x \succ 0 \end{cases} \quad \text{for } \varepsilon = -1 \\ u(0,x) &= \begin{cases} 1 & \text{for } x \leqslant 0 \\ 0 & \text{for } x \succ 0 \end{cases} \quad \text{for } \varepsilon = 1 \end{aligned} \tag{45}$$

Table 2
The values of the data points close to the shock at $t = 8$.

x_i	7.50	7.52	7.54	7.56	7.58	7.60	7.62	7.64	7.66	7.68
u_i	1	1	1	1	0.999999	0.580211	0.000001	0	0	0

Table 3
The values of the data points close to the shock at $t = 16$.

x_i	15.84	15.86	15.88	15.90	15.92	15.94	15.96	15.98	16.00	16.02
u_i	1	1	1	1	0.999999	0.702009	0.000017	0	0	0

Table 4
The values of the data points close to the shock at $t = 24$.

x_i	23.72	23.74	23.76	23.78	23.80	23.82	23.84	23.86	23.88	23.90
u_i	1	1	1	1	0.999995	0.410988	0.000001	0	0	0

To ensure the scheme (36) is generalized multi-symplectic, we let the step length $\Delta t = \Delta x = 0.02$ according to Fig. 6. Using the scheme (36), we can get the wave form of the shock, see Fig. 7.

To investigate the local form of the shocks, we present the shocks at different time with $\varepsilon = 1$, see Fig. 8, from which, we can conclude that the scheme (36) can capture the shock wave in the compound KdV–Burgers equation accurately.

The number of the data points on the shocks is a focus on the simulation of shocks, thus, we give the data points on the shock with $\varepsilon = 1$ at different time to illustrate this issue, see Fig. 9, and list the values of the data points in Tables 2–4 at $t = 8$, $t = 16$ and $t = 24$.

From the results, we can find that there is only one data point related to the shocks at certain time, which implies that the generalized multi-symplectic scheme (36) is a high-resolution shock-capturing scheme that can preserve the local properties of the shock excellently and the generalized multi-symplectic method is a effective way to study the local properties of the complex fluid with small viscosity.

6. Conclusions

Focusing on the local properties of the complex fluid, a new theoretical framework of generalized multi-symplectic integrator concept and approach in Hamiltonian space based on the multi-symplectic idea is presented in this paper. Taking an example for the compound KdV–Burgers equation, the generalized multi-symplectic formulation is introduced. Then a twelve-point generalized multi-symplectic scheme is constructed, which satisfies the discrete local momentum conservation law exactly as well as two discrete modified conservation laws well: discrete generalized multi-symplectic conservation law and discrete modified local energy conservation law. From the numerical results, we can conclude:

1. The generalized multi-symplectic scheme can simulate the travelling front solution (44) accurately with small numerical error in the generalized multi-symplectic conservation law and the modified local energy, which implies the good conservation properties of the generalized multi-symplectic method;
2. The generalized multi-symplectic scheme can capture the shock structure within one data point and track the shock wave for a long time excellently, which implies the excellent long-time numerical behavior as well as the good conservation property of the generalized multi-symplectic method. With these remarkable advantages, the generalized multi-symplectic method can be used to exposit some specific phenomena existed in the complex fluid.

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