

A NEW CLASS STRUCTURE PRESERVING ALGORITHM FOR
MULTI-SYMPLECTIC PDES

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ABSTRACT

A NEW CLASS STRUCTURE PRESERVING ALGORITHM FOR MULTI-SYMPLECTIC PDEs

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In this thesis, several novel systematic algorithms for numerical solution of general multi-symplectic Hamiltonian PDEs are developed including a local energy-preserving algorithm, a local momentum-preserving algorithm and a global energy-preserving algorithm. All these structure-preserving algorithms are original and never studied in the literature before.

Local structure-preserving algorithms are constructed by using the combination of the Partitioned Average Vector Field (PAVF) method with implicit midpoint rule for spatial and temporal discretization. It is proven that local-structure preserving algorithms preserve the discrete local-energy and discrete local-momentum of a multi-symplectic PDE exactly. It is also proven that the local structure-preserving algorithms possesses the discrete global energy conservation and discrete global-momentum conservation under the periodic boundary conditions.

A class of global energy-preserving algorithm is developed by discretizing the spatial and temporal derivatives of a general multi-symplectic Hamiltonian PDEs by an anti-symmetric differentiation matrix and the PAVF method, respectively. It is proven that the discretization preserves the discrete global-energy of a multi-symplectic Hamiltonian PDEs exactly.

All these new novel algorithms are applied successfully to the nonlinear Dirac equation and the nonlinear complex modified Korteweg-de Vries equation. Many numerical experiments are presented to demonstrate the conservative properties of the proposed numerical methods.

In addition to new local structure-preserving algorithms based on the multi-symplectic formulation, some new structure-preserving schemes are also proposed for the numerical solution of the one-dimensional and two-dimensional Schrödinger-Boussinesq equation based on finite dimensional Hamiltonian formulation. Numerical results showed that this new methods capture some features of the Schrödinger-Boussinesq equation such as energy and mass conservation.

Keywords: Multi-Symplectic PDEs, Local Structure-Preserving Methods, Hamiltonian system, Coupled Schrödinger-Boussinesq Equation , Complex Modified Korteweg de Vries Equation, Nonlinear Dirac Equation

ÖZ

ÇOKLU-SİMPLEKTİK KİSMİ TÜREVLİ DİFERANSİYEL DENKLEMLER İÇİN YAPI KORUYAN YENİ BİR SINIF ALGORİTMA

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Bu tezde, genel çoklu-simplektik Hamilton kısmi diferansiyel denklemlerinin sayısal çözümü için yerel enerji koruyan bir algoritma, yerel momentum koruyan bir algoritma ve global enerji koruyan bir algoritma olmak üzere çeşitli yeni sistematik algoritmalar geliştirilmiştir. Tüm bu yapı koruyan algoritmalar özgündür ve literatürde daha önce hiç çalışılmamıştır.

Yerel yapı-koruyan algoritmalar, Bölümlü Ortalama Vektör Alanı (PAVF) yönteminin, mekansal ve zamansal ayırıklaştırma için örtük orta nokta kuralıyla birleştirilmesiyle oluşturulmuştur. Yerel yapı-koruma algoritmalarının, çoklu-simplektik bir kısmi diferansiyel denklemin ayırık yerel enerjisini ve ayırık yerel momentumunu tam olarak koruduğu kanıtlanmıştır. Ayrıca, yerel yapı-koruyan algoritmaların periyodik sınır koşulları altında ayırık global enerji korunumu-na ve ayırık global momentum korunumuna sahip olduğu da kanıtlanmıştır.

Global enerji-koruyan algoritma, genel çoklu-simplektik Hamilton kısmi diferansiyel denklemlerinin uzaysal ve zamansal türevlerinin sırasıyla antisimetrik bir diferansiyel matris ve PAVF yöntemi ile ayırıklaştırılmasıyla geliştirilmiştir. Ayırıklaştırmanın, çoklu-simplektik Hamilton kısmi diferansiyel denklemlerinin ayırık global enerjisini

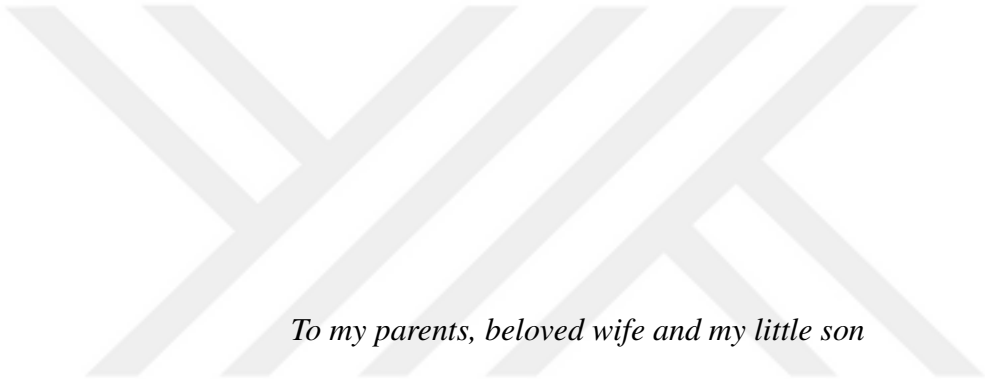
tam olarak koruduğu kanıtlanmıştır.

Tüm bu yeni algoritmalar, doğrusal olmayan Dirac denklemine ve doğrusal olmayan kompleks modifiye Korteweg-de Vries denklemine başarıyla uygulanmıştır. Önerilen sayısal yöntemlerin korunum özelliklerini göstermek için birçok sayısal deney sunulmuştur.

Çoklu-simplektik formülasyona dayalı yeni yerel yapı-koruyan algoritmalar ek olarak, Schrödinger-Boussinesq denkleminin sonlu boyutlu Hamilton formülasyonuna dayalı sayısal çözümü için bazı yeni yapı-koruyan şema-lar da önerilmiştir. Sayısal sonuçlar, bu yeni yöntemlerin Schrödinger-Boussinesq denkleminin dikkat çekici özel-liklerini yakaladığını göstermiştir.

Çoklu simplektik formülasyona dayalı yeni yerel yapı-koruyan algoritmalar ek olarak, sonlu boyutlu Hamilton formülasyonuna dayalı tek boyutlu ve iki boyutlu Schrödinger-Boussinesq denkleminin sayısal çözümü için bazı yeni yapı koruma şema-ları da önerilmiştir. Sayısal sonuçlar, bu yeni yöntemlerin Schrödinger-Boussinesq denkleminin enerji ve kütle korunumu gibi bazı özelliklerini yakaladığını göstermiştir.

Anahtar Kelimeler: Çoklu-Simplektik Kısmi Türevli Diferansiyel Denklemler, Lokal Yapı-Koruyan yöntemler, Hamilton sistem, İkili Schrödinger-Boussinesq Denklemi, Modifiye Kompleks Korteweg-de Vries Denklemi, Doğrusal Olmayan Dirac Denklemi



To my parents, beloved wife and my little son

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LIST OF SYMBOLS

$\mathbb{N}$	:	the set of natural numbers
$\mathbb{N}_0$	:	the set of non-negative integers
$\mathbb{Z}$	:	the set of integers
$\mathbb{R}$	:	the set of real numbers
$\mathbb{R}^n$	:	the n -dimensional vector space
$\langle x, y \rangle$	:	standard inner product of the vectors $x, y \in \mathbb{R}^n$
J	:	the canonical structure matrix
$\mathcal{J}$	:	the skew-adjoint operator
N	:	the spatial mesh points
M	:	the time mesh points
$\nabla_z S(z)$	:	Gradient of function $S(z)$
L	:	Skew-symmetric matrix
K	:	Skew-symmetric matrix

CHAPTER 1

HAMILTONIAN SYSTEMS

1.1 Introduction

We start by introducing some notation. Let Ω be a nonempty open and connected subset which represents the domain of the problems in the Euclidean space $\mathbb{R}^{2d}$ of the points $(p, q) = (p_1, \dots, p_d, q_1, \dots, q_d)$, where $d \geq 1$ is a positive integer. The open interval of the real line $\mathbb{R}$ of the variable t is denoted by $\mathcal{I}$, where $\mathcal{I} = (a, b)$, such that $0 \leq a < b$. Suppose that the function $H = H(p, q, t)$ is a sufficiently smooth and real function defined in the extended phase space product; $\Omega \times \mathcal{I}$, then the Hamiltonian H with the Hamiltonian system of differential equations is given by definition as

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}, \quad \frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}, \quad i = 1, \dots, d \quad (1.1)$$

where d represents the degree of freedom. As an application to mechanics, usually the q variables $(q_1, \dots, q_d)$ refer to generalized coordinates, while the p variables $(p_1, \dots, p_d)$ refer to conjugate generalized momenta, and H refers to the total mechanical energy.

In many Hamiltonian system problems, the Hamiltonian H does not depend directly on t , which shows that the system (1.1) is an autonomous system of differential equation, and for this reason we will consider H as a function defined in the phase space Ω more than a function defined in the extended phase space $\Omega \times \mathbb{R}$ and also independent of the last variable. It is useful to consider the phase space Ω as an even dimension; for that, we set $y = (p, q)^T$, and consider the Hamiltonian system (1.1) in a simple form

$$\frac{dy}{dt} = J^{-1} \nabla H, \quad (1.2)$$

where $y \in \mathbb{R}^m$, $m = 2d$ and ∇ is the gradient operator and J is the $m \times m$ skew-symmetric matrix (*canonical structure matrix*)

$$J := \begin{bmatrix} 0_d & I_d \\ -I_d & 0_d \end{bmatrix} \quad (1.3)$$

where 0_d is the zero matrix, and I_d is the $d \times d$ identity matrix. The term *canonical* is reserved for Hamiltonian systems on an even-dimensional Euclidean space. If the Hamiltonian is *autonomous*, that is, If the vector field is formally independent of time, then

$$\frac{dH}{dt} = (\nabla H)^T J^{-1} \nabla H = 0.$$

The Hamiltonian H is a conserved quantity that is constant along the solutions of the system. As an application, this usually corresponds to energy conservation. Time-dependent or *non-autonomous* Hamiltonian systems $H = H(z, t)$ also arise frequently in applications.

1.2 Examples of Hamiltonian systems

In this section, we give some examples of canonical Hamiltonian systems arising in the literature.

1.2.1 The Harmonic Oscillator

We know that a Hamiltonian system can be represented by the potential energy added to the kinetic energy. *i.e.*,

$$H = T + V, \quad T = p_1^2/2\xi, \quad V = kq_1^2/2.$$

Systems that require d ($d \geq 1$ is a positive integer) independent coordinates to describe their motion are called n degree of freedom systems. This is the well-known system with one degree of freedom ($d = 1$), where T and V are the kinetic and potential energies, respectively, ξ and k are positive constants that, for the common example of a material point coupled to a spring, respectively, correspond to a mass and energy constant ([61]). In this case when $d = 1$, it is undoubtedly practical to use the notation p and q for the dependent variables, so that the equation (1.1) for the harmonic

oscillator becomes,

$$\dot{p} = -kq, \quad \dot{q} = \frac{p}{\xi}, \quad (1.4)$$

where dots represent the derivatives of the dependent variables with respect to t .

The general solution for q is an oscillation given by

$$q(t) = c_1 \sin(\omega t + c_2), \quad \omega = \sqrt{k/\xi}.$$

Here, ω is the angular frequency, $\mathcal{T} = 2\pi/\omega$, is the period. $\nu = 1/\mathcal{T} = \omega/2\pi$, is the frequency and c_1, c_2 are integral constants.

In a similar way p is given by

$$p(t) = \xi\omega c_1 \cos(\omega t + c_2).$$

It is easy to write the particular solution that take the initial condition $(p(0), q(0))$ at $t = 0$ in a matrix representation as follows,

$$\begin{bmatrix} p(t) \\ q(t) \end{bmatrix} = \begin{bmatrix} \cos(\omega t) & -(\xi\omega)\sin(\omega t) \\ (\xi\omega)^{-1}\sin(\omega t) & \cos(\omega t) \end{bmatrix} \begin{bmatrix} p(0) \\ q(0) \end{bmatrix}. \quad (1.5)$$

When (1.5) plotted in the (p, q) -phase plane, $(p(t), q(t))$ parametric curves comparable to the ellipses

$$H(p, q) = p^2/2\xi + kq^2/2 = \text{constant}.$$

These are circles when $\xi k = 1$.

1.2.2 The Double Harmonic Oscillators

This system has two degree of freedom ($d = 2$) and

$$H = T + V, \quad T = (\omega_1 p_1^2 + \omega_2 p_2^2)/2, \quad V(q) = (\omega_1 q_1^2 + \omega_2 q_2^2)/2.$$

Since we consider two uncoupled harmonic oscillators, the variables (p_1, q_1) in the equations of motion $\dot{p}_1 = -\omega_1 q_1$, $\dot{q}_1 = \omega_1 p_1$, $\dot{p}_2 = -\omega_2 q_2$, $\dot{q}_2 = \omega_2 p_2$ are not coupled to the variables. (p_2, q_2) . The projections of the double harmonic oscillator solutions onto the (p_i, q_i) -plane correspond to circles and have an angular frequency of $\omega_i > 0$, in accordance with our earlier explanation of the harmonic oscillators. The trajectory returns to its initial position in the four dimensional phase space after having completed r cycles of the (p_1, q_1) variables and s cycles of the (p_2, q_2) variables, if

ω_1/ω_2 is a rational number r/s . If this is the case, then the solutions of the double harmonic oscillators are periodic with period $\mathcal{T} = 2\pi r/\omega_1 = 2\pi s/\omega_2$. On the other hand, the trajectory never returns to its starting point if ω_1/ω_2 is irrational.

A geometric image is utilized. The system has two conserved quantities

$$H_1 = \frac{\omega_1}{2}(p_1^2 + q_1^2) \quad \text{and} \quad H_2 = \frac{\omega_2}{2}(p_2^2 + q_2^2),$$

which represent the energies in each of the two uncoupled oscillators.

1.3 Symplectic Map and The Wedge Product

In this section, we review some basic definitions and theorem from [51]. First, definition of the symplecticity of a Smooth mapping $\Psi : \mathbb{R}^{2d} \rightarrow \mathbb{R}^{2d}$ and its implication for the solution behavior of canonical Hamiltonian systems are discussed.

Definition: A smooth map $\Psi : U \rightarrow \mathbb{R}^{2d}$ (where $U \subset \mathbb{R}^{2d}$ is an open set) is called a *symplectic map* if its Jacobian $\Psi_z(z)$ satisfies:

$$[\Psi_z(z)]^T J [\Psi_z(z)] = J, \quad (1.6)$$

for all z in the domain of definition of Ψ . If J is the canonical structure matrix given in (1.2), the term *canonical map* can be used as a synonym for the term *symplectic map*. For a linear transformation $\Psi(z) = Bz$, the condition of symplecticness reduces to

$$B^T J B = J,$$

and B is referred to as a *symplectic matrix*.

A symplectic matrix B preserves the bilinear form $\langle x, y \rangle_J = x^T J y$, that is, $\langle Bx, By \rangle_J = \langle x, y \rangle_J$ for all $x, y \in \mathbb{C}^{2d \times 2d}$ [31].

Theorem 1.3.1 [51] *Let $\Psi : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ be a symplectic map in the plane. Then the determinant of the Jacobian matrix of the symplectic map Ψ is 1, i.e.*

$$\det [\Psi_z(z)] = 1. \quad (1.7)$$

Proof. We write the Jacobian $\Psi_z(z)$ as

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

Using the symplecticity condition (1.6), we obtain

$$ad - bc = 1.$$

This proves condition (1.7). □

Symplectic planar map preserves the area. Let D be a bounded subset of phase space. The oriented area of the region D in the (p, q) -Cartesian coordinate system is defined by the double integral

$$Area(D) = \iint_D dpdq \quad (1.8)$$

Let $\hat{D}$ denote the image of D under the symplectic map Ψ i.e. $\hat{D} = \Psi(D)$. Then, the standard rules for changing variables in an integral gives

$$\begin{aligned} Area(\hat{D}) &= \iint_{\hat{D}} d\hat{p}d\hat{q} \\ &= \iint_{\hat{D}} \det[\Psi_z(z)] dpdq \\ &= \iint_D dpdq \\ &= Area(D). \end{aligned}$$

Thus, a symplectic map in $\mathbb{R}^2$ is area preserving.

Now, we discuss the symplectic structure in term of two-forms associated to $2d$ -dimensional phase space.

Definition 1.3.2 A two-form on $\mathbb{R}^{2d}$ is a skew-symmetric bilinear function $\Omega(\xi, \eta)$ with arguments $\xi, \eta \in \mathbb{R}^{2d}$. Bilinearity means that the function is linear in each of its two arguments separately, i.e.,

$$\begin{aligned} \Omega(a\xi_1 + b\xi_2, \eta) &= a\Omega(\xi_1, \eta) + b\Omega(\xi_2, \eta) \\ \Omega(\xi, a\eta_1 + b\eta_2) &= a\Omega(\xi, \eta_1) + b\Omega(\xi, \eta_2), \quad a, b \in \mathbb{R}, \end{aligned}$$

and skew-symmetry means

$$\Omega(\xi, \eta) = -\Omega(\eta, \xi), \quad \forall \xi, \eta \in \mathbb{R}^{2d}.$$

Theorem 1.3.3 *The symplectic structure matrix (1.3), that is*

$$J = \begin{pmatrix} 0_d & I_d \\ -I_d & 0_d \end{pmatrix},$$

introduces the two-form Ω on the phase space, $\mathbb{R}^{2d}$,

$$\Omega(\xi, \eta) := \xi^T J \eta, \quad \xi, \eta \in \mathbb{R}^{2d}, \quad (1.9)$$

which is equivalent to

$$\Omega(\xi, \eta) = \xi_1 \eta_2 - \xi_2 \eta_1, \quad \xi, \eta \in \mathbb{R}^2. \quad (1.10)$$

for $d = 1$.

Proof. The proof will be given for case $d = 1$, for simplicity. Let $\xi = (\xi_1, \xi_2)^T, \xi' = (\xi'_1, \xi'_2)^T, \eta = (\eta_1, \eta_2)^T$ be vectors in $\mathbb{R}^2$. Then the symplectic form (1.9) takes the form

$$\Omega(\xi, \eta) = \xi^T J \eta = \xi_1 \eta_2 - \xi_2 \eta_1, \quad \xi, \eta \in \mathbb{R}^2 \quad (1.11)$$

Bilinearity:

$$\begin{aligned} \Omega(a\xi + b\xi', \eta) &= (a\xi + b\xi')^T J \eta \\ &= -a\xi_2 \eta_1 - b\xi'_2 \eta_1 + a\xi_1 \eta_2 + b\xi'_1 \eta_2 \\ &= a(\xi_1 \eta_2 - \xi_2 \eta_1) + b(\xi'_1 \eta_2 - \xi'_2 \eta_1) \\ &= a\Omega(\xi, \eta) + b\Omega(\xi', \eta), \end{aligned}$$

for all $\xi, \xi', \eta \in \mathbb{R}^2$.

$\Omega(\xi, a\eta + b\eta') = a\Omega(\xi, \eta) + b\Omega(\xi, \eta')$, for all $\xi, \eta, \eta' \in \mathbb{R}^2$ can be shown similarly.

Skew-symmetry:

$$\begin{aligned} \Omega(\xi, \eta) &= \xi_1 \eta_2 - \xi_2 \eta_1 \\ &= -(\eta_1 \xi_2 - \eta_2 \xi_1) \\ &= -\Omega(\eta, \xi), \end{aligned}$$

for all $\xi, \eta \in \mathbb{R}^2$. □

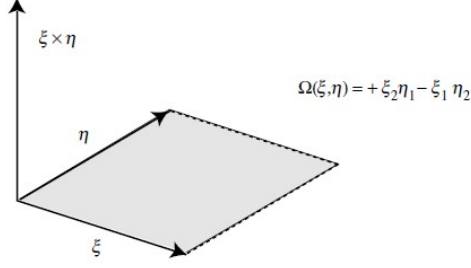


Figure 1.1: The two-form $\Omega(\xi, \eta)$ for $d = 1$ is the oriented area of the parallelogram spanned by the vectors $\xi, \eta \in \mathbb{R}^2$. (The picture is copied from [51])

Geometrically, for $d = 1$, the two-form $\Omega(\xi, \eta)$ in (1.9) is either the area spanned by the vectors $\xi, \eta \in \mathbb{R}^2$, or is the negative of this area. Viewing the two planar vectors $\xi, \eta \in \mathbb{R}^2$ embedded in $\mathbb{R}^3$, the two-form $\Omega(\xi, \eta)$ is nothing but the z -coordinate of the cross product of the two vectors as shown in Fig 1.1.

For $d > 1$, we project $\xi \in \mathbb{R}^{2d}$ and $\eta \in \mathbb{R}^{2d}$ down on to the q_i, p_i -coordinate planes, $i = 1 \cdots, d$. Denote the corresponding vectors in $\mathbb{R}^{2d}$ by $\xi^{(i)}, \eta^{(i)}$ respectively, $i = 1 \cdots, d$. Then $\Omega(\xi, \eta)$ is equivalent to the sum of the oriented areas of the parallelograms spanned by the pair of vectors $\xi^{(i)}$ and $\eta^{(i)}$. If Ω_0 denotes the standard two-form of a pair of vectors in the plane, then

$$\Omega(\xi, \eta) = \sum_i \Omega_0(\xi^{(i)}, \eta^{(i)}), \quad \xi^{(i)}, \eta^{(i)} \in \mathbb{R}^2. \quad (1.12)$$

The definition (1.9) is not always the most convenient way to check the symplecticness of the map Ψ if the map is implicit. In this case, the symplecticness can be checked by using the differential one-form and two-form. This section is devoted to the introduction of some basic materials of one-form and two-form.

It is known from the calculus that if $f : \mathbb{R}^m \rightarrow \mathbb{R}$ is a smooth function, then the directional derivative of f at the point $z \in \mathbb{R}^m$ along a vector $\xi \in \mathbb{R}^m$, denoted by $df(\xi)$, is given by

$$df(\xi) := D_\xi f(z) = \nabla f(z) \cdot \xi = \frac{\partial f}{\partial z_1} \xi_1 + \cdots + \frac{\partial f}{\partial z_m} \xi_m. \quad (1.13)$$

It can be seen that $df(\xi)$ is linear in ξ . The linear functional $df(\cdot)$ is called the *differential* of f at z and is an example of a *differential one-form*.

If f is the coordinate function, that is $f(z) = z_i$, then from (1.13), it can be shown that

$$df(\xi) = \frac{\partial z_i}{\partial z_1} \xi_1 + \cdots + \frac{\partial z_i}{\partial z_i} \xi_i + \cdots + \frac{\partial z_i}{\partial z_m} \xi_m,$$

that is

$$dz_i(\xi) = \xi_i, \quad i = 1, 2, \dots, m. \quad (1.14)$$

Thus, the differential df in (1.13) can be written in term of the differentials (1.14) as

$$df(\xi) = \frac{\partial f}{\partial z_1} dz_1(\xi) + \cdots + \frac{\partial f}{\partial z_m} dz_m(\xi),$$

and consequently,

$$df = \frac{\partial f}{\partial z_1} dz_1 + \cdots + \frac{\partial f}{\partial z_m} dz_m.$$

Let $\xi, \eta \in \mathbb{R}^{2d}$. Consider the ordering of vectors ξ, η into a sequence of projections $\xi^{(i)}, \eta^{(i)}$ on the (q_i, p_i) -coordinate planes. From (1.12) we can write

$$\Omega(\xi, \eta) = \sum_i \Omega_0(\xi^{(i)}, \eta^{(i)}) = \sum_i [dp_i(\xi) dq_i(\eta) - dq_i(\xi) dp_i(\eta)].$$

Using (1.14), $dp_i(\xi) = \xi_2^{(i)}, dq_i(\eta) = \eta_1^{(i)}, dq_i(\xi) = \xi_1^{(i)}, dp_i(\eta) = \eta_2^{(i)}$, we can write this as

$$\Omega(\xi, \eta) = \sum_i [\xi_2^{(i)} \eta_1^{(i)} - \xi_1^{(i)} \eta_2^{(i)}]. \quad (1.15)$$

Definition 1.3.4 *The wedge product of two differentials df and dg is defined by*

$$(df \wedge dg)(\xi, \eta) := dg(\xi) df(\eta) - df(\xi) dg(\eta), \quad \xi, \eta \in \mathbb{R}^2 \quad (1.16)$$

Using the definition (1.16), the the two-form (1.15) can be written as

$$\Omega = \sum_i dq_i \wedge dp_i,$$

or, in vector notation,

$$\Omega = dq \wedge dp. \quad (1.17)$$

Properties of the wedge product:

Let dp, dq and dz be k -vectors of differential one-forms on $\mathbb{R}^k$. Then the following properties hold.

- *Bilinearity*: $dz \wedge (\alpha dp + \beta dq) = \alpha dz \wedge dp + \beta dz \wedge dq$, for all $\alpha, \beta \in \mathbb{R}$.
- *Skew-symmetry*: $dp \wedge dq = -dq \wedge dp$.
- *Rule of matrix multiplication*: $dp \wedge (Adq) = (A^T dp \wedge dq)$, for all $k \times k$ matrix A .

Theorem 1.3.5 [51]: *The conservation of symplecticness, under a transformation*

$$\hat{q} = \Psi^1(q, p), \quad \hat{p} = \Psi^2(q, p),$$

reduces to

$$d\hat{q} \wedge d\hat{p} = dq \wedge dp, \quad (1.18)$$

where

$$\begin{aligned} d\hat{q} &= \Psi_q^1(q, p)dq + \Psi_p^1(q, p)dp \\ d\hat{p} &= \Psi_q^2(q, p)dq + \Psi_p^2(q, p)dp. \end{aligned}$$

1.4 Symplecticness of Hamiltonian Flow Maps

This section is devoted to the implications of the symplecticness for the solution behavior of canonical Hamiltonian systems.

Theorem 1.4.1 [11] *Let $(q, p) \in \mathbb{R}^{2d}$ be canonical coordinates and let $H : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ be a smooth function. The continuous-time Hamiltonian system (1.1), that is*

$$\begin{aligned} p_t &= -\nabla_q H(q, p) \\ q_t &= \nabla_p H(q, p) \end{aligned} \quad (1.19)$$

preserves exactly the symplectic form $\omega = dp \wedge dq$; i.e.,

$$\frac{d}{dt}\omega = 0 \quad (1.20)$$

for all time t .

Proof. The differential of (1.19) yields

$$\begin{aligned} dp_t &= -H_{qq}(q, p)dq - H_{qp}(q, p)dp \\ dq_t &= H_{pq}(q, p)dq + H_{pp}(q, p)dp. \end{aligned}$$

Taking the wedge product with dp and dq , respectively, gives

$$\begin{aligned} dp_t \wedge dq &= -H_{qq}(q, p)dq \wedge dq - H_{qp}(q, p)dp \wedge dq \\ dp \wedge dq_t &= H_{pq}(q, p)dp \wedge dq + H_{pp}(q, p)dp \wedge dp. \end{aligned}$$

Adding these lines leads to

$$dp_t \wedge dq + dp \wedge dq_t = -H_{qp}(q, p)dp \wedge dq + H_{pq}(q, p)dp \wedge dq$$

where $dp \wedge dp = dq \wedge dq = 0$. This implies $\frac{d}{dt}\omega = 0$ as desired. $\square$

Symplecticity of the Hamiltonian system (1.19) can also be shown by using the flow map of the Hamiltonian system. The flow $\varphi_t : U \rightarrow \mathbb{R}^{2d}$ of the Hamiltonian system (1.19) is the mapping that advances the solution by time t , i.e.,

$$\varphi_t(p_0, q_0) = (p(t, p_0, q_0), q(t, p_0, q_0)),$$

where $p(t, p, q)$ and $q(t, p, q)$ are the solutions of the Hamiltonian system (1.19) at the time t corresponding to the initial conditions $p(t_0) = p_0$ and $q(t_0) = q_0$.

Theorem 1.4.2 (Poincaré) [38] *Let the Hamiltonian $H(q, p)$ of the system (1.19) be a twice continuously differentiable function on $U \subset \mathbb{R}^{2d}$. Then the flow φ_t satisfies the symplecticness condition (1.6), that is,*

$$\left(\frac{\partial \varphi_t}{\partial(p_0, q_0)} \right)^T J \left(\frac{\partial \varphi_t}{\partial(p_0, q_0)} \right) = J \quad (1.21)$$

for each fixed t , wherever it is defined.

We illustrate this theorem with the harmonic oscillator problem (see Sec.1.2.1). Let us recall the general solution of the equations (1.4) of the Harmonic oscillator problem (1.2.1)

$$\begin{pmatrix} p(t) \\ q(t) \end{pmatrix} = \begin{pmatrix} \cos \omega t & -(m\omega) \sin \omega t \\ (m\omega)^{-1} \sin \omega t & \cos \omega t \end{pmatrix} \begin{pmatrix} p(0) \\ q(0) \end{pmatrix}.$$

The flow of the Hamiltonian system (1.4) is the mapping

$$\varphi_t(t, p_0, q_0) = \begin{pmatrix} \cos \omega t & -(m\omega) \sin \omega t \\ (m\omega)^{-1} \sin \omega t & \cos \omega t \end{pmatrix}. \quad (1.22)$$

Computing the derivative $\frac{\partial \varphi_t}{\partial(p_0, q_0)}$, one can show that the symplecticity condition (1.21) is satisfied.

Let $\varphi_t : \mathbb{R}^2 \rightarrow \mathbb{R}^2$ be a symplectic map in the plane. We write the Jacobian $\frac{\partial \varphi_t}{\partial(p_0, q_0)}$ as

$$\frac{\partial \varphi_t}{\partial(p_0, q_0)} = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

If we use this matrix in the symplecticness condition (1.21) then we obtain the expression

$$ad - cb$$

and conclude that

$$\det[\varphi_t(p_0, q_0)] = 1. \quad (1.23)$$

Thus, for a planar map $\varphi_t(p_0, q_0)$, the condition of symplecticness (1.21) is that the determinant of Jacobian $\varphi_t(p_0, q_0)$ is equal to one everywhere .

The condition (1.23) can be easily verified in the harmonic oscillator problem (1.4). The determinant of the flow map (1.22) leads to

$$\det \left[\frac{\partial \varphi_t}{\partial(p_0, q_0)} \right] = \cos^2(\omega t) + \sin^2(\omega t) = 1,$$

which verifies the symplecticness of the flow φ_t .

1.4.1 Some Elementary Symplectic Integrators

First, we consider the first-order differential equation, the so-called *Cauchy problem*, which takes the form

$$\begin{cases} y'(t) = f(t, y(t)), & \forall t \in I \subset \mathbb{R} \\ y(t_0) = y_0. \end{cases} \quad (1.24)$$

where $f : I \times \mathbb{R} \rightarrow \mathbb{R}$ is a given function, $I = [t_0, T]$ with $T < \infty$, y' denotes the derivative of the function y with respect to time t , t_0 is a given point of I and y_0 is a given value which is called the initial data.

Unfortunately, an explicit or implicit solution is available only for some special types of ordinary differential equations. Moreover, as in the case of the differential equation $y' = e^{t^2}$, a solution can only be expressed through a series expansion. For all these

reasons, a numerical solution is essential to approximate the solution of *every family* of ordinary differential equations for which the solution does not exist.

The strategy of the finite difference methods consists of subdividing the interval of integration I into N subintervals of length $h = \Delta t = (T - t_0)/N$ is called the discretization step size. Then at each *node* $t_n = t_0 + nh$, $n = 1, 2, \dots, N$, we seek the unknown value y_n which approximates the exact value $y(t_n)$. The set $y_0, y_1, y_2, \dots, y_N$ represents the *numerical solution*.

Now we confine ourselves to the symplecticness of the Hamiltonian system. Since symplecticity is a geometric property of Hamiltonian systems (1.19), it is natural to preserve this property in numerical solutions. This subsection is devoted to some well-known symplectic integrators arising in the literature.

Definition 1.4.3 [38] *A numerical one-step method is called symplectic if the one-step method*

$$y_{n+1} = \Phi(y_n) \quad (1.25)$$

is symplectic whenever the method is applied to a smooth Hamiltonian (1.19).

That is, a numerical one-step method applied to (1.1) is called a *symplectic integrator* if the discrete version of the symplecticness condition (1.21), i.e.

$$\left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right)^T J \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)} \right) = J \quad (1.26)$$

is satisfied. Symplecticness of a numerical method can also be shown by using the wedge product (1.20). A numerical one-step method is called a *symplectic integrator* if the symplecticness condition

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n \quad (1.27)$$

is preserved exactly [51].

Theorem 1.4.4 [38] *For the numerical solution of equations (1.19), the so-called Euler-A method*

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_{n+1}, q_n) \\ q_{n+1} &= q_n + hH_p(p_{n+1}, q_n) \end{aligned} \quad (1.28)$$

or the Euler-B method

$$\begin{aligned} p_{n+1} &= p_n - hH_q(p_n, q_{n+1}) \\ q_{n+1} &= q_n + hH_p(p_n, q_{n+1}) \end{aligned} \quad (1.29)$$

are both *symplectic methods* of order 1.

Proof. We will prove the symplecticness of the Euler-A method. Symplecticness of the Euler-B method can be proven similarly.

We consider the method (1.28) with $d = 1$ for simplicity. We will show that the symplecticness condition (1.26) is satisfied by computing the derivative $\left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right)$. Differentiating (1.28) with respect to p_n and q_n yields

$$\begin{aligned} \frac{\partial p_{n+1}}{\partial p_n} &= 1 - h \left(H_{qq} \frac{\partial q_{n+1}}{\partial p_n} + H_{qp} \right), & \frac{\partial p_{n+1}}{\partial q_n} &= -h H_{qq} \frac{\partial q_{n+1}}{\partial q_n} \\ \frac{\partial q_{n+1}}{\partial p_n} &= h \left(H_{pq} \frac{\partial q_{n+1}}{\partial p_n} + H_{pp} \right), & \frac{\partial q_{n+1}}{\partial q_n} &= 1 + h H_{pq} \frac{\partial q_{n+1}}{\partial q_n}, \end{aligned} \quad (1.30)$$

where H_{pp} , H_{qq} and H_{pq} denote the second-order partial derivatives evaluated at (p_{n+1}, q_n) .

Inserting these derivatives into the symplecticness condition (1.26), we get

$$\begin{aligned} \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right)^T J \left(\frac{\partial(p_{n+1}, q_{n+1})}{\partial(p_n, q_n)}\right) &= \begin{pmatrix} 0 & -\frac{\partial q_{n+1}}{\partial p_n} \frac{\partial p_{n+1}}{\partial q_n} + \frac{\partial p_{n+1}}{\partial p_n} \frac{\partial q_{n+1}}{\partial q_n} \\ -\frac{\partial q_{n+1}}{\partial q_n} \frac{\partial p_{n+1}}{\partial p_n} \frac{\partial p_{n+1}}{\partial q_n} \frac{\partial q_{n+1}}{\partial p_n} & 0 \end{pmatrix} \\ &= \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \\ &= J. \end{aligned}$$

Thus, the symplecticness of the Euler-A method (1.28) has been shown. $\square$

The symplecticness of the Euler-A method (1.28) can be also shown by using the wedge product notation (1.27) [51].

Taking the wedge product of the first equation in (1.28) with dq_n from the right, we have

$$\begin{aligned} dp_{n+1} \wedge dq_n &= (dp_n - hH_{qp}dp_{n+1} - hH_{qq}dq_n) \wedge dq_n \\ &= dp_n \wedge dq_n - hH_{qp}dp_{n+1} \wedge dq_n \\ &= \left(\frac{1}{1 + hH_{qp}}\right) dp_n \wedge dq_n. \end{aligned} \quad (1.31)$$

Now, the wedge product of the second equation in (1.28) with dp_{n+1} from the left

yields

$$\begin{aligned}
dp_{n+1} \wedge dq_{n+1} &= dp_{n+1} \wedge (dq_n + hH_{pp}dp_{n+1} + hH_{pq}dq_n) \\
&= dp_{n+1} \wedge dq_n + hH_{pq}dp_{n+1} \wedge dq_n \\
&= (1 + hH_{pq})dp_{n+1} \wedge dq_n.
\end{aligned} \tag{1.32}$$

Substituting $dp_{n+1} \wedge dq_n$ from (1.31) into (1.32) implies that

$$dp_{n+1} \wedge dq_{n+1} = dp_n \wedge dq_n. \tag{1.33}$$

Hence, the symplectic Euler method (1.28) is a two-dimensional symplectic map, i.e., an area preserving map of the plane.

For the Euler-A method (1.28), notice that the variable p is treated by the implicit Euler method and the variable q by the explicit Euler method. However, for the Euler-B method (1.29), the variable q is treated by the implicit Euler method and the variable p by the explicit Euler method.

Theorem 1.4.5 [38] *The implicit midpoint rule*

$$y_{n+1} = y_n + hJ \nabla H\left(\frac{y_{n+1} + y_n}{2}\right) \tag{1.34}$$

applied to the autonomous Hamiltonian system

$$y'(t) = J \nabla H(y)$$

is a symplectic method of order 2.

Proof. Differentiating both sides of (1.34) with respect to y_n yields

$$\left(I - \frac{h}{2}J \nabla^2 H(y^{n+\frac{1}{2}})\right) \left(\frac{\partial y_{n+1}}{\partial y_n}\right) = \left(I + \frac{h}{2}J \nabla^2 H(y^{n+\frac{1}{2}})\right) \tag{1.35}$$

where $y^{n+\frac{1}{2}} = (y_{n+1} + y_n)/2$ and $\nabla^2 H$ is the symmetric Hessian matrix. Then, after a tedious computation, it can be shown that

$$\left(\frac{\partial y_{n+1}}{\partial y_n}\right)^T J \left(\frac{\partial y_{n+1}}{\partial y_n}\right) = J.$$

□

1.5 Infinite-Dimensional Hamiltonian Systems

An essential tool for describing phenomena that arise in the physical sciences is the partial differential equation (PDE). A unique subset of PDEs that do more than just model systems with conserved quantities are those with Hamiltonian structure (such as energy and momentum), and also have a variety of unique strategies for their simulation and analysis. Major advancements have been made and are still being made in this dynamic area of research on both the mathematics and computational sides. These advancements not only advance the field as a whole but also advance a wide spectrum of other scientific disciplines. Numerical solutions to Hamiltonian partial differential equations (PDEs) may provide certain obstacles, the reason is by the generalization of the underlying phase space from finite to infinite dimensions. Most frequently, the methods of lines are used to consider Hamiltonian PDEs. In these methods, a PDE is first discretized in space to produce a sizable system of Hamiltonian ordinary differential equations (ODEs). The resulting system of ODEs is then integrated using a numerical technique that preserves structure.

The general form of Hamiltonian PDEs is

$$\frac{\partial u}{\partial t} = \mathcal{J} \frac{\delta H}{\delta u}, \quad (1.36)$$

where the domain is $\Gamma = (x, t) = \mathbb{R} \times \mathbb{R}$. Here, $\mathcal{H} = \int_{\Gamma} H(u, u_x, u_{xx}, \dots) dx$ and $\mathcal{J}$ is the skew-adjoint operator. Also the last term of (1.36) is called the variational derivative, which is given by

$$\frac{\delta H}{\delta u} = \frac{\partial H}{\partial u} - \frac{\partial}{\partial x} \left(\frac{\partial H}{\partial u_x} \right) + \frac{\partial^2}{\partial x^2} \left(\frac{\partial H}{\partial u_{xx}} \right) - \dots \quad (1.37)$$

In the Hamiltonian PDEs, the conservation of energy and other PDE integrals are crucial. Several energy or integral-preserving techniques for ODEs and PDEs have already been developed in recent years by using of discrete gradients and discrete variational derivatives [51]. The following finite dimensional Hamiltonian system is created after the skew-adjoint operators and Hamiltonian in (1.36) are sufficiently spatially discretized

$$\frac{du}{dt} = J(u) \frac{\partial H}{\partial u}, \quad (1.38)$$

where J is the $N \times N$ skew-symmetric matrix that corresponds to the discretization of the skew-adjoint operator $\mathcal{J}$.

Hamiltonian PDEs arises in various filed in science such as fluid mechanics, plasma physics, and nonlinear optics. In the following section, we will consider the nonlinear Schrödinger equation (NLS) and Boussinesq equation as a Hamiltonian PDE and see how they can be converted into finite-dimensional Hamiltonian ODEs.

1.5.1 The Nonlinear Schrödinger Equation

The one-dimensional nonlinear Schrödinger equation is of the form

$$iu_t + u_{xx} + k|u|^2 u = 0, \quad (1.39)$$

where $i = \sqrt{-1}$ and $u(x, t)$ is a complex-valued function. The non-linear Schrödinger equation have drawn a lot of attention from mathematicians, particularly because of its applications of small amplitude gravity on the surface of zero viscosity, the langmuir waves in hot plasmas and the propagation of plane diffracted wave beams in the focusing regions of the ionosphere and also in the application of non linear optics. The NLS equation is a completely integrable Hamiltonian system, and to solve (1.39) we can consider an infinite dimensional system by letting $u = p + iq$, where $p(x, t)$ and $q(x, t)$ are real valued functions. The formulation of the Hamiltonian of (1.39) can be expressed as follows

$$\frac{dz}{dt} = J \frac{\delta H(z, z_x)}{\delta u}. \quad (1.40)$$

where

$$z = (p, q), \quad J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix},$$

and the Hamiltonian is

$$\mathcal{H}(z, z_x) = \int \frac{1}{2} \left[p_x^2 + q_x^2 - \frac{1}{2}(p^2 + q^2)^2 \right] dx.$$

A finite-dimensional Hamiltonian system can be obtained by discretizing the spatial derivatives in (1.40). We suppose that outside the region $x_L \leq x \leq x_R$, the solutions to (1.40) are extremely small. Let

$$P = [p_1, p_2, \dots, p_N]^T, \quad Q = [q_1, q_2, \dots, q_N]^T$$

where N is the number of spatial grid points. To get the semi-discrete system, we can discretize the spatial derivatives of (1.39) using central difference approximation with

accuracy of $O(\Delta^{2m})$

$$\frac{d}{dt} \begin{bmatrix} P \\ Q \end{bmatrix} = \begin{bmatrix} 0 & I_N \\ -I_N & 0 \end{bmatrix} \begin{bmatrix} M(2m) & 0 \\ 0 & M(2m) \end{bmatrix} \begin{bmatrix} P \\ Q \end{bmatrix}. \quad (1.41)$$

where $M(2m)$ is an $N \times N$ matrix and I is the $N \times N$ identity matrix. The matrix $M(2m)$ can be written as the sum of two matrices $M(2m) = B(2m) + D$, where D is a diagonal matrix

$$D = \text{diag}(-k(p_1^2 + q_1^2), \dots, -k(p_N^2 + q_N^2)).$$

For the spatial discretization we can use the second-order and fourth-order central difference approximations. Once we use these two approximations, we get the following matrices

$$M(2) = B(2) + D$$

where

$$B(2) = -\frac{1}{\Delta x^2} \begin{bmatrix} -2 & 1 & 0 & \dots & 0 \\ 1 & -2 & 1 & \dots & 0 \\ & \ddots & \ddots & \ddots & \\ 0 & \dots & 1 & -2 & 1 \\ 0 & \dots & 0 & 1 & -2 \end{bmatrix},$$

and

$$M(4) = B(4) + D,$$

where

$$B(4) = -\frac{1}{12\Delta x^2} \begin{bmatrix} -30 & 16 & -1 & 0 & \dots & 0 \\ 16 & -30 & 16 & -1 & \dots & 0 \\ & \ddots & \ddots & \ddots & \ddots & \\ 0 & \dots & -1 & 16 & -30 & 16 \\ 0 & \dots & 0 & -1 & 16 & -30 \end{bmatrix}.$$

The system (1.41) is a finite-dimensional Hamiltonian system. Assuming that $Z = (P^T, Q^T)^T$ and

$$J = \begin{bmatrix} 0 & I \\ -I & 0 \end{bmatrix},$$

then (1.41) can be written as

$$\frac{dZ}{dt} = J \nabla_z H(Z), \quad (1.42)$$

with Hamiltonian

$$H(P, Q) = \frac{1}{2} \left[P^T B(2m)P + Q^T B(2m)Q \right] - \frac{\alpha}{4} \sum_{i=1}^N (p_i^2 + q_i^2)^2. \quad (1.43)$$

Now, the time derivative in (1.42) can be discretized by any energy-preserving scheme [66].

1.5.2 Boussinesq Equation

Long waves or shallow water waves are formed when the water depth is much lesser compared to the wavelength. Boussinesq equations describe behaviour of water waves when they approach shallow water areas such as the surf zone, coast, or beach; the water depth is usually constant. The earlier work of the French mathematician Joseph Boussinesq was very instrumental in solitary wave theory along the ones of Russell, Airy, Stokes, and others [29]. The Boussinesq equation includes the weak non-linear and dispersive effects, which can successfully remedy the problem where the shallow water equation is unable to directly handle the dispersion wave. It still ignores the effects of non-linearity and bottom friction during transoceanic spreading and only includes them in the calculation process during spreading on the coast and climbing. Its fundamental principle is equivalent to that of the equation of shallow water long wave. The general Boussinesq equation is

$$u_{tt} + a(u^n)_{xx} + b(u^l)_{xxxx} = 0, \quad l, n \in \mathbb{R}, \quad (1.44)$$

for simplicity, we will consider the case that $l = 1$ and getting the following equation

$$u_{tt} + a(u^n)_{xx} + b(u)_{xxxx} = 0, \quad (1.45)$$

in the region $D = [(x, t) \in \mathbb{R}^2 : x_L \leq x \leq x_R, t \geq 0]$, with initial condition

$$u(x, 0) = u_0(x), \quad u_t(x, 0) = \tilde{u}_0(x), \quad (1.46)$$

and periodic boundary condition

$$u(x_L, t) = u(x_R, t), \quad t \in [0, T]. \quad (1.47)$$

Equation (1.45) can be written as infinite-dimensional Hamiltonian system by introducing

$$-v_t = [a(u^n)_x + b(u)_{xxx}], \quad u_t = v_x, \quad (1.48)$$

we get

$$\begin{bmatrix} u_t \\ v_t \end{bmatrix} = \begin{bmatrix} 0 & \partial_x \\ \partial_x & 0 \end{bmatrix} \begin{bmatrix} -a(u^n) - b(u)_{xx} \\ v \end{bmatrix} = \begin{bmatrix} 0 & \partial_x \\ \partial_x & 0 \end{bmatrix} \begin{bmatrix} \delta H_u \\ \delta H_v \end{bmatrix}. \quad (1.49)$$

Setting $n = p$, the Hamiltonian form is

$$\mathcal{H}(u, v) = \int_{-\infty}^{\infty} \left[\frac{1}{2} v^2 - \frac{a}{p+1} u^{p+1} + \frac{b}{2} (u_x)^2 \right] dx. \quad (1.50)$$

The system (1.48) is discretized for the spatial derivatives, and for that we will use central difference approximation to get the following discrete system

$$\begin{aligned} \frac{du_i(t)}{dt} &= \frac{1}{2\Delta x} [v_{i+1} - v_i], \\ \frac{dv_i(t)}{dt} &= \frac{-a}{2\Delta x} [u_{i+1}^p - u_{i-1}^p] - \frac{b}{2\Delta x^3} [u_{i+2} - 2u_{i+1} + 2u_{i-1} - u_{i-2}], \end{aligned} \quad (1.51)$$

With a discrete Hamiltonian

$$\mathcal{H}(u, v) = \sum_{i=1}^N \left[\frac{1}{2} v_i^2 - \frac{a}{p+1} u_i^{p+1} + \frac{b}{2} \left(\frac{u_{i+1} - u_i}{\Delta x} \right)^2 \right]. \quad (1.52)$$

Now, the time derivative in (1.51) can be discretized by any energy preserving scheme.

1.5.3 Klein-Gordon Schrödinger Equation

The Schrödinger equation is a fundamental equation in non-relativistic quantum mechanics. On the other hand, The Klein–Gordon (KG) equation describes the behavior of particles that moves at high speeds without spinning. These two equations are combined to study the behavior of particles in relativistic quantum mechanics [60]. These equations are essential tools for studying the behavior of fundamental particles and their interactions in various physical systems. Consider the following Klein-Gordon Schrödinger (KGS) equation [19]

$$\begin{aligned} i\psi_t + \frac{1}{2}\psi_{xx} + \psi\varphi &= 0 \\ \varphi_{tt} - \varphi_{xx} + \varphi - |\psi|^2 &= 0, \end{aligned} \quad (1.53)$$

where $(x, t) \in \mathbb{R}^2$, $x_L \leq x \leq x_R$, and $t \geq 0$. This system of PDEs describes the collision between a conservative complex neutron field and a neutron meson field. The complex unknown function $\psi(x, t)$ represents the scalar neutron field, while the real unknown function $\varphi(x, t)$ represents the scalar neutral meson field. The system (1.53) shows the

main success of quantum mechanics in the quantitative description.

To determine the solution of (1.53), the initial and boundary conditions are given by

$$\psi(x, 0) = \psi_0(x), \quad \varphi(x, 0) = \varphi_0(x), \quad \varphi_t(x, 0) = \varphi_1(x). \quad (1.54)$$

$$\lim_{|x| \rightarrow \infty} \psi(x, t) = 0, \quad \lim_{|x| \rightarrow \infty} \varphi(x, t) = 0. \quad (1.55)$$

Now, introducing $\psi(x, t) = p(x, t) + iq(x, t)$, $\varphi(x, t) = 2v$, where both $p(x, t)$ and $q(x, t)$ are real valued functions, the KGS equation (1.53) can be written as follows

$$\begin{aligned} q_t &= \frac{1}{2} p_{xx} + \varphi p \\ p_t &= -\frac{1}{2} q_{xx} - \varphi q \\ v_t &= \frac{1}{2} (\varphi_{xx} - \varphi + p^2 + q^2) \\ \varphi_t &= 2v. \end{aligned} \quad (1.56)$$

Letting $z = [p, q, v, \varphi]^T$, equation (1.56) has an infinite Hamiltonian PDE

$$z_t = \mathcal{J} \frac{\delta \mathcal{H}(z)}{\delta z} \quad (1.57)$$

$$\text{where } \mathcal{J} = \begin{bmatrix} 0_{2 \times 2} & J_{2 \times 2} \\ -J_{2 \times 2} & 0_{2 \times 2} \end{bmatrix}, \quad J_{2 \times 2} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

and the Hamiltonian is defined by

$$\mathcal{H}(z(t)) = \int_{x_L}^{x_R} \left[\frac{1}{2} \varphi (p^2 + q^2) - \frac{1}{4} (\varphi^2 + \varphi_x^2 + p_x^2 + q_x^2) - v^2 \right] dx. \quad (1.58)$$

Besides the Hamiltonian, $H(z(t)) = H(z(0))$, the KGS (1.56) has also mass conservation.

$$\mathcal{M}(z(t)) = \int_{x_L}^{x_R} (p^2 + q^2) dx = \mathcal{M}(z(0)). \quad (1.59)$$

The spatial derivatives in (1.56) will be discretized by using second order central difference approximation, while the time derivative can be discretized by any energy preserving scheme.

1.6 Operator Splitting Methods

Operator splitting is a classical and intuitive approach. In cases where a (PDE) or a system of PDEs comprises distinct terms representing different physical phenomena,

it is often advantageous to employ specialized numerical methods tailored to each individual process. This strategy not only enhances computational efficiency but also contributes to the simplification of the overall solution procedure. This technique is commonly referred to as operator splitting, fractional step methods, or split-step methods. Within the framework of nonlinear differential equations, operator splitting proves particularly useful for isolating nonlinear components, thereby facilitating the development of more tractable and efficient solution strategies.

1.6.1 Ordinary Operator Splitting for ODEs

Consider first an ODE such that the right-hand side can be split into two terms

$$u' = f_0(u) + f_1(u). \quad (1.60)$$

In case f_0 and f_1 are linear functions of u , $f_0 = au$ and $f_1 = bu$, we have $u(t) = Ae^{(a+b)t}$, if $u(0) = A$. When going on one time step of length Δt from t_n to t_{n+1} , we have

$$u(t_{n+1}) = u(t_n)e^{(a+b)\Delta t}$$

. This expression can be also written as

$$u(t_{n+1}) = u(t_n)e^{a\Delta t}e^{b\Delta t}$$

, or

$$u^* = u(t_n)e^{a\Delta t}, \quad (1.61)$$

$$u(t_{n+1}) = u^*e^{b\Delta t}, \quad (1.62)$$

The first step (1.61) corresponds to solving the differential equation $u' = f_0$ over a time interval Δt , using $u(t_n)$ as the initial condition. The subsequent step (1.62) involves solving $u' = f_1$ over the same time interval, where the initial condition is given by the terminal value obtained from the first step. In other words, the full time step is decomposed into two successive substeps, each governed by a distinct ordinary differential equation (ODE), namely $u' = f_0$ and $u' = f_1$.

The sequence in which these equations are solved is not essential; as shown in the preceding derivation, one may equivalently reverse the order and solve $u' = f_1$ prior to $u' = f_0$. This operator splitting method yields an exact solution when the ODEs are

linear. However, in the case of nonlinear ODEs, the method is only approximate and introduces a local error of order (Δt) .

Moreover, this approach is amenable to generalization: the system can be partitioned into an arbitrary number of subsystems, allowing for the solution of a larger system of partial differential equations (PDEs) through a sequence of simpler subproblems.

1.6.2 Introduction to Splitting Methods

The idea is simple: divide and conquer. It is probably the most important systematic technique for the development of algorithms in general. Suppose that the differential equation is of the form

$$\frac{dz}{dt} = f(z) \equiv f_0(z) + f_1(z),$$

where each of two differential equations

$$\frac{dz}{dt} = f_0(z)$$

and

$$\frac{dz}{dt} = f_1(z)$$

are completely integrable. We first note that any point in the phase space, the vector field can be broken up into the two components f_0 and f_1 . A method can then be constructed by stepping forward along first one, then a second, solution curve, each time for a small time step τ .

That is, we start from some points z_n and solve first the initial value problem

$$\frac{dz}{dt} = f_0(z), \quad z(0) = z_n$$

for a time τ . This means to compute the exact solution of this part of the system, which is possible, since f_0 is assumed integrable. This takes us to the point $z^* = z_0(\tau, z_n)$, where z_0 represents the exact solution of the differential equations on vector field f_0 . Next we start from z^* and solve the second differential equation initial value problem

$$\frac{dz}{dt} = f_1(z), \quad z(0) = z^*$$

for a time τ . This takes us to the point $z_{n+1} = z_1(\tau, z^*)$. Denoting the flow maps of the vector fields f_0 and f_1 as Ψ_{t,f_0} and Ψ_{t,f_1} , we have just computed $z_{n+1} = \Psi_{\tau,f_1}(\Psi_{\tau,f_0}(z_0)) = (\Psi_{\tau,f_1} \circ \Psi_{\tau,f_0})(z_0)$. Such a method is referred to as a splitting method.

1.6.3 Linear ODEs

As a first step to understanding splitting methods, we consider the system of linear ODE

$$\frac{dy}{dt} = Ay$$

Let $A = B + C$, where A is $N \times M$ matrix, then the splitting method defined by solving first

$$\frac{dy}{dt} = By$$

followed by

$$\frac{dy}{dt} = Cy$$

can be written

$$\Psi_\tau(y) = e^{C\tau} e^{B\tau}.$$

The local error is

$$le(y, \tau) = \Psi_\tau(y) - \zeta_\tau(y) = e^{C\tau} e^{B\tau} - e^{A\tau}.$$

Let us work on these formulas in order to estimate the local error. Using the exponential series, we have

$$\begin{aligned} le(y, \tau) &= (I + A\tau + \frac{1}{2}A^2\tau^2 + \dots) - (I + C\tau + \frac{1}{2}C^2\tau^2 + \dots)(I + B\tau + \frac{1}{2}B^2\tau^2 + \dots) \\ &= (I + A\tau + \frac{1}{2}A^2\tau^2)(I + \tau(B + C) + \tau^2(CB + \frac{1}{2}C^2 + \frac{1}{2}B^2)) + O(\tau^3) \\ &= \tau^2(\frac{1}{2}(C + B)^2 - (CB + \frac{1}{2}C^2 + \frac{1}{2}B^2)) + O(\tau^3) \\ &= \tau^2[\frac{1}{2}C^2 + \frac{1}{2}CB + \frac{1}{2}BC + \frac{1}{2}B^2 - CB - \frac{1}{2}C^2 - \frac{1}{2}B^2] + O(\tau^3) \\ &= \frac{\tau^2}{2}(BC - CB) + O(\tau^3) \\ &= \frac{\tau^2}{2}[B, C] + O(\tau^3) \end{aligned}$$

The matrix $[B, C] = BC - CB$ is called the "commutator" of the matrices B and C . If the commutator is zero, we say that the matrices commute. In that case, it can be shown that not only the 2nd order term in the local error vanishes, but moreover

$$e^{C\tau} e^{B\tau} = e^{A\tau}$$

i.e. the splitting method is exact.

1.6.4 Nonlinear ODEs

Now let $f = f_0 + f_1$ be a real valued function. We will denote the flow map on f by $\Psi_{\tau,f}$ and on each of the two parts by Ψ_{τ,f_0} and Ψ_{τ,f_1} . The question we would like to answer is : what is the local error associated to the map

$$\Psi_{\tau,f} = \Psi_{\tau,f_1} \circ \Psi_{\tau,f_0}?$$

As before, $z(\tau) = (\Psi_{\tau,f_1} \circ \Psi_{\tau,f_0})(y) = \Psi_{\tau,f_1}(\Psi_{\tau,f_0}(y))$. Noting that $\Psi_0(y) = y$, we see that

$$z(0) = y.$$

We know that

$$\Psi_{\tau,f_0}(y) = y + hf_0(y) + \frac{1}{2}\tau^2 f_0'(y)f_0(y) + \dots$$

and

$$\Psi_{\tau,f_1}(y) = y + hf_1(y) + \frac{1}{2}\tau^2 f_1'(y)f_1(y) + \dots$$

Hence

$$\begin{aligned} \Psi_{\tau,f_1}(\Psi_{\tau,f_0}(y)) &= [y + \tau f_0(y) + O(\tau^2)] + \tau f_1[y + \tau f_0(y) + O(\tau^2)] + O(\tau^2) \\ &= y + \tau f_0(y) + \tau f_1(y) + O(\tau^2), \end{aligned}$$

that is,

$$z(\tau) = y + hf(y) + O(\tau^2),$$

which shows that the method is at least first order.

1.6.5 Strang Splitting for ODEs

The accuracy of the splitting method in the section (Ordinary Operator Splitting for ODEs) can be improved from $O(\Delta t)$ to $O(\Delta t^2)$ using the so-called Strang splitting, where we take half a step with the f_0 operator, a full step with the f_1 operator, and finally half another step with the f_0 operator. During a time interval Δt the algorithm can be written as follows:

$$\begin{aligned} \frac{du^*}{dt} &= f_0(u^*), & u^*(t_n) &= u(t_n), & t &\in [t_n, t_n + \frac{1}{2}\Delta t], \\ \frac{du^{***}}{dt} &= f_1(u^{***}), & u^{***}(t_n) &= u^*(t_{n+\frac{1}{2}}), & t &\in [t_n, t_n + \Delta t], \\ \frac{du^{**}}{dt} &= f_0(u^{**}), & u^{**}(t_n + \frac{1}{2}) &= u^{***}(t_{n+\frac{1}{2}}), & t &\in [t_n + \frac{1}{2}\Delta t, t_n + \Delta t]. \end{aligned}$$

The global solution is set as $u(t_{n+1}) = u^{**}(t_{n+1})$.

1.7 Adjoint Method, Symmetric Method

Closely linked to the notion of symmetry is the concept of the adjoint of a numerical method [38]. For an autonomous dynamical system described by $\dot{x} = f(x)$, the flow map ψ_t satisfies the relation

$$\psi_{-t}^{-1} = \psi_t,$$

which reflects the time-reversal symmetry intrinsic to the continuous system. However, this property does not generally hold for the discrete maps ψ_h associated with many numerical integrators. Typically, if $\psi_h(x) = x + hf(x) + O(h^2)$, then the map defined by

$$\psi_h^* \equiv \psi_{-h}^{-1}$$

serves as the adjoint of ψ_h , and is itself a numerical method of at least first order accuracy. This adjoint method effectively reverses the numerical step, with forward iteration of ψ_h corresponding to a backward step via ψ_h^* .

A numerical method ψ_h is classified as symmetric if it satisfies the relation

$$\psi_h = \psi_{-h}^{-1}.$$

By this definition, the scheme

$$x_{n+1} = \psi_h(x_n)$$

is symmetric if and only if, upon interchanging $h \leftrightarrow -h$ and $x_n \leftrightarrow x_{n+1}$, the same relation is preserved, i.e.,

$$\psi_{-h}(x_{n+1}) = x_n.$$

Utilizing the concept of the adjoint, it becomes straightforward to construct symmetric methods. Given an arbitrary integrator ψ_h of order $r \geq 1$, the compositions

$$\psi_{h/2} \circ \psi_{h/2}^* \quad \text{and} \quad \psi_{h/2}^* \circ \psi_{h/2}$$

generate symmetric methods of at least order $r \geq 2$. Furthermore, it can be rigorously demonstrated that symmetric methods inherently possess even-order accuracy.

Definition 1.7.1 The adjoint method ϕ_τ^* of the method ϕ_τ is the inverse map of ϕ_τ with reverse time step $-h$, i.e.

$$\phi_\tau^* = \phi_{-\tau}^{-1}$$

The method is symmetric if $\phi_\tau^* = \phi_\tau$.

It is well known that the implicit Euler method is the adjoint method of the explicit Euler method. The adjoint of the adjoint method is the original method, that is $(\phi_\tau^*)^* = \phi_\tau$.

1.8 The Average Vector Field (AVF) Method

Consider the system of ODE

$$\frac{dx}{dt} = S(x)\nabla H(x) \quad (1.63)$$

where $x \in \mathbb{R}^n$, $S(x)$ is a skew-symmetric matrix, i.e. $S(x)^T = -S(x)$ and ∇H is the gradient of the Hamiltonian H .

Definition 1.8.1 [36] (Discrete Gradient) A discrete gradient is denoted by $\bar{\nabla}H(x_n, x_{n+1})$ and defined by

$$\begin{aligned} (x_{n+1} - x_n) \cdot \bar{\nabla}H(x_n, x_{n+1}) &= H(x_{n+1}) - H(x_n) \\ \lim_{x_{n+1} \rightarrow x_n} \bar{\nabla}H(x_n, x_{n+1}) &= \nabla H(x_n) \end{aligned} \quad (1.64)$$

Theorem 1.8.2 Let $\bar{\nabla}H$ be a discrete gradient. Then the discretization

$$\frac{x_{n+1} - x_n}{\Delta t} = S(x_n)\bar{\nabla}H(x_n, x_{n+1}) \quad (1.65)$$

is an energy-preserving scheme for the system (1.63), that is $H(x_{n+1}) = H(x_n)$.

Proof.

$$\begin{aligned} H(x_{n+1}) - H(x_n) &= \bar{\nabla}H(x_n, x_{n+1}) \cdot (x_{n+1} - x_n), \text{ by defn.} \\ &= \bar{\nabla}H(x_n, x_{n+1}) \cdot \Delta t S(x_n) \bar{\nabla}H(x_n, x_{n+1}) \\ &= 0, \quad \text{by skew-symmetry of } S(x). \end{aligned}$$

□

Discrete gradient (1.64) is not unique. Several discrete gradients are known in the literature such as the midpoint discrete gradient [36] and the mean value discrete gradient [40].

Theorem 1.8.3 [40] (*Average Value Discrete Gradient, or Mean Value Discrete Gradient*)

$$\bar{\nabla}H(x_n, x_{n+1}) = \int_0^1 \nabla H(\xi x_{n+1} + (1 - \xi)x_n) d\xi \quad (1.66)$$

is a discrete gradient.

Proof. Multiplying equation (1.66) by $(x_{n+1} - x_n)^T$ from the left and using the Fundamental Theorem of Calculus, we obtain

$$\begin{aligned} (x_{n+1} - x_n)^T \bar{\nabla}H(x_n, x_{n+1}) &= \int_0^1 (x_{n+1} - x_n)^T \nabla H(\xi x_{n+1} + (1 - \xi)x_n) d\xi \\ &= \int_0^1 \frac{d}{d\xi} H(\xi x_{n+1} + (1 - \xi)x_n) d\xi \\ &= \nabla H(\xi x_{n+1} + (1 - \xi)x_n) \Big|_{\xi=0}^{\xi=1} \\ &= H(x_{n+1}) - H(x_n). \end{aligned}$$

The limit of $\bar{\nabla}H(x_n, x_{n+1})$ is

$$\lim_{x_{n+1} \rightarrow x_n} \bar{\nabla}H(x_n, x_{n+1}) = \int_0^1 \lim_{x_{n+1} \rightarrow x_n} \nabla H(\xi x_{n+1} + (1 - \xi)x_n) d\xi = \nabla H(x_n)$$

Therefore, (1.66) is a discrete gradient by definition (1.64). $\square$

Both the mean value and the midpoint discrete gradient are second-order approximations to the value of the gradient at the midpoint of $x_{n+1/2} := \frac{x_{n+1} + x_n}{2}$, being exact on linearly varying ∇H [57].

Definition 1.8.4 *For an ODE*

$$\frac{dx}{dt} = f(x),$$

the method defined by

$$\frac{x_{n+1} - x_n}{\Delta x} = \int_0^1 f(\xi x_{n+1} + (1 - \xi)x_n) d\xi, \quad (1.67)$$

is called as the average vector field (AVF) method [57].

Here we list the application of AVF method (1.67) to some polynomial vector field $f(x)$.

If $f(x) = x$ then

$$\int_0^1 (\xi x_{n+1} + (1 - \xi)x_n) d\xi = \frac{x_{n+1} + x_n}{2}$$

and the AVF method (1.67) becomes

$$\frac{x_{n+1} - x_n}{\Delta x} = \frac{x_{n+1} + x_n}{2},$$

which is nothing but the well-known implicit midpoint rule [47]. It can be shown that when the vector field $f(x)$ is linear, the AVF method (1.67) yields a linearly implicit method that can be solved easily. Otherwise, the evaluation of (1.67) yields a nonlinear system of equations in x_{n+1} which requires an iterative method for the solution, such as the Newton-Raphson method or fixed point iteration. For instance, for the quadratic and cubic vector fields, we have the following schemes:

If $f(x) = x^2$ then

$$\int_0^1 (\xi x_{n+1} + (1 - \xi)x_n)^2 d\xi = \frac{1}{3} (x_{n+1}^2 + x_{n+1}x_n + x_n^2)$$

and the AVF method (1.67) becomes

$$\frac{x_{n+1} - x_n}{\Delta x} = \frac{1}{3} (x_{n+1}^2 + x_{n+1}x_n + x_n^2).$$

If $f(x) = x^3$ then

$$\int_0^1 (\xi x_{n+1} + (1 - \xi)x_n)^3 d\xi = \frac{1}{4} (x_{n+1}^3 + x_{n+1}^2x_n + x_{n+1}x_n^2 + x_n^3)$$

and the AVF method (1.67) becomes

$$\frac{x_{n+1} - x_n}{\Delta x} = \frac{1}{4} (x_{n+1}^3 + x_{n+1}^2x_n + x_{n+1}x_n^2 + x_n^3).$$

Theorem 1.8.5 [21] *Let J be any constant skew-symmetric matrix, and Hamiltonian $H(x) : \mathbb{R}^n \rightarrow \mathbb{R}$ be a sufficiently differentiable function. Let x_n be the solution of the average vector field method*

$$\frac{x_{n+1} - x_n}{\Delta x} = J \int_0^1 \nabla H(\xi x_{n+1} + (1 - \xi)x_n) d\xi \quad (1.68)$$

applied to the Hamiltonian system of ODEs $\frac{dx}{dt} = J\nabla H(x)$. Then the energy is preserved exactly, that is

$$H(x_{n+1}) = H(x_n). \quad (1.69)$$

Proof. Taking the scalar product of both sides of (1.68) with

$$\left(\int_0^1 \nabla H(\xi x_{n+1} + (1-\xi)x_n) d\xi \right)^T$$

and using the skew-symmetry of the matrix S and the Fundamental Theorem of Calculus, we obtain

$$\begin{aligned} 0 &= \left(\int_0^1 \nabla H(\xi x_{n+1} + (1-\xi)x_n) d\xi \right)^T J \int_0^1 \nabla H(\xi x_{n+1} + (1-\xi)x_n) d\xi \\ &= \left(\int_0^1 \nabla H(\xi x_{n+1} + (1-\xi)x_n) d\xi \right)^T \left(\frac{x_{n+1} - x_n}{\Delta t} \right) \\ &= \frac{1}{\Delta t} \int_0^1 \frac{d}{d\xi} [\nabla H(\xi x_{n+1} + (1-\xi)x_n)]^T d\xi \\ &= \frac{1}{\Delta t} (H(x_{n+1}) - H(x_n)). \end{aligned} \quad (1.70)$$

Thus, (1.69) holds. $\square$

In contrast to the constant matrix J in (1.68), for Hamiltonian systems with non-canonical structure matrix, i.e., $J = J(x)$, the AVF method (1.67) applied to

$$\frac{dx}{dt} = J(x)\nabla H(x)$$

can be implemented as [27]

$$\frac{z_{n+1} - z_n}{\tau} = J\left(\frac{z_{n+1} + z_n}{2}\right) \int_0^1 \nabla H((1-\xi)z_n + \xi z_{n+1}) d\xi. \quad (1.71)$$

The scheme (1.71) exactly preserves Hamiltonian H and quadratic Casimir functions; they are symmetric and of order 2 [27]. In recent years, there has been an increased emphasis on constructing numerical methods to preserve the energy using the AVF method (1.68).

1.9 Multisymplectic PDEs

In this section, we introduce multisymplectic PDEs and its local and global structure preservation properties.

Consider the spatial-temporal domain $(x, t) = [x_L, x_R] \times [0, T]$. A wide range of PDEs can be written as a multisymplectic system [11]

$$Lz_t + Kz_x = \nabla_z S(z), \quad z \in \mathbb{R}^d, t \in \mathbb{R}, \quad (1.72)$$

where M and K are two skew-symmetric matrices and $S : \mathbb{R}^d \mapsto \mathbb{R}$ is a scalar-valued smooth function. The system (1.72) has three local conservation laws, namely, the multisymplectic conservation law

$$\partial_t \omega + \partial_x \kappa = 0, \quad \omega = dz \wedge L_+ dz, \quad \kappa = dz \wedge K_+ dz, \quad (1.73)$$

the local energy conservation law (LECL)

$$E_t + F_x = 0, \quad E = S(z) + z_x^T K_+ z, \quad F = -z_t^T K_+ z, \quad (1.74)$$

the local momentum conservation law (LMCL)

$$I_t + G_x = 0, \quad G = S(z) + z_t^T L_+ z, \quad I = -z_x^T L_+ z, \quad (1.75)$$

where L_+ and K_+ satisfy

$$L = L_+ - L_+^T, \quad K = K_+ - K_+^T.$$

We note that different splittings produce different local conservation laws. We notice that these local conservation laws are independent of boundary conditions.

For periodic boundary condition $z(x_L, t) = z(x_R, t)$ or homogeneous boundary conditions $z(x_L, t) = z(x_R, t) = 0$, the local conservation laws can be integrated in x to obtain global conservation of energy and momentum

$$\frac{d\mathcal{E}}{dt} = 0, \quad \frac{d\mathcal{I}}{dt} = 0 \quad (1.76)$$

respectively, where

$$\mathcal{E}(z(t)) = \int_{x_l}^{x_r} E(z(x, t)) dx, \quad \mathcal{I}(z(t)) = \int_{x_l}^{x_r} I(z(x, t)) dx.$$

In the following section, we introduce numerical methods that preserve the local structures (1.74) and (1.75) as well as the global structures (1.76).

Before developing structure-preserving algorithms, we introduce some notations.

Consider the multisymplectic PDE (1.72) in the spatial domain $x = [x_L, x_R]$. Let $x_j = x_L + hj$, $t_n = n\tau$, $j = 0, 1, 2, \dots, N-1$; $n = 0, 1, 2, \dots$ where $h = L/J$ and τ are spatial length and temporal step length, respectively, and $L = x_R - x_L$. The approximation of the value of the function $f(x, t)$ at the node (x_j, t_n) is denoted by f_j^n .

Introduce the finite difference operators

$$\begin{aligned}\delta_t f_j^n &= \frac{f_j^{n+1} - f_j^n}{\tau}, & \delta_x f_j^n &= \frac{f_{j+1}^n - f_j^n}{h} \\ A_t f_j^n &= \frac{f_j^{n+1} + f_j^n}{2}, & A_x f_j^n &= \frac{f_{j+1}^n + f_j^n}{2}.\end{aligned}\tag{1.77}$$

Now we give the following result.

Lemma 1.9.1 *The operators (1.77) obey the commutative laws*

$$\delta_t \delta_x f_j^n = \delta_x \delta_t f_j^n, \quad A_t A_x f_j^n = A_x A_t f_j^n, \quad \delta_t A_x f_j^n = A_x \delta_t f_j^n, \quad A_t \delta_x f_j^n = \delta_x A_t f_j^n \tag{1.78}$$

and satisfy the discrete Leibniz rule,

$$\delta_x (f \cdot g)_j^n = (\epsilon f_{j+1}^n + (1 - \epsilon) f_j^n) \cdot \delta_x g_j^n + \delta_x f_j^n \cdot ((1 - \epsilon) g_{j+1}^n + \epsilon g_j^n), \quad \forall \quad 0 \leq \epsilon \leq 1.$$

Proof. The proof of these equalities can be obtained in the Appendix □

Special cases for the Leibniz rule are the following:

$$\begin{aligned}\epsilon &= 0 & \delta_x (f \cdot g)_j^n &= f_j^n \cdot \delta_x g_j^n + \delta_x f_j^n \cdot g_{j+1}^n \\ \epsilon &= \frac{1}{2} & \delta_x (f \cdot g)_j^n &= A_x f_j^n \cdot \delta_x g_j^n + \delta_x f_j^n \cdot A_x g_j^n \\ \epsilon &= 1 & \delta_x (f \cdot g)_j^n &= f_{j+1}^n \cdot \delta_x g_j^n + \delta_x f_j^n \cdot g_j^n.\end{aligned}\tag{1.79}$$

Discrete Leibniz rules in the time direction can be obtained analogously.

1.9.1 Literature Review About Local Structure Preserving Algorithms For Multi-symplectic PDEs

In this section, we review the most recent novel approaches that preserve local structures of general multi-symplectic PDEs.

A Novel Local Structure-Preserving Approach for MS PDEs I: In [35], the author propose new multi-symplectic integrators based on an implicit midpoint Average

Vector Field (AVF) discretization. The authors argue that many existing structure-preserving methods focus exclusively on global conservation properties tied to boundary conditions, failing to preserve local conservation laws such as energy or momentum flux. Their schemes are designed to be more general, applying to a wide class of multi-symplectic PDE formulations.

For the local energy- preserving, one can discretize the multisymplectic equation (1.72) in spatial direction by the implicit midpoint rule (1.34) and in temporal direction by the AVF method (1.67) and obtain the scheme

$$L\delta_t A_x Z_j^n + K\delta_x A_t Z_j^n = \int_0^1 \nabla_z S((1-\xi)A_x Z_j^n + \xi A_x Z_j^{n+1}) d\xi. \quad (1.80)$$

The local conservation laws of energy (1.74) is evaluated from the residual

$$(R_E)_{j+1/2}^{n+1/2} = \delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2}, \quad (1.81)$$

where

$$E_{j+1/2}^n = S(A_x Z_j^n) + (\delta_x Z_j^n)^T K_+ A_x Z_j^n, \quad F_j^{n+1/2} = -(\delta_t Z_j^n)^T K_+ A_t Z_j^n. \quad (1.82)$$

In addition to the discrete local energy (1.81), the global energy is evaluated according to

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_{j+1/2}^n. \quad (1.83)$$

The scheme (1.80) preserves exactly the local energy (1.81).

For the periodic boundary condition $z(x+l, t) = z(x, t)$, the scheme (1.80) possesses the discrete global energy conservation law

$$\mathcal{E}^{n+1} = \mathcal{E}^n, \quad (1.84)$$

where

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_{j+1/2}^n.$$

For the local-momentum preserving algorithm, the AVF method (1.67) can be used in space discretization and implicit midpoint scheme (1.34) can be used in time discretization. Thus, one can obtain a full-discrete scheme

$$L\delta_t A_x z_j^n + K\delta_x A_t z_j^n = \int_0^1 \nabla_z S((1-\xi)A_t z_j^n + \xi A_t z_{j+1}^n) d\xi. \quad (1.85)$$

The local conservation laws of energy (1.75) is evaluated from the residual

$$(R_M)_{j+1/2}^{n+1/2} = \delta_t I_{j+1/2}^n + \delta_x G_j^{n+1/2}, \quad (1.86)$$

where

$$G_j^{n+1/2} = S(A_t Z_j^n) + (\delta_t Z_j^n)^T L_+ A_t Z_j^n, \quad I_{j+1/2}^n = -(\delta_x Z_j^n)^T L_+ A_x Z_j^n. \quad (1.87)$$

The scheme (1.85) exactly preserves the discrete local momentum (1.86).

For the periodic boundary conditions $z(x+l, t) = z(x, t)$, the scheme (1.85) conserves the discrete global momentum conservation law

$$I^{n+1} = I^n \quad (1.88)$$

where

$$I^n = h \sum_{j=0}^{N-1} I_{j+1/2}^n \quad (1.89)$$

For the global energy-preserving algorithm, the first-order spatial derivative ∂_x in multisymplectic PDE (1.72) is discretized by an anti-symmetric differential matrix denoted by D_1 such as the second-order central finite difference approximation [47]

$$D_1 = \frac{1}{2h} \begin{pmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 0 & 1 \\ 1 & & & -1 & 0 \end{pmatrix}. \quad (1.90)$$

Then, discretizing the temporal derivative by the AVF method (1.67), we have

$$L \delta_t z_j^n + K(D_1 A_t z_j^n)_j = \int_0^1 \nabla_z S((1-\xi)z_j^n + \xi z_j^{n+1}) d\xi. \quad (1.91)$$

Local conservation laws of energy and momentum are evaluated according to residuals,

$$(R_E)_j^n = \delta_t E_j^n + (D_1 F^{n+1/2})_j, \quad (R_M)_j^n = \delta_t I_j^n + (D_1 G_j^{n+1/2}), \quad (1.92)$$

respectively, and the discrete global energy and momentum are defined as

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_j^n, \quad (1.93)$$

$$\mathcal{I}^n = h \sum_{j=0}^{N-1} I_j^n, \quad (1.94)$$

where

$$\begin{aligned} E_j^n &= S(Z_j^n) + (D_1 Z_j^n)^T K_+ Z_j^n, & F_j^{n+1/2} &= -(\delta_t Z_j^n)^T K_+ A_t Z_j^n \\ G_j^{n+1/2} &= S(A_t Z_j^n) + (\delta_t Z_j^n)^T L_+ A_t Z_j^n, & I_j^n &= -(D_1 Z_j^n)^T L_+ Z_j^n. \end{aligned}$$

The scheme (1.91) exactly preserves the global energy (1.93).

The above methods will be explained in detail in the next chapter.

A Novel Local Structure-Preserving Approach for MS PDEs II: In [17], the authors systematically develop local energy- and momentum-preserving schemes for general multi-symplectic Hamiltonian PDEs. By leveraging discrete gradient and AVF methods, the authors construct robust integrators that respect local conservation laws even under non-trivial boundary conditions, by considering the multisymplectic Hamiltonian form [12]

$$L \partial_t z + \sum_{l=1}^d K_l \partial_{x_l} z = \nabla_z S(z), \quad z \in \mathbb{R}^d, \quad (1.95)$$

where M and K_l , $l = 1, 2, \dots, d$, are constant $d_1 \times d_1$ skew-symmetric matrices, $x = (x_1, x_2, \dots, x_d)$ is a state variable, $z = z(t, x)$, and $S : \mathbb{R}^{d_1} \rightarrow \mathbb{R}$ is a scalar-valued smooth function, such as the Sine-Gordon equation [52], the Korteweg-de Vries (KdV) equation [5], the Camassa-Holm equation [28], the regularized long-wave (RLW) equation [14], the nonlinear Schrödinger (NLS) equation [23] [15], Maxwell's equations [16] [50], and so on.

It is well-known that the solution z of (1.95) admits a multi-symplectic conservation law (MSCL):

$$\partial_t \omega + \sum_{l=1}^d \partial_{x_l} \kappa_l = 0, \quad (1.96)$$

with the differential 2-forms $\omega = dz \wedge L dz$ and $\kappa_l = dz \wedge K_l dz$, where matrices L and K_l satisfy

$$L = L_+ - L_+^T, \quad K_l = K_{+l} - K_{+l}^T. \quad (1.97)$$

For the local energy-preserving method, let K be a splitting matrix of L , satisfying the relation (1.97). For the 1-D multi-symplectic Hamiltonian PDE (1.72), we make

a spatial discretization as follows:

$$L \frac{d}{dt} z_j + K_+ \delta_x^+ z_j - K_+^T \delta_x^- z_j = \nabla_z S(z_j), \quad j = 0, 1, \dots, J-1. \quad (1.98)$$

Taking the inner product of (1.98) with $\frac{dz_j}{dt}$ on both sides together with the vanishment of $\left(\frac{dz_j}{dt}\right)^T L \frac{dz_j}{dt}$, we have

$$\left(\frac{d}{dt} z_j\right)^T K_+ \delta_x^+ z_j - \left(\frac{d}{dt} z_j\right)^T K_+^T \delta_x^- z_j = \frac{d}{dt} S(z_j). \quad (1.99)$$

The left-hand terms can be reformed into

$$\delta_x^+ \left(\frac{dz_{j-1}}{dt}\right)^T K_+ z_j - \frac{d}{dt} \left((\delta_x^- z_j)^T K_+ z_j\right).$$

And thus it follows from (1.99) that

$$\frac{dE_j}{dt} + \delta_x^+ F_j = 0, \quad (1.100)$$

where

$$E_j = S(z_j) + (\delta_x^- z_j)^T K_+ z_j, \quad F_j = -\left(\frac{dz_{j-1}}{dt}\right)^T K_+ z_j.$$

This is a local property, independent of boundary conditions, which shows that the semi-discrete system (1.98) conserves the semi-discrete energy conservation law exactly.

Next, an application of a DG method to (1.98) gives a fully discrete scheme

$$L \delta_t^+ z_j^n + K_+ + A_t \delta_x^+ z_j^n - K_+^T A_t \delta_x^- z_j^n = \nabla_z S(z_j^{n+1}, z_j^n), \quad (1.101)$$

where ∇_z is a DG of S , that is, a continuous function of $(\hat{z}, z)$ satisfying

$$\nabla_z S(\hat{z}, z)^T (\hat{z} - z) = S(\hat{z}) - S(z) \quad \text{and} \quad \nabla_z S(z, z) = \nabla_z S(z).$$

Theorem 1.9.2 [17] *The method (1.101) possesses a discrete local energy conservation law*

$$\delta_t^+ E_j^n + \delta_x^+ F_j^{n+\frac{1}{2}} = 0, \quad (1.102)$$

where

$$E_j^n = S(z_j^n) + (\delta_x^- z_j^n)^T K_+ z_j^n, \quad F_j^{n+\frac{1}{2}} = -\left(\delta_t^+ z_{j-1}^n\right)^T K_+ (A_t z_j^n).$$

Proof. Left-multiplying (1.101) with $(\delta_t^+ z_j^n)^T$ on both sides reads

$$(\delta_t^+ z_j^n)^T (KA_t \delta_x^+ z_j^n - K^T A_t \delta_x^- z_j^n) = (\delta_t^+ z_j^n)^T \nabla_z S(z_j^{n+1}, z_j^n). \quad (1.103)$$

The right-hand term can be written as $\delta_t^+ S(z_j^n)$, and by the discrete Leibniz rules, the left-hand term becomes

$$\begin{aligned} & (\delta_t^+ z_j^n)^T KA_t \delta_x^+ z_j^n - \delta_t^+ ((\delta_x^- z_j^n)^T K z_j^n) + (\delta_t^+ \delta_x^- z_j^n)^T KA_t z_j^n \\ &= \delta_x^+ ((\delta_t^+ z_{j-1}^n)^T KA_t z_j^n) - \delta_t^+ ((\delta_x^- z_j^n)^T K z_j^n). \end{aligned}$$

This completes the proof.

In particular, integrating (1.98) by the second-order AVF method gives a discrete scheme

$$L\delta_t^+ z_j^n + KA_t \delta_x^+ z_j^n - K^T A_t \delta_x^- z_j^n = \int_0^1 \nabla_z S((1-\xi)z_j^n + \xi z_j^{n+1}) d\xi. \quad (1.104)$$

□

Corollary 1.9.3 *If the multi-symplectic Hamiltonian (1.72) is subjected to appropriate boundary conditions, such as periodic or homogeneous boundary conditions, the proposed LEP scheme will preserve a discrete global energy conservation law*

$$E^n = h \sum_j E_j^n = E^{n-1} = \dots = E^0.$$

For the local momentum-preserving method, let M_+ be a splitting matrix of M , satisfying (1.97), and then make a temporal semi-discretization

$$L\delta_t^+ z^n - L^T \delta_t^- z^n + K \frac{d}{dx} z^n = \nabla_z S(z^n), \quad (1.105)$$

for the system (1.72). It is easy to show that the semi-discrete scheme (1.105) has a local energy conservation law (LMCL)

$$\delta_t^+ I^n + \frac{d}{dx} G^n = 0, \quad I^n = -\left(\frac{d}{dx} z^{n-1}\right)^T L z^n, \quad G^n = S(z^n) + (\delta_t^- z^n)^T L z^n, \quad (1.106)$$

which is independent of boundary conditions.

For the semi-discrete system (1.105), an application of the AVF method in space yields

$$L\delta_t^+ A_x z_j^n - L^T \delta_t^- A_x z_j^n + K\delta_x^+ z_j^n = \int_0^1 \nabla_z S((1-\xi)z_j^n + \xi z_{j+1}^n) d\xi. \quad (1.107)$$

It is worthy to note that the nonlinear term only contains the values of the numerical solution at the n -th time level. Thus it is an explicit scheme. As in the proof of Theorem (1.9.2), it is easy to prove the scheme (1.107) has the following discrete LECL.

Theorem 1.9.4 [17] *The method (1.107) is local-momentum-preserving, which satisfies a discrete local energy conservation law (LMCL)*

$$\delta_t^+ I_j^{n+1/2} + \delta_x^+ G_j^n = 0,$$

where

$$I_j^{n+1/2} = -(\delta_x^+ z_j^{n-1})^T M A_x z_j^n$$

and

$$G_j^n = S(z_j^n) + (\delta_t^- z_j^n)^T M z_j^n.$$

Corollary 1.9.5 *If the multi-symplectic Hamiltonian PDE (1.72) is subjected to periodic or homogeneous boundary conditions, the LMP integrator (1.107) conserves a discrete global momentum conservation law*

$$I^n = h \sum_j I_j^{n+1/2} = I^{n-1} = \dots = I^0.$$

A Novel Local Structure-Preserving Approach for MS PDEs III: In [53], the authors propose and investigate a general approach to construct local energy-preserving algorithms which can be of arbitrarily high order in time for solving Hamiltonian PDEs. This approach is based on the temporal discretization using continuous Runge-Kutta type methods, and the spatial discretization using pseudospectral methods or Gauss-Legendre collocation methods.

Consider autonomous ODEs together with initial conditions:

$$\frac{dy(t)}{dt} = f(y(t)), \quad y \in \mathbb{R}^d, \quad y(t_0) = y_0. \quad (1.108)$$

Hairer's approach can be regarded as a continuous Runge–Kutta method:

$$\begin{cases} y_\tau = y_0 + h \int_0^1 A_{\tau,\sigma} f(y_\sigma) d\sigma, \\ y_1 = y_0 + h \int_0^1 B_\sigma f(y_\sigma) d\sigma, \\ B_\sigma \equiv 1, \quad A_{\tau,\sigma} = \sum_{i=1}^s \frac{1}{b_i} \int_0^\tau l_i(\alpha) d\alpha l_i(\sigma), \end{cases} \quad (1.109)$$

where h is the stepsize, $\{l_i(\tau)\}_{i=1}^s$ are Lagrange interpolating polynomials based on the s distinct points $c_1, c_2, \dots, c_s$, $b_i = \int_0^1 l_i(\tau) d\tau$ for $i = 1, 2, \dots, s$, and y_τ approximates the value of $y(t_0 + \tau h)$ for $\tau \in [0, 1]$.

The continuous RK method can be expressed in a Butcher tableau as:

$$\begin{array}{c|c} C_\tau & A_{\tau,\sigma} \\ \hline & B_\tau \end{array},$$

with

$$C_\tau = \int_0^1 A_{\tau,\sigma} d\sigma = \tau$$

If $f(y) = J^{-1} \nabla H(y)$, where J is a constant skew-symmetric matrix, then this method preserves the Hamiltonian: $H(y_1) = H(y_0)$.

Let r be the order of the quadrature formula $(b_i, c_i)_{i=1}^s$, then this continuous method has order:

$$\begin{cases} 2s, & \text{for } r \geq 2s - 1 \\ 2r - 2s + 2, & \text{for } r \leq 2s - 2. \end{cases} \quad (1.110)$$

For pseudospectral spatial discretization, the PDE with one spatial variable

$$Lz_t + Kz_x = \nabla_z S(z, x). \quad (1.111)$$

For the classical multi-symplectic PDE (1.72), the Hamiltonian S is independent of the variable x . It should be noticed that (1.111) does not have the MSCL and the MCL, but the local energy conservation still holds:

$$\partial_t E + \partial_x F = 0, \quad (1.112)$$

where

$$E = S(z, x) - \frac{1}{2} z^\top K z_x,$$

and

$$F = \frac{1}{2} z^\top K z_t.$$

Thus, local energy-preserving methods can be more widely used than classical multi-symplectic methods. Most multi-symplectic methods can be constructed by concatenating two ODE methods in time and space, respectively. The temporal method is always symplectic, while the spatial one may not be. However, in our new schemes, we use the continuous Runge–Kutta (CRK) method instead of the symplectic method for the time integration.

In this subsection, we consider a class of convenient methods for the spatial discretization under the periodic boundary condition. They are the Fourier spectral, the pseudospectral, and the wavelet collocation methods (see, e.g., [12] [22] [77]). A common characteristic of these three methods is the substitution of a skew-symmetric differential matrix D for the operator ∂_x . For example, assuming $z(x_0, t) = z(x_0 + l, t)$, equation (1.111) becomes a system of ODEs in time after the pseudospectral spatial discretization.

$$L \frac{d}{dt} z_j + K \sum_{k=0}^{N-1} D_{jk} z_k = \nabla_z S(z_j, x_j), \quad (1.113)$$

for $j = 0, 1, \dots, N-1$, where N is an even integer, $x_j = x_0 + j \Delta x$, $\Delta x = \frac{l}{N}$, $z_j \approx z(x_j, t)$, and D is a skew-symmetric matrix whose entries are determined by (see, e.g., [22])

$$D_{jk} = \begin{cases} \frac{\pi}{l} (-1)^{j+k} \cot\left(\frac{\pi(x_j - x_k)}{l}\right), & j \neq k, \\ 0, & j = k. \end{cases}$$

Multiplying both sides of (1.113) by $\frac{d}{dt} z_j^\top$, we get N semi-discrete energy conservation laws (ECLs)

$$\frac{d}{dt} E_j + \sum_{k=0}^{N-1} D_{jk} F_{jk} = 0, \quad (1.114)$$

for $j = 0, 1, \dots, N-1$, where

$$E_j = S(z_j, x_j) - \frac{1}{2} z_j^\top K \sum_{k=0}^{N-1} D_{jk} z_k$$

$$F_{jk} = \frac{1}{2} z_k^\top K \frac{d}{dt} z_j + \frac{1}{2} z_j^\top K \frac{d}{dt} z_k.$$

The term $\sum_{k=0}^{N-1} D_{jk} F_{jk}$ can be considered as the discrete $\partial_x F(z(x_j, t))$:

$$\begin{aligned} \sum_{k=0}^{N-1} D_{jk} F_{jk} &= \frac{1}{2} \delta_x z_j^\top K \frac{d}{dt} z_j + \frac{1}{2} z_j^\top K \frac{d}{dt} \delta_x z_j \\ &\approx \frac{1}{2} \partial_x z(x_j, t)^\top K \frac{d}{dt} z(x_j, t) + \frac{1}{2} z(x_j, t)^\top K \frac{d}{dt} \partial_x z(x_j, t) \\ &= \partial_x F(z(x_j, t)), \end{aligned} \quad (1.115)$$

where $\sum_{k=0}^{N-1} D_{jk} z_k = \delta_x z_j \approx \partial_x z(x_j, t)$.

If S is independent of the variable x , then N semi-discrete multi-symplectic conservation laws (MSCLs) (see, e.g., [12], [22]) also hold:

$$\begin{aligned} \frac{d}{dt} \omega_j + \sum_{k=0}^{N-1} D_{jk} \kappa_{jk} &= 0, \\ \omega_j &= \frac{1}{2} dz_j \wedge L dz_j, \quad \kappa_{jk} = \frac{1}{2} (dz_j \wedge K dz_k + dz_k \wedge K dz_j), \end{aligned}$$

for $j = 0, 1, \dots, N-1$. Here $\sum_{k=0}^{N-1} D_{jk} \kappa_{jk}$ (the discrete $\partial_x \kappa(z(x_j, t))$) can be understood in a similar way to (1.115).

After the temporal discretization using the CRK method (1.109), the fully discrete scheme can be written as follows:

$$\begin{cases} z_j^\tau = z_j^0 + \Delta t \int_0^1 A_{\tau, \sigma} \delta_t z_j^\sigma d\sigma \\ z_j^1 = z_j^0 + \Delta t \int_0^1 \delta_t z_j^\sigma d\sigma \\ \delta_x z_j^\tau = \sum_{k=0}^{N-1} D_{jk} z_k^\tau \\ M \delta_t z_j^\tau + K \delta_x z_j^\tau = \nabla_z S(z_j^\tau, x_j) \end{cases} \quad (1.116)$$

for $j = 0, 1, \dots, N-1$, where $z_j^\tau \approx z(x_j, t_0 + \tau \Delta t)$ and $\delta_t z_j^\tau \approx \partial_t z(x_j, t_0 + \tau \Delta t)$ are polynomials in τ .

For the energy-preserving property of the CRK method, we expect this scheme to preserve some discrete ECLs. Note that

$$b_i = \int_0^1 l_i(\tau) d\tau.$$

For convenience, we denote

$$f_i = \frac{1}{b_i} \int_0^1 l_i(\tau) f(\tau) d\tau$$

the weighted average of a function f with weight $l_i(\tau)$ as $\langle f_i \rangle$. Obviously, the operator $\langle \cdot \rangle_i$ is linear.

The next theorem shows the N -discrete local energy conservation law of (1.116).

Theorem 1.9.6 *The scheme (1.116) exactly conserves the N -discrete local energy conservation law:*

$$\frac{E_j^1 - E_j^0}{\Delta t} + \sum_{k=0}^{N-1} D_{jk} \bar{F}_{jk} = 0, \quad (1.117)$$

for $j = 0, 1, \dots, N-1$, where

$$E_j^\alpha = S(z_j^\alpha, x_j) - \frac{1}{2} z_j^{\alpha\top} K \delta_x z_j^\alpha, \quad \alpha = 0, 1$$

and

$$\bar{F}_{jk} = \frac{1}{2} \sum_{i=1}^s b_i (z_j^{i\top} K \delta_t z_k^i + z_k^{i\top} K \delta_t z_j^i).$$

By summing the identities (1.117) from $j = 0$ to $N-1$, and noting that $\bar{F}_{jk}$ is symmetric in j, k while D_{jk} is antisymmetric, the discrete ECLs lead to the global energy conservation:

$$\Delta x \sum_{j=0}^{N-1} E_j^1 - \Delta x \sum_{j=0}^{N-1} E_j^0 = -\Delta x \Delta t \sum_{j=0}^{N-1} \sum_{k=0}^{N-1} D_{jk} \bar{F}_{jk}. \quad (1.118)$$

If we evaluate the integrals of $\bar{F}_{jk}$ by the generating quadrature formula of the CRK method, we have

$$\bar{F}_{jk} \approx \frac{1}{2} \sum_{i=1}^s b_i (z_j^{c_i\top} K \delta_t z_k^{c_i} + z_k^{c_i\top} K \delta_t z_j^{c_i}).$$

The previous approach can also be easily generalized to high dimensional problems. For example, we consider the following equation:

$$Lz_t + Kz_x + Lz_y = \nabla_z S(z, x, y). \quad (1.119)$$

The energy conservation law (ECL) of this equation is:

$$\partial_t E + \partial_x F + \partial_y G = 0, \quad (1.120)$$

where

$$E = S(z, x, y) - \frac{1}{2}z^\top K z_x - \frac{1}{2}z^\top L z_y, \quad F = \frac{1}{2}z^\top K z_t$$

and

$$G = \frac{1}{2}z^\top L z_t.$$

As an introduction of the local structure preserving algorithms in [72], consider the nonlinear Klein-Gordon equation

$$\partial_{tt}u = \partial_{xx}u - F(u), \quad (x, t) \in \Omega \subset \mathbb{R}^2, \quad (1.121)$$

where the subscript denotes differentiation and $F(u) : \mathbb{R} \rightarrow \mathbb{R}$ is a smooth nonlinear function.

The initial conditions are

$$u(x, 0) = u_1(x), \quad u_t(x, 0) = u_2(x), \quad (1.122)$$

and we need some boundary conditions to well-pose the problem.

Under appropriate boundary conditions such as homogeneous or periodic boundary conditions, we can rewrite the above equation in the form of the Hamiltonian system:

$$\frac{dz}{dt} = J^{-1} \frac{\delta H(z)}{\delta z}, \quad z = \begin{pmatrix} v \\ u \end{pmatrix} = \begin{pmatrix} u_t \\ u \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad (1.123)$$

where $H(z) = \frac{v^2}{2} + \frac{u_x^2}{2} + F(u)$, $\delta H / \delta z$ is the variational derivative, and the variable $v = u_t$ is implied in (1.123).

Equation (1.123) has the following symplectic conservation law:

$$\frac{\partial \omega}{\partial t} = 0; \quad \omega = du \wedge dv \, dx, \quad (1.124)$$

where $\wedge$ denotes the wedge product between the differential one-forms du and dv .

An algorithm is called a symplectic algorithm for (1.121) or (1.123) if it preserves the discrete form of the symplectic conservation law (4), i.e., the discrete form of ω at the n -th time level equals that at the $(n + 1)$ -th time level:

$$\omega_D^n = \omega_D^{n+1}, \quad \omega_D = \sum_i du_i \wedge dv_i.$$

The simplest symplectic algorithm for (1.121) is

$$D_t^2 u_i^j - D_x^2 u_i^j + F(u_i^j) = 0, \quad (1.125)$$

where

$$D_t^2 u_i^j = \frac{u_i^{j+1} - 2u_i^j + u_i^{j-1}}{\tau^2}, \quad D_x^2 u_i^j = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2},$$

and $u_i^j \approx u(x_i, t_j)$, τ and h are the time step and space step, respectively.

Under homogeneous or periodic boundary conditions, (1.121) also has the energy conservation law:

$$\frac{dE}{dt} = 0; \quad E = \int \frac{1}{2}(v^2 + w^2) + F(u) dx, \quad w = u_x. \quad (1.126)$$

An algorithm is called an energy-conserving algorithm if it preserves the discrete form of (1.126), i.e., the discrete energy is the same on all time levels.

An example of an energy-conserving algorithm is

$$D_t^2 u_i^j - D_x^2 u_i^j + \frac{F(u_i^{j+1}) - F(u_i^{j-1})}{u_i^{j+1} - u_i^{j-1}} = 0. \quad (7)$$

The corresponding discrete energy at the m -th time level is

$$E_D^m = \sum_i \frac{h}{2} \left[\left(\frac{u_i^{m+1} - u_i^m}{\tau} \right)^2 + \frac{u_{i+1}^{m+1} - u_i^{m+1}}{h} \cdot \frac{u_{i+1}^m - u_i^m}{h} + F(u_i^{m+1}) + F(u_i^m) \right].$$

Also under homogeneous or periodic boundary conditions, (1.121) may have the momentum conservation law:

$$\frac{dM}{dt} = 0; \quad E = \int wv dx. \quad (1.127)$$

An algorithm is called a momentum-conserving algorithm if it preserves the discrete form of (1.127). An example of the momentum-conserving algorithms for (1.121) is

$$D_t^2 u_i^j - D_x^2 u_i^j + \frac{F(u_{i+1}^j) - F(u_{i-1}^j)}{u_{i+1}^j - u_{i-1}^j} = 0, \quad (1.128)$$

and the corresponding discrete momentum at the m -th time level is

$$M_D^m = \sum_i \left[\frac{u_i^{m+1} - u_i^m}{\tau} \cdot \frac{u_{i+1}^m - u_i^m}{h} \right].$$

In this thesis, we offer an original contribution to the numerical treatment of Multi-symplectic (MS) partial differential equations (PDEs) by proposing new local structure-preserving schemes based on the partitioned average vector field (PAVF) method. We propose the following three new schemes:

Local Energy-Preserving PAVF Scheme for MS PDEs

- Uses the PAVF method in time with the implicit midpoint rule in space.
- Proven to exactly satisfy a discrete local energy conservation law consistent with the multisymplectic PDE's underlying structure.
- Also ensures global energy conservation under suitable boundary conditions.

Global Energy-Preserving PAVF Scheme for MS PDEs

- Employs an antisymmetric differentiation matrix for spatial discretization and the PAVF method in time.
- Leads to a fully discrete scheme that conserves global energy exactly.
- Demonstrates that our discretization faithfully reflects the Hamiltonian structure of the continuous system.

Local Momentum-Preserving PAVF Scheme for MS PDEs

- Applies the PAVF method in space and the implicit midpoint rule in time.
- Ensures a discrete local momentum conservation law analogous to the continuous multisymplectic formulation.
- Also yields global momentum conservation under appropriate boundary conditions.

Each scheme is rigorously derived, and their conservative properties are established via discrete calculus, inner product arguments, and the property of skew-symmetric matrix structures. By avoiding the fully implicit nonlinear systems of traditional AVF

methods, our PAVF-based approaches maintain structure preservation with reduced computational complexity.

These new schemes extend the range of practical structure-preserving integrators for multisymplectic PDEs and offer promising tools for the accurate and efficient simulation of Hamiltonian wave phenomena.



CHAPTER 2

A NOVEL STRUCTURE-PRESERVING AVF SCHEME FOR MULTISYMPLECTIC PDEs

2.1 Introduction

Over the last tens of years, there have been a great deal of work on the structure-preserving algorithms [38]. A numerical method preserving at least one structural property of systems is called a geometric integrator or structure-preserving algorithm. Most of the existing structure preserving algorithms for PDE preserve only the global structures such as global energy or global momentum which depends on boundary conditions. However, many PDEs admit the local conservation laws which are independent of boundary conditions, such as multisymplectic conservation law [11]. Therefore, it is natural to develop a scheme preserving the local structure of the underlying differential equation.

Recently, the so-called Average Vector Field (AVF) method [57] is used as a kind of structure-preserving method for the numerical solution of the finite-dimensional Hamiltonian system. Higher order energy-preserving AVF methods have been proposed in [57]. It has been proved by plenty of numerical results that the structure preserving algorithms are more stable and accurate for long-time computations than other algorithms [33]. Boundary conditions play a crucial role in the application of structure preserving algorithms. The applications of the the structure preserving algorithms to the PDEs depend on the homogeneous and periodic boundary conditions.

Multisymplectic integrators are a kind of structure-preserving algorithms that preserves the multisymplectic structure of the PDEs but ignores the local preservation,

such as local energy and local momentum conservation laws. Although, there has been a lot of previous works on numerical methods preserving the multisymplectic structure, little attention has been given to developing numerical method that preserves the local structures of multisymplectic Hamiltonian PDEs. Gong et.al [35] studied several novel methods for general multisymplectic formulations of Hamiltonian PDEs, including a local energy-preserving algorithm, a class of global energy-preserving algorithms, and a local momentum-preserving algorithm. The approach is based on spatial and temporal discretization using second order implicit midpoint rule and the AVF method. In this chapter, we review some material from [35].

We introduce a local structure-preserving method developed in [35]. The idea of the developed methods comes from the Average Vector Field (AVF) method.

2.2 Local Energy-Preserving AVF Method for Multisymplectic PDEs

This section is devoted to local energy-preserving method for the multisymplectic PDE (1.72). The basic idea lying in this type of methods is to apply the implicit midpoint scheme in space and the AVF method in time. Then, one can show that the method obtained in this way preserves the discrete version of local energy (1.74).

We discretize the multisymplectic equation (1.72) in spatial direction by the implicit midpoint rule (1.34) and in temporal direction by the AVF method (1.67) and obtain the scheme

$$L\delta_t A_x Z_j^n + K\delta_x A_t Z_j^n = \int_0^1 \nabla_Z S((1-\xi)A_x Z_j^n + \xi A_x Z_j^{n+1}) d\xi. \quad (2.1)$$

The local conservation laws of energy (1.74) and momentum (1.75) are evaluated from the residuals

$$(R_E)_{j+1/2}^{n+1/2} = \delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2}, \quad (2.2)$$

and

$$(R_M)_{j+1/2}^{n+1/2} = \delta_t I_{j+1/2}^n + \delta_x G_j^{n+1/2}, \quad (2.3)$$

respectively, where

$$E_{j+1/2}^n = S(A_x Z_j^n) + (\delta_x Z_j^n)^T K_+ A_x Z_j^n, \quad F_j^{n+1/2} = -(\delta_t Z_j^n)^T K_+ A_t Z_j^n, \quad (2.4)$$

and

$$G_j^{n+1/2} = S(A_t Z_j^n) + (\delta_t Z_j^n)^T L_+ A_t Z_j^n, \quad I_{j+1/2}^n = -(\delta_x Z_j^n)^T L_+ A_x Z_j^n. \quad (2.5)$$

In addition to the discrete local energy (2.2) and discrete local momentum (2.3), the discrete global energy and momentum are

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_{j+1/2}^n, \quad \mathcal{I}^n = h \sum_{j=0}^{N-1} I_{j+1/2}^n, \quad (2.6)$$

respectively.

Theorem 2.2.1 [35] *The scheme (2.1) admits the discrete local energy conservation law*

$$\delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2} = 0. \quad (2.7)$$

where $E_{j+1/2}^n$ and $F_j^{n+1/2}$ are defined in (2.4).

Proof. We take the inner product of both sides of (2.1) with $(\delta_t A_x Z_j^n)^T$. Using the skew-symmetric properties of the matrix L ,

$$(\delta_t A_x Z_j^n)^T L (\delta_t A_x Z_j^n) = 0,$$

we obtain

$$(\delta_t A_x Z_j^n)^T K \delta_x A_t Z_j^n = (\delta_t A_x Z_j^n)^T \int_0^1 \nabla_Z S((1-\xi)A_x Z_j^n + \xi A_x Z_j^{n+1}) d\xi. \quad (2.8)$$

Splitting of matrix $K = K_+ - K_+^T$, the left-hand side of the equality (2.8) can be written as

$$(\delta_t A_x Z_j^n)^T K \delta_x A_t Z_j^n = (\delta_t A_x Z_j^n)^T K_+ \delta_x A_t Z_j^n - (\delta_x A_t Z_j^n)^T K_+ \delta_t A_x Z_j^n. \quad (2.9)$$

From the commutative law (1.78) and discrete Leibniz rules, we obtain

$$(\delta_t A_x Z_j^n)^T K \delta_x A_t Z_j^n = (\delta_t \delta_x Z_j^n)^T K_+ A_t A_x Z_j^n + (\delta_x A_t Z_j^n)^T K_+ \delta_t A_x Z_j^n, \quad (2.10)$$

which can be written as

$$(\delta_t A_x Z_j^n)^T K \delta_x A_t Z_j^n = (\delta_t \delta_x Z_j^n)^T K_+ A_t A_x Z_j^n + (\delta_t A_x Z_j^n)^T K_+ \delta_x A_t Z_j^n. \quad (2.11)$$

The right-hand side of the equality (2.8) can be written as

$$\begin{aligned}
& (\delta_t A_x Z_j^n)^T \int_0^1 \nabla_Z S((1-\xi)A_x Z_j^n + \xi A_x Z_j^{n+1}) d\xi \\
&= (\delta_t A_x Z_j^n)^T \int_0^1 \nabla_Z S((1-\xi)A_x Z_j^n + \xi A_x Z_j^{n+1}) d\xi \\
&= \frac{1}{\tau} \int_0^1 \frac{d}{d\xi} S((1-\xi)A_x Z_j^n + \xi A_x Z_j^{n+1}) d\xi \\
&= \delta_t S(A_x Z_j^n).
\end{aligned} \tag{2.12}$$

Then, substituting (2.11) and (2.12) into (2.8), we get

$$\delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2} = \delta_t S(A_x Z_j^n) + \delta_t ((\delta_x Z_j^n)^T K_+ A_x Z_j^n) - \delta_x ((\delta_t Z_j^n)^T K_+ A_t Z_j^n) = 0.$$

□

Corollary 2.2.2 *For the periodic boundary condition $z(x+L, t) = z(x, t)$, the scheme (2.1) possesses the discrete global energy conservation law*

$$\mathcal{E}^{n+1} = \mathcal{E}^n \tag{2.13}$$

where

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_{j+1/2}^n$$

2.3 Local Momentum-Preserving AVF Method for Multisymplectic PDEs

In this section, we investigate a local momentum-preserving algorithm for multisymplectic PDEs. An algorithm is called a local momentum-preserving algorithm if it can preserve the discrete form of local momentum (1.75), i.e., the discrete momentum is the same on all the time levels. Momentum Conservation law is also an important invariant in physics. In the literature, structure-preserving methods such as methods that preserve symplectic or multisymplectic structure and methods that preserve energy of the system under consideration are frequently used. On the other hand, little attention has been paid for momentum-preserving algorithms. This section is devoted to investigate local momentum conserving algorithm for multisymplectic PDEs (1.72).

We use the AVF method (1.67) in space and implicit midpoint scheme (1.34) in time and obtain a full-discrete scheme

$$L\delta_t A_x z_j^n + K\delta_x A_t z_j^n = \int_0^1 \nabla_z S((1-\xi)A_t z_j^n + \xi A_t z_{j+1}^n) d\xi, \quad (2.14)$$

for the multisymplectic Hamiltonian system (1.72). The residuals of energy and momentum of the scheme (2.14) are also defined as (2.2) and (2.3).

Theorem 2.3.1 [35] *The scheme (2.14) conserves the discrete local momentum conservation law*

$$\delta_t I_{j+1/2}^n + \delta_x G_j^{n+1/2} = 0,$$

where

$$G_j^{n+1/2} = S(A_t Z_j^n) + (\delta_t Z_j^n)^T L_+ A_t Z_j^n, \quad I_{j+1/2}^n = -(\delta_x Z_j^n)^T L_+ A_x Z_j^n. \quad (2.15)$$

Proof. Multiplying both sides of (2.14) with $(\delta_x A_t z_j^n)$, and using the skew-symmetry of the matrix K

$$(\delta_x A_t z_j^n)^T K \delta_x A_t z_j^n = 0,$$

we have

$$(\delta_x A_t z_j^n)^T L \delta_t A_x z_j^n = (\delta_x A_t z_j^n)^T \int_0^1 \nabla_z S((1-\xi)A_t z_j^n + \xi A_t z_{j+1}^n) d\xi. \quad (2.16)$$

Using the Fundamental Theorem of Calculus, the right-hand side of (2.16) can be written as

$$(\delta_x A_t z_j^n)^T \int_0^1 \nabla_z S((1-\xi)A_t z_j^n + \xi A_t z_{j+1}^n) d\xi = \delta_x S(A_t z_j^n). \quad (2.17)$$

Moreover, by using the splitting of the matrix $L = L_+ - L_+^T$, we obtain

$$\delta_x S(A_t z_j^n) = (\delta_x A_t z_j^n)^T L_+ \delta_t A_x z_j^n - (\delta_t A_x z_j^n)^T L_+ \delta_x A_t z_j^n. \quad (2.18)$$

Therefore, (2.16) becomes

$$(\delta_x A_t z_j^n)^T L \delta_t A_x z_j^n = (\delta_x A_t z_j^n)^T L_+ \delta_t A_x z_j^n - (\delta_t A_x z_j^n)^T L_+ \delta_x A_t z_j^n. \quad (2.19)$$

According to commutative law (1.78) and discrete Leibniz rules, we can deduce

$$\delta_t((\delta_x z_j^n)^T L_+ A_x z_j^n) = (\delta_t \delta_x z_j^n)^T L_+ A_t A_x z_j^n + (\delta_x A_t z_j^n)^T L_+ \delta_t A_x z_j^n, \quad (2.20)$$

and hence

$$\delta_x((\delta_t z_j^n)^T L_+ A_t z_j^n) = (\delta_t \delta_x z_j^n)^T L_+ A_t A_x z_j^n + (\delta_t A_x z_j^n)^T L_+ \delta_x A_t z_j^n. \quad (2.21)$$

Using (2.18), (2.20) and (2.21), we obtain

$$-\delta_t((\delta_x z_j^n)^T L_+ A_x z_j^n) + \delta_x S(A_t z_j^n) + \delta_x((\delta_t z_j^n)^T L_+ A_t z_j^n) = 0.$$

Therefore (2.15) holds. $\square$

Corollary 2.3.2 *For the periodic boundary conditions $z(xL, t) = z(x, t)$, the scheme (2.14) conserves the discrete global-momentum conservation law*

$$\mathcal{I}^{n+1} = \mathcal{I}^n, \quad (2.22)$$

where

$$\mathcal{I}^n = h \sum_{j=0}^{N-1} I_{j+1/2}^n. \quad (2.23)$$

2.4 Global Energy-Preserving AVF Method for Multisymplectic PDEs

This section is devoted to introduce a global energy-preserving method for multisymplectic PDEs (1.72). Under periodic boundary condition, the preservation of the global energy $\mathcal{E}^n$ in (2.6) will be investigated.

The first-order spatial derivative ∂x in multisymplectic PDE (1.72) is discretized by an antisymmetric differential matrix D_1 such as the second-order central finite difference approximation [47]

$$D_1 = \frac{1}{2h} \begin{pmatrix} 0 & 1 & & -1 \\ -1 & 0 & 1 & \\ & \ddots & \ddots & \ddots \\ & & -1 & 0 & 1 \\ 1 & & & -1 & 0 \end{pmatrix} \quad (2.24)$$

or the first-order Fourier pseudospectral differentiation matrix [68]

$$(D_1)_{j,k} = \begin{cases} \frac{1}{2} \mu (-1)^{j+k} \cot(\mu \frac{x_j - x_k}{2}), & j \neq k \\ 0, & j = k. \end{cases} \quad (2.25)$$

and obtain a semi-discrete system for Eq. (1.72)

$$L\partial_t z_j + K(D_1 z)_j = \nabla_z S(z), \quad j = 0, 1, 2, \dots, N-1 \quad (2.26)$$

where $z = (z_0, z_1, \dots, z_{N-1})^T$ and $(D_1 z)_j = \sum_{k=0}^{N-1} (D_1)_{j,k} z_k$. Then, discretizing the temporal derivative by the AVF method (1.67) for (2.26), we have

$$L\delta_t z_j^n + K(D_1 A_t z^n)_j = \int_0^1 \nabla_z S((1-\xi)z_j^n + \xi z_j^{n+1}) d\xi. \quad (2.27)$$

Local conservation laws of energy and momentum are evaluated according to residuals

$$(R_E)_j^n = \delta_t E_j^n + (D_1 F^{n+1/2})_j, \quad (R_M)_j^n = \delta_t I_j^n + (D_1 G_j^{n+1/2})_j, \quad (2.28)$$

respectively, and the discrete global energy and momentum are defined as

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_j^n, \quad (2.29)$$

and

$$\mathcal{I}^n = h \sum_{j=0}^{N-1} I_j^n, \quad (2.30)$$

where

$$\begin{aligned} E_j^n &= S(Z_j^n) + (D_1 Z^n)_j^T K_+ Z_j^n, & F_j^{n+1/2} &= -(\delta_t Z_j^n)^T K_+ A_t Z_j^n, \\ G_j^{n+1/2} &= S(A_t Z_j^n) + (\delta_t Z_j^n)^T L_+ A_t Z_j^n, & I_j^n &= -(D_1 Z^n)_j^T L_+ Z_j^n. \end{aligned}$$

Theorem 2.4.1 *The scheme (2.27) possesses the discrete global energy conservation law*

$$\mathcal{E}^{n+1} = \mathcal{E}^n, \quad (2.31)$$

where

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_j^n.$$

Proof. Multiplying both sides of (2.27) with $(\delta_t z_j^n)^T$, using the skew-symmetry of the matrix L we have

$$(\delta_t z_j^n)^T L \delta_t z_j^n = 0$$

and

$$\begin{aligned} (\delta_t z_j^n)^T K(D_1 A_t z^n)_j &= (\delta_t z_j^n)^T \int_0^1 \nabla_z S((1-\xi)z_j^n + \xi z_j^{n+1}) d\xi \\ &= \delta_t S(z_j^n). \end{aligned} \quad (2.32)$$

Splitting of the matrix $K = K_+ - K_+^T$, the left-hand side of Eq. (2.32) can be written as

$$\delta_t S(z_j^n) = (\delta_t z_j^n)^T K_+ (D_1 A_t z_j^n) - (D_1 A_t z_j^n)^T K_+ \delta_t z_j^n. \quad (2.33)$$

From commutative law and discrete Leibniz rules (1.79) with $\epsilon = 1/2$, we have

$$\delta_t ((D_1 z^n)^T K_+ z_j^n) = (D_1 \delta_t z^n)^T K_+ A_t z_j^n + (D_1 A_t z^n)^T K_+ \delta_t z_j^n. \quad (2.34)$$

From (2.33) and (2.34) we have

$$\begin{aligned} \delta_t E_j^n &= \delta_t S(z_j^n) + \delta_t ((D_1 z^n)^T K_+ z_j^n) \\ &= (\delta_t z^n)^T_j K_+ (D_1 A_t z^n)_j + (D_1 \delta_t z^n)^T_j K_+ A_t z_j^n \\ &= \sum_{k=0}^{N-1} (D_1)_{j,k} A_{j,k}, \end{aligned}$$

where $A_{j,k} = (\delta_t z^n)^T_j K_+ A_t z_k^n + (\delta_t z^n)^T_j K_+ A_t z_j^n$. Notice that D_1 is anti-symmetric and $A_{j,k} = A_{k,j}$. We can get

$$\sum_{j=0}^{N-1} \delta_t E_j^n = 0,$$

which implies the discrete global energy conservation law (2.31). $\square$

Theorem 2.4.2 [35]. *If D_1 satisfies the discrete Leibniz rule*

$$D_1(u^n \cdot v^n) = u^n \cdot D_1 v^n + v^n \cdot D_1 u^n, \quad (2.35)$$

where $u^n \cdot v^n = (u_0^n v_0^n, u_1^n v_1^n, \dots, u_{N-1}^n v_{N-1}^n)^T$, the scheme (2.27) conserves the discrete local energy conservation law

$$\delta_t E_j^n + (D_1 F^{n+1/2})_j = 0. \quad (2.36)$$

Proof. See [35]. $\square$

Remark 2.4.3 [35] *Differential matrix (2.24) and (2.25) don't satisfy the discrete Leibnitz rule (2.35). Therefore, the method (2.27) does not conserve the discrete local energy conservation law (2.31).*

2.5 Local and Global Structure-Preserving AVF Method for the NLS equation

In this section, we review the local energy-preserving algorithm (2.1), the local momentum-preserving algorithm (2.14), and the global energy-preserving algorithm (2.27) proposed in [35] for the nonlinear Schrödinger (NLS) equation. Consider the NLS equation [66, 65]

$$iu_t + u_{xx} + \beta|u|^2u = 0, \quad x_l \leq x \leq x_r, \quad 0 < t \leq T, \quad (2.37)$$

with the initial condition

$$u(x, 0) = u_0(x), \quad x_l \leq x \leq x_r \quad (2.38)$$

and periodic boundary condition

$$u(x_l, t) = u(x_r, t), \quad 0 < t \leq T \quad (2.39)$$

where $u(x, t)$ is the complex-valued function, $u_0(x)$ is the smooth known function, and β is defined as the birefringent optical parameter. For the implementation of the structure-preserving algorithm described in this chapter, we write the NLS equation (2.37) in multisymplectic form. To do this, we decompose $u = p + iq$ and separate (2.37) into two parts: real and imaginary parts. Then, introducing $v = p_x$, $w = q_x$, we have the following first-order system

$$\begin{aligned} q_t - v_x &= a(p^2 + q^2)p \\ -pt - w_x &= a(p^2 + q^2)q \\ p_x &= v \\ q_x &= w, \end{aligned} \quad (2.40)$$

which can be written as a multisymplectic PDE of the form (1.72) with

$$z = \begin{pmatrix} p \\ q \\ v \\ w \end{pmatrix} \quad M = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

and Hamiltonian $S(z) = \frac{1}{2}(v^2 + w^2 + \frac{a}{2}(p^2 + q^2)^2)$. The local energy conservation law (1.74) and local momentum conservation law (1.75) associated to the multisymplectic formulation (2.40) can be written as

$$\frac{\partial}{\partial t} \left[\frac{1}{2} \left(\frac{a}{2}(p^2 + q^2)^2 - v^2 - w^2 \right) \right] + \frac{\partial}{\partial x} (vp_t + wq_t) = 0 \quad (2.41)$$

and

$$\frac{\partial}{\partial t}(pw - qv) + \frac{\partial}{\partial x} \left[\frac{a}{2}(p^2 + q^2)^2 + v^2 + w^2 - pq_t + qp_t \right] = 0. \quad (2.42)$$

In addition, the global energy and global momentum conservation laws (1.76) are given as

$$\begin{aligned} \mathcal{E}(t) &= \frac{1}{2} \int_0^L \left(\frac{a}{2}(p^2 + q^2)^2 - v^2 - w^2 \right) dx, \\ \mathcal{I}(t) &= \int_0^L (pw - qv) dx. \end{aligned}$$

Applying local energy-preserving method (2.1) for multi-symplectic formulation (2.40) of the NLS equation, we have

$$\begin{aligned} \delta_t A_x q_j^n - \delta_x A_t v_j^n &= f(A_x p_j^{n+1}, A_x p_j^n, A_x q_j^{n+1}, A_x q_j^n) \\ -\delta_t A_x p_j^n - \delta_x A_t w_j^n &= f(A_x q_j^{n+1}, A_x q_j^n, A_x p_j^{n+1}, A_x p_j^n) \\ \delta_x A_t p_j^n &= A_t A_x v_j^n \\ \delta_x A_t q_j^n &= A_t A_x w_j^n. \end{aligned} \quad (2.43)$$

where

$$f(r, u, v, w) = a \left[\frac{1}{4}(r + u).(r^2 + u^2 + v^2 + w^2) + \frac{1}{6}(v - w).(r.w - u.v) \right].$$

Eliminating the auxiliary variables v and w and using $u = p + iq$, the system (2.43) can be written as a single equation

$$i\delta_t A_x^2 u_{j-1}^n + \delta_x^2 A_t u_{j-1}^n + A_x g(A_x u_{j-1}^{n+1}, A_x u_{j-1}^n, A_x p_{j-1}^{n+1}, A_x p_{j-1}^n), \quad (2.44)$$

where

$$g(\phi, \varphi, r, u) = a \left[\frac{1}{4}(\phi + \varphi).(|\phi|^2 + |\varphi|^2) + \frac{1}{6}(\phi - \varphi).(u.\phi - r.\varphi) \right].$$

The residuals $(R_E)_{j+1/2}^{n+1/2}$ and $(R_M)_{j+1/2}^{n+1/2}$ in (2.2) for the scheme (2.44) is evaluated according to

$$\begin{aligned} E_{j+1/2}^n &= \frac{1}{2} \left(\frac{a}{2}((A_x p_j^n)^2 + (A_x q_j^n)^2) - (A_x v_j^n)^2 - (A_x w_j^n)^2 \right), \\ F_j^{n+1/2} &= A_t v_j^n . \delta_t p_j^n + A_t w_j^n . \delta_t q_j^n, \\ I_{j+1/2}^n &= A_x p_j^n . A_x w_j^n - A_x q_j^n . A_x v_j^n, \\ G_j^{n+1/2} &= \frac{a}{2} \left((A_t p_j^n)^2 + (A_t q_j^n)^2 \right) + (A_t v_j^n)^2 + (A_t w_j^n)^2 - A_t p_j^n . \delta_t q_j^n + A_t q_j^n . \delta_t p_j^n. \end{aligned}$$

The corresponding discrete global energy is calculated from $\mathcal{E}^n = h \sum_{j=0}^{N-1} E_{j+1/2}^n$, the global momentum is calculated from $\mathcal{I}^n = h \sum_{j=0}^{N-1} I_{j+1/2}^n$.

Applying global energy-preserving method (2.27) for the multi-symplectic formulation(2.40) of the NLS equation, we obtain

$$\begin{aligned}
\delta_t q_j^n - (D_1 A_t v^n)_j &= f(p_j^{n+1} \cdot p_j^n, q_j^{n+1} \cdot q_j^n) \\
-\delta_t p_j^n - (D_1 A_t w^n)_j &= f(q_j^{n+1} \cdot q_j^n, p_j^{n+1} \cdot p_j^n) \\
(D_1 A_t p^n)_j &= A_t v_j^n \\
(D_1 A_t q^n)_j &= A_t w_j^n,
\end{aligned} \tag{2.45}$$

which can be recombined into a single equation as

$$i\delta_t \Psi_j^n + (D_1^2 A_t \Psi^n)_j + g(\Psi_j^{n+1}, \Psi_j^n, p_j^{n+1}, p_j^n) = 0. \tag{2.46}$$

The corresponding discrete LECL for the scheme (2.45) or (2.46) is

$$\begin{aligned}
(R_E)_j^n &= \delta_t E_j^n + (D_1 F^{n+1/2})_j, \\
E_j^n &= \frac{1}{2} \left(\frac{a}{2} ((p_j^n)^2 + (A_x q_j^n)^2) - (v_j^n)^2 - (w_j^n)^2 \right), \\
F_j^{n+1/2} &= A_t v_j^n \cdot \delta_t p_j^n + A_t w_j^n \cdot \delta_t q_j^n
\end{aligned}$$

and the discrete LMCL is

$$\begin{aligned}
(R_M)_j^n &= \delta_t I_j^n + (D_1 G^{n+1/2})_j \\
I_j^n &= p_j^n \cdot w_j^n - q_j^n \cdot v_j^n \\
G_j^{n+1/2} &= \frac{a}{2} \left((A_t p_j^n)^2 + (A_t q_j^n)^2 \right) + (A_t v_j^n)^2 + (A_t w_j^n)^2 - A_t p_j^n \cdot \delta_t q_j^n + A_t q_j^n \cdot \delta_t p_j^n.
\end{aligned}$$

Moreover, the corresponding discrete total energy is $\mathcal{E}^n = h \sum_{j=0}^{N-1} E_j^n$, the total momentum, $\mathcal{I}^n = h \sum_{j=0}^{N-1} I_j^n$, and the total normal is $\mathcal{N}^n = \frac{1}{2} h \sum_{j=0}^{N-1} ((p_j^n)^2 + (q_j^n)^2)$.

Applying local momentum-preserving method (2.14) for the multi-symplectic formulation (2.40) of the NLS equation, we obtain

$$\begin{aligned}
\delta_t A_x q_j^n - \delta_x A_t v_j^n &= f(A_t p_{j+1}^n, A_t p_j^n, A_t q_{j+1}^n, A_t q_j^n), \\
-\delta_t A_x p_j^n - \delta_x A_t w_j^n &= f(A_t q_{j+1}^n, A_t q_j^n, A_t p_{j+1}^n, A_t p_j^n), \\
\delta_x A_t p_j^n &= A_t A_x v_j^n, \\
\delta_x A_t q_j^n &= A_t A_x w_j^n,
\end{aligned} \tag{2.47}$$

which can be recombined into a single equation as

$$i\delta_t A_x^2 \psi_{j-1}^n + \delta_x^2 A_t \psi_{j-1}^n + A_x g(A_t \psi_j^n, A_t \psi_{j-1}^n, A_t p_j^n, A_t p_{j-1}^n) \tag{2.48}$$

The corresponding discrete conservation laws for the scheme (2.47) or (2.48) can be defined as the same as that of the LEP method.

2.6 Local and Global Structure-Preserving AVF Method for the KdV equation

Consider the Korteweg-de Vries equation

$$u_t + \eta u u_x + \mu^2 u_{xxx} = 0, \quad (2.49)$$

where η and μ are two real parameters. By introducing the potential $\phi_x = u$, momenta $v = \mu u_x$ and variable $w = \frac{1}{2}\phi_t + \mu v_x + \eta u^2/2$ and using the covariant Legendre transform from the Lagrangian, we obtain the system

$$\begin{cases} \frac{1}{2}u_t + w_x = 0, \\ -\frac{1}{2}\phi_t - \mu v_x = -w + \frac{\eta}{2}u^2, \\ \mu u_x = v, \\ -\phi_x = -u. \end{cases} \quad (2.50)$$

We can write the system (2.50) in standard multi-symplectic form with

$$z = \begin{pmatrix} \phi \\ u \\ v \\ w \end{pmatrix}, \quad M = \begin{pmatrix} 0 & \frac{1}{2} & 0 & 0 \\ -\frac{1}{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -\mu & 0 \\ 0 & \mu & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}$$

and $S(z) = \frac{1}{2}v^2 - uw + \eta u^3/6$. The corresponding energy and momentum conservation laws are

$$\frac{\partial}{\partial t} \left(-\frac{1}{2}v^2 + \frac{1}{6}\eta u^3 \right) + \frac{\partial}{\partial x} (-w\phi_t + \mu v u_t) = 0 \quad (2.51)$$

and

$$\frac{\partial}{\partial t} \left(-\frac{1}{2}u^2 \right) + \frac{\partial}{\partial x} \left(\frac{1}{2}v^2 - uw + \frac{1}{6}\eta u^3 + \frac{1}{2}u\phi_t \right) = 0. \quad (2.52)$$

By using the periodic boundary condition, we can integrate the above local conservation laws in x -direction to obtain the total energy conservation law

$$\mathcal{E}(t) = \int_0^L \left(-\frac{1}{2}v^2 + \frac{1}{6}\eta u^3 \right) dx = \text{const.},$$

and total momentum conservation law

$$\mathcal{I}(t) = -\frac{1}{2} \int_0^L u^2 dx = \text{const.}$$

Applying the LEP method (2.1) for the multi-symplectic formulation (2.50) of the KDV equation, we obtain

$$\begin{cases} \frac{1}{2}\delta_t A_x u_j^n + \delta_x A_t w_j^n = 0 \\ -\frac{1}{2}\delta_t A_x \phi_j^n - \mu \delta_x A_t v_j^n = -A_t A_x w_j^n + f(A_x u_j^{n+1}, A_x u_j^n) \\ \mu \delta_x A_t u_j^n = A_t A_x v_j^n \\ -\delta_x A_t \phi_j^n = -A_t A_x u_j^n, \end{cases} \quad (2.53)$$

where $f(r, s) = \frac{\eta}{6}(r^2 + r.s + s^2)$. By eliminating the auxiliary variables, ϕ , v , and w , we obtain

$$\delta_t A_t A_x^3 u_{j-2}^n + \delta_x A_t A_x f(A_x u_{j-2}^{n+1}, A_x u_{j-2}^n) + \mu^2 \delta_x^3 A_t^2 u_{j-2}^n = 0. \quad (2.54)$$

Since equations $\mu u_x = v$, and $\phi_x = u$ in (2.50) contain no time derivatives, we can omit the average operator A_t in the corresponding equations and obtain a two-time-levels scheme for (2.49):

$$\delta_t A_x^3 u_{j-2}^n + \delta_x A_x f(A_x u_{j-2}^{n+1}, A_x u_{j-2}^n) + \mu^2 \delta_x^3 A_t u_{j-2}^n = 0. \quad (2.55)$$

Applying the GEP method (2.27) for the multi-symplectic formulation (2.50) of the KdV equation, we obtain

$$\begin{aligned} \frac{1}{2}\delta_t u_j^n + (D_1 A_t w^n)_j &= 0 \\ -\frac{1}{2}\delta_t \phi_j^n - \mu(D_1 A_t v^n)_j &= -A_t w_j^n + f(u_j^{n+1}, u_j^n) \\ \mu(D_1 A_t u^n)_j &= A_t v_j^n \\ -(D_1 A_t \phi^n)_j &= -A_t u_j^n, \end{aligned} \quad (2.56)$$

Moreover, eliminating the the auxiliary variables ϕ , v and w , equation (2.56) is written as

$$\delta_t A_t u_j^n + A_t (D_1 f(u_j^{n+1}, u_j^n))_j + \mu^2 A_t^2 (D_1^3 u^n)_j = 0. \quad (2.57)$$

Similarly, we can obtain a two-time-level scheme for (2.49)

$$\delta_t u_j^n + (D_1 f(u_j^{n+1}, u_j^n))_j + \mu^2 A_t (D_1^3 u^n)_j = 0. \quad (2.58)$$

Applying the LMP method (2.14) for the multi-symplectic formulation (2.50) of the

KdV equation, we obtain

$$\begin{cases} \frac{1}{2}\delta_t A_x u_j^n + \delta_x A_t w_j^n = 0 \\ -\frac{1}{2}\delta_t A_x \phi_j^n - \mu \delta_x A_t v_j^n = -A_t A_x w_j^n + f(A_t u_{j+1}^n, A_t u_j^n) \\ \mu \delta_x A_t u_j^n = A_t A_x v_j^n \\ -\delta_x A_t \phi_j^n = -A_t A_x u_j^n, \end{cases} \quad (2.59)$$

Eliminating the auxiliary variables ϕ, v and w , Eq. (2.59) is equivalent to

$$\delta_t A_t A_x^3 u_{j-2}^n + \delta_x A_t A_x f(A_t u_{j-1}^n, A_t u_{j-2}^n) + \mu^2 \delta_x^3 A_t^2 u_{j-2}^n = 0. \quad (2.60)$$

Similarly, we can obtain a two-time-level scheme for (2.49):

$$\delta_t A_x^3 u_{j-2}^n + \delta_x A_x f(A_t u_{j-1}^n, A_t u_{j-2}^n) + \mu^2 \delta_x^3 A_t u_{j-2}^n = 0. \quad (2.61)$$

In the numerical experiments, one can use the two-time-level schemes (2.55), (2.58), (2.61) to give the initial datum for the second level values of the three-time-level schemes (2.54), (2.57) and (2.60), respectively.

CHAPTER 3

A NOVEL STRUCTURE-PRESERVING PAVF SCHEME FOR MULTISYMPLECTIC PDEs

This chapter of the thesis contains the original contribution to the literature. In this chapter, we propose a new novel local energy-preserving algorithm, a class of global energy-preserving methods, and a local momentum-preserving algorithm for the multisymplectic PDEs. Gong et. al. [35] proposed several novel local structure preserving methods and a global energy-preserving method for general multisymplectic PDEs based on the AVF method as described in Chapter 2. In this thesis, based on spatial and temporal discretization using the second-order implicit midpoint rule and the first-order partitioned average vector field (PAVF) method, we propose novel local energy, local momentum, and global energy-preserving algorithms for general multisymplectic PDEs.

The most important structures of a Hamiltonian system are conservation of symplecticity and conservation of energy [38]. The AVF method applied to a Hamiltonian system preserves the Hamiltonian. However, the AVF method leads to a fully implicit nonlinear algebraic system of equations. In order to address this drawback, and maintain the energy conservation property, Cai et.al.[19] proposed a first-order partitioned AVF (PAVF) method, which divides the variables of the Hamiltonian system into groups and then applies the AVF method step-by-step. Then, using the adjoint method of the PAVF method, they presented the second-order PAVF composition (PAVF-C) method and the PAVF plus (PAVF-P) method.

Before starting the structure-preserving PAVF method for multisymplectic PDEs, first we present the PAVF method.

3.1 The Partitioned Average Vector Field (PAVF) Method

Let $H : \mathbb{R}^{2d} \rightarrow \mathbb{R}$ be a sufficiently differentiable function. Consider the Hamiltonian system of the form

$$\frac{dz}{dt} = J_{2d} \nabla H(z), \quad (3.1)$$

where $z \in \mathbb{R}^{2d}$ and J_{2d} is a $2d \times 2d$ skew-symmetric constant matrix, and $H(z)$ is the Hamiltonian. Without loss of generality, we can group the variable z by choosing $z = (\mathbf{a}, \mathbf{b})^T$ where $\mathbf{a} = (z_1, z_2, \dots, z_d)^T$, $\mathbf{b} = (z_{d+1}, z_{d+2}, \dots, z_{2d})^T$. Then the canonical Hamiltonian system (3.1) can be written as

$$\frac{d}{dt} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = J_{2d} \begin{pmatrix} \nabla_{\mathbf{a}} H(\mathbf{a}, \mathbf{b}) \\ \nabla_{\mathbf{b}} H(\mathbf{a}, \mathbf{b}) \end{pmatrix}, \quad \mathbf{a}, \mathbf{b} \in \mathbb{R}^d. \quad (3.2)$$

To see the difference between the AVF method and the PAVF method, we recall the energy preserving AVF integrator (1.67). The AVF method for canonical Hamiltonian equation (3.2) is given by

$$\frac{1}{\tau} \begin{pmatrix} \mathbf{a}^{n+1} - \mathbf{a}^n \\ \mathbf{b}^{n+1} - \mathbf{b}^n \end{pmatrix} = J_{2d} \begin{pmatrix} \int_0^1 \nabla_{\mathbf{a}} H(\xi \mathbf{a}^{n+1} + (1-\xi) \mathbf{a}^n, \xi \mathbf{b}^{n+1} + (1-\xi) \mathbf{b}^n) d\xi \\ \int_0^1 \nabla_{\mathbf{b}} H(\xi \mathbf{a}^{n+1} + (1-\xi) \mathbf{a}^n, \xi \mathbf{b}^{n+1} + (1-\xi) \mathbf{b}^n) d\xi \end{pmatrix}. \quad (3.3)$$

Theorem 3.1.1 [20] *The scheme (3.3) is energy-preserving, which possesses discrete energy (4.17), i.e.*

$$H(\mathbf{a}^n, \mathbf{b}^n) = H(\mathbf{a}^{n-1}, \mathbf{b}^{n-1}) = \dots = H(\mathbf{a}^0, \mathbf{b}^0) \quad (3.4)$$

Proof. If we take the inner product of both sides of (3.3) with

$$\begin{pmatrix} \int_0^1 \nabla_{\mathbf{a}} H(\xi \mathbf{a}^{n+1} + (1-\xi) \mathbf{a}^n, \xi \mathbf{b}^{n+1} + (1-\xi) \mathbf{b}^n) d\xi \\ \int_0^1 \nabla_{\mathbf{b}} H(\xi \mathbf{a}^{n+1} + (1-\xi) \mathbf{a}^n, \xi \mathbf{b}^{n+1} + (1-\xi) \mathbf{b}^n) d\xi \end{pmatrix}^T$$

, the right-hand side of (3.3) vanishes due to the skew-symmetry of J_{2d} . Then we use the fundamental theorem of calculus in the left-hand side of (3.3) and obtain

$$\frac{1}{\tau} (H(\mathbf{a}^{n+1}, \mathbf{b}^{n+1}) - H(\mathbf{a}^n, \mathbf{b}^n)) = 0$$

that is, the energy H is precisely conserved at every time step. This completes the proof. $\square$

For a polynomial Hamiltonian, the integral can be evaluated exactly, and the implementation is comparable to that of the implicit mid-point rule. When the Hamiltonian energy is a quadratic function, the resulting AVF scheme is linearly implicit and therefore can be efficiently solved. But this is not the case to reflect the merit of the AVF method since any symplectic Runge–Kutta method can also achieve the energy conservation for quadratic Hamiltonians [39]. Under most circumstances, the evaluation of the integration in (3.3) leads to a nonlinear function, z^{n+1} , which further constitutes a fully implicit numerical scheme. The iterative processes are then inevitably required, such that the computational complexity will be evidently increased, especially for the application on Hamiltonian PDEs.

Cai et.al. [19] defined the so-called partitioned AVF (PAVF) method for the Hamiltonian system (3.2) which has a remarkable advantage over the AVF method. The one-step, first-order PAVF method for the Hamiltonian system (3.2) is written as

$$\frac{1}{\tau} \begin{pmatrix} \mathbf{a}^{n+1} - \mathbf{a}^n \\ \mathbf{b}^{n+1} - \mathbf{b}^n \end{pmatrix} = J_{2d} \begin{pmatrix} \int_0^1 \nabla_{\mathbf{a}} H(\xi \mathbf{a}^{n+1} + (1 - \xi) \mathbf{a}^n, \mathbf{b}^n) \\ \int_0^1 \nabla_{\mathbf{b}} H(\mathbf{a}^{n+1}, \xi \mathbf{b}^{n+1} + (1 - \xi) \mathbf{b}^n) \end{pmatrix}. \quad (3.5)$$

Theorem 3.1.2 [19] *The PAVF method (3.5) preserves the Hamiltonian $H(\mathbf{a}, \mathbf{b})$ of the system (3.2) exactly and satisfies*

$$H(\mathbf{a}^n, \mathbf{b}^n) = H(\mathbf{a}^{n-1}, \mathbf{b}^{n-1}) = \cdots = H(\mathbf{a}^0, \mathbf{b}^0). \quad (3.6)$$

Proof. If we take the inner product of both sides of (3.5) with

$$\begin{pmatrix} \int_0^1 \nabla_{\mathbf{a}} H(\xi \mathbf{a}^{n+1} + (1 - \xi) \mathbf{a}^n, \mathbf{b}^n) \\ \int_0^1 \nabla_{\mathbf{b}} H(\mathbf{a}^{n+1}, \xi \mathbf{b}^{n+1} + (1 - \xi) \mathbf{b}^n) \end{pmatrix}^T$$

the right-hand side of (3.5) vanishes due to the skew-symmetry of J_{2d} . Then we use

the fundamental theorem of calculus on the left-hand side of (3.5) and obtain

$$\begin{aligned}
& \frac{1}{\tau} \int_0^1 \nabla_{\mathbf{a}} H(\xi \mathbf{a}^{n+1} + (1 - \xi) \mathbf{a}^n, \mathbf{b}^n)^T d\xi (\mathbf{a}^{n+1} - \mathbf{a}^n) \\
& + \frac{1}{\tau} \int_0^1 \nabla_{\mathbf{b}} H(\mathbf{a}^{n+1}, \xi \mathbf{b}^{n+1} + (1 - \xi) \mathbf{b}^n)^T d\xi (\mathbf{b}^{n+1} - \mathbf{b}^n) \\
& = \frac{1}{\tau} \int_0^1 \frac{d}{d\xi} [H(\xi \mathbf{a}^{n+1} + (1 - \xi) \mathbf{a}^n, \mathbf{b}^n) + H(\mathbf{a}^{n+1}, \xi \mathbf{b}^{n+1} + (1 - \xi) \mathbf{b}^n)] d\xi \\
& = \frac{1}{\tau} [H(\mathbf{a}^{n+1}, \mathbf{b}^n) - H(\mathbf{a}^n, \mathbf{b}^n) + H(\mathbf{a}^{n+1}, \mathbf{b}^{n+1}) - H(\mathbf{a}^{n+1}, \mathbf{b}^n)] \\
& = \frac{1}{\tau} (H(\mathbf{a}^{n+1}, \mathbf{b}^{n+1}) - H(\mathbf{a}^n, \mathbf{b}^n)) = 0
\end{aligned}$$

This completes the proof. $\square$

Adjoint method can be used to increase the order of a method.

Definition 3.1.3 [39] *The adjoint φ_τ^* of the method φ_τ is the inverse map of the original method with reversed time step $-\tau$.*

The adjoint of the explicit Euler method is the implicit Euler method. The adjoint method of the implicit midpoint rule is the implicit midpoint rule itself; that is, the implicit midpoint rule is symmetric. Accordingly, reversing the path order in (3.5), the adjoint method of the PAVF method is written as [19]

$$\frac{1}{\tau} \begin{pmatrix} \mathbf{a}^{n+1} - \mathbf{a}^n \\ \mathbf{b}^{n+1} - \mathbf{b}^n \end{pmatrix} = J \begin{pmatrix} \int_0^1 \nabla_{\mathbf{a}} \bar{H}(\xi \mathbf{a}^{n+1} + (1 - \xi) \mathbf{a}^n, \mathbf{b}^{n+1}) \\ \int_0^1 \nabla_{\mathbf{b}} \bar{H}(\mathbf{a}^n, \xi \mathbf{b}^{n+1} + (1 - \xi) \mathbf{b}^n) \end{pmatrix}. \quad (3.7)$$

The adjoint method has the same order as the original method. In the following, we consider the composition of the PAVF method (3.5) and the adjoint method (3.7) with the same step size. This allows an order increase for the odd order method. In particular, if Φ_τ is the method (3.5) and Φ_τ^* is the adjoint method (3.7) then the composition method [19]

$$\Psi_h = \Phi_{\frac{\tau}{2}} \circ \Phi_{\frac{\tau}{2}}^* \quad (3.8)$$

is the second-order method and conserves the Hamiltonian exactly. Analogously, taking the average of the Φ_τ and Φ_τ^* , we can write the plus method [19]

$$\hat{\Psi}_h = \frac{1}{2} (\Phi_\tau + \Phi_\tau^*) \quad (3.9)$$

3.2 Local Energy-Preserving PAVF Method for Multisymplectic PDEs

In this section, we apply the PAVF method in time and the implicit midpoint rule in space to construct a new local energy preserving algorithm for multisymplectic PDEs (1.72).

We take $z = (z_1, z_2, \dots, z_d)^T$ in (1.72) and apply the implicit midpoint rule in space and obtain the semi-discrete system

$$\frac{d}{dt} \mathbf{L} \begin{pmatrix} A_x z_{1j} \\ A_x z_{2j} \\ \vdots \\ A_x z_{dj} \end{pmatrix} + \mathbf{K} \begin{pmatrix} \delta_x z_{1j} \\ \delta_x z_{2j} \\ \vdots \\ \delta_x z_{dj} \end{pmatrix} = \begin{pmatrix} S_{z_1}(A_x z_{1j}, A_x z_{1j}, \dots, A_x z_{dj}) \\ S_{z_2}(A_x z_{1j}, A_x z_{1j}, \dots, A_x z_{dj}) \\ \vdots \\ S_{z_d}(A_x z_{1j}, A_x z_{1j}, \dots, A_x z_{dj}) \end{pmatrix}. \quad (3.10)$$

We use the PAVF method (3.5) for the semi-discrete system (3.10) and obtain the full-discrete system

$$\begin{aligned} & \mathbf{L} \begin{pmatrix} \delta_t A_x z_{1j} \\ \delta_t A_x z_{2j} \\ \vdots \\ \delta_t A_x z_{dj} \end{pmatrix} + \mathbf{K} \begin{pmatrix} \delta_x A_t z_{1j} \\ \delta_x A_t z_{2j} \\ \vdots \\ \delta_x A_t z_{dj} \end{pmatrix} \\ &= \begin{pmatrix} \int_0^1 S_{z_1}(\xi A_x z_{1j}^{n+1} + (1-\xi)A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ \int_0^1 S_{z_2}(A_x z_{1j}^{n+1}, \xi A_x z_{2j}^{n+1} + (1-\xi)A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ \vdots \\ \int_0^1 S_{z_d}(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, \xi A_x z_{dj}^{n+1} + (1-\xi)A_x z_{dj}^n) d\xi \end{pmatrix} \end{aligned} \quad (3.11)$$

The local conservation laws of energy (1.74) and momentum (1.75) are evaluated from the residuals

$$(R_E)_{j+1/2}^{n+1/2} = \delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2}, \quad (3.12)$$

and

$$(R_M)_{j+1/2}^{n+1/2} = \delta_t I_{j+1/2}^n + \delta_x G_j^{n+1/2}, \quad (3.13)$$

respectively, where

$$E_{j+1/2}^n = S(A_x Z_j^n) + (\delta_x Z_j^n)^T L A_x Z_j^n, \quad F_j^{n+1/2} = -(\delta_t Z_j^n)^T L A_t Z_j^n, \quad (3.14)$$

and

$$G_j^{n+1/2} = S(A_t Z_j^n) + (\delta_t Z_j^n)^T K_+ A_t Z_j^n, \quad I_{j+1/2}^n = -(\delta_x Z_j^n)^T K_+ A_x Z_j^n. \quad (3.15)$$

In addition to the discrete local energy (2.2) and discrete local momentum (2.3), the discrete global energy and momentum are

$$\mathcal{E}^n = h \sum_{j=0}^{N-1} E_{j+1/2}^n, \quad \mathcal{I}^n = h \sum_{j=0}^{N-1} I_{j+1/2}^n, \quad (3.16)$$

respectively.

Remark 3.2.1 *Note that, we use the same residuals $(R_E)_{j+1/2}^{n+1/2}$ and $(R_M)_{j+1/2}^{n+1/2}$ with the residuals of AVF scheme (2.2) and (2.3).*

Now, we analyze the conservation property of our new scheme (3.11).

Theorem 3.2.2 *The scheme (3.11) conserves the local energy*

$$\delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2} = 0 \quad (3.17)$$

of the multisymplectic PDE (1.72) where

$$E_{j+1/2}^n = S(A_x z_j^n) + (\delta_x z_j^n)^T \mathbf{L}_+ A_x z_j^n, \quad F_j^{n+1/2} = -(\delta_t z_j^n)^T \mathbf{L}_+ A_t z_j^n$$

Proof. We multiply both sides of (3.11) by

$$\begin{pmatrix} \delta_t A_x z_{1j} \\ \delta_t A_x z_{2j} \\ \vdots \\ \delta_t A_x z_{dj} \end{pmatrix}^T$$

and obtain that the first term in (3.11) vanishes since

$$\begin{pmatrix} \delta_t A_x z_{1j} \\ \delta_t A_x z_{2j} \\ \vdots \\ \delta_t A_x z_{dj} \end{pmatrix}^T \mathbf{L} \begin{pmatrix} \delta_x A_t z_{1j} \\ \delta_x A_t z_{2j} \\ \vdots \\ \delta_x A_t z_{dj} \end{pmatrix} = 0 \quad (3.18)$$

by the skew-symmetry property of $\mathbf{L}$. For simplicity, we write the second term of (3.11) as

$$\begin{pmatrix} \delta_t A_x z_{1j} \\ \delta_t A_x z_{2j} \\ \vdots \\ \delta_t A_x z_{dj} \end{pmatrix}^T \mathbf{K} \begin{pmatrix} \delta_x A_t z_{1j} \\ \delta_x A_t z_{2j} \\ \vdots \\ \delta_x A_t z_{dj} \end{pmatrix} = (\delta_t A_x z_j^n)^T \mathbf{K} (\delta_t A_x z_j^n) \quad (3.19)$$

Splitting the matrix $\mathbf{K} = \mathbf{K}_+ - \mathbf{K}_+^T$, we obtain

$$(\delta_t A_x z_j^n)^T \mathbf{K} (\delta_x A_t z_j^n) = (\delta_t A_x z_j^n)^T \mathbf{K}_+ (\delta_x A_t z_j^n) - (\delta_x A_t z_j^n)^T \mathbf{K}_+ (\delta_t A_x z_j^n). \quad (3.20)$$

According to the commutativity law and the discrete Leibniz rule, (3.20) can be written as

$$(\delta_t A_x z_j^n)^T \mathbf{K} (\delta_t A_x z_j^n) = -\delta_t \left[(\delta_x z_j^n)^T \mathbf{K}_+ A_x z_j^n \right] + \delta_x \left[(\delta_t z_j^n)^T \mathbf{K}_+ A_t z_j^n \right]. \quad (3.21)$$

By using the properties of the integral, the right-hand side of the equation (3.11) can be written as

$$\begin{aligned} & \begin{pmatrix} \delta_t A_x z_{1j} \\ \delta_t A_x z_{2j} \\ \vdots \\ \delta_t A_x z_{dj} \end{pmatrix}^T \begin{pmatrix} \int_0^1 S_{z_1}(\xi A_x z_{1j}^{n+1} + (1-\xi)A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ \int_0^1 S_{z_2}(A_x z_{1j}^{n+1}, \xi A_x z_{2j}^{n+1} + (1-\xi)A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ \vdots \\ \int_0^1 S_{z_d}(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, \xi A_x z_{dj}^{n+1} + (1-\xi)A_x z_{dj}^n) d\xi \end{pmatrix} \\ &= (\delta_t A_x z_{1j}^n) \int_0^1 S_{z_1}(\xi A_x z_{1j}^{n+1} + (1-\xi)A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ &+ (\delta_t A_x z_{2j}^n) \int_0^1 S_{z_2}(A_x z_{1j}^{n+1}, \xi A_x z_{2j}^{n+1} + (1-\xi)A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ &\quad \vdots \\ &+ (\delta_t A_x z_{dj}^n) \int_0^1 S_{z_d}(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, \xi A_x z_{dj}^{n+1} + (1-\xi)A_x z_{dj}^n) d\xi \\ &= \frac{1}{\tau} (A_x z_{1j}^{n+1} - A_x z_{1j}^n) \int_0^1 S_{z_1}(\xi A_x z_{1j}^{n+1} + (1-\xi)A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ &+ \frac{1}{\tau} (A_x z_{2j}^{n+1} - A_x z_{2j}^n) \int_0^1 S_{z_2}(A_x z_{1j}^{n+1}, \xi A_x z_{2j}^{n+1} + (1-\xi)A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ &\quad \vdots \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{\tau} (A_x z_{dj}^{n+1} - A_x z_{dj}^n) \int_0^1 S_{z_d}(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, \xi A_x z_{dj}^{n+1} + (1-\xi) A_x z_{dj}^n) d\xi \\
& = \frac{1}{\tau} \left[\int_0^1 \frac{d}{d\xi} \left(S_{z_1}(\xi A_x z_{1j}^{n+1} + (1-\xi) A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) \right. \right. \\
& \quad + S_{z_2}(A_x z_{1j}^{n+1}, \xi A_x z_{2j}^{n+1} + (1-\xi) A_x z_{2j}^n, \dots, A_x z_{dj}^n) \\
& \quad + \dots + S_{z_d}(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, \xi A_x z_{dj}^{n+1} + (1-\xi) A_x z_{dj}^n) \left. \right) d\xi \\
& = \frac{1}{\tau} [S(A_x z_{1j}^{n+1}, A_x z_{2j}^n, \dots, A_x z_{dj}^n) - S(A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) \\
& \quad + S(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, A_x z_{dj}^n) - S(A_x z_{1j}^{n+1}, A_x z_{2j}^n, \dots, A_x z_{dj}^n) \\
& \quad \vdots \\
& \quad + S(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, A_x z_{dj}^{n+1}) - S(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, A_x z_{dj}^n) \\
& = \frac{1}{\tau} [S(A_x z_{1j}^{n+1}, A_x z_{2j}^{n+1}, \dots, A_x z_{dj}^{n+1}) - S(A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n)] \\
& = \delta_t S(A_x z_j^n)
\end{aligned} \tag{3.22}$$

where we have used the Fundamental Theorem of Calculus. Combining (3.18), (3.21) and (3.22) we have

$$\delta_t [S(A_x z_j^n) + (\delta_x z_j^n)^T \mathbf{K}_+ A_x z_j^n] + \delta_x [-(\delta_t z_j^n)^T \mathbf{K}_+ A_t z_j^n] = 0$$

which is the local energy conservation

$$\delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2} = 0$$

with

$$E_{j+1/2}^n = S(A_x z_j^n) + (\delta_x z_j^n)^T \mathbf{K}_+ A_x z_j^n, \quad F_j^{n+1/2} = -(\delta_t z_j^n)^T \mathbf{K}_+ A_t z_j^n$$

□

Remark: We notice that the local conservation (3.17) is same as the local energy conservation law (2.7) [35].

Corollary 3.2.3 *For the periodic boundary condition $z(x_L, t) = z(x_R, t)$ or homogeneous boundary condition, $z(x_L, t) = z(x_R, t) = 0$ the scheme (3.17) satisfies the discrete global energy conservation law*

$$\mathcal{E}^{n+1} = \mathcal{E}^n \tag{3.23}$$

where

$$\mathcal{E}^n = h \sum_{j=0}^{J-1} E_{j+1/2}^n.$$

Remark: We notice that the global conservation (3.23) is the same as the global energy conservation law (2.13) [35].

3.3 Global Energy-Preserving PAVF Method for Multisymplectic PDEs

In this section, we give another novel global energy-preserving method for the multisymplectic PDEs (1.72). To do this, we discretized the first-order spatial derivative ∂_x in (1.72) with an antisymmetric differentiation matrix D_1 and applied the PAVF method (3.5) in time to construct the global energy preserving scheme.

We take $z = (z_1, z_2, \dots, z_d)^T$ in (1.72) and discretized in space by an antisymmetric differentiation matrix D_1 to obtain the semi-discrete system

$$\frac{d}{dt} \mathbf{L} \begin{pmatrix} z_{1j} \\ z_{2j} \\ \vdots \\ z_{dj} \end{pmatrix} + \mathbf{K} \begin{pmatrix} D_1 z_{1j} \\ D_1 z_{2j} \\ \vdots \\ D_1 z_{dj} \end{pmatrix} = \begin{pmatrix} S_{z_1}(z_{1j}, z_{1j}, \dots, z_{dj}) \\ S_{z_2}(z_{1j}, z_{1j}, \dots, z_{dj}) \\ \vdots \\ S_{z_d}(z_{1j}, z_{1j}, \dots, z_{dj}) \end{pmatrix}. \quad (3.24)$$

We discretized this semi-discrete system in time by using the PAVF method (3.5) and obtain the full-discrete system

$$\begin{aligned} & \mathbf{L} \begin{pmatrix} \delta_t z_{1j} \\ \delta_t z_{2j} \\ \vdots \\ \delta_t z_{dj} \end{pmatrix} + \mathbf{K} \begin{pmatrix} D_1 A_t z_{1j} \\ D_1 A_t z_{2j} \\ \vdots \\ D_1 A_t z_{dj} \end{pmatrix} \\ &= \begin{pmatrix} \int_0^1 S_{z_1}(\xi z_{1j}^{n+1} + (1-\xi)z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n) d\xi \\ \int_0^1 S_{z_2}(z_{1j}^{n+1}, \xi z_{2j}^{n+1} + (1-\xi)z_{2j}^n, \dots, z_{dj}^n) d\xi \\ \vdots \\ \int_0^1 S_{z_d}(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, \xi z_{dj}^{n+1} + (1-\xi)z_{dj}^n) d\xi \end{pmatrix} \end{aligned} \quad (3.25)$$

To evaluate the local energy conservation law (1.74), we use the discretizations of the form

$$(RE)_j^n = \delta_t E_j^n + (D_1 F^{n+1/2})_j \quad (3.26)$$

where

$$E_j^n = S(z_j^n) + (D_1 z_j^n)^T L_+ z_j^n, \quad F_j^{n+1/2} = -(\delta_t z_j^n)^T L_+ (A_t z_j^n). \quad (3.27)$$

To evaluate the local momentum conservation law (1.75), we use the discretizations of the form

$$(RM)_j^n = \delta_t I_j^n + (D_1 G^{n+1/2})_j \quad (3.28)$$

where

$$G_j^n = S(A_t z_j^n) + (\delta_t z_j^n)^T L_+ (A_t z_j^n), \quad I_j^{n+1/2} = -(D_1 z_j^n)^T L_+ z_j^n. \quad (3.29)$$

$(RE)_j^n$ and $(RM)_j^n$ are called the residuals of LECL (1.74) and LMCL (1.75), respectively. We also define the discrete global energy conservation law and global momentum conservation law (1.76) as follows:

$$\mathcal{E} = h \sum_{j=1}^{J-1} E_j^n,$$

and

$$\mathcal{I} = h \sum_{j=1}^{J-1} I_j^n.$$

Now, we focus on the discrete global energy conservation of the scheme (3.25).

Theorem 3.3.1 *The scheme (3.25) possesses the discrete global energy conservation law*

$$\mathcal{E}^{n+1} = \mathcal{E}^n \quad (3.30)$$

where

$$\mathcal{E} = h \sum_{j=1}^{J-1} E_j^n$$

Proof. We multiply both sides of (3.25) by

$$\begin{pmatrix} \delta_t z_{1j} \\ \delta_t z_{2j} \\ \vdots \\ \delta_t z_{dj} \end{pmatrix}^T$$

and obtain that the first term in (3.25) vanishes since

$$\begin{pmatrix} \delta_t z_{1j} \\ \delta_t z_{2j} \\ \vdots \\ \delta_t z_{dj} \end{pmatrix}^T \mathbf{L} \begin{pmatrix} \delta_t z_{1j} \\ \delta_t z_{2j} \\ \vdots \\ \delta_t z_{dj} \end{pmatrix} = 0 \quad (3.31)$$

by the skew-symmetry property of $\mathbf{K}$. For simplicity, we write the second term of (3.25) as

$$\begin{pmatrix} \delta_t z_{1j} \\ \delta_t z_{2j} \\ \vdots \\ \delta_t z_{dj} \end{pmatrix}^T \mathbf{K} \begin{pmatrix} D_1 A_t z_{1j} \\ D_1 A_t z_{2j} \\ \vdots \\ D_1 A_t z_{dj} \end{pmatrix} = (\delta_t z_j^n)^T \mathbf{K} (D_1 A_t z_j^n) \quad (3.32)$$

Splitting the matrix $\mathbf{K} = \mathbf{K}_+ - \mathbf{K}_+^T$, we obtain

$$(\delta_t z_j^n)^T \mathbf{K} (D_1 A_t z_j^n) = (\delta_t z_j^n)^T \mathbf{K}_+ (D_1 A_t z_j^n) - (D_1 A_t z_j^n)^T \mathbf{K}_+ (\delta_t z_j^n). \quad (3.33)$$

The right-hand side of (3.25) can be written as

$$\begin{aligned} & \begin{pmatrix} \delta_t z_{1j} \\ \delta_t z_{2j} \\ \vdots \\ \delta_t z_{dj} \end{pmatrix}^T \begin{pmatrix} \int_0^1 S_{z_1}(\xi z_{1j}^{n+1} + (1-\xi)z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n) d\xi \\ \int_0^1 S_{z_2}(z_{1j}^{n+1}, \xi z_{2j}^{n+1} + (1-\xi)z_{2j}^n, \dots, z_{dj}^n) d\xi \\ \vdots \\ \int_0^1 S_{z_d}(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, \xi z_{dj}^{n+1} + (1-\xi)z_{dj}^n) d\xi \end{pmatrix} \\ &= (\delta_t z_{1j}^n) \int_0^1 S_{z_1}(\xi z_{1j}^{n+1} + (1-\xi)z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n) d\xi \\ &+ (\delta_t z_{2j}^n) \int_0^1 S_{z_2}(z_{1j}^{n+1}, \xi z_{2j}^{n+1} + (1-\xi)z_{2j}^n, \dots, z_{dj}^n) d\xi \\ &\quad \vdots \\ &+ (\delta_t z_{dj}^n) \int_0^1 S_{z_d}(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, \xi z_{dj}^{n+1} + (1-\xi)z_{dj}^n) d\xi \\ &= \frac{1}{\tau} (z_{1j}^{n+1} - z_{1j}^n) \int_0^1 S_{z_1}(\xi z_{1j}^{n+1} + (1-\xi)z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n) d\xi \\ &+ \frac{1}{\tau} (z_{2j}^{n+1} - z_{2j}^n) \int_0^1 S_{z_2}(z_{1j}^{n+1}, \xi z_{2j}^{n+1} + (1-\xi)z_{2j}^n, \dots, z_{dj}^n) d\xi \\ &\quad \vdots \end{aligned}$$

$$\begin{aligned}
& + \frac{1}{\tau} (z_{dj}^{n+1} - z_{dj}^n) \int_0^1 S_{z_d}(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, \xi z_{dj}^{n+1} + (1-\xi)z_{dj}^n) d\xi \\
& = \frac{1}{\tau} \left[\int_0^1 \frac{d}{d\xi} \left(S_{z_1}(\xi z_{1j}^{n+1} + (1-\xi)z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n) \right. \right. \\
& \quad + S_{z_2}(z_{1j}^{n+1}, \xi z_{2j}^{n+1} + (1-\xi)z_{2j}^n, \dots, z_{dj}^n) \\
& \quad + \dots + S_{z_d}(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, \xi z_{dj}^{n+1} + (1-\xi)z_{dj}^n) \left. \right] d\xi \\
& = \frac{1}{\tau} [S(z_{1j}^{n+1}, z_{2j}^n, \dots, z_{dj}^n) - S(z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n) \\
& \quad + S(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, z_{dj}^n) - S(z_{1j}^{n+1}, z_{2j}^n, \dots, z_{dj}^n) \\
& \quad \vdots \\
& \quad + S(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, z_{dj}^{n+1}) - S(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, z_{dj}^n) \\
& = \frac{1}{\tau} [S(z_{1j}^{n+1}, z_{2j}^{n+1}, \dots, z_{dj}^{n+1}) - S(z_{1j}^n, z_{2j}^n, \dots, z_{dj}^n)] \\
& = \delta_t S(z_j^n)
\end{aligned} \tag{3.34}$$

where we have used the Fundamental Theorem of Calculus. Combining (3.31), (3.33) and (3.34) we obtain

$$[(\delta_t z_j^n)^T \mathbf{K}_+ (D_1 A_t z_j^n) - (D_1 A_t z_j^n)^T \mathbf{K}_+ (\delta_t z_j^n)] = \delta_t S(z_j^n). \tag{3.35}$$

According to the commutativity law and the discrete Leibnitz rule,

$$\delta_t (f g)_j^n = (\delta_t f_j^n)(A_t g_j^n) + (A_t f_j^n)(\delta_t g_j^n)$$

we obtain that

$$\delta_t [(D_1 z_j^n)^T \mathbf{K}_+ z_j^n] = (D_1 \delta_t z_j^n)^T \mathbf{K}_+ (A_t z_j^n) + (D_1 A_t z_j^n)^T \mathbf{K}_+ (\delta_t z_j^n). \tag{3.36}$$

Substituting $(D_1 A_t z_j^n)^T \mathbf{K}_+ (\delta_t z_j^n)$ into (3.35), we have

$$[(\delta_t z_j^n)^T \mathbf{K}_+ (D_1 A_t z_j^n) + (\delta_t D_1 z_j^n)^T \mathbf{K}_+ (A_t z_j^n)] = \delta_t [S(z_j^n) + (D_1 z_j^n)^T \mathbf{K}_+ z_j^n]. \tag{3.37}$$

Noting that

$$\sum_{k=0}^{N-1} (D_1)_{j,k} A_{j,k} = (\delta_t z_j^n)^T \mathbf{K}_+ (D_1 A_t z_j^n) + (D_1 \delta_t z_j^n)^T \mathbf{K}_+ A_t z_j^n \tag{3.38}$$

where

$$A_{j,k} = (\delta_t z_j^n)^T \mathbf{K}_+ A_t z_k^n + (\delta_t z_j^n)^T \mathbf{K}_+ A_t z_j^n$$

since D_1 is anti-symmetric and $A_{j,k} = A_{k,j}$, we have

$$\begin{aligned} \delta_t \left[S(z_j^n) + (D_1 z_j^n)^T \mathbf{K}_+ z_j^n \right] &= 0 \\ \sum_{j=0}^{N-1} \delta_t E_j^n &= 0 \end{aligned} \quad (3.39)$$

where

$$E_j^n = S(z_j^n) + (D_1 z_j^n)^T \mathbf{K}_+ z_j^n.$$

□

3.4 Local Momentum-Preserving PAVF Method for Multisymplectic PDEs

In this section, we apply the PAVF method in space and the implicit midpoint rule in time to construct a new local momentum-preserving algorithm for multisymplectic PDEs (1.72).

We take $z = (z_1, z_2, \dots, z_d)^T$ in (1.72) and apply the implicit midpoint rule in time and obtain the semi-discrete system

$$\mathbf{L} \begin{pmatrix} \delta_t z_1^n \\ \delta_t z_2^n \\ \vdots \\ \delta_t z_d^n \end{pmatrix} + \frac{d}{dx} \mathbf{K} \begin{pmatrix} A_t z_1^n \\ A_t z_2^n \\ \vdots \\ A_t z_d^n \end{pmatrix} = \begin{pmatrix} S_{z_1}(A_t z_1^n, A_t z_1^n, \dots, A_t z_d^n) \\ S_{z_2}(A_t z_1^n, A_t z_1^n, \dots, A_t z_d^n) \\ \vdots \\ S_{z_d}(A_t z_1^n, A_t z_1^n, \dots, A_t z_d^n) \end{pmatrix}. \quad (3.40)$$

We use the PAVF method (3.5) for the semi-discrete system (3.40) and obtain the full-discrete system

$$\begin{aligned} & \mathbf{L} \begin{pmatrix} \delta_t A_x z_{1j}^n \\ \delta_t A_x z_{2j}^n \\ \vdots \\ \delta_t A_x z_{dj}^n \end{pmatrix} + \mathbf{K} \begin{pmatrix} \delta_x A_t z_{1j}^n \\ \delta_x A_t z_{2j}^n \\ \vdots \\ \delta_x A_t z_{dj}^n \end{pmatrix} \\ &= \begin{pmatrix} \int_0^1 S_{z_1}(\xi A_x z_{1j+1}^n + (1-\xi) A_x z_{1j}^n, A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ \int_0^1 S_{z_2}(A_x z_{1j+1}^n, \xi A_x z_{2j+1}^n + (1-\xi) A_x z_{2j}^n, \dots, A_x z_{dj}^n) d\xi \\ \vdots \\ \int_0^1 S_{z_d}(A_x z_{1j+1}^n, A_x z_{2j+1}^n, \dots, \xi A_x z_{dj+1}^n + (1-\xi) A_x z_{dj}^n) d\xi \end{pmatrix} \end{aligned} \quad (3.41)$$

Theorem 3.4.1 *The scheme (3.41) satisfies the discrete local momentum conservation law:*

$$\delta_t I_{j+\frac{1}{2}}^n + \delta_x G_j^{n+\frac{1}{2}} = 0, \quad (3.42)$$

where

$$I_{j+\frac{1}{2}}^n = -(\delta_x z_j^n)^T L_+ A_x z_j^n, \quad G_j^{n+\frac{1}{2}} = S(A_t z_j^n) + (\delta_t z_j^n)^T L_+ A_t z_j^n.$$

Proof. Consider the PDE in multisymplectic form:

$$Lz_t + Kz_x = \nabla_z S(z).$$

For simplicity, let $z = (u, v, w)$. Applying the implicit midpoint rule in time, we get:

$$L \begin{pmatrix} A_x u \\ A_x v \\ A_x w \end{pmatrix}_t + K \begin{pmatrix} \delta_x u \\ \delta_x v \\ \delta_x w \end{pmatrix}_x = \begin{pmatrix} S_u(A_t u, A_t v, A_t w) \\ S_v(A_t u, A_t v, A_t w) \\ S_w(A_t u, A_t v, A_t w) \end{pmatrix}$$

Now, applying the PAVF method in space:

$$L \begin{pmatrix} \delta_t A_x u \\ \delta_t A_x v \\ \delta_t A_x w \end{pmatrix}_t + K \begin{pmatrix} A_t \delta_x u \\ A_t \delta_x v \\ A_t \delta_x w \end{pmatrix}_x = \begin{pmatrix} \int_0^1 S_u(\xi A_t u_{j+1}^n + (1-\xi)A_t u_j^n, A_t v_j^n, A_t w_j^n) d\xi \\ \int_0^1 S_v(A_t u_{j+1}^n, \xi A_t v_{j+1}^n + (1-\xi)A_t v_j^n, A_t w_j^n) d\xi \\ \int_0^1 S_w(A_t u_{j+1}^n, A_t v_{j+1}^n, \xi A_t w_{j+1}^n + (1-\xi)A_t w_j^n) d\xi \end{pmatrix} \quad (3.43)$$

Taking the inner product of both sides of equation (3.43) with $(\delta_x A_t z_j^n)^T$, noting that:

$$(\delta_x A_t z_j^n)^T K \delta_x A_t z_j^n = 0,$$

we have

$$(\delta_x A_t u, \delta_x A_t v, \delta_x A_t w) L \begin{pmatrix} A_x \delta_t u \\ A_x \delta_t v \\ A_x \delta_t w \end{pmatrix}_t \quad (3.44)$$

$$= (\delta_x A_t u, \delta_x A_t v, \delta_x A_t w) \begin{pmatrix} \int_0^1 S_u(\xi A_t u_{j+1}^n + (1-\xi)A_t u_j^n, A_t v_j^n, A_t w_j^n) d\xi \\ \int_0^1 S_v(A_t u_{j+1}^n, \xi A_t v_{j+1}^n + (1-\xi)A_t v_j^n, A_t w_j^n) d\xi \\ \int_0^1 S_w(A_t u_{j+1}^n, A_t v_{j+1}^n, \xi A_t w_{j+1}^n + (1-\xi)A_t w_j^n) d\xi \end{pmatrix} \quad (3.45)$$

The right-hand side simplifies to:

$$\begin{aligned}
& (\delta_x A_t u_j^n) \int_0^1 S_u \left(\xi A_t u_{j+1}^n + (1 - \xi) A_t u_j^n, A_t v_j^n, A_t w_j^n \right) d\xi \\
& + (\delta_x A_t v_j^n) \int_0^1 S_v \left(A_t u_{j+1}^n, \xi A_t v_{j+1}^n + (1 - \xi) A_t v_j^n, A_t w_j^n \right) d\xi \\
& + (\delta_x A_t w_j^n) \int_0^1 S_w \left(A_t u_{j+1}^n, A_t v_{j+1}^n, \xi A_t w_{j+1}^n + (1 - \xi) A_t w_j^n \right) d\xi \\
& = \frac{1}{h} \left(A_t u_{j+1}^n - A_t u_j^n \right) \int_0^1 S_u \left(\xi A_t u_{j+1}^n + (1 - \xi) A_t u_j^n, A_t v_j^n, A_t w_j^n \right) d\xi \\
& + \frac{1}{h} \left(A_t v_{j+1}^n - A_t v_j^n \right) \int_0^1 S_v \left(A_t u_{j+1}^n, \xi A_t v_{j+1}^n + (1 - \xi) A_t v_j^n, A_t w_j^n \right) d\xi \\
& + \frac{1}{h} \left(A_t w_{j+1}^n - A_t w_j^n \right) \int_0^1 S_w \left(A_t u_{j+1}^n, A_t v_{j+1}^n, \xi A_t w_{j+1}^n + (1 - \xi) A_t w_j^n \right) d\xi \quad (3.46) \\
& = \frac{1}{h} \int_0^1 \frac{d}{d\xi} \left[S \left(\xi A_t u_{j+1}^n + (1 - \xi) A_t u_j^n, A_t v_j^n, A_t w_j^n \right) \right. \\
& \quad + S \left(A_t u_{j+1}^n, \xi A_t v_{j+1}^n + (1 - \xi) A_t v_j^n, A_t w_j^n \right) \\
& \quad \left. + S \left(A_t u_{j+1}^n, A_t v_{j+1}^n, \xi A_t w_{j+1}^n + (1 - \xi) A_t w_j^n \right) \right] d\xi \\
& = \frac{1}{h} \left[S \left(A_t u_{j+1}^n, A_t v_j^n, A_t w_j^n \right) - S \left(A_t u_j^n, A_t v_j^n, A_t w_j^n \right) \right. \\
& \quad + S \left(A_t u_{j+1}^n, A_t v_{j+1}^n, A_t w_j^n \right) - S \left(A_t u_{j+1}^n, A_t v_j^n, A_t w_j^n \right) \\
& \quad \left. + S \left(A_t u_{j+1}^n, A_t v_{j+1}^n, A_t w_{j+1}^n \right) - S \left(A_t u_{j+1}^n, A_t v_{j+1}^n, A_t w_j^n \right) \right] \\
& = \frac{1}{h} \left[S \left(A_t u_{j+1}^n, A_t v_{j+1}^n, A_t w_{j+1}^n \right) - S \left(A_t u_j^n, A_t v_j^n, A_t w_j^n \right) \right] = \delta_x S \left(A_t z_j^n \right)
\end{aligned}$$

Combining equations (3.44) and (3.46), and noting the decomposition $L = L_+ - L_+^T$, we obtain:

$$\delta_x \left[S \left(A_t z_j^n \right) + (\delta_t z_j^n)^T L_+ A_t z_j^n \right] + \delta_t \left[-(\delta_x z_j^n)^T L_+ A_x z_j^n \right] = 0,$$

which completes the proof.

Corollary 3.4.2 *For the periodic boundary condition $z(x_L, t) = z(x_R, t)$ or homogeneous boundary condition, $z(z_L, t) = z(x_R, t) = 0$ the scheme (3.42) satisfies the discrete global energy conservation law*

$$\mathcal{I}^{n+1} = \mathcal{I}^n \quad (3.47)$$

where

$$\mathcal{I}^n = h \sum_{j=0}^{J-1} I_{j+1/2}^n.$$

Remark: We notice that the global conservation (3.47) is the same as the global momentum conservation law (2.22) [35].

3.5 Local Energy-Preserving PAVF Method for Nonlinear Schrödinger equation

In this section, we propose a new local energy preserving method for the nonlinear Schrödinger equation

$$i\psi_t + \psi_{xx} + a|\psi|^2\psi = 0, \quad a > 0. \quad (3.48)$$

Decompose $\psi = p + iq$ to get the real-valued equations

$$\begin{aligned} q_t - p_{xx} &= a(p^2 + q^2)p \\ -p_t - q_{xx} &= a(p^2 + q^2)q \end{aligned} \quad (3.49)$$

Then introducing $p_x = v$ and $q_x = w$, we get the first-order nonlinear system of PDEs

$$\begin{aligned} q_t - v_x &= a(p^2 + q^2)p \\ -p_t - w_x &= a(p^2 + q^2)q \\ p_x &= v \\ q_x &= w \end{aligned} \quad (3.50)$$

which can be written as MS equation (1.72) with

$$\mathbf{K} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \mathbf{L} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \mathbf{z} = \begin{pmatrix} p \\ q \\ v \\ w \end{pmatrix}$$

$$\text{and } S(\mathbf{z}) = \frac{a}{2} \left(\frac{1}{2}(p^2 + q^2)^2 + v^2 + w^2 \right)$$

Space discretization by Implicit Midpoint rule:

$$\begin{aligned} A_x \dot{q}_j - \delta_x v_j &= S_p(A_x p_j, A_x q_j, A_x v_j, A_x w_j) = a \left[(A_x p_j)^2 + (A_x q_j)^2 \right] A_x p_j \\ -A_x \dot{p}_j - \delta_x w_j &= S_q(A_x p_j, A_x q_j, A_x v_j, A_x w_j) = a \left[(A_x p_j)^2 + (A_x q_j)^2 \right] A_x q_j \\ \delta_x p_j &= S_v(A_x p_j, A_x q_j, A_x v_j, A_x w_j) = A_x v_j \\ \delta_x q_j &= S_w(A_x p_j, A_x q_j, A_x v_j, A_x w_j) = A_x w_j \end{aligned} \quad (3.51)$$

Time discretization by PAVF Method:

$$\begin{aligned}
\delta_t A_x q_j^n - A_t \delta_x v_j &= S_p(\xi A_x p_j^{n+1} + (1 - \xi) A_x p_j^n, A_x q_j^n, A_x v_j^n, A_x w_j^n) \\
-\delta_t A_x p_j - A_t \delta_x w_j &= S_q(A_x p_j^{n+1}, \xi A_x q_j^{n+1} + (1 - \xi) A_x q_j^n, A_x v_j^n, A_x w_j^n) \\
A_t \delta_x p_j &= S_v(A_x p_j^{n+1}, A_x q_j^{n+1}, \xi A_x v_j^{n+1} + (1 - \xi) A_x v_j^n, A_x w_j^n) \\
A_t \delta_x q_j &= S_w(A_x p_j^{n+1}, A_x q_j^{n+1}, A_x v_j^{n+1}, \xi A_x w_j + (1 - \xi) A_x w_j^n)
\end{aligned} \tag{3.52}$$

where

$$\begin{aligned}
&S_p(\xi A_x p_j^{n+1} + (1 - \xi) A_x p_j^n, A_x q_j^n, A_x v_j^n, A_x w_j^n) \\
&= \int_0^1 a \left[(\xi A_x p_j^{n+1} + (1 - \xi) A_x p_j^n)^2 + A_x q_j^n \right] (\xi A_x p_j^{n+1} + (1 - \xi) A_x p_j^n) d\xi \\
&= \frac{a}{4} \left[A_x p_j^{n+1} + A_x p_j^n \right] \left[(A_x p_j^{n+1})^2 + (A_x p_j^n)^2 + 2(A_x q_j^n)^2 \right].
\end{aligned} \tag{3.53}$$

$$\begin{aligned}
&S_q(A_x p_j^{n+1}, \xi A_x q_j^{n+1} + (1 - \xi) A_x q_j^n, A_x v_j^n, A_x w_j^n) \\
&= \int_0^1 a \left[A_x p_j^{n+1} + (\xi A_x q_j^{n+1} + (1 - \xi) A_x q_j^n)^2 \right] (\xi A_x q_j^{n+1} + (1 - \xi) A_x q_j^n) d\xi \\
&= \frac{a}{4} \left[A_x q_j^{n+1} + A_x q_j^n \right] \left[(A_x q_j^{n+1})^2 + (A_x q_j^n)^2 + 2(A_x p_j^{n+1})^2 \right].
\end{aligned} \tag{3.54}$$

$$\begin{aligned}
&S_v(A_x p_j^{n+1}, A_x q_j^{n+1}, \xi A_x v_j^{n+1} + (1 - \xi) A_x v_j^n, A_x w_j^n) \\
&= \int_0^1 \left[(\xi A_x v_j^{n+1} + (1 - \xi) A_x v_j^n) \right] d\xi \\
&= \frac{1}{2} (A_x v_j^{n+1} + A_x v_j^n) = A_t A_x v_j^n.
\end{aligned} \tag{3.55}$$

$$\begin{aligned}
&S_w(A_x p_j^{n+1}, A_x q_j^{n+1}, A_x v_j^{n+1}, \xi A_x w_j + (1 - \xi) A_x w_j^n) \\
&= \int_0^1 \left[(\xi A_x w_j^{n+1} + (1 - \xi) A_x w_j^n) \right] d\xi \\
&= \frac{1}{2} (A_x w_j^{n+1} + A_x w_j^n) = A_t A_x w_j^n.
\end{aligned} \tag{3.56}$$

$$\begin{aligned}
\delta_t A_x q_j^n - A_t \delta_x v_j &= f(A_x p_j^{n+1}, A_x p_j^n, A_x q_j^n) \\
-\delta_t A_x p_j - A_t \delta_x w_j &= f(A_x q_j^{n+1}, A_x q_j^n, A_x p_j^{n+1}) \\
A_t \delta_x p_j &= A_t A_x v_j^n \\
A_t \delta_x q_j &= A_t A_x w_j^n
\end{aligned} \tag{3.57}$$

where

$$f(r, u, v) = \frac{a}{4}(r + u)(r^2 + u^2 + 2v^2)$$

which can be combined into the real-valued coupled equations as

$$\begin{aligned}
\delta_t A_x^2 q_j^n - A_t \delta_x^2 p_j &= A_x f(A_x p_j^{n+1}, A_x p_j^n, A_x q_j^n) \\
-\delta_t A_x^2 p_j - A_t \delta_x^2 q_j &= A_x f(A_x q_j^{n+1}, A_x q_j^n, A_x p_j^{n+1})
\end{aligned} \tag{3.58}$$

which is the corresponding discretization to (3.49).

CHAPTER 4

NEW CONSERVATIVE PARTITIONED AVERAGE VECTOR FIELDS SCHEMES FOR SCHRÖDINGER - BOUSSINESQ EQUATIONS

In this chapter, some new structure-preserving schemes are proposed for the numerical solution of the Schrödinger-Boussinesq equation. The methods are fully implicit and semi-explicit. It has been found that the first-order method is also mass-conserving. Concrete schemes have been applied to simulate the soliton solution of the Schrödinger-Boussinesq equation. Numerical results show that the proposed methods capture the remarkable features of the Schrödinger-Boussinesq equation. We obtained that the semi-explicit methods are more efficient than the fully implicit methods. Numerical results also show that the new energy-preserving schemes can well simulate the soliton evolution of the Schrödinger-Boussinesq equation

The result of this chapter is published in [8, 9]

4.1 Introduction

the coupled partial differential equations, such as Schrödinger-KDV equations [73], N-coupled nonlinear Schrödinger equations [6], and the coupled Gross-Pitaevskii equations [71] play a crucial role in applied mathematics, engineering, and physics, many of which are the models of the various nonlinear phenomena. In this thesis, we consider the coupled nonlinear Schrödinger- Boussinesq (CNSB) equations

$$\begin{aligned}
iu_t &= \gamma \Delta u + \xi uv, \quad i^2 = -1, \quad \mathbf{x} \in \mathbb{R}^d, t > 0 \\
v_t &= \Delta \phi, \quad \mathbf{x} \in \mathbb{R}^d, t > 0 \\
\phi_t &= -\alpha \Delta v + v + f(v) + \omega |u|^2, \quad \mathbf{x} \in \mathbb{R}^d, t > 0
\end{aligned} \tag{4.1}$$

with initial conditions

$$u(\mathbf{x}, 0) = u_0(\mathbf{x}), \quad v(\mathbf{x}, 0) = v_0(\mathbf{x}), \quad \phi(\mathbf{x}, 0) = \phi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^d, \quad \mathbf{x} \in \Omega \tag{4.2}$$

and $(l_1, \dots, l_d)$ -periodic boundary conditions

$$\begin{aligned}
u(\mathbf{x}, t) &= u(\mathbf{x} + l_1, \dots, x_d, t), \quad \dots, \quad u(\mathbf{x}, t) = u(x_1, \dots, x + l_d, t), \\
v(\mathbf{x}, t) &= v(\mathbf{x} + l_1, \dots, x_d, t), \quad \dots, \quad v(\mathbf{x}, t) = v(x_1, \dots, x + l_d, t), \\
\phi(\mathbf{x}, t) &= \phi(\mathbf{x} + l_1, \dots, x_d, t), \quad \dots, \quad \phi(\mathbf{x}, t) = \phi(x_1, \dots, x + l_d, t).
\end{aligned} \tag{4.3}$$

In the system (4.1), the complex function $u(x, t)$ describes the electrical field of Langmuir oscillations, real valued function $v(x, t)$ represents the low-frequency density perturbation where $\mathbf{x} = (x_1, \dots, x_d)^T \in \mathbb{R}^d$, $t = [0, T]$, the parameters $\gamma, \xi, \omega, \alpha > 0$ are constants, Δ is the Laplacian operator, and $f(x)$ is a sufficiently smooth real function with $f(0) = 0$.

The periodic-initial value problem (4.1)-(4.3) conserves the Langmuir plasmon number

$$M(t) := \int_{\Omega} |u(x, t)|^2 dx \equiv M(0) \tag{4.4}$$

and the total energy

$$E(t) := \int_{\Omega} \left(\frac{2\gamma\omega}{\xi} |\nabla u|^2 + \alpha |\nabla v|^2 + |\nabla \phi|^2 + v^2 + 2F(v) + 2\omega v |u|^2 \right) dx \equiv E(0) \tag{4.5}$$

where $F(v)$ is the primitive function of $f(v)$. The CNSB equations (4.1) are conservative systems. Therefore, proper discretization is required to reflect the conservation properties (4.4)-(4.5). In general, a conservative numerical scheme exhibits better numerical performance on long-time integration than a nonconservative one [39]. The CNSB equations (4.1) have been solved numerically by several authors. In a multisymplectic Hamiltonian formulation has been presented for the CNSB. Liao et al. proposed two conserved compact finite difference schemes for solving the nonlinear CNSB equations [54]. Bai et al. proposed a quadratic B-spline finite element scheme for the CNSB equations [46]. Zhang et al. studied the implicit conservative difference

scheme and obtained an optimal error estimate [74]. Bai et al. studied the CNSB equations by the time-splitting Fourier spectral method [10]. All these numerical methods for the CNSB equations are obtained by constructing the appropriate discretization. However, these methods for high-dimensional CNSB equations ($d \geq 2$) are time-consuming and difficult since the resulting schemes are fully coupled and nonlinearly implicit. Few numerical methods are available in the literature for the numerical solution of multi-dimensional ($d \geq 2$) CNSB equations. Liao et al. [55] proposed a time-splitting exponential wave integrator method based on Gautschi-type quadrature and Fourier pseudo-spectral discretization for solving Boussinesq-like equations and then presented the time-splitting Fourier spectral discretization for Schrödinger-like equations. Two efficient compact finite difference schemes are introduced. By a combination of the Crank-Nicolson method and Leap-Frog scheme for temporal discretization and a second-order centered difference scheme for spatial approximations, a linear Energy and Mass Preserving Finite Difference Method (EMP-FDM) is devised for 1-D CSBEs. Cai et al. [18] developed second- and fourth-order energy-preserving wavelet collocation schemes for CNSB equations based on the Hamiltonian structure and composition technique. The proposed method is energy-preserving but does not preserve mass. In many cases, the conservation of energy is more important than the conservation of mass. Recently, extensive structure-preserving numerical methods have been carried out for the numerical solution of dispersive/dissipative partial differential equations in the literature. For instance, a fourth-order compact and energy-conservative difference scheme is proposed for solving the two-dimensional nonlinear Schrödinger equation, and convergence analysis of the method has been carried out in. The numerical study of fractional differential equations is also a challenging problem for many authors. For instance, the Schrodinger equation with the variable-order fractional operator has been solved numerically. In that study, an implicit fully discrete continuous Galerkin finite element method was developed to tackle this equation while the fractional operator was expressed with a nonsingular Mittag-Leffler kernel. Quispel et al. [57] developed the so-called Average Vector Field (AVF) method for ordinary differential equations (ODEs) which is energy preserving for the Hamiltonian vector fields. Under most circumstances, the second-order AVF method yields a fully implicit numerical scheme that requires a nonlinear solver such as Newton's iteration. Cai et al. [19] developed a more efficient AVF-based method and call this method a

partitioned AVF (PAVF) method, which can also automatically preserve the arbitrary Hamiltonian energy of a Hamiltonian system. An explicit scheme has been developed for the Zakharov equation using the PAVF method. The main purpose of this study is to develop a new energy-preserving scheme for the CNSB equations (4.1) based on the PAVF method. Firstly, the equations (4.1) are written in an infinite Hamiltonian form. Then, the second-order central difference is employed for the spatial discretization to cast the CNSB equations (4.1) into a finite-dimensional Hamiltonian equation. We use the PAVF method for time integration to develop the energy-preserving scheme. The proposed scheme is semi-implicit, which has a significant advantage over the AVF method. In conjunction with the adjoint method, we further present the PAVF composition (PAVF-C) method and the PAVF plus (PAVF-P) method for the CNSB equations (4.1).

4.2 Construction of Finite Difference Method

Many evolution PDEs can be written as an infinite-dimensional Hamiltonian system of the form [51]

$$\frac{dz}{dt} = \mathcal{D} \frac{\delta \mathcal{H}}{\delta z} \quad (4.6)$$

where $z = z(x, t) \in \mathbb{R}^d \times \mathbb{R}$, and $\mathcal{D}$ is a constant linear differential operator. For example, if $d = 1$, and $z(x, t)$ belongs to the Hilbert space $L^2(\Omega)$, the Hamiltonian $\mathcal{H}$ and the variational derivative are

$$\mathcal{H}(z) = \int_{\Omega} H(x, z, z_x, z_{xx}, \dots) dx, \quad (4.7)$$

$$\frac{\delta \mathcal{H}}{\delta z} = \frac{\partial H}{\partial z} + \partial_x \left(\frac{\partial H}{\partial z_x} \right) - \partial_{xx} \left(\frac{\partial H}{\partial z_{xx}} \right) - \dots \quad (4.8)$$

where Ω is the subset of $\mathbb{R} \times \mathbb{R}$ and $z(x, t)$ satisfies homogenous or periodic boundary conditions. For two-dimension $d = 2$ i.e., $x = (x, y)^T$, $\Omega = [x_L, x_R] \times [y_L, y_R]$, the Hamiltonian $\mathcal{H}$ and the variational derivative are

$$\mathcal{H}[z] = \int \int_{\Omega} H(x, y, z, z_x, z_y, z_{xx}, \dots) dx dy, \quad (4.9)$$

$$\frac{\delta \mathcal{H}}{\delta z} = \frac{\partial H}{\partial z} + \partial_x \left(\frac{\partial H}{\partial z_x} \right) + \partial_y \left(\frac{\partial H}{\partial z_y} \right) - \partial_{xx} \left(\frac{\partial H}{\partial z_{xx}} \right) - \dots \quad (4.10)$$

By decomposing $u(x, t) = p(x, y, t) + iq(x, y, t)$ in real and imaginary components, the CNSB equations (4.1) in two space dimensions can be written as a first-order system of equations

$$\begin{aligned} p_t &= -\gamma(q_{xx} + q_{yy}) + \xi qv \\ q_t &= \gamma(p_{xx} + p_{yy}) - \xi pv \\ v_t &= \phi_{xx} + \phi_{yy} \\ \phi_t &= v - \alpha(v_{xx} + v_{yy}) + f(v) + \omega(p^2 + q^2) \end{aligned} \quad (4.11)$$

which can be written as infinite-dimensional Hamiltonian system (4.6) with the state variable $z(t) = (p(x, y, t), q(x, y, t), v(x, y, t), \phi(x, y, t))^T$, the differential operator

$$\mathcal{D} = \begin{pmatrix} 0 & \xi/(4\omega) & 0 & 0 \\ -\xi/(4\omega) & 0 & 0 & 0 \\ 0 & 0 & 0 & -1/2 \\ 0 & 0 & 1/2 & 0 \end{pmatrix}$$

and the Hamiltonian

$$H(t) := \int_{\Omega} \int_{\Omega} \left(\frac{2\gamma\omega}{\xi} |\nabla u|^2 + \alpha |\nabla v|^2 + |\nabla \phi|^2 + v^2 + 2F(v) + 2\omega v |u|^2 \right) dx dy. \quad (4.12)$$

We can find that the Hamiltonian $H(t)$ is the total energy (4.5) of the system (4.1). In the following sections, we propose a nonlinear two-level, conservative, and second order accurate finite difference scheme for the problem (4.1)-(4.3)

Now, we consider the spatial discretization of the problem (4.1)-(4.3). For simplicity of notations, we shall consider the CNSB system (4.1) in one space dimension. Extension to higher dimensions is straightforward. The domain $(x, t) \in \Omega \times [0, T]$ is discretized into grids by the set (x_j, t_n) of nodes, in which $x = x_L + jh, 0 \leq j \leq N+1, t_n = n\tau, 0 \leq n \leq M$, where $h = (x_R - x_L)/N, \tau = T/M$, and M and N are positive integers. Let p_j^n, q_j^n, v_j^n and ϕ_j^n be the approximations to $p(x, t), q(x, t), v(x, t)$ and $\phi(x, t)$ at the grid (x_j, t_n) , respectively. For convenience, we introduce some notations:

$$\begin{aligned} \delta_t z_j^n &= \frac{z_j^{n+1} - z_j^n}{\tau}, & \delta_x^+ z_j^n &= \frac{z_{j+1}^n - z_j^n}{h}, & \delta_x^\pm z_j^n &= \delta^+(\delta^- z_j^n) = \frac{z_{j+1}^n - 2z_j^n + z_{j-1}^n}{h^2} \\ \delta_x^- z_j^n &= \frac{z_j^n - z_{j-1}^n}{h}, & z_j^{n+1/2} &= \frac{z_j^{n+1} + z_j^n}{2}. \end{aligned} \quad (4.13)$$

Discrete periodic boundary conditions are treated as

$$z_j = z_{N+j}, \quad j = \dots, -2, -1, 0, 1, 2, \dots$$

Consider the spatial discretization of (4.11) in one space dimension

$$\begin{aligned}
\frac{d}{dt}p_j &= -\gamma(\delta_x^{+-}q_j) + q_jv_j, \\
\frac{d}{dt}q_j &= \gamma(\delta_x^{+-}p_j) - p_jv_j, \\
\frac{d}{dt}v_j &= \delta_x^{+-}\phi_j, \\
\frac{d}{dt}\phi_j &= -\alpha(\delta_x^{+-}v_j) + v_j + \frac{1}{2}v_j^2 + \frac{1}{2}(p_j^2 + q_j^2).
\end{aligned} \tag{4.14}$$

where $j = 1, \dots, N$. The equation (4.14) can be written as a finite-dimensional canonical Hamiltonian system

$$\frac{d}{dt}Z = \overline{\mathcal{D}}\nabla\overline{H}(Z) \tag{4.15}$$

where $Z = (\mathbf{p}^T, \mathbf{q}^T, \mathbf{v}^T, \phi^T)^T$, $\mathbf{p}, \mathbf{q}, \mathbf{v}, \phi \in \mathbb{R}^N$ with entries $\mathbf{p} = (p_1, \dots, p_N)^T$, $\mathbf{q} = (q_1, \dots, q_N)^T$, $\mathbf{v} = (v_1, \dots, v_N)^T$, and $\phi = (\phi_1, \dots, \phi_N)^T$, respectively,

$$\overline{\mathcal{D}} = \begin{pmatrix} 0 & \frac{\xi}{4\omega}I & 0 & 0 \\ -\frac{\xi}{4\omega}I & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{1}{2}I \\ 0 & 0 & \frac{1}{2}I & 0 \end{pmatrix} \tag{4.16}$$

where I is an $N \times N$ identity matrix, and O is an $N \times N$ zero matrix and the discrete Hamiltonian is

$$\overline{H} = \sum_{i=1}^N \left(\frac{2\gamma\omega}{\xi} ((\delta_x^+ p_j)^2 + (\delta_x^+ q_j)^2) + \alpha(\delta_x^+ v_j)^2 + (\delta_x^+ \phi_j)^2 + v_j^2 + 2F(v_j) + 2\omega v_j |u_j|^2 \right) h \tag{4.17}$$

For system (4.15) we have,

$$\frac{d\overline{H}(Z(t))}{dt} = \nabla\overline{H}(Z(t)) \frac{dZ(t)}{dt} = \nabla\overline{H}(Z(t)) \overline{\mathcal{D}} \nabla\overline{H}(Z(t)) = 0. \tag{4.18}$$

due to the skew-symmetric property of the matrix $\overline{\mathcal{D}}$. Therefore, the flow of the semi-discrete system (4.15) preserves the Hamiltonian $\overline{H}(Z)$ exactly. The Hamiltonian system (4.15) also possesses symplecticity. Conservation of energy is as important as conservation of symplectic structure in numerical simulations. Therefore, it is natural to consider the temporal discretization of (4.15) with a conservative method. In the following sections, energy-preserving AVF and PAVF methods have been considered for temporal discretization of (4.15).

4.3 Average Vector Field Methods for CSB System.

Consider the Hamiltonian differential equation (4.15). We present the conventional second-order AVF method (3.3) for (4.1) [8]. To obtain the AVF integrator, we apply the AVF method to time integration for the semi-discrete system (4.15) as follows

$$\begin{aligned}
\delta_t p_j^n &= -\gamma \delta_x^{+-}(q_j^{n+1/2}) + \xi \left(\frac{1}{3} q_j^{n+1} v_j^{n+1} + \frac{1}{6} q_j^{n+1} v_j^n + \frac{1}{6} q_j^n v_j^{n+1} + \frac{1}{3} q_j^n v_j^n \right), \\
\delta_t q_j^n &= \gamma \delta_x^{+-}(p_j^{n+1/2}) - \xi \left(\frac{1}{3} p_j^{n+1} v_j^{n+1} + \frac{1}{6} p_j^{n+1} v_j^n + \frac{1}{6} p_j^n v_j^{n+1} + \frac{1}{3} p_j^n v_j^n \right), \\
\delta_t v_j^n &= \delta_x^{+-}(\phi_j^{n+1/2}), \\
\delta_t \phi_j^n &= -\alpha \delta_x^{+-}(v_j^{n+1/2}) + v_j^{n+1/2} + \hat{f}(v_j^{n+1}, v_j^n) + \frac{\omega}{6} \left((p_j^{n+1})^2 + p_j^{n+1} p_j^n \right. \\
&\quad \left. + (p_j^n)^2 + (q_j^{n+1})^2 + q_j^{n+1} q_j^n + (q_j^n)^2 \right).
\end{aligned} \tag{4.19}$$

where $\hat{f}(v_j^{n+1}, v_j^n) = \int_0^1 f(\xi v_j^{n+1} + (1-\xi)v_j^n) d\xi$. We see that the scheme (4.19) is fully implicit, which requires a time-consuming iterative method such as the Newton-Raphson method. Now, we propose a more efficient energy-preserving method for CNSB equations (4.1).

4.4 Partitioned Average Vector Field Methods for CSB System.

To apply the PAVF method (3.5) for the system (4.15), first we group the variable Z by choosing $Z = (\mathbf{a}, \mathbf{b})^T$ where

$$\begin{aligned}
\mathbf{a} &= (p_1, \dots, p_N, q_1, \dots, q_N) \\
\mathbf{b} &= (v_1, \dots, v_N, \phi_1, \dots, \phi_N)^T.
\end{aligned}$$

Then the canonical Hamiltonian system (4.15) can be written as

$$\frac{d}{dt} \begin{pmatrix} \mathbf{a} \\ \mathbf{b} \end{pmatrix} = \overline{\mathcal{D}} \begin{pmatrix} \nabla_{\mathbf{a}} \overline{H}(\mathbf{a}, \mathbf{b}) \\ \nabla_{\mathbf{b}} \overline{H}(\mathbf{a}, \mathbf{b}) \end{pmatrix}. \tag{4.20}$$

Upon applying the PAVF method (3.5) to the semi-discrete system (4.20), we obtain

$$\begin{aligned}
\delta_t(p_j^n) &= -\gamma\delta_x^{+-}(q_j^{n+1/2}) + \frac{\xi}{2}(q_j^{n+1}v_j^n + q_j^n v_j^n), \\
\delta_t(q_j^n) &= \gamma\delta_x^{+-}(p_j^{n+1/2}) - \frac{\xi}{2}(p_j^{n+1}v_j^n + p_j^n v_j^n), \\
\delta_t(v_j^n) &= \delta_x^{+-}(\phi_j^{n+1/2}), \\
\delta_t(\phi_j^n) &= -\alpha\delta_x^{+-}(v_j^{n+1/2}) + v_j^{n+1/2} + \hat{f}(v_j^{n+1}, v_j^n) + \omega((p_j^{n+1})^2 + (q_j^{n+1})^2).
\end{aligned} \tag{4.21}$$

The PAVF method (4.21) is simpler than the AVF method (4.19). The first two equations in (4.21) are linearly implicit according to the variables p^{n+1} and q^{n+1} . Once the values p_j^n, q_j^n, v_j^n and ϕ_j^n are known, the values p_j^{n+1} and q_j^{n+1} can be found from the first two equations of (4.21) and substituted into the last two equations. Then the values ϕ_j^{n+1} and v_j^{n+1} can be approximated from the last two equations by using an iterative method such as Newton's method. On the other hand, the AVF method (4.19) is fully implicit, which requires more cost per time step than the PAVF method (4.21).

Remark: In contrast to the semi-implicit structure of the PAVF method (4.21) for the CNSB equations, Cai et. al. [19] have constructed the PAVF method for non-linear Klein-Gordon-Schrödinger equations that require solving two sets of nonlinear algebraic equations.

In addition to the conservation of energy, the conservation of mass (4.4), which is a quadratic invariant, also plays an important role in physics. Therefore, it is natural to discuss the mass conservation of the method (4.21).

Theorem 4.4.1 *The difference scheme(4.21) is conservative; that is, the mass (4.4) is conserved in the sense that*

$$M^n = \sum_{k=1}^N ((p_k^n)^2 + (q_k^n)^2)h = M^{n-1} = \dots = M^0 \tag{4.22}$$

where $M^n = M(p^n, q^n)$.

Proof. Multiplying both sides of the first line of equation (4.21) with $(p_j^{n+1} + p_j^n)^T$ yields

$$\frac{1}{\tau}(p_j^{n+1} + p_j^n)^T(p_j^{n+1} - p_j^n) = (p_j^{n+1} + p_j^n)^T \left(-\gamma\delta_x^{+-}q_j^n + \frac{1}{2}(q_j^{n+1}v_j^n + q_j^n v_j^n) \right) \tag{4.23}$$

and multiplying both sides of the second line of equation (4.21) with $(q_j^{n+1} + q_j^n)^T$ yields

$$\frac{1}{\tau}(q_j^{n+1} + q_j^n)^T(q_j^{n+1} - q_j^n) = (q_j^{n+1} + q_j^n)^T \left(\gamma \delta_x^{+-} p_j^n - \frac{1}{2}(p_j^{n+1} v_j^n + p_j^n v_j^n) \right). \quad (4.24)$$

Then, adding (4.23) to (4.24), we have

$$\frac{1}{\tau} \sum_{j=1}^N \left((p_j^{n+1})^2 + (q_j^{n+1})^2 \right) = \frac{1}{\tau} \sum_{j=1}^N \left((p_j^n)^2 + (q_j^n)^2 \right).$$

which completes the proof. □

The adjoint PAVF method for (4.20) is

$$\begin{aligned} \delta_t(p_j^n) &= -\gamma \delta_x^{+-} (q_j^{n+1/2}) + \frac{\xi}{2} (q_j^{n+1} v_j^{n+1} + q_j^n v_j^{n+1}), \\ \delta_t(q_j^n) &= \gamma \delta_x^{+-} (p_j^{n+1/2}) - \frac{\xi}{2} (p_j^{n+1} v_j^{n+1} + p_j^n v_j^{n+1}), \\ \delta_t(v_j^n) &= \delta_x^{+-} (\phi_j^{n+1/2}), \\ \delta_t(\phi_j^n) &= -\alpha \delta_x^{+-} (v_j^{n+1/2}) + v_j^{n+1/2} + \hat{f}(v_j^{n+1}, v_j^n) + \omega \left((p_j^n)^2 + (q_j^n)^2 \right). \end{aligned} \quad (4.25)$$

We can see that the adjoint scheme (4.25) is semi-implicit due to the nonlinear term $\hat{f}(v_j^{n+1}, v_j^n)$. The values v_j^{n+1} and ϕ_j^{n+1} can be approximated from the last two equations of (4.25) using an iterative method. Then v_j^{n+1} and ϕ_j^{n+1} can be substituted into the first two equations of (4.25) and p_j^{n+1} and q_j^{n+1} can be approximated. Using the PAVF method (4.21) with the adjoint method (4.25), we can write the energy-preserving

composition (PAVF-C) method (3.8) as follows

$$\begin{aligned}
\frac{2}{\tau}(p_j^* - p_j^n) &= -\gamma\delta_x^{+-}(q_j^* + q_j^n) + \xi(q_j^*v_j^n + q_j^n v_j^n), \\
\frac{2}{\tau}(q_j^* - q_j^n) &= \gamma\delta_x^{+-}(p_j^* + p_j^n) - \xi(p_j^*v_j^n + p_j^n v_j^n), \\
\frac{2}{\tau}(v_j^* - v_j^n) &= \delta_x^{+-}(\phi_j^* + \phi_j^n), \\
\frac{2}{\tau}(\phi_j^* - \phi_j^n) &= -\alpha\delta_x^{+-}(v_j^* + v_j^n) + (v_j^* + v_j^n) + 2\omega((p_j^*)^2 + (q_j^*)^2) \\
&\quad + 2\hat{f}(v_j^*, v_j^n) \\
\frac{2}{\tau}(p_j^{n+1} - p_j^*) &= -\gamma\delta_x^{+-}(q_j^{n+1} + q_j^*) + \xi(q_j^{n+1}v_j^{n+1} + q_j^*v_j^{n+1}), \\
\frac{2}{\tau}(q_j^{n+1} - q_j^*) &= \gamma\delta_x^{+-}(p_j^{n+1} + p_j^*) - \xi(p_j^{n+1}v_j^{n+1} + p_j^*v_j^{n+1}), \\
\frac{2}{\tau}(v_j^{n+1} - v_j^*) &= \delta_x^{+-}(\phi_j^{n+1} + \phi_j^*), \\
\frac{2}{\tau}(\phi_j^{n+1} - \phi_j^*) &= -\alpha\delta_x^{+-}(v_j^{n+1} + v_j^*) + (v_j^{n+1} + v_j^*) + 2\omega((p_j^*)^2 + (q_j^*)^2) \\
&\quad + 2\hat{f}(v_j^{n+1}, v_j^*)
\end{aligned} \tag{4.26}$$

We can see that PAVF-C method (4.26) inherits the semi-implicit property. If the values p_j^n , q_j^n , v_j^n and ϕ_j^n are known, the values p_j^* and q_j^* can be found from the first two equations of (4.26) and substituted into the third and fourth equations, which are nonlinear in terms of the unknowns ϕ_j^* and v_j^* . Thus, ϕ_j^* and v_j^* can be approximated using an iterative method. Here, Newton's method is used as a nonlinear solver. Then, ϕ_j^* , v_j^* , ϕ_j^* and v_j^* can be substituted into the last two equations in (4.26) and ϕ_j^{n+1} and v_j^{n+1} can be approximated using Newton's method. Finally, ϕ_j^{n+1} and v_j^{n+1} can be substituted into the fifth and sixth equations, and p_j^{n+1} and q_j^{n+1} can be approximated by using the semi-implicit property of these two equations.

With the adjoint scheme (4.25), we can directly write down the corresponding the plus scheme (PAVF-P)

$$\begin{aligned}
\delta_t(p_j^n) &= -\gamma\delta_x^{+-}(q_j^n) - \frac{\xi}{4}(q_j^{n+1}v_j^n + q_j^n v_j^n + q_j^{n+1}v_j^{n+1} + q_j^n v_j^{n+1}), \\
\delta_t(q_j^n) &= \gamma\delta_x^{+-}(p_j^n) - \frac{\xi}{4}(p_j^{n+1}v_j^n + p_j^n v_j^n + p_j^{n+1}v_j^{n+1} + p_j^n v_j^{n+1}), \\
\delta_t(v_j^n) &= \delta_x^{+-}\phi_j^n, \\
\delta_t(\phi_j^n) &= -\alpha\delta_x^{+-}v_j^n + v_j^{n+1/2} + \hat{f}(v_j^n, v_j^{n+1}) + \frac{\omega}{2}((p_j^{n+1})^2 + (q_j^{n+1})^2 \\
&\quad + (p_j^n)^2 + (q_j^n)^2).
\end{aligned} \tag{4.27}$$

Obviously, the scheme (4.27) is implicit and nonlinear. In order to obtain the numerical solution p_j^{n+1} , q_j^{n+1} , ϕ_j^{n+1} and v_j^{n+1} , we need an iterative algorithm which increase the computational time. Here Newton's method is used as a nonlinear solver.

4.5 Numerical Results

In this section, we present some numerical experiments to verify theoretical results and to demonstrate the effectiveness of the conservative schemes (4.21), (4.26), and (4.27). $L_\infty^n(\tau)$ and $L_2^n(\tau)$ errors for temporal accuracy is defined by

$$\begin{aligned} L_\infty^n &= \max_{1 \leq n \leq M} \left\{ |u(x_j, t_n) - u_j^n| + |v(x_j, t_n) - v_j^n| \right\} \\ L_2^n &= \left(h \sum_{j=1}^N |u(x_j, t_n) - u_j^n|^2 \right)^{1/2} + \left(h \sum_{j=1}^N |v(x_j, t_n) - v_j^n|^2 \right)^{1/2}. \end{aligned} \quad (4.28)$$

L_∞^j and L_2^j errors for spatial accuracy can be defined analogously. The preservation of the mass and energy are monitored by the relative errors

$$GE = \frac{|H^n - H^0|}{|H^0|}, \quad GM = \frac{|M^n - M^0|}{|M^0|}$$

where

$$H^n = \sum_{i=1}^N \left(\frac{2\gamma\omega}{\xi} ((\delta_x^+ p_j^n)^2 + (\delta_x^+ q_j^n)^2) + \alpha (\delta_x^+ v_j^n)^2 + (\delta_x^+ \phi_j^n)^2 + (v_j^n)^2 + 2F(v_j^n) + 2\omega v_j^n |u_j^n|^2 \right) h. \quad (4.29)$$

denote the Hamiltonian corresponding to (4.17), and M^n is the mass (4.22) at $t = t^n$. The rate of convergence in time discretization is obtained by using

$$\text{order} \approx \log(L(\tau_1)/L(\tau_2)) / \log(\tau_1/\tau_2)$$

where L represents L_∞^n and L_2^n errors at the time steps τ_1 and τ_2 . The rate of convergence in space discretization can be defined analogously. To demonstrate the long-time behavior of the energy-preserving schemes, we take the periodic boundary conditions $u(x_L, t) = u(x_R, t)$, and $v(x_L, t) = v(x_R, t)$. For simplicity, we present the wave profiles of the PAVF (4.25) scheme in all computations, since the other schemes, AVF (4.19), PAVF-C (4.26) and PAVF-P (4.27) produce the same profile.

4.5.1 One-dimensional CSB Equation.

In this section, we report some numerical results to exhibit the performance of the PAVF schemes (4.21), (4.26), and (4.27) and verify the energy and mass conservation. Performance of the PAVF schemes (4.21), (4.26) and (4.27) are compared with the fully implicit AVF scheme (4.19) [8]. An analytical solution has been given in [70]

$$\begin{aligned} u(x, t) &= \frac{9}{10} \operatorname{sech}^2 \left(\frac{\sqrt{15}}{10} \left(x - \frac{\sqrt{10}}{5} t \right) \right) \exp \left(i \left(\frac{\sqrt{10}}{10} x + \frac{1}{2} t \right) \right), \\ v(x, t) &= \frac{9}{10} \operatorname{sech}^2 \left(\frac{\sqrt{15}}{10} \left(x - \frac{\sqrt{10}}{5} t \right) \right), \\ v_t(x, t) &= \frac{9}{10} \operatorname{sech}^2 \left(\frac{\sqrt{15}}{10} \left(x - \frac{\sqrt{10}}{5} t \right) \right) \tanh \left(\frac{\sqrt{15}}{10} \left(x - \frac{\sqrt{10}}{5} t \right) \right). \end{aligned} \quad (4.30)$$

Accuracy test: First, the correctness of the numerical schemes are examined. The spatial domain has been chosen large enough that solitary wave propagation do not effect the propagation of wave. The initial conditions are taken from the exact solution (4.30)

$$u(x, 0) = u_0(x), \quad v(x, 0) = v_0(x), \quad v_t(x, 0) = v_{t,0}(x). \quad (4.31)$$

Table (4.1) represents L_∞^j and L_2^j errors and convergence order in space. We note that all method are both of second order in space

Table (4.2) lists the L_∞^j and L_2^j errors and convergence order in time. From the table, we see that all methods reach the second order in time except the PAVF method, which is only first-order. From (4.1) and (4.2), we can see that the PAVF-P method has higher accuracy than the PAVF and PAVF-C methods. Table 4.3 and Figure (4.1) represent the CPU time of the four methods with different temporal steps. All computations were done on a custom computer with $i7 - 1.80GHz$ processor. To estimate how long a portion of our algorithm takes to run we used Matlab's stopwatch timer function, "tic" and "toc". The Matlab (R2024b) built-in functions "tic" and "toc" are used to measure the performance of the algorithms. These functions return wall-clock time. Since the PAVF method and PAVF-C method are semi-implicit, they require a solution of two linear systems of equations as well as the solution of two nonlinear systems

Table 4.1: The L_∞ and L_2 errors and convergence orders in space of the proposed methods for Schrödinger-Boussinesq equation (4.1) on the interval $-16 \leq x \leq 16$ with $\tau = 0.00025$ at $t = 1$

	h	0.5	0.25	0.125
AVF	L_∞^j	error	1.174×10^{-2}	3.014×10^{-3}
		order	–	1.96
	L_2^j	error	1.739×10^{-2}	4.371×10^{-3}
		order	–	1.99
PAVF	L_∞^j	error	1.175×10^{-2}	3.030×10^{-3}
		order	–	0.95
	L_2^j	error	1.741×10^{-2}	4.392×10^{-3}
		order	–	1.99
PAVF-C	L_∞^j	error	1.174×10^{-2}	3.014×10^{-3}
		order	–	1.96
	L_2^j	error	1.135×10^{-2}	4.371×10^{-3}
		order	–	1.99
PAVF-P	L_∞^j	error	7.501×10^{-3}	1.892×10^{-3}
		order	–	1.99
	L_2^j	error	4.240×10^{-3}	1.122×10^{-3}
		order	–	1.91

of equations. On the other hand, fully implicit PAVF-P and AVF methods require the solution of four nonlinear systems of equations.

Table 4.2: The L_∞ and L_2 errors and convergence orders in space of the proposed methods for Schrödinger-Boussinesq equation (4.1) on the interval $-16 \leq x \leq 16$ with $\tau = 0.00025$ at $t = 1$

	τ	0.5	0.25	0.125
AVF	L_∞^n	error	2.889×10^{-3}	7.274×10^{-4}
		order	—	1.99
	L_2^n	error	4.902×10^{-3}	1.243×10^{-3}
		order	—	1.98
PAVF	L_∞^n	error	1.966×10^{-2}	1.061×10^{-2}
		order	—	0.89
	L_2^n	error	3.238×10^{-2}	1.725×10^{-2}
		order	—	0.91
PAVF-C	L_∞^n	error	2.078×10^{-3}	5.116×10^{-4}
		order	—	2.02
	L_2^n	error	3.456×10^{-3}	8.685×10^{-4}
		order	—	1.99
PAVF-P	L_∞^n	error	2.086×10^{-3}	5.409×10^{-4}
		order	—	1.99
	L_2^n	error	3.277×10^{-3}	8.441×10^{-4}
		order	—	1.96

Table 4.3: Computation time for $-32 \leq x \leq 32$ at $t = 1$.

	PAVF		PAVF-C		PAV-P		AVF	
τ	$h = 0.1$	$h = 0.05$	$h = 0.1$	$h = 0.05$	$h = 0.1$	$h = 0.05$	$h = 0.1$	$h = 0.05$
0.1	0.083	0.137	0.129	0.239	0.165	0.350	0.249	0.405
0.05	0.121	0.240	0.217	0.263	0.220	0.479	0.240	0.509
0.01	0.509	1.138	0.994	2.206	0.987	2.087	1.097	2.218
0.005	1.002	3.123	2.027	6.132	1.995	5.528	2.026	4.590

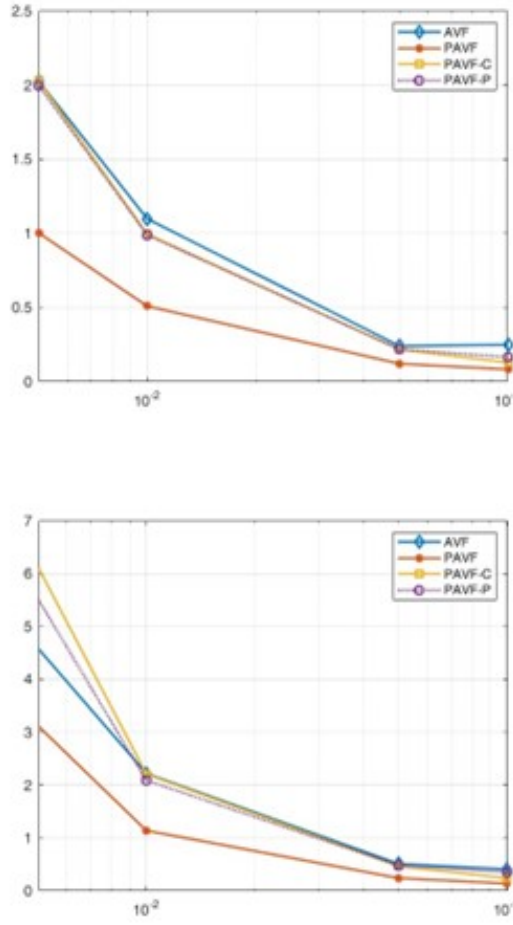


Figure 4.1: Computation time for $-32 \leq x \leq 32$ at $t = 1$.

Accordingly, the PAVF method is more efficient than the AVF method. Figure (4.1) verifies this fact. Table 4.3 also shows that the computational cost of the PAVF and PAVF-C is less than that of the fully implicit PAVF-P and AVF methods. In addition, we notice that the computational times of the PAVF-C and PAVF-P methods are slightly less than twice that of PAVF although the PAVF-C method is the composition of the PAVF method and its adjoint method, and the PAVF-P method is fully implicit. In addition, the PAVF-C and PAVF-P methods have the same accuracy as the AVF method, but they are more efficient than the AVF method. Finally, we can say that the PAVF-P is the most efficient method among the methods we have considered.

Next, we test the stability of the scheme concerning the initial data. We consider the perturbed initial data $u_{noise}(x, 0) = u_0(x)(1 + \mu\theta)$, $v_{noise}(x, 0) = v_0(x)(1 + \mu\theta)$, $u_{t,noise}(x, 0) = u_{t,0}(x)(1 + \mu\theta)$, where μ is the percentage of the noise and θ is the random variable gen-

erated from a uniform distribution in the interval $[-0.5, 0.5]$. We denote the perturbed solution as U_p and V_p . Figure (4.2) represents the solitary wave obtained by the PAVF scheme (4.21) with noise using the perturbed initial condition with $\mu = 0.2$. Similar results have been obtained for the PAVF-C and PAVF-P methods which are not shown here. From the figure, we see that the small perturbation in the initial data does not yield any significant effect on the wave propagation, which confirms the stability of the methods.

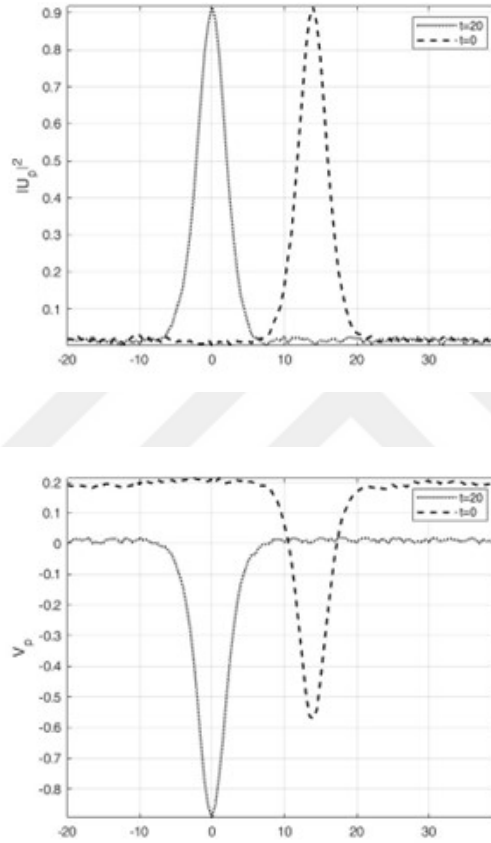


Figure 4.2: Solitary wave propagation with noise $\tau = 0.001$, $h = 0.5$

Single solitary wave. In this subsection, we examine the long-time solitary wave simulation. We solve the SB equations (4.1) in the spatial interval $[-64, 64]$ and temporal interval $[0, 40]$. We choose the spatial interval large enough so that solitary wave propagation and conservation properties are not affected by the boundary conditions. We can see that solitons move forward without any changes in shape as shown in Fig 4.3. The corresponding errors of total energy H^n and mass M^n are represented

Table 4.4: Computation time for $h_x = h_y = 0.25$, $-10 \leq x, y \leq 10$ at $t = 1$.

τ	PAVF	PAVF-C	PAV-P	AVF
0.1	3.609	6.575	13.794	8.552
0.05	5.160	9.670	18.047	15.798
0.01	28.731	57.022	97.931	66.328
0.005	58.076	116.404	200.128	131.089

by Figure (4.3). From the figure, we see that the errors are small during long-time integration which confirms theoretical results. The left figure of Figure (4.3) represents that all four methods preserve the discrete energy up to round-off errors. From the right figure of Figure (4.3) we can see that, the AVF method cannot preserve the mass, but the relative error is bounded. On the other hand, we can see the excellent mass preservation of the other three methods during time integration. Numerical

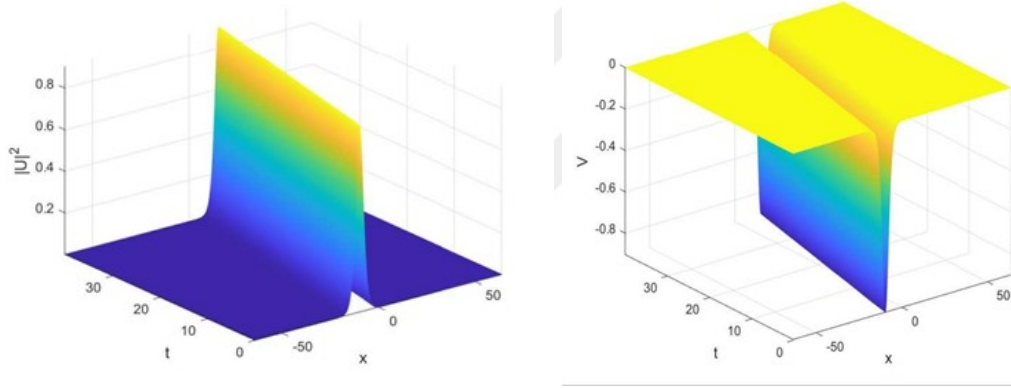


Figure 4.3: Evolution of PAVF solution for $\tau = 0.001$, $h = 0.2$

results show that the proposed schemes have excellent conservation properties and stability even for long time integration.

4.5.2 Two-dimensional Schrödinger-Boussinesq Equation

The advantage of the PAVF method becomes more evident in two-dimensional problems [19]. In this subsection, we consider the two-dimensional SB equations (4.1) with $d = 2$, and $f(v) = \sin(v)$ ([18], [54]). We choose the parameters

$\gamma = \alpha = -1$ and $\xi = \omega = -1/10$. The analytical solution of two-dimensional SB

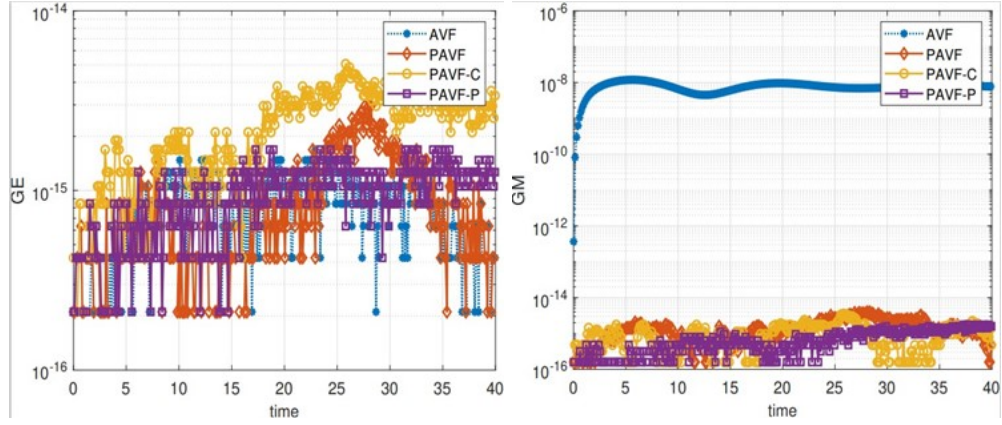


Figure 4.4: Relative errors in total energy H^n and the mass M^n for $\tau = 0.01$, $h = 0.2$

equation is not available. The initial data are taken as

$$\begin{aligned} u_0(x, y) &= \frac{2}{e^{x^2+2y^2} + e^{-x^2} + 2y^2} e^5 i / \cosh(\sqrt{4x^2 + y^2}) \\ v_0(x, y) &= e^{-x^2} + 2y^2 \\ \phi_0(x, y) &= \frac{1}{2} e^{-x^2} + 2y^2. \end{aligned} \quad (4.32)$$

Table (4.4) indicates the computational times obtained by four energy-preserving methods in the spatial domain $\Omega = (-10 \times 10) \times (-10 \times 10)$ with $h_x = h_y = 0.1$ for the different temporal step sizes. Here, h_x and h_y are step size in x -direction and y -direction, respectively. From the table, we see that PAVF method requires smaller computational time than the AVF method, as expected. Moreover, as in the one-dimensional case, the computational time of PAVF-C method is much less than twice that of PAVF. In addition, it can be seen that the PAVF-P method is the method with the most CPU time.

Figure (4.5) shows the surfaces of $|u|$, v and ϕ at the initial time $t = 0$ and the final time $t = 1$. the spatial interval is set to $\Omega = [-16 \times 16] \times [-16 \times 16]$. the step sizes taken as $\tau = 0.01$ and $h_x = h_y = 0.25$

From the left plot of the figure, one can see the initial hump collapses as time evolves many spikes appear at the end. From the middle plot, one can see that the initial hump collapses as time evolves, and a hole appears inside the hump. In addition, there are spikes from under the horizontal plane. The right graph displays the evolution of the plane ϕ . From the right figure, one can see that again the initial hump collapses, but

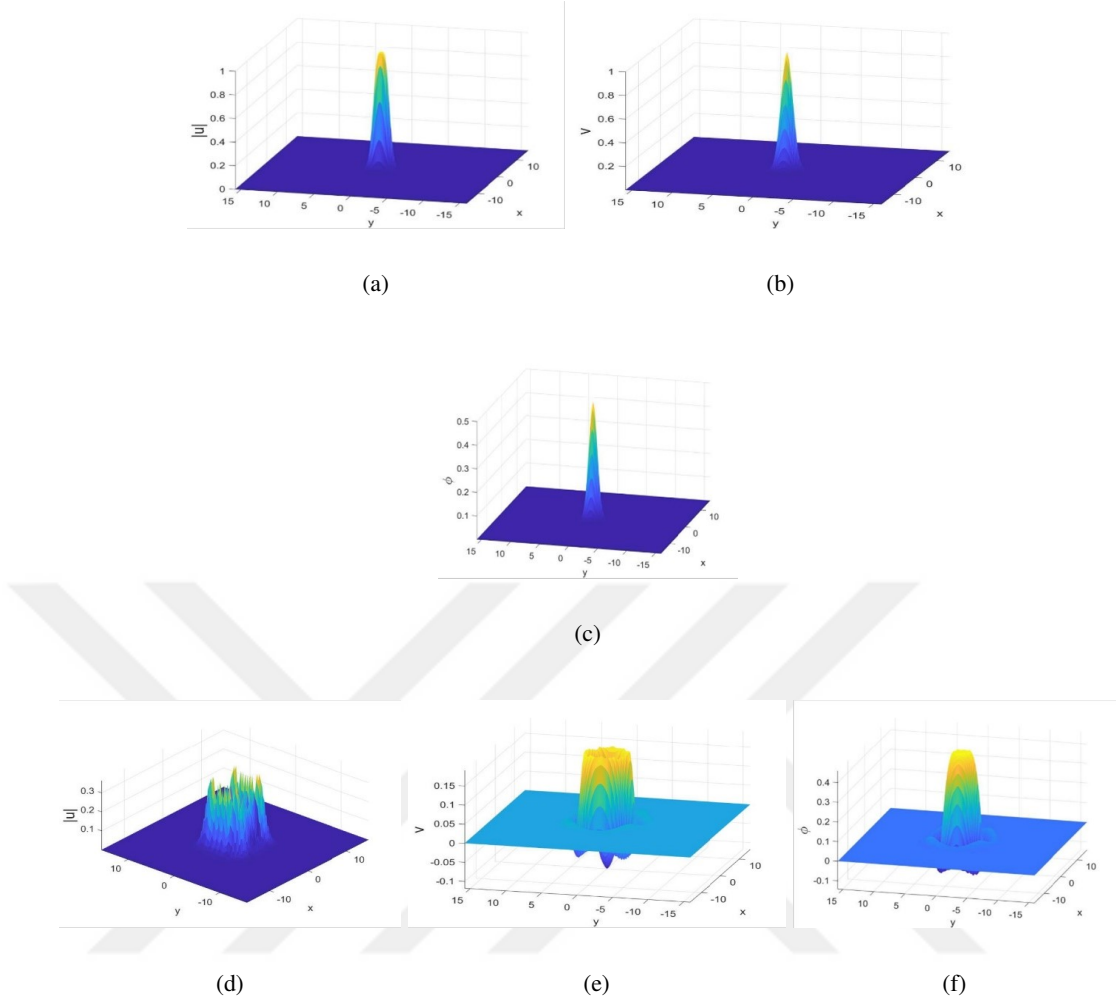
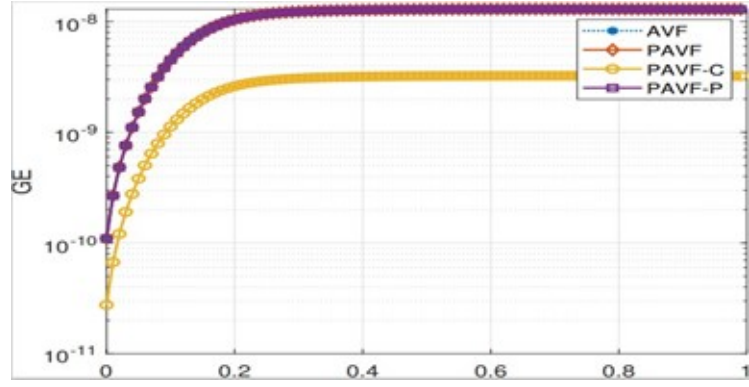


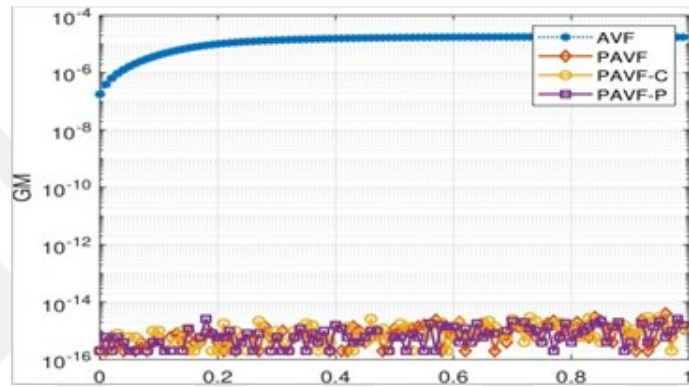
Figure 4.5: Evolution of PAVF solution for $\tau = 0.01$, $h_x = h_y = 0.25$.

no hole appears. Moreover, spikes from under the horizontal plane. The energy and mass conservation are depicted in Fig.5. From the figure, one can find that PAVF-C preserves the total energy better than the other methods. Moreover, all PAVF methods preserve the mass better than the AVF method.

Conclusion. In this study, we applied the energy-preserving PAVF method to the one-dimensional and two-dimensional CNSB equations. The method leads to semi-implicit algebraic equations for the CNSB equations. In addition, we find that the new energy-preserving scheme preserves the mass of the equations. In conjunction with the adjoint method of the PAVF method, we further introduce the conservative PAVF composition (PAVF-C) method and PAVF plus (PAVF-P) method. Some numerical results are presented to demonstrate the accuracy and efficiency of the method for the



(a)



(b)

Figure 4.6: Error in total energy H^n and Langmuir plasmon number L^n for $\tau = 0.01$, $h = 0.25$.

numerical solution of the CNSB equations. Numerical results confirm the theoretical results. Errors in the methods and computational times are compared with the AVF method. Numerical results verify that the applied schemes simulate both one- and two-dimensional CNSB system well.

CHAPTER 5

NEW CONSERVATIVE PARTITIONED AVERAGE VECTOR FIELDS SCHEMES FOR NONLINEAR DIRAC EQUATION

Introduction

In this chapter, we consider the non-linear Dirac equation [45]

$$\begin{aligned}\psi_t &= A\psi_x + if(|\psi_1|^2 - |\psi_2|^2)B\psi \\ \psi_1(x, 0) &= \phi_1(x), \quad \psi_2(x, 0) = \phi_2(x)\end{aligned}\tag{5.1}$$

where $\psi = [\psi_1, \psi_2]^T$ is a spinor wave function representing a particle with spin $-1/2$. In this context, ψ_1 and ψ_2 are complex-valued functions, $f(s)$ is a real-valued function of a real variable s , and A and B are matrices given by

$$A = \begin{bmatrix} 0 & -1 \\ -1 & 0 \end{bmatrix}, \quad B = \begin{bmatrix} -1 & 0 \\ 0 & 1 \end{bmatrix}$$

Several numerical techniques have been developed to solve the nonlinear Dirac (NLD) equation (5.1), including spectral methods [30] and finite difference methods [2],[4] and [3]. In [69], finite volume methods on fine computational grids were introduced to explore the dynamics of Dirac solitary wave interactions. High-order accurate Runge-Kutta discontinuous Galerkin methods were proposed in [62], [63] and [64] to simulate solitary wave interactions governed by the NLD equation. More recently, an integrating-factor approach tailored for the NLD equation was suggested in [32].

This study focuses on developing efficient multisymplectic numerical schemes for the NLD equation. Multi-symplectic methods are specifically designed to preserve the multi-symplectic structure inherent in Hamiltonian PDEs under suitable discretiza-

tion, providing improved performance in long-term simulations compared to conventional methods [12], similar to the well-known symplectic methods [49], [37], [34] and [75]. Interest in such methods has grown considerably in recent years [13].

Various multi-symplectic schemes have been formulated for Hamiltonian PDEs, including the multi-symplectic Preissmann scheme [12], [49] [37], [34] [75], [13] and [46], multi-symplectic Runge-Kutta methods [58], spectral discretizations [12], Fourier pseudospectral techniques [22] and [24], and wavelet collocation methods [77], [76], [77] and [25]. However, most of these schemes are implicit and can be computationally inefficient. To address this challenge, splitting methods have been introduced. For instance, [59] presents a splitting strategy that simplifies the implementation of multi-symplectic methods. The practical efficiency of these splitting-based approaches is demonstrated numerically in [44], [50] and [26]. Furthermore, explicit multi-symplectic schemes have been constructed for the wave and Klein-Gordon-Schrödinger equations using symplectic Runge-Kutta-Nyström and symplectic Runge-Kutta-type methods [43] and [42].

In [41], the NLD equation is reformulated into a multi-symplectic structure, and based on this framework, multi-symplectic Runge-Kutta (MSRK) methods are theoretically analyzed. Numerical simulations confirm the effectiveness of these MSRK methods for the NLD equation. However, MSRK methods are implicit and require fixed-point iterations to solve the resulting nonlinear systems, which increases computational complexity.

Now, we consider the nonlinear Dirac (NLD) equation (5.1) [45]

$$\begin{aligned} \frac{\partial \Psi_1}{\partial t} + \frac{\partial \Psi_2}{\partial x} + im\Psi_1 + 2i\lambda(|\Psi_2|^2 - |\Psi_1|^2)\Psi_1 &= 0, \quad x_L \leq x \leq x_r, \quad 0 < t \leq T, \\ \frac{\partial \Psi_2}{\partial t} + \frac{\partial \Psi_1}{\partial x} - im\Psi_2 + 2i\lambda(|\Psi_1|^2 - |\Psi_2|^2)\Psi_2 &= 0, \quad x_L < x < x_r, \quad 0 < t \leq T, \end{aligned} \quad (5.2)$$

with initial condition

$$\Psi_1(x, 0) = \psi_1(x), \quad \Psi_2(x, 0) = \psi_2(x), \quad x_L \leq x \leq x_r, \quad (5.3)$$

and periodic boundary condition

$$\Psi_1(x_L, t) = \Psi_1(x_r, t), \quad \Psi_2(x_L, t) = \Psi_2(x_r, t), \quad 0 < t \leq T, \quad (5.4)$$

where $\Psi = (\Psi_1, \Psi_2)^T$ is a spinorial wave function of a particle with the spin $(-\frac{1}{2})$; Ψ_1 and Ψ_2 are complex-valued functions describing the up and down state of the spin

$(-\frac{1}{2})$ particle, respectively [45]. By letting $\Psi_1 = q_1 + iq_2$ and $\Psi_2 = q_3 + iq_4$, we decompose the Dirac equation (5.2) into real and imaginary parts. Then we have the following system

$$\begin{aligned} \frac{\partial q_2}{\partial t} + \frac{\partial q_4}{\partial x} &= -mq_1 - 2\lambda(q_3^2 + q_4^2 - q_1^2 - q_2^2)q_1, \\ -\frac{\partial q_1}{\partial t} - \frac{\partial q_3}{\partial x} &= -mq_2 - 2\lambda(q_3^2 + q_4^2 - q_1^2 - q_2^2)q_2, \\ \frac{\partial q_4}{\partial t} + \frac{\partial q_2}{\partial x} &= mq_3 + 2\lambda(q_3^2 + q_4^2 - q_1^2 - q_2^2)q_3, \\ -\frac{\partial q_3}{\partial t} - \frac{\partial q_1}{\partial x} &= mq_4 + 2\lambda(q_3^2 + q_4^2 - q_1^2 - q_2^2)q_4. \end{aligned} \quad (5.5)$$

The system (5.5) can be written in a multisymplectic Hamiltonian PDE (1.72)

$$Mz_t + Kz_x = \nabla_z S(z) \quad (5.6)$$

where

$$M = \begin{pmatrix} 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \end{pmatrix}, \quad K = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{pmatrix}, \quad z = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \\ q_4 \end{pmatrix}$$

and

$$S(Z) = \frac{1}{2} \left[\lambda(q_1^2 + q_2^2 - q_3^2 - q_4^2) - m \right] [q_1^2 + q_2^2 - q_3^2 - q_4^2].$$

The NLD equation in multi-symplectic form (5.6) satisfies the multi-symplectic conservation law (1.73) together with a local energy conservation law (LECL) $E_t + F_x = 0$ (1.74) with

$$E(z) = S(z) + \frac{\partial q_1}{\partial x} q_4 - \frac{\partial q_2}{\partial x} q_3, \quad F(z) = \frac{\partial q_1}{\partial t} q_4 - \frac{\partial q_2}{\partial t} q_3, \quad (5.7)$$

and local momentum conservation laws $I_t + G_x = 0$ (1.75) with

$$I(z) = -\frac{\partial q_1}{\partial x} q_2 - \frac{\partial q_3}{\partial x} q_4, \quad G(z) = S(z) - \frac{\partial q_1}{\partial t} q_2 - \frac{\partial q_3}{\partial t} q_4 \quad (5.8)$$

5.1 Local Energy-Preserving AVF Method for Dirac Equation

In this section, we present the second-order local energy preserving AVF scheme (2.1) for the Dirac equation (5.5). Applying local energy-preserving method (2.1) for the

multisymplectic formulation (5.6) of the Dirac equation (5.2) we obtain

$$\begin{aligned}
\delta_t A_x q_{2j}^n - \delta_x A_t q_{4j}^n - m A_x A_t q_{1j}^n - \frac{1}{2} \lambda F_1(a, b) + \frac{1}{6} \lambda G_1(a, b, c, d, e, f, g, h) &= 0 \\
- \delta_t A_x q_{1j}^n - \delta_x A_t q_{3j}^n + m A_x A_t q_{2j}^n - \frac{1}{2} \lambda F_2(c, d) + \frac{1}{6} \lambda G_2(a, b, c, d, e, f, g, h) &= 0 \\
\delta_t A_x q_{4j}^n + \delta_x A_t q_{2j}^n - m A_x A_t q_{3j}^n - \frac{1}{2} \lambda F_3(e, f) + \frac{1}{6} \lambda G_3(a, b, c, d, e, f, g, h) &= 0 \\
\delta_t A_x q_{3j}^n - \delta_x A_t q_{1j}^n - m A_x A_t q_{4j}^n - \frac{1}{2} \lambda F_4(g, h) + \frac{1}{6} \lambda G_4(a, b, c, d, e, f, g, h) &= 0.
\end{aligned} \tag{5.9}$$

where

$$F_1(a, b) = a^3 + a^2b + ab^2 + b^3, \quad F_2(c, d) = c^3 + c^2d + cd^2 + d^3, \quad F_3(e, f) = e^3 + e^2f + ef^2 + f^3 \text{ and } F_4(g, h) = g^3 + g^2h + gh^2 + h^3.$$

The functions G_1, G_2, G_3 and G_4 will take the forms

$$\begin{aligned}
G_1(a, b, c, d, e, f, g, h) &= -3ac^2 - ad^2 - c^2b - 3bd - 2acd - 2cdb + 3ae^2 + af^2 \\
&\quad + 4e^2b + 2aef + 2ebf + 5ag^2 + ah^2 + 3bh^2 + 2agh \\
G_2(a, b, c, d, e, f, g, h) &= -3da^2 - cb^2 - a^2c + 3db^2 + 2cab + 2ad + 3ce^2 + cf^2 \\
&\quad + e^2d + 3df^2 + 2cef + 2edf + 3cg^2 + ch^2 + g^2d + 3dh^2 + 2cgh + 2gdh \\
G_3(a, b, c, d, e, f, g, h) &= 3ea^2 + eb^2 + a^2f + 3fb^2 + 2eab + 2afb + 3ec^2 + ed^2 + c^2f \\
&\quad + 3fd^2 + ecd + 2cfd - 3eg^2 - eh^2 - g^2f - 3fh^2 - 2egh - 2gfh
\end{aligned}$$

and

$$\begin{aligned}
G_4(a, b, c, d, e, f, g, h) &= 3ga^2 + gb^2 + a^2h + 3hb^2 + 2gab + 2ahd + 3gc^2 + gd^2 + c^2h + \\
&\quad + 3hd^2 + 2gcd + 2chd - 3ge^2 - gf^2 - e^2h - 3hf^2 + 2gef + 2ehf.
\end{aligned}$$

5.2 Local Energy-Preserving PAVF Methods for Dirac Equation

In this section, we present a new local energy-preserving algorithm for the nonlinear Dirac equation (5.5) based on Sec. 3.2. We introduce our new local energy preserving method (3.11) for the multisymplectic formulation (5.6) of the Dirac equation (5.2) and

obtain

$$\begin{aligned}
\delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \lambda G_1(a, b, d, f, h) - \frac{1}{2} \lambda F_1(a, b) &= 0 \\
-\delta_t A_x q_1^n - \delta_x A_t q_3^n + m A_x A_t q_2^n + \lambda G_2(a, c, d, f, h) - \frac{1}{2} \lambda F_1(c, d) &= 0 \\
\delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \lambda G_3(a, c, e, f, h) - \frac{1}{2} \lambda F_3(e, f) &= 0 \\
-\delta_t A_x q_3^n - \delta_x A_t q_1^n + m A_x A_t q_4^n - \lambda G_4(a, c, e, g, h) - \frac{1}{2} \lambda F_4(g, h) &= 0.
\end{aligned} \tag{5.10}$$

The special function F in (5.10), (5.11) and (5.13) will be the same, so there is no need to repeat it, while G of equation (5.10) takes the forms

$$G_1(a, b, d, f, h) = (f^2 + h^2 - d^2)(a + b)$$

$$G_2(a, c, d, f, h) = (f^2 + h^2 - a^2)(c + d)$$

$$G_3(a, c, e, f, h) = (h^2 - a^2 - e^2)(e + f)$$

and

$$G_4(a, c, e, g, h) = (e^2 - a^2 - c^2)(g + h).$$

We notice that the local energy-preserving AVF scheme (5.9) and the local energy preserving PAVF scheme (5.10) are nonlinear systems of equations that require an iterative method. In this thesis we use Newton-Raphson's method as an iterative solver. We also note that our new local energy preserving PAVF scheme (5.10) is simpler than the local energy preserving AVF scheme (5.9). To derive the second-order local energy preserving PAVF methods, including the PAVF composition (PAVF-C) and PAVF plus (PAVF-P) methods, we first present the adjoint of the PAVF (PAVF-ADJ) scheme (5.10) for the Dirac equation:

$$\begin{aligned}
\delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \lambda G_1(a, b, c, e, g) - \frac{1}{2} F_1(a, b) &= 0 \\
-\delta_t A_x q_1^n - \delta_x A_t q_3^n + m A_x A_t q_2^n + \lambda G_2(a, c, d, e, g) - \frac{1}{2} \lambda F_2(c, d) &= 0 \\
\delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \lambda G_3(b, d, e, f, g) - \frac{1}{2} F_3(e, f) &= 0 \\
-\delta_t A_x q_3^n - \delta_x A_t q_1^n + m A_x A_t q_4^n - \lambda G_4(b, d, f, g, h) - \frac{1}{2} \lambda F_4(g, h) &= 0,
\end{aligned} \tag{5.11}$$

where

$$G_1(a, b, c, e, g) = (e^2 + g^2 - c^2)(a + b),$$

$$G_2(a, c, d, e, g) = (e^2 + g^2 - a^2)(c + d),$$

$$G_3(b, d, e, f, g) = (g^2 - b^2 - d^2)(e + f),$$

and

$$G_4(b, d, f, g, h) = (f^2 - b^2 - d^2)(g + h).$$

With the adjoint scheme (5.11), we can directly write down the corresponding PAVF-C scheme (3.8). For this, we denote the LEP-PAVF scheme (5.10) by Φ_τ and the corresponding adjoint scheme (5.11) by Φ_τ^* and then write the PAVF-C scheme for Dirac equation (5.2) as

$$\Psi_\tau = \Phi_{\frac{\tau}{2}} \circ \Phi_{\frac{\tau}{2}}^*. \quad (5.12)$$

Finally, the PAVF-P method (3.9) for the Dirac equation (5.2) can be written as

$$\begin{aligned} \delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \frac{1}{2} G_1(a, b, c, d, e, f, g, h) - \frac{1}{2} \lambda F_1(a, b) &= 0 \\ -\delta_t A_x q_1^n - \delta_x A_t q_3^n + m A_x A_t q_2^n + \frac{1}{2} G_2(a, b, c, d, e, f, g, h) - \frac{1}{2} \lambda F_2(c, d) &= 0 \\ \delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \frac{1}{2} \lambda G_3(a, b, c, d, e, f, g, h) - \frac{1}{2} \lambda F_3(e, f) &= 0 \\ -\delta_t A_x q_3^n - \delta_x A_t q_1^n + m A_x A_t q_4^n - \frac{1}{2} G_4(a, b, c, d, e, f, g, h) - \frac{1}{2} \lambda F_4(g, h) &= 0 \end{aligned} \quad (5.13)$$

where

$$G_1(a, b, c, d, e, f, g, h) = (e^2 + f^2 + g^2 + h^2 - c^2 - d^2)(a + b)$$

$$G_2(a, b, c, d, e, f, g, h) = (e^2 + f^2 + g^2 + h^2 - a^2 - b^2)(c + d)$$

$$G_3(a, b, c, d, e, f, g, h) = (g^2 + h^2 - a^2 - b^2 - c^2 - d^2)(e + h)$$

and

$$G_4(a, b, c, d, e, f, g, h) = (e^2 + f^2 - a^2 - b^2 - c^2 - d^2)(g + h).$$

5.3 Local Momentum-Preserving AVF Method for Dirac Equation

In this section, we present the second-order local momentum preserving AVF scheme (2.14) for the multisymplectic formulation (5.6) of the Dirac equation (5.2). Applying local momentum-preserving method (2.14) for the multisymplectic formulation (5.6) of the Dirac equation (5.2), we obtain

$$\begin{aligned} \delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \frac{1}{12} A_x \lambda G_1(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_1(a, b) &= 0 \\ \delta_t A_x q_1^n + \delta_x A_t q_3^n - m A_x A_t q_2^n - \frac{1}{12} A_x \lambda G_2(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_2(c, d) &= 0 \\ \delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \frac{1}{12} A_x \lambda G_3(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_3(e, f) &= 0 \\ \delta_t A_x q_3^n + \delta_x A_t q_1^n - m A_x A_t q_4^n + \frac{1}{12} A_x \lambda G_4(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_4(g, h) &= 0, \end{aligned} \quad (5.14)$$

where

$$F_1 = \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right]$$

$$F_2 = \left[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3 \right]$$

$$F_3 = \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right]$$

$$G_1 = (a + b) \left[(Be + Bf)^2 + (Be + Bf)(e + f) + (e + f)^2 + (Bg + Bh)^2 + (Bg + Bh)(g + h) + (g + h)^2 - (Bc + Bd)^2 - (Bc + Bd)(c + d) - (c + d)^2 \right]$$

$$G_2 = (c + d) \left[(Be + Bf)^2 + (Be + Bf)(e + f) + (e + f)^2 + (Bg + Bh)^2 + (Bg + Bh)(g + h) + (g + h)^2 - (Ba + Bb)^2 - (Ba + Bb)(a + b) - (a + b)^2 \right]$$

$$G_3 = (e + f) \left[(Bg + Bh)^2 + (Bg + Bh)(g + h) + (g + h)^2 - (Bc + Bd)^2 - (Bc + Bd)(c + d) - (c + d)^2 - (Ba + Bb)^2 - (Ba + Bb)(a + b) - (a + b)^2 \right]$$

and

$$G_4 = (g + h) \left[(Be + Bf)^2 + (Be + Bf)(e + f) + (e + f)^2 - (Bc + Bd)^2 - (Bc + Bd)(c + d) - (c + d)^2 - (Ba + Bb)^2 - (Ba + Bb)(a + b) - (a + b)^2 \right]$$

5.4 Local Momentum-Preserving PAVF Methods for Dirac Equation

In this section, we present a new local momentum-preserving algorithm (3.41) for the Dirac equation (5.2) based on sec. (3.4). Now, we introduce our new LMP method

$$\begin{aligned} \delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \frac{1}{4} \lambda A_x G_1(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_1(a, b) &= 0 \\ \delta_t A_x q_1^n + \delta_x A_t q_3^n - m A_x A_t q_2^n - \frac{1}{4} \lambda A_x G_2(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_2(Bc, Bd, c, d) &= 0 \\ \delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \frac{1}{4} \lambda A_x G_3(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_3(e, f) &= 0 \\ \delta_t A_x q_3^n + \delta_x A_t q_1^n - m A_x A_t q_4^n + \frac{1}{4} \lambda A_x G_4(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_4(g, h) &= 0, \end{aligned} \quad (5.15)$$

where

$$F_1 = \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right]$$

$$F_2 = \left[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3 \right]$$

$$F_3 = \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right].$$

$$G_1 = (a + b) \left[(e + f)^2 + (g + h)^2 - (c + d)^2 \right]$$

$$G_2 = (c + d) \left[(e + f)^2 + (g + h)^2 - (Ba + Bb)^2 \right]$$

$$G_3 = (e + f) \left[(g + h)^2 - (Ba + Bb)^2 - (Bc + Bd)^2 \right]$$

and

$$G_4 = (g + h) \left[(Be + Bf)^2 - (Ba + Bb)^2 - (Bc + Bd)^2 \right]$$

We notice that the local momentum-preserving AVF scheme (5.14) and the local energy-preserving PAVF scheme (5.15) are nonlinear systems of equations that require an iterative method. We also note that our new local momentum preserving PAVF scheme (5.15) is simpler than the local momentum preserving AVF scheme (5.14). To derive the second-order local momentum preserving PAVF methods, including the PAVF composition (PAVF-C) and PAVF plus (PAVF-P) methods, we first present the adjoint of the PAVF (PAVF-ADJ) scheme (5.15) for the Dirac equation:

$$\begin{aligned} \delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \frac{1}{4} \lambda A_x G_1(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_1(a, b) &= 0 \\ \delta_t A_x q_1^n + \delta_x A_t q_3^n - m A_x A_t q_2^n - \frac{1}{4} \lambda A_x G_2(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_2(c, d) &= 0 \\ \delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \frac{1}{4} \lambda G_3(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_3(e, f) &= 0 \\ \delta_t A_x q_3^n + \delta_x A_t q_1^n - m A_x A_t q_4^n + \frac{1}{4} \lambda A_x G_3(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_4(g, h) &= 0, \end{aligned} \quad (5.16)$$

where

$$F_1 = \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right]$$

$$F_2 = \text{Big}[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3]$$

$$F_3 = \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right].$$

$$G_1 = (a + b) \left[(Be + Bf)^2 + (Bg + Bh)^2 - (Bc + Bd)^2 \right]$$

$$G_2 = (c + d) \left[(Be + Bf)^2 + (Bg + Bh)^2 - (a + b)^2 \right]$$

$$G_3 = (e + f) \left[(Bg + Bh)^2 - (a + b)^2 - (c + d)^2 \right]$$

and

$$G_4 = (g + h) \left[(e + f)^2 - (a + b)^2 - (c + d)^2 \right]$$

The PAVF-P method is written as

$$\begin{aligned}
\delta_t A_x q_2^n + \delta_x A_t q_4^n + m A_x A_t q_1^n + \frac{1}{8} \lambda A_x G_1(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F_1(a, b) &= 0 \\
\delta_t A_x q_1^n + \delta_x A_t q_3^n - m A_x A_t q_2^n - \frac{1}{8} \lambda A_x G_2(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_2(c, d) &= 0 \\
\delta_t A_x q_4^n + \delta_x A_t q_2^n - m A_x A_t q_3^n - \frac{1}{8} \lambda A_x G_3(a, b, c, d, e, f, g, h) - \frac{1}{16} \lambda F(e, f) &= 0 \\
\delta_t A_x q_3^n + \delta_x A_t q_1^n - m A_x A_t q_4^n + \frac{1}{8} \lambda A_x G_4(a, b, c, d, e, f, g, h) + \frac{1}{16} \lambda F_g, h &= 0,
\end{aligned} \tag{5.17}$$

where

$$F_1 = \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right]$$

$$F_2 = \left[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3 \right]$$

$$F_3 = \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right]$$

$$G_1 = \left[(Be + Bf)^2 + (Bg + Bh)^2 - (Bc + Bd)^2 + (e + f)^2 + (g + h)^2 - (c + d)^2 \right]$$

$$G_2 = (c + d) \left[(Be + Bf)^2 + (Bg + Bh)^2 - (a + b)^2 + (e + f)^2 + (g + h)^2 - (Ba + Bb)^2 \right]$$

$$G_3 = (e + f) \left[(Bg + Bh)^2 - (a + b)^2 - (c + d)^2 + (g + h)^2 - (Ba + Bb)^2 - (Bc + Bd)^2 \right]$$

and

$$G_4 = (g + h) \left[(e + f)^2 - (a + b)^2 - (c + d)^2 + (Be + Bf)^2 - (Ba + Bb)^2 - (Bc + Bd)^2 \right]$$

5.5 Global Energy-Preserving AVF Method for Dirac Equation

In this section, we present the global energy preserving AVF scheme (2.27) for the Dirac equation (5.5). Applying global energy-preserving method (2.27) for the multisymplectic formulation (5.6) of the Dirac equation (5.2), we get

$$\begin{aligned}
\delta_t q_{2_j}^n - DA_t q_{4_j}^n - mA_t q_{1_j}^n - \frac{1}{2} \lambda F_1(a, b) + \frac{1}{6} \lambda G_1(a, b, c, d, e, f, g, h) &= 0 \\
-\delta_t q_{1_j}^n - DA_t q_{3_j}^n + mA_t q_{2_j}^n - \frac{1}{2} \lambda F_2(c, d) + \frac{1}{6} \lambda G_2(a, b, c, d, e, f, g, h) &= 0 \\
\delta_t q_{4_j}^n + DA_t q_{2_j}^n - mA_t q_{3_j}^n - \frac{1}{2} \lambda F_3(e, f) + \frac{1}{6} \lambda G_3(a, b, c, d, e, f, g, h) &= 0 \\
\delta_t q_{3_j}^n - DA_t q_{1_j}^n - mA_t q_{4_j}^n - \frac{1}{2} \lambda F_4(g, h) + \frac{1}{6} \lambda G_4(a, b, c, d, e, f, g, h) &= 0,
\end{aligned} \tag{5.18}$$

where

$$F_1 = \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right]$$

$$F_2 = \left[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3 \right]$$

$$F_3 = \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right]$$

$$G_1 = \left[-3ac^2 - ad^2 - c^2b - 3bd^2 - 2acd - 2cbd + 3ae^2 + af^2 + e^2b + 3bf^2 + 2aef + 2ebf + 3ag^2 + ah^2 + g^2b + 3bh^2 + 2agh + 2gbh \right]$$

$$G_2 = \left[-3da^2 - cb^2 - a^2c + 3db^2 + 2cab + 2adb + 3ce^2 + cf^2 + e^2d + 3df^2 + 2cef + 2edf + 3cg^2 + ch^2 + g^2d + 3dh^2 + 2cgh + 2gdh \right]$$

$$G_3 = \left[3ea^2 + eb^2 + a^2f + 3fb^2 + 2eab + 2afb + 3ec^2 + ed^2 + c^2f + 3fd^2 + 2ecd + 2cfd - 3eg^2 - eh^2 - g^2f - 3fh^2 - 2egh - 2ghf \right]$$

and

$$G_4 = \left[3ga^2 + gb^2 + a^2h + 3hb^2 + 2gab + 2ahb + 3gc^2 + gd^2 + c^2h + 3hd^2 + 2gcd + 2chd - 3ge^2 - gf^2 - e^2h - 3hf^2 + 2gef + 2ehf \right].$$

5.6 Global Energy-Preserving PAVF Methods for Dirac Equation

In this section, we present a new local energy-preserving algorithm for the nonlinear Dirac equation (5.5) based on the Sec. 3.3. We introduce our new global energy preserving method (3.25) for the multisymplectic formulation (5.6) of the Dirac equation (5.2) and obtain

$$\begin{aligned} \delta_t q_2^n + DA_t q_4^n + mA_t q_1^n + \lambda G_1(a, b, d, f, h) - \frac{1}{2} \lambda F_1(a, b) &= 0 \\ -\delta_t q_1^n - DA_t q_3^n + mA_t q_2^n + \lambda G_2(a, c, d, f, h) - \frac{1}{2} \lambda F_2(c, d) &= 0 \\ \delta_t q_4^n + DA_t q_2^n - mA_t q_3^n - \lambda G_3(a, c, e, f, h) - \frac{1}{2} \lambda F_3(e, f) &= 0 \\ -\delta_t q_3^n - DA_t q_1^n + mA_t q_4^n - \lambda G_4(a, c, e, g, h) - \frac{1}{2} \lambda F_4(g, h) &= 0, \end{aligned} \tag{5.19}$$

where

$$F_1 = \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right]$$

$$F_2 = \left[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3 \right]$$

$$F_3 = \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right]$$

$$G_1 = [f^2 + h^2 - d^2](a + b)$$

$$G_2 = [f^2 + h^2 - a^2](c + d)$$

$$G_3 = [h^2 - a^2 - c^2](e + f)$$

and

$$G_4 = [e^2 - a^2 - c^2](g + h).$$

To derive the second-order local energy preserving PAVF methods, including the PAVF composition (PAVF-C) and PAVF plus (PAVF-P) methods, we first present the adjoint of the PAVF (PAVF-ADJ) scheme (5.19) for the Dirac equation:

$$\begin{aligned} \delta_t q_2^n + DA_t q_4^n + mA_t q_1^n + \lambda G_1(a, b, c, e, g) - \frac{1}{2} \lambda F_1(a, b) &= 0 \\ -\delta_t q_1^n - DA_t q_3^n + mA_t q_2^n + \lambda G_2(a, c, d, e, g) - \frac{1}{2} \lambda F_3(c, d) &= 0 \\ \delta_t q_4^n + DA_t q_2^n - mA_t q_3^n - \lambda G_3(b, d, e, f, g) - \frac{1}{2} \lambda F_3(e, f) &= 0 \\ -\delta_t q_3^n - DA_t q_1^n + mA_t q_4^n - \lambda G_4(b, d, f, g, h) - \frac{1}{2} \lambda F_4(g, h) &= 0, \end{aligned} \quad (5.20)$$

where

$$F_1 = [(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3]$$

$$F_2 = [(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3]$$

$$F_3 = [(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3]$$

and

$$F_4 = [(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3]$$

$$G_1 = [e^2 + g^2 - c^2](a + b)$$

$$G_2 = [e^2 + g^2 - a^2](c + d)$$

$$G_3 = [g^2 - b^2 - d^2](e + f)$$

and

$$G_4 = [f^2 - b^2 - d^2](g + h).$$

With the adjoint scheme (5.20), we can directly write down the corresponding PAVF-C scheme (3.8). For this, we denote the GEP-PAVF scheme (5.19) by Φ_τ and the corresponding adjoint scheme (5.20) by Φ_τ^* and then write the PAVF-C scheme for Dirac equation (5.2) as

$$\Psi_\tau = \Phi_{\frac{\tau}{2}} \circ \Phi_{\frac{\tau}{2}}^* \quad (5.21)$$

Finally, the PAVF-P method (3.9) for the Dirac equation (5.2) can be written as

$$\begin{aligned}
\delta_t q_2^n + DA_t q_4^n + mA_t q_1^n + \frac{1}{2}\lambda G_1(a, b, c, d, e, f, g, h) - \frac{1}{2}\lambda F_1(a, b) &= 0 \\
-\delta_t q_1^n - DA_t q_3^n + mA_t q_2^n + \frac{1}{2}\lambda G_2(a, b, c, d, e, f, g, h) - \frac{1}{2}\lambda F_2(c, d) &= 0 \\
\delta_t q_4^n + DA_t q_2^n - mA_t q_3^n - \frac{1}{2}\lambda G_3(a, b, c, d, e, f, g, h) - \frac{1}{2}\lambda F_3(e, f) &= 0 \\
-\delta_t q_3^n - DA_t q_1^n + mA_t q_4^n - \frac{1}{2}\lambda G_4(a, b, c, d, e, f, g, h) - \frac{1}{2}\lambda F_4(g, h) &= 0,
\end{aligned} \tag{5.22}$$

where

$$\begin{aligned}
F_1 &= \left[(Ba + Bb)^3 + (Ba + Bb)^2(a + b) + (Ba + Bb)(a + b)^2 + (a + b)^3 \right] \\
F_2 &= \left[(Bc + Bd)^3 + (Bc + Bd)^2(c + d) + (Bc + Bd)(c + d)^2 + (c + d)^3 \right] \\
F_3 &= \left[(Be + Bf)^3 + (Be + Bf)^2(e + f) + (Be + Bf)(e + f)^2 + (e + f)^3 \right]
\end{aligned}$$

and

$$F_4 = \left[(Bg + Bh)^3 + (Bg + Bh)^2(g + h) + (Bg + Bh)(g + h)^2 + (g + h)^3 \right]$$

$$G_1 = \frac{1}{2}\lambda \left[f^2 + h^2 - d^2 \right] (a + b) + \frac{1}{2}\lambda \left[e^2 + g^2 - c^2 \right] (a + b)$$

$$G_2 = \frac{1}{2}\lambda \left[f^2 + h^2 - a^2 \right] (c + d) + \frac{1}{2}\lambda \left[e^2 + g^2 - b^2 \right] (c + d)$$

$$G_3 = \frac{1}{2}\lambda \left[h^2 - a^2 - c^2 \right] (e + f) - \frac{1}{2}\lambda \left[g^2 - b^2 - d^2 \right] (e + f)$$

and

$$G_4 = \frac{1}{2}\lambda \left[e^2 - a^2 - c^2 \right] (g + h) - \frac{1}{2}\lambda \left[f^2 - b^2 - d^2 \right] (g + h).$$

5.7 Numerical Results

In this section, we implement several local energy-preserving, global energy-preserving, and local momentum-preserving methods for the nonlinear Dirac equation (5.2). We note that the discrete systems are nonlinear. We used the Newton-Raphson's method to solve nonlinear system of equations.

To evaluate the local conservation laws of energy, we use the residual (3.12)

$$(R_E)_{j+1/2}^{n+1/2} = \delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2} \tag{5.23}$$

where

$$\begin{aligned}
E_{j+1/2}^n &= S(A_x z_j^n) + (\delta_x q_1)_j^n (A_x q_4)_j^n - (\delta_x q_2)_j^n (A_x q_3)_j^n \\
F_j^{n+1/2} &= -(\delta_t q_1)_j^n (A_x q_4)_j^n + (\delta_t q_2)_j^n (A_x q_3)_j^n.
\end{aligned} \tag{5.24}$$

Moreover, to evaluate the local conservation laws of momentum, we use the residual (3.13)

$$(R_M)_{j+1/2}^{n+1/2} = \delta_t I_{j+1/2}^n + \delta_x G_j^{n+1/2} \quad (5.25)$$

where

$$\begin{aligned} I_{j+1/2}^n &= -(\delta_x q_1)_j^n (A_x q_2)_j^n - (\delta_x q_3)_j^n (A_x q_4)_j^n \\ G_j^{n+1/2} &= S(A_t z_j^n) + (\delta_t q_1)_j^n (A_t q_2)_j^n + (\delta_t q_3)_j^n (A_t q_4)_j^n \end{aligned} \quad (5.26)$$

The corresponding discrete total energy is

$$\mathcal{E}^n = h \sum_{j=0}^{J-1} E_{j+1/2}^n \quad (5.27)$$

and the total momentum is

$$\mathcal{I}^n = h \sum_{j=0}^{J-1} I_{j+1/2}^n. \quad (5.28)$$

To justify the efficiency of the presents methods, we also report the relative errors of the total energy and total momentum defined by

$$\mathcal{E}_{\text{Relative error}} = \frac{\mathcal{E}^n - \mathcal{E}^0}{\mathcal{E}^0}, \quad \mathcal{I}_{\text{Relative error}} = \frac{\mathcal{I}^n - \mathcal{I}^0}{\mathcal{I}^0}. \quad (5.29)$$

The nonlinear Dirac equation (5.2) has the following theoretical solitary wave solution [45]

$$\begin{aligned} \Psi_1(x, t) &= |1 + a| \sqrt{2(1 - a)} \frac{\cosh((1 - a^2)x)}{1 + a \cosh(2\sqrt{1 - a^2}x)} e^{-iat} \\ \Psi_2(x, t) &= |1 + a| \sqrt{2(1 - a)} \frac{\sinh((1 - a^2)x)}{1 + a \cosh(2\sqrt{1 - a^2}x)} e^{-iat} \end{aligned} \quad (5.30)$$

The initial conditions (5.3) are taken form the exact solution (5.30)

$$\begin{aligned} \Psi_1(x, 0) &= |1 + a| \sqrt{2(1 - a)} \frac{\cosh((1 - a^2)x)}{1 + a \cosh(2\sqrt{1 - a^2}x)}, \\ \Psi_2(x, 0) &= |1 + a| \sqrt{2(1 - a)} \frac{\sinh((1 - a^2)x)}{1 + a \cosh(2\sqrt{1 - a^2}x)}. \end{aligned} \quad (5.31)$$

We take the constant $m = 1$ and $\lambda = \frac{1}{2}$ in the Dirac equation (5.2). All of the solutions are computed with the space and time step sizes $h = k = 0.1$. A periodic boundary condition is imposed in all simulations. We solve the problem in the spatial interval $-24 \leq x \leq 24$ for $0 \leq t \leq 30$.

Table 5.1: The L_∞ and L_2 errors and convergence orders in space of the LEP methods with fixed time step $\tau = 0.001$, $-35 \leq x \leq 35$, at $t = 1$

		h	1/4	1/8	1/12
AVF	L_∞	error	8.73e-4	2.14e-4	9.48e-5
		order	–	2.00	2.01
	L_2	error	1.22e-3	2.98e-4	1.32e-4
		order	–	2.00	2.01
PAVF	L_∞	error	8.57e-4	1.99e-4	7.95e-5
		order	–	2.1	2.3
	L_2	error	1.19e-3	2.83e-4	1.20e-4
		order	–	2.1	2.1
PAVF-C	L_∞	error	3.04e-4	7.5e-5	3.4e-5
		order	–	2.02	1.95
	L_2	error	4.14e-4	1.03e-4	4.65e-5
		order	–	2.01	1.96
PAVF-P	L_∞	error	8.73e-4	2.14e-4	9.48e-5
		order	–	2.00	2.01
	L_2	error	1.22e-3	2.98e-4	1.32e-4
		order	–	2.00	2.01

5.7.1 Numerical Experiment for Local Energy-Preserving Schemes

Our objective in this section is to demonstrate the effectiveness of the local energy preserving AVF (LEP-AVF) method (5.9), local energy preserving PAVF (LEP-PAVF) method (5.10), local energy preserving PAVF composition (LEP-PAVF-C) method (5.12), and local energy preserving PAVF plus (LEP-PAVF-P) method (5.13). As stated in (2.13) and (3.23), these methods preserve the global energy under periodic boundary conditions.

In all numerical simulation of local energy preserving algorithms, we represent the numerical solitary wave solutions $q_1(x, t)$, $q_2(x, t)$, $q_3(x, t)$, and $q_4(x, t)$, obtained by the LEP-PAVF scheme (5.10). The results of AVF method (5.9), the PAVF-C method (5.12) and the PAVF-P method (5.13) are very similar. For this reason they are not shown.

Accuracy test: First, the correctness of the numerical schemes are examined. The spatial domain has been chosen large enough that solitary wave propagation do not effect the propagation of wave. Table 5.1 gives some errors of the difference solutions with different step sizes which verify the second-order convergence and good stability of the numerical methods.

Fig. 5.1 represents the numerical solution obtained by the LEP-PAVF scheme (5.10). From the figure, we can see that the time interval $[0, 30]$ contains almost 4 periods. The LEP-PAVF scheme shows periodic behavior almost perfectly. Fig. 5.2 represents the solitary waves $\Psi_1(x, t) = \sqrt{q_1(x, t)^2 + q_2(x, t)^2}$ and $\Psi_2(x, t) = \sqrt{q_3(x, t)^2 + q_4(x, t)^2}$ obtained by the LEP-PAVF scheme (5.10). From the figure, we see that the LEP-PAVF scheme (5.10) well simulates the solitary waves. The residuals (5.23) in the local energy conservation laws of the schemes PAVF method (5.10), PAVF-C method (5.12), the PAVF-P (5.13) method and the AVF method (5.9) are depicted in Fig. 5.3, respectively. We can see that four algorithms preserve the local energy within the roundoff errors of the computer. Fig. 5.4 represents the local momentum conservation of the four algorithms. The relative errors (5.29) in the global conservation of energy and momentum are plotted in Fig. 5.5 and Fig. 5.6, respectively.

Remark 5.7.1 *From the figures Fig. 5.3 and Fig. 5.5, we can see that the local energy and global energy are conserved up to the accuracy of the LEP methods, supporting Theorem 2.2.1, Corollary 2.2.2, Theorem 3.2.2 and the Corollary 2.2.2.*

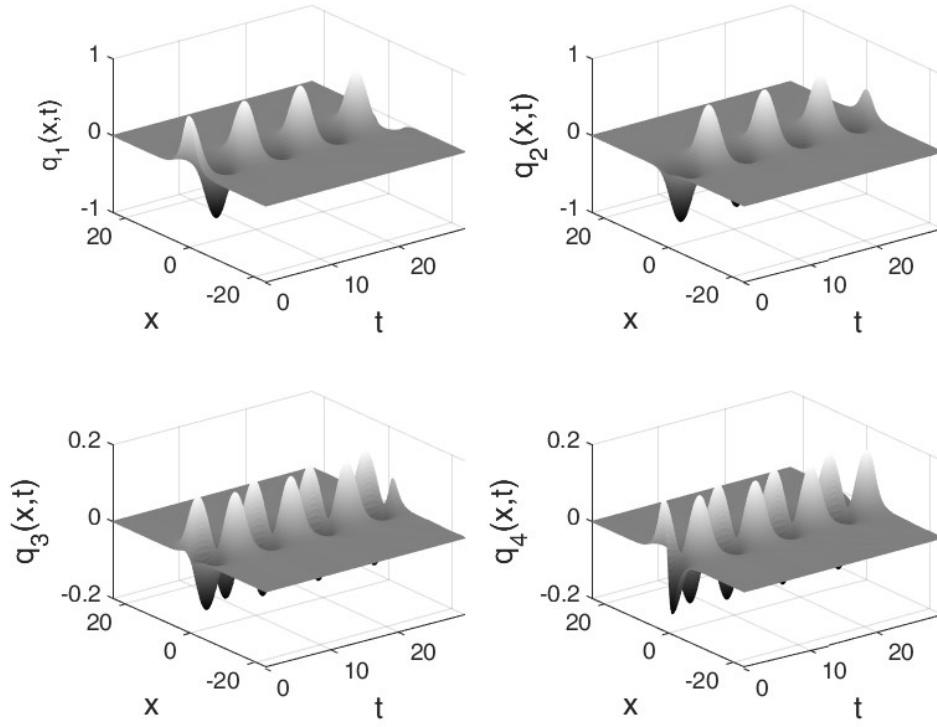


Figure 5.1: LEP scheme (5.10) for Dirac Equation (5.2). The four numerical solitary wave solutions obtained by using LEP-PAVF method (5.10)

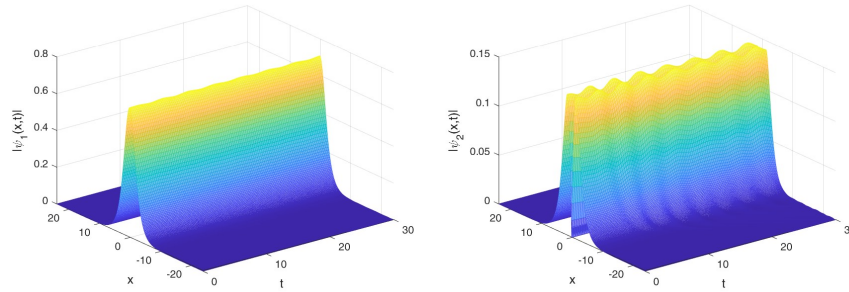


Figure 5.2: The solitary wave solutions $|\Psi_1(x,t)|$ and $|\Psi_2(x,t)|$ of the Dirac equation (5.2) obtained by using LEP-PAVF method (5.10)

Figure 5.7 shows the numerical results for the Dirac equation by the four numerical schemes. From the figure, we can see that both the local and global energies and global momentum are preserved exactly since their errors are always in the scale of the round-off error of the machine throughout computations. From the figure, we can say that there is no visible difference in absolute maximal error in local energy conservation. However, we can say the LEP-PAVF-P scheme (5.13) preserves the

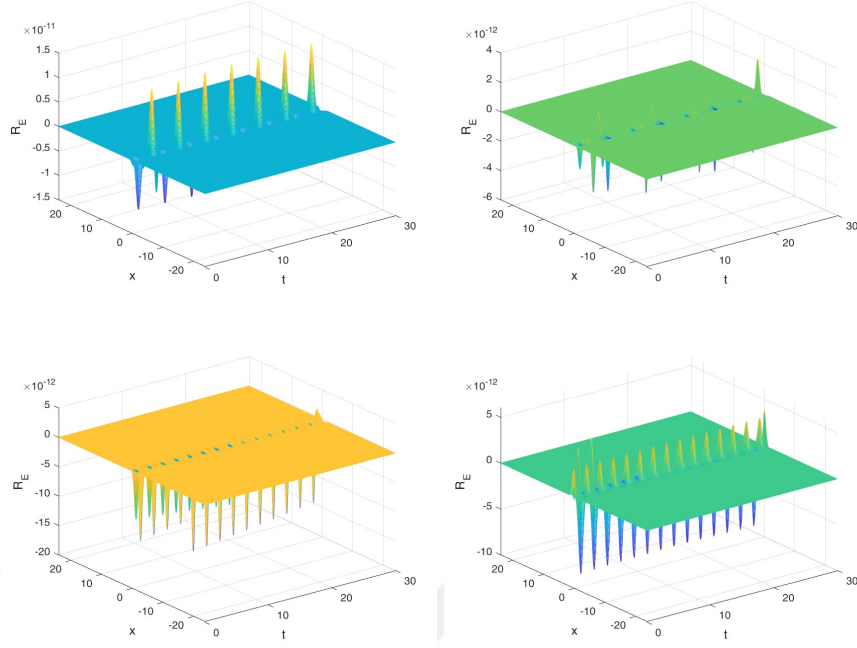


Figure 5.3: Residuals (5.23) in local energy conservation obtained by LEP schemes. The left-top one is PAVF method (5.10), the right-top is the PAVF-C method (5.12), and the left-bottom is the PAVF-P (5.13) method and right-bottom is the AVF method (5.9), respectively.

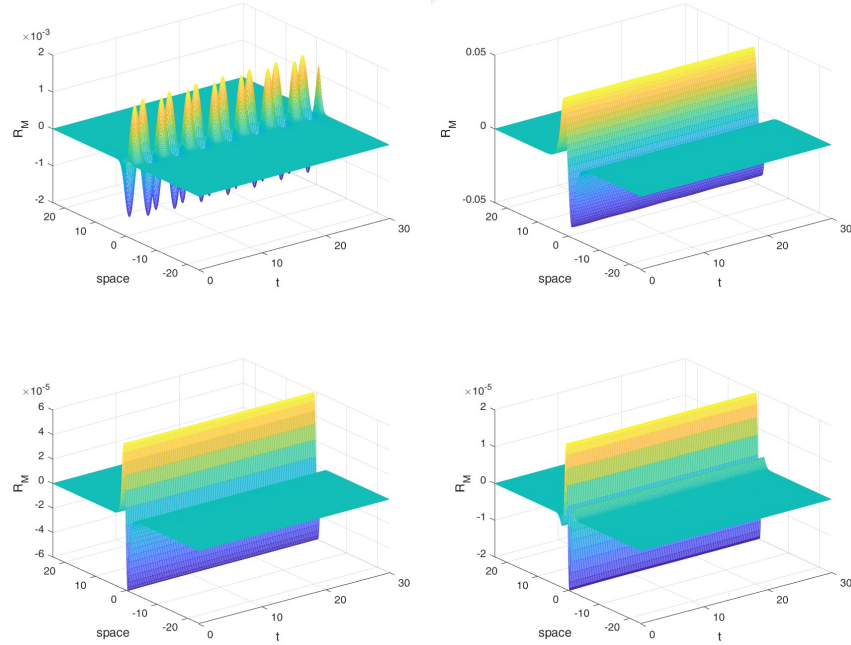


Figure 5.4: Residuals (5.25) in local momentum conservation obtained by LEP schemes. The left-top one is PAVF method (5.10), the right-top is the PAVF-C method (5.12), and the left-bottom is the PAVF-P method (5.13) and right-bottom is the AVF method (5.9), respectively.

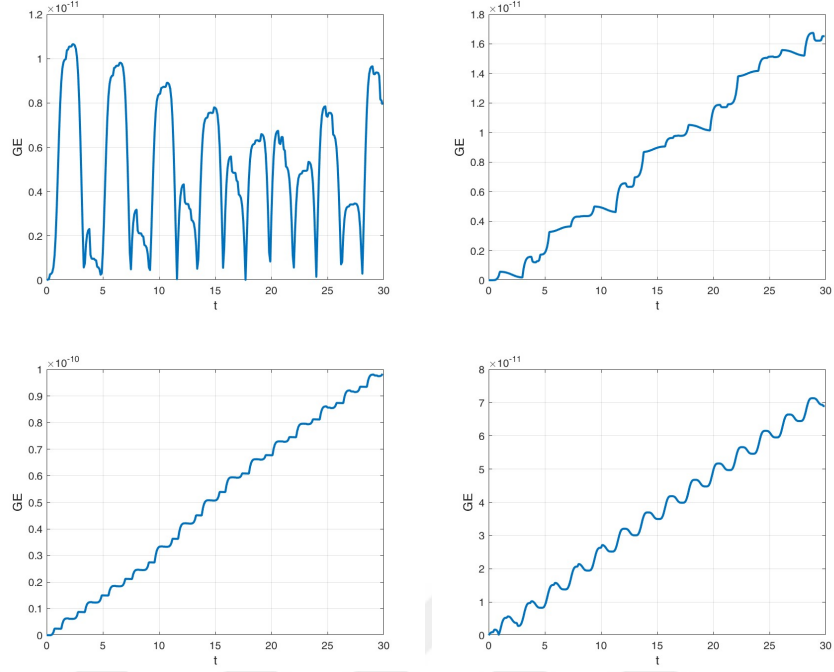


Figure 5.5: Relative errors in total energy conservation (5.27) obtained by LEP schemes. The left-top one is PAVF method (5.10), the right-top is the PAVF-C method (5.12), and the left-bottom is the PAVF-P (5.13) method and right-bottom is the AVF method (5.9), respectively.

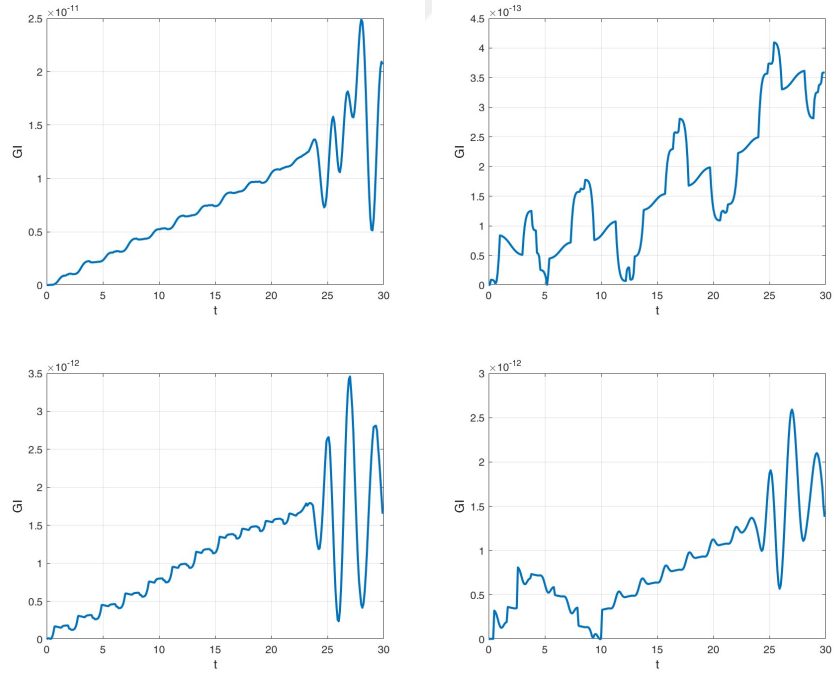


Figure 5.6: Relative errors in total momentum conservation (5.28) obtained by LEP schemes. The left-top one is PAVF method (5.10), the right-top is the PAVF-C method (5.12), and the left-bottom is the PAVF-P method (5.13) and right-bottom is the AVF method (5.9), respectively.

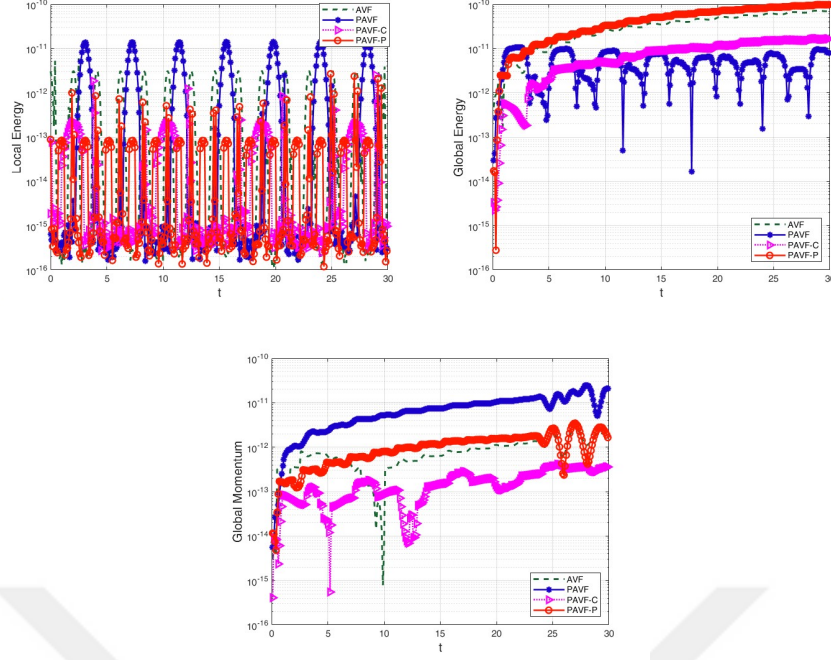


Figure 5.7: Numerical solution of the Dirac equation obtained by the LEP-PAVF scheme (5.10), LEP-PAVF-C scheme (5.12), LEP-PAVF-P scheme (5.13) and LEP-AVF scheme (5.9). The left-top is maximal absolute error in local energy conservation (5.23), the right-top is relative errors in conservation of global energy $\mathcal{E}^n$ in (5.29), bottom is errors in conservation of global momentum $\mathcal{I}^n$ in (5.29),

global energy better than the other schemes. On the other hand, global momentum is preserved better by the LEP-PAVF-C scheme (5.12).

5.7.2 Numerical Experiment for Local Momentum-Preserving Schemes

Our object in this section is to demonstrate the effectiveness of the local momentum preserving AVF (LMP-AVF) method (5.14), local momentum preserving PAVF (LMP-PAVF) method (5.15), local momentum preserving PAVF adjoint (LMP-PAVF-ADJ) method (5.16), and local momentum preserving PAVF plus (LMP-PAVF-P) method (5.17). As stated in (2.22) and (3.47), these methods preserves the global momentum under periodic boundary conditions.

In all numerical simulation of local momentum preserving algorithms, we represent the numerical solitary wave solutions $q_1(x, t)$, $q_2(x, t)$, $q_3(x, t)$, and $q_4(x, t)$, obtained by the LMP-PAVF scheme (5.15). The results of local momentum preserving AVF method (5.14), the PAVF-ADJ method (5.16) and the PAVF-P method (5.17) are sim-

ilar. For this reason they are not shown.

Table 5.2 gives the errors of the difference solution which verifies the second-order convergence except the PAVF method which is only first-order. The table also shows good stability of the numerical solutions. Fig. 5.8 represents the numerical solution obtained by the LMP-PAVF scheme (5.15). From the figure, we can see that the time interval $[0, 30]$ contains almost 4 periods. The LMP-PAVF scheme show periodic behavior almost perfectly. Fig. 5.9 represents the solitary waves $\Psi_1(x, t) = \sqrt{q_1(x, t)^2 + q_2(x, t)^2}$ and $\Psi_2(x, t) = \sqrt{q_3(x, t)^2 + q_4(x, t)^2}$ obtained by the LMP-PAVF scheme (5.15). From the figure, we see that the LMP-PAVF scheme (5.15) well simulates the solitary waves. The residuals (5.25) in the local momentum conservation laws of the schemes PAVF method (5.15), PAVF-ADJ method (5.16), and the PAVF-P (5.17) method are depicted in Fig. 5.10, respectively. We can see that the algorithms preserve the local momentum within the roundoff errors of the computer. The relative errors (5.29) in the total conservation of momentum are plotted in Fig. 5.11.

Table 5.2: The L_∞ and L_2 errors and convergence orders in space of the LMP methods with fixed time step $\tau = 0.001$, $-35 \leq x \leq 35$, at $t = 1$

		h	1/4	1/8	1/12
AVF	L_∞	error	9.82e-4	2.39e-4	1.06e-4
		order	–	2.00	2.00
	L_2	error	1.31e-3	3.2e-4	1.41e-4
		order	–	2.00	2.00
PAVF	L_∞	error	7.43e-3	3.52e-3	2.3e-3
		order	–	1.07	1.04
	L_2	error	1.13e-2	5.59e-3	3.7e-3
		order	–	1.01	1.01
PAVF-P	L_∞	error	1.03e-3	2.52e-4	1.12e-4
		order	–	2.03	1.99
	L_2	error	1.44e-3	3.52e-4	1.55e-4
		order	–	2.03	2.02

Remark 5.7.2 From the Fig. 5.10 and Fig. 5.11, we can see that the local momentum and global momentum are conserved up to the accuracy of the LMP methods, supporting Theorem 2.3.1, Corollary 2.3.2, Theorem 3.4.1 and the Corollary 3.4.2.

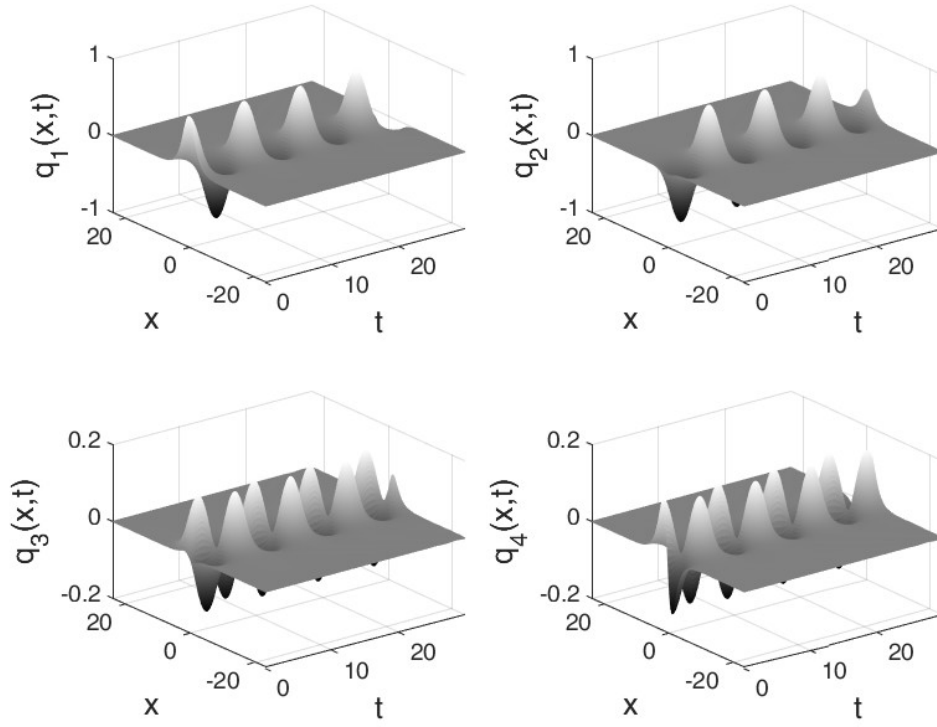


Figure 5.8: LMP scheme for Dirac Equation. The four numerical solitary wave solutions obtained by using LMP-PAVF method (5.15)

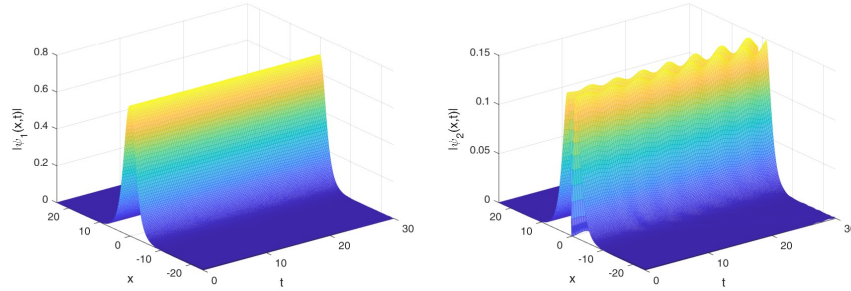


Figure 5.9: The solitary wave solutions $|\psi_1(x, t)|$ and $|\psi_2(x, t)|$ obtained by using LMP-PAVF method (5.15)

First, we show the accuracy and the correctness of the schemes by testing the convergence order in space. Table 5.3 gives some errors of the difference schemes. From the table, we can see that convergence order in space is 2 which is the order of the second-order central difference approximation of second derivative. We found that as the spatial step size decrease the convergence order is becoming more and more clear.

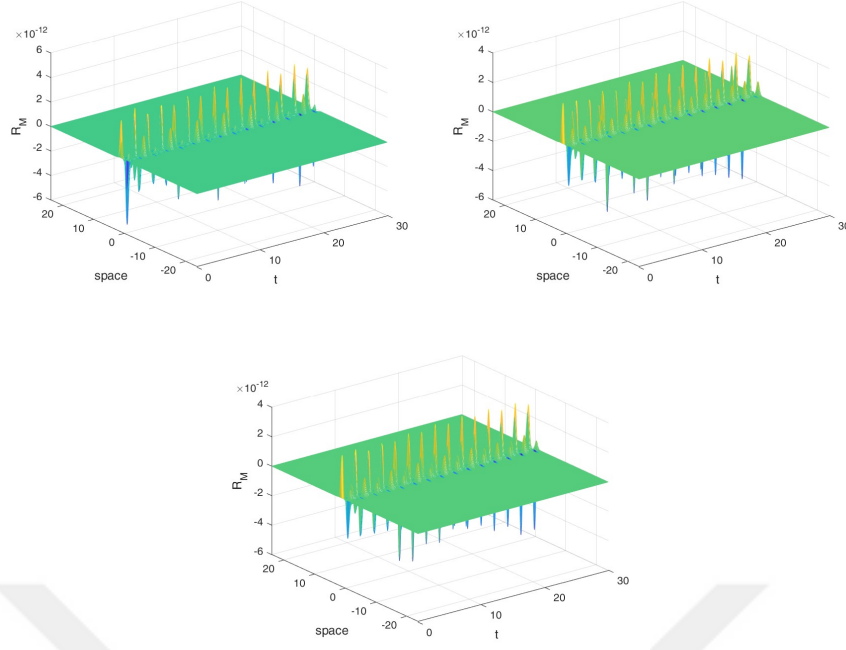


Figure 5.10: Residuals in local momentum conservation obtained by LMP schemes. The left-top one is PAVF method (5.15), the right-top is the PAVF-ADJ method, the left-bottom is the PAVF-P method, respectively.

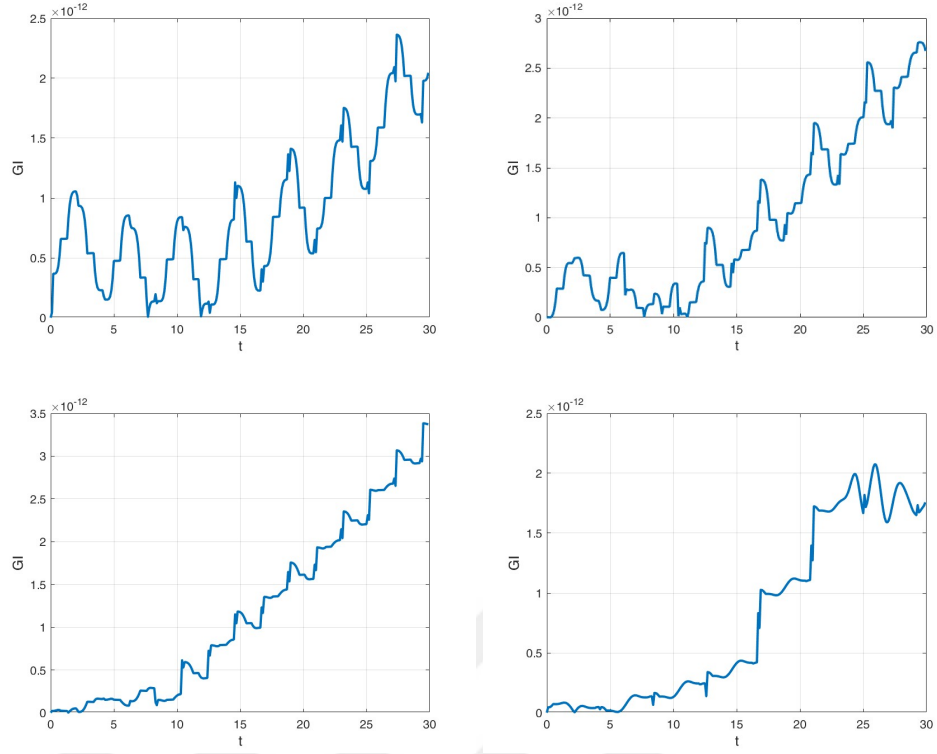


Figure 5.11: LMP scheme for Dirac Equation. Relative Errors in Global Momentum Conservation obtained by LMP schemes. The left-top one is PAVF method (5.15), the right-top is the PAVF-ADJ method, the left-bottom is the PAVF-P method, the right-bottom is the AVF method (5.14), respectively.

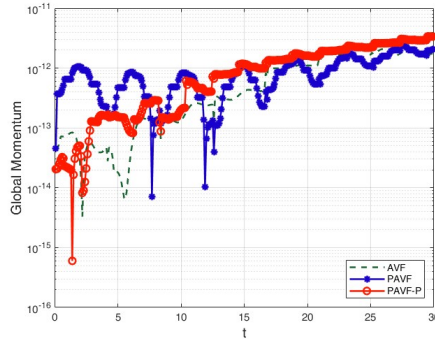


Figure 5.12: LMP scheme for Dirac Equation. Relative errors in conservation of global energy $\mathcal{I}^n$ in (5.29)

Figure 5.12 represents the relative errors in global conservation of momentum. From the figure we can see that LMP-PAVF method (5.15) preserves the discrete global momentum better than the LMP-AVF method and the LMP-PAVF-P method in long time integration.

5.7.3 Numerical Experiment for Global Energy-Preserving Schemes

Our objective in this section is to demonstrate the effectiveness of the global energy preserving AVF (GEP-AVF) method (5.18), global energy preserving PAVF (GEP-PAVF) method (5.19), global energy preserving PAVF composition (GEP-PAVF-C) method (5.21), and global energy preserving PAVF plus (GEP-PAVF-P) method (5.22). As stated in (2.13) and (3.23), these methods preserve the global energy under periodic boundary conditions.

In all numerical simulation of global energy preserving algorithm, we represent the numerical solitary wave solutions $q_1(x, t)$, $q_2(x, t)$, $q_3(x, t)$, and $q_4(x, t)$, obtained by the GEP-PAVF scheme (5.19). The results of AVF method (5.18), the PAVF-C method (5.21) and the PAVF-P method (5.22) are similar. For this reason they are not shown.

First we examine the accuracy of the GEP methods. We set $\tau = 0.001$ so that the error that comes from the temporal discretization is negligible. The results are listed in Table 5.3. The table indicates that the order of convergence is almost equal to 2 in the spatial direction. The table shows the correctness of our scheme.

Fig. 5.13 represents the numerical solution obtained by the GEP-PAVF scheme (5.19). From the figure, we can see that the time interval $[0, 30]$ contains almost 4 periods. The GEP-PAVF scheme show periodic behavior almost perfectly. Fig. 5.14 represents the solitary waves $\Psi_1(x, t) = \sqrt{q_1(x, t)^2 + q_2(x, t)^2}$ and $\Psi_2(x, t) = \sqrt{q_3(x, t)^2 + q_4(x, t)^2}$ obtained by the GEP-PAVF scheme (5.19). From the figure, we see that the GEP-PAVF scheme (5.19) well simulates the solitary waves. The relative errors (5.29) in the total conservation of energy are plotted in Fig. 5.15. From the figure, we can see that total energy is conserved exactly by all methods.

Figure 5.16 represent the relative errors in conservation of global energy $\mathcal{E}^n$ momentum $\mathcal{I}^n$ in (5.29) obtained by the GEP schemes. From the figure, we can see that while global energy is well preserved by GEP-AVF method and GEP-PAVF-P method, the PAVF-C method has a significant advantage over other methods in preserving momentum.

According to the results of the LEP schemes, LMP schemes and GEP schemes, it

is not possible to say that there is a prominent method for the numerical solution of the nonlinear Dirac equation. Among the LEP schemes, the composition method preserves the local energy better than the other methods. PAVF method preserves the global energy and global momentum better than the other methods. Among the LMP schemes, PAVF preserves the global momentum better than the other methods. Among the GEP methods PAVF and PAVF-P methods preserve the global energy better than the other methods.

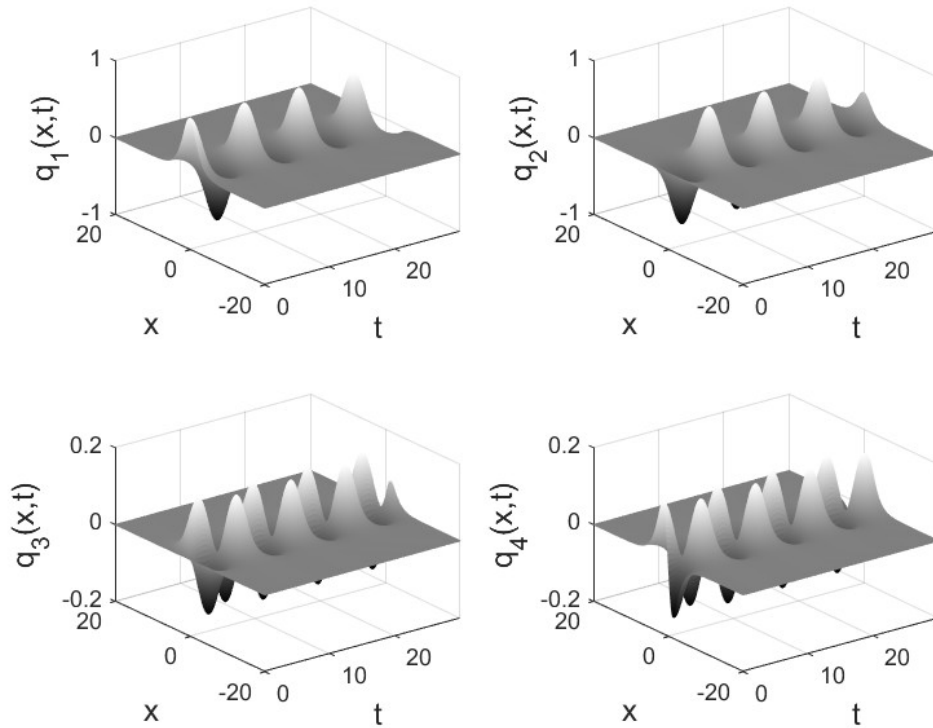


Figure 5.13: GEP scheme (5.19) for Dirac Equation (5.2). The four numerical solitary wave solutions obtained by using GEP-PAVF method (5.19)

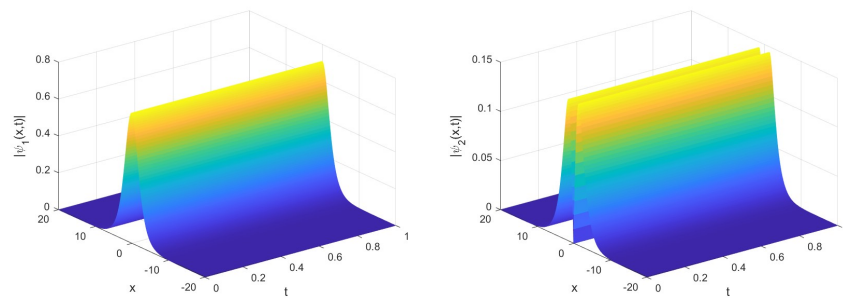


Figure 5.14: The solitary wave solutions $|\Psi_1(x, t)|$ and $|\Psi_2(x, t)|$ of the Dirac equation (5.2) obtained by using GEP-PAVF method (5.19)

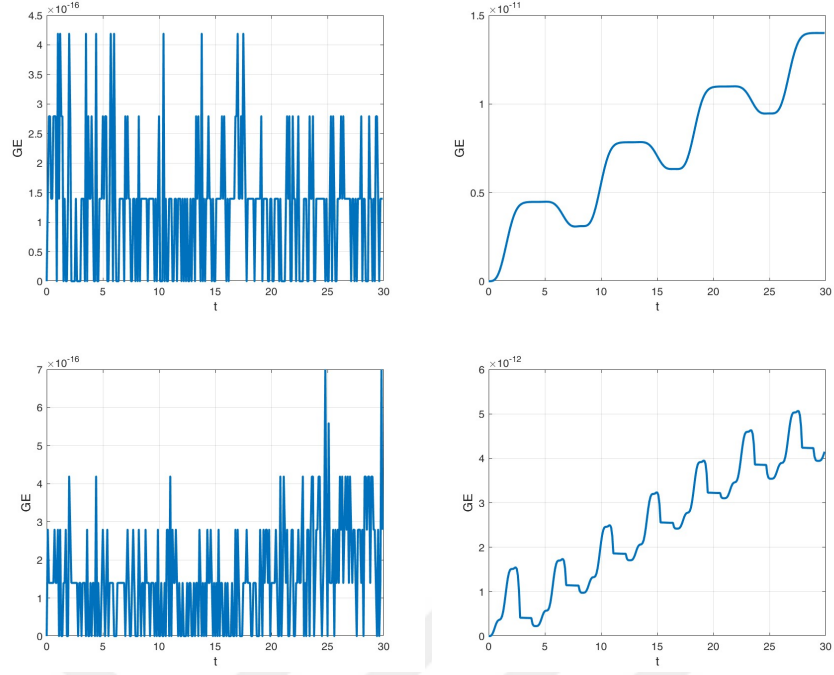


Figure 5.15: GEP scheme for Dirac Equation. Relative Errors in Global Energy Conservation obtained by GEP schemes. The left-top one is PAVF method (5.19), the right-top is the PAVF-C method, and the left-bottom is the PAVF-P (5.22) method and right-bottom is the AVF method (5.18), respectively.

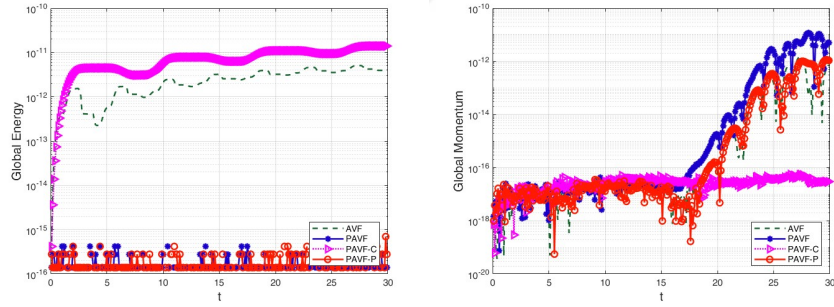


Figure 5.16: Numerical solution of the Dirac equation obtained by the GEP-PAVF scheme (5.19), GEP-PAVF-C scheme (5.21), GEP-PAVF-P scheme (5.22) and GEP-AVF scheme (5.18). The relative errors in conservation of global energy $\mathcal{E}^n$ in (5.29) (left), and relative errors in conservation of global momentum $\mathcal{I}^n$ in (5.29) (right)

Table 5.3: The L_∞ and L_2 errors and convergence orders in space of the GEP methods with fixed time step $\tau = 0.001$, $-35 \leq x \leq 35$, at $t = 1$

		h	1/4	1/8	1/12
AVF	L_∞	error	1.98e-3	5.15e-4	2.31e-4
		order	–	1.94	1.98
	L_2	error	3.23e-3	8.24e-4	3.68e-4
		order	–	1.97	1.99
PAVF	L_∞	error	1.98e-3	5.27e-4	2.42e-4
		order	–	1.91	1.92
	L_2	error	3.23e-3	8.29e-4	3.73e-4
		order	–	1.96	1.97
PAVF-C	L_∞	error	5.68e-4	1.50e-4	6.81e-5
		order	–	1.92	1.95
	L_2	error	1e-3	2.58e-4	1.15e-4
		order	–	1.95	1.99
PAVF-P	L_∞	error	1.98e-3	5.14e-4	2.31e-4
		order	–	1.95	1.97
	L_2	error	3.23e-3	8.24e-4	3.68e-4
		order	–	1.97	1.99

CHAPTER 6

NEW CONSERVATIVE PARTITIONED AVERAGE VECTOR FIELDS SCHEMES FOR COMPLEX MODIFIED KORTEWEG-de VRIES EQUATIONS

This chapter is devoted to proposing several new local and global structure-preserving algorithms for the numerical integration of the complex modified Korteweg–de Vries (CMKdV) equation

$$\frac{\partial \psi}{\partial t} + \frac{\partial^3 \psi}{\partial x^3} + \alpha \frac{\partial(|\psi|^2 \psi)}{\partial x} = 0, \quad x_L \leq x \leq x_R, \quad 0 < t \leq T \quad (6.1)$$

with the initial condition

$$\psi(x, 0) = \psi_0(x), \quad x_L \leq x \leq x_R, \quad (6.2)$$

and periodic boundary condition

$$\psi(x_L, t) = \psi(x_R, t), \quad 0 < t \leq T, \quad (6.3)$$

where $\psi(x, t)$ is a complex-valued function of $\{x, t\}$ and α is a real constant. Introducing $\psi(x, t) = u(x, t) + iv(x, t)$, we can decompose the equation (6.1) into its real and imaginary parts

$$\begin{aligned} u_t + u_{xxx} + \alpha[(u^2 + v^2)u]_x &= 0 \\ v_t + v_{xxx} + \alpha[(u^2 + v^2)v]_x &= 0. \end{aligned} \quad (6.4)$$

The coupled nonlinear system of equations (6.4) describe the interaction of two orthogonally polarized transverse waves [67], where $u(x, t)$ and $v(x, t)$ represent y-polarized and z-polarized transverse waves, respectively, propagating in the x -direction in an xyz coordinate system [56]. The equation (6.1) is one of the well-known and completely

integrable equations in soliton theory, which possesses all the basic characters of integrable models. From a physical point of view, the above equation has been derived for, e.g., fluid dynamics, plasma physics, ultra-short pulses in nonlinear optics, nonlinear transmission lines, and so on [1].

The numerical solution of the CMKdV equation (6.1) has been the subject of many studies in recent years. Muslu et al. [56] and Taha [67] solved this equation using a split-step Fourier method. Ismail [48] used a Petrov–Galerkin method with a cubic B-splines as test functions and linear B-splines as trial functions. These methods solves the equation numerically but ignore the structure-preservation of the equation. Aydin et.al [7] solved the equation using two multisymplectic integrators namely an eight-point Preissman box scheme and a narrow box scheme for numerical integration of the equation. This method preserves the multisymplectic structure of the equation but ignore the local structure preservation such as local energy preservation and local momentum preservation of the equation. In this thesis, we propose a novel local structure preserving algorithm based on the PAVF method of the multisymplectic formulation of the equation.

To construct the multisymplectic formulation of the CMKdV equation (6.4), we introduce new variables $u_x = a$, $v_x = b$, $u_t = -p_x$, $v_t = -q_x$, $c_x = -\frac{1}{2}u$ and $f_x = -\frac{1}{2}v$. Using these variables, we can write the equation (6.4) as a first-order system of equations

$$\begin{aligned}
 -c_t + a_x &= \frac{1}{2}p - \alpha(u^2 + v^2)u \\
 -f_t + b_x &= \frac{1}{2}q - \alpha(u^2 + v^2)v \\
 u_t + p_x &= 0 \\
 v_t + q_x &= 0 \\
 -u_x &= -a \\
 -v_x &= -b \\
 -c_x &= \frac{1}{2}u \\
 -f_x &= \frac{1}{2}v.
 \end{aligned} \tag{6.5}$$

The system (6.5) can be written as a multisymplectic PDE of form (1.72)

$$Lz_t + Kz_x = \nabla_z S(z) \tag{6.6}$$

where

$$L = \begin{pmatrix} 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}, K = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \end{pmatrix},$$

$$z = \left(u, v, c, f, a, b, p, q \right)^T \text{ and } S(z) = \frac{1}{2}(up + vq) - \frac{1}{2}(a^2 + b^2) - \frac{\alpha}{4}(u^2 + v^2)^2.$$

The CMKDV equation in multi-symplectic form (6.6) satisfies the multi-symplectic conservation law (1.73) together with a local energy conservation law (LECL) $E_t + F_x = 0$ (1.74) with

$$E(z) = \frac{1}{2} \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial x} \right)^2 \right] - \frac{\alpha}{4} [u^2 + v^2]^2, \quad F(z) = -\frac{\partial u}{\partial t} a - \frac{\partial v}{\partial t} b - \frac{\partial c}{\partial t} p - \frac{\partial f}{\partial t} q \quad (6.7)$$

and local momentum conservation laws $I_t + G_x = 0$ (1.75) with

$$I(z) = \frac{\partial u}{\partial x} c + \frac{\partial v}{\partial x} f, \quad G(z) = S(z) - \frac{\partial u}{\partial t} c - \frac{\partial v}{\partial t} f \quad (6.8)$$

After the multi-symplectic formulation (6.6), one can construct a multisymplectic scheme for the numerical integration of the CMKDV equation (6.1). One of the most popular multi-symplectic integrator is the Preissmann scheme [11], which corresponds to the midpoint discretization in space and time variables. The eight-point Preissman box scheme and a narrow box scheme are considered for numerical integration of the CMKDV equation (6.1) in [7]. However, these scheme preserves the discrete multi-symplectic structure but ignore the local conservations. In the following sections, we propose new local structure-preserving algorithms for the numerical solution of the CMKDV equation (6.1) which are never studied in the literature before.

6.1 Local Energy-Preserving AVF Method for CMKDV Equation

In this section, we present the second-order local energy-preserving AVF scheme (2.1) for the CMKDV (6.1). Applying local energy preserving method (2.1) for the multi-

symplectic formulation (6.6) of the CMKDV equation (6.1) we obtain

$$\begin{aligned}
-(\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2}(A_t A_x p_j^n) - \frac{\alpha}{4} \left[(A_x u_j^{n+1})^3 (A_x u_j^{n+1})^2 (A_x u_j^n) + (A_x u_j^{n+1})(A_x u_j^n)^2 + (A_x u_j^n)^3 \right] \\
&\quad - \frac{\alpha}{12} [3(A_x u_j^{n+1})(A_x v_j^{n+1})^2 + (A_x u_j^{n+1})(A_x v_j^n)^2 + (A_x v_j^{n+1})^2 (A_x u_j^n) \\
&\quad + 3(A_x u_j^n)(A_x v_j^n)^2 + 2(A_x u_j^{n+1})(A_x v_j^{n+1})(A_x v_j^n) + 2(A_x v_j^{n+1})(A_x u_j^n)(A_x v_j^n)] \\
-(\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2}(A_t A_x q_j^n) - \frac{\alpha}{4} \left[(A_x v_j^{n+1})^3 (A_x v_j^{n+1})^2 (A_x v_j^n) + (A_x v_j^{n+1})(A_x v_j^n)^2 + (A_x v_j^n)^3 \right] \\
&\quad - \frac{\alpha}{12} [3(A_x v_j^{n+1})(A_x u_j^{n+1})^2 + (A_x v_j^{n+1})(A_x u_j^n)^2 + (A_x u_j^{n+1})^2 (A_x v_j^n) \\
&\quad + 3(A_x v_j^n)(A_x u_j^n)^2 + 2(A_x v_j^{n+1})(A_x u_j^{n+1})(A_x u_j^n) + 2(A_x u_j^{n+1})(A_x v_j^n)(A_x u_j^n)] \\
(\delta_t A_x u_j^n) + (\delta_x A_t p_j^n) &= 0 \\
(\delta_t A_x v_j^n) + (\delta_x A_t q_j^n) &= 0 \\
-(\delta_x A_t a_j^n) &= -(A_t A_x a_j^n) \\
-(\delta_x A_t b_j^n) &= -(A_t A_x b_j^n) \\
-(\delta_x A_t c_j^n) &= \frac{1}{2}(A_t A_x u_j^n) \\
-(\delta_x A_t f_j^n) &= \frac{1}{2}(A_t A_x v_j^n)
\end{aligned} \tag{6.9}$$

Eliminating the auxiliary variables a, b, c, f, p, q , we obtain

$$\begin{aligned}
(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) + \delta_x A_t A_x F(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^{n+1}, A_x v_j^n) &= 0 \\
(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) + \delta_x A_t A_x F(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^{n+1}, A_x u_j^n) &= 0,
\end{aligned} \tag{6.10}$$

a three time level scheme that requires two initial conditions. Since the last four equations of (6.9) contain no time derivative, we can omit the average vector A_t in the corresponding equations. Applying the same procedure for (6.9), we get

$$\begin{aligned}
(\delta_t A_x^3 u_j^n) + (\delta_x^3 A_t u_j^n) + \delta_x A_x F(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^{n+1}, A_x v_j^n) &= 0 \\
(\delta_t A_x^3 v_j^n) + (\delta_x^3 A_t v_j^n) + \delta_x A_x F(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^{n+1}, A_x u_j^n) &= 0,
\end{aligned} \tag{6.11}$$

which is a two-time level scheme for the CMKDV equation (6.1).

6.2 Local Energy-Preserving PAVF Methods for CMKDV Equation

In this section, we present a new local energy preserving algorithm for the CMKDV equation (6.1) based on Sec. 3.2. We introduce our new local energy preserving method (3.11) for the multisymplectic formulation (6.6) of the CMKDV equation (6.1)

and obtain

$$\begin{aligned}
-(\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2}(A_x p_j^n) - f(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^n, A_x A_t u_j^n) \\
-(\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2}(A_x q_j^n) - f(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^{n+1}, A_x A_t v_j^n) \\
(\delta_t A_x u_j^n) + (\delta_x A_t p_j^n) &= 0 \\
(\delta_t A_x v_j^n) + (\delta_x A_t q_j^n) &= 0 \\
-(\delta_x A_t u_j^n) &= -(A_t A_x a_j^n) \\
-(\delta_x A_t v_j^n) &= -(A_t A_x b_j^n) \\
-(\delta_x A_t c_j^n) &= \frac{1}{2}(A_x u_j^{n+1}) \\
-(\delta_x A_t f_j^n) &= \frac{1}{2}(A_x v_j^{n+1})
\end{aligned} \tag{6.12}$$

where $f(\xi, \beta, \eta, \phi) = -\frac{\alpha}{4}(\xi^3 + \xi^2\beta + \xi\beta^2 + \beta^3) - \alpha\eta^2\phi$. Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned}
(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) + \delta_x A_x A_t f(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^n, A_x A_t u_j^n) &= 0 \\
(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) + \delta_x A_x A_t f(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^{n+1}, A_x A_t v_j^n) &= 0
\end{aligned} \tag{6.13}$$

The adjoint-PAVF scheme for CMKDV system (6.5) is given by

$$\begin{aligned}
-(\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2}(A_x p_j^{n+1}) - f(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^{n+1}, A_x A_t u_j^n) \\
-(\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2}(A_x q_j^{n+1}) - f(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^{n+1}, A_x A_t v_j^n) \\
(\delta_t A_x u_j^n) + (\delta_x A_t p_j^{n+1}) &= 0 \\
(\delta_t A_x v) + (\delta_x A_t q_j^{n+1}) &= 0 \\
-(\delta_x A_t u_j^n) &= -(A_t A_x a_j^n) \\
-(\delta_x A_t v_j^n) &= -(A_t A_x b_j^n) \\
-(\delta_x A_t c_j^n) &= \frac{1}{2}(A_x u_j^n) \\
-(\delta_x A_t f_j^n) &= \frac{1}{2}(A_x v_j^n)
\end{aligned} \tag{6.14}$$

where $f(\xi, \beta, \eta, \phi) = -\frac{\alpha}{4}(\xi^3 + \xi^2\beta + \xi\beta^2 + \beta^3) - \alpha\eta^2\phi$. Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned}
(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) + \delta_x A_x A_t f(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^{n+1}, A_x A_t u_j^n) &= 0 \\
(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) + \delta_x A_x A_t f(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^n, A_x A_t v_j^n) &= 0.
\end{aligned} \tag{6.15}$$

With the adjoint scheme (6.15), we can directly write down the corresponding PAVF-C scheme (3.8). For this, we denote the LEP-PAVF scheme (6.13) by Φ_τ and the

corresponding adjoint scheme (6.15) by Φ_τ^* and then write the PAVF-C scheme for CMKDV equation (6.1) as

$$\Psi_{E,\tau} = \Phi_{E,\frac{\tau}{2}} \circ \Phi_{E,\frac{\tau}{2}}^* \quad (6.16)$$

The PAVF-P scheme for the CMKDV system (6.5) is

$$\begin{aligned} -(\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2}(A_x A_t p_j^n) - f(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^n, A_x v_j^{n+1}, A_x A_t u_j^n) \\ -(\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2}(A_x A_t q_j^n) - f(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^n, A_x u_j^{n+1}, A_x A_t v_j^n) \\ (\delta_t A_x A_t u_j^n) + (\delta_x A_t^2 p_j^n) &= 0 \\ (\delta_t A_x A_t v_j^n) + (\delta_x A_t^2 q_j^n) &= 0 \\ -(\delta_x A_t u_j^n) &= -(A_t A_x a_j^n) \\ -(\delta_x A_t v_j^n) &= -(A_t A_x b_j^n) \\ -(\delta_x A_t c_j^n) &= \frac{1}{2}(A_x A_t u_j^n) \\ -(\delta_x A_t f_j^n) &= \frac{1}{2}(A_x A_t v_j^n) \end{aligned} \quad (6.17)$$

where $f(\xi, \beta, \eta, \phi, \zeta) = -\frac{\alpha}{4}(\xi^3 + \xi^2\beta + \xi\beta^2 + \beta^3) - \frac{1}{2}\alpha\zeta(\eta^2 + \phi^2)$. Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned} (\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) + \delta_x A_x A_t f(A_x u_j^{n+1}, A_x u_j^n, A_x v_j^n, A_x v_j^{n+1}, A_x A_t u_j^n) &= 0 \\ (\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) + \delta_x A_x A_t f(A_x v_j^{n+1}, A_x v_j^n, A_x u_j^n, A_x u_j^{n+1}, A_x A_t v_j^n) &= 0. \end{aligned} \quad (6.18)$$

6.3 Local Momentum-Preserving AVF Method for CMKDV Equation

In this section, we present the second-order local momentum preserving AVF scheme (2.14) for the multisymplectic formulation (6.6) of the CMKDV equation (6.1). Applying local momentum preserving method (2.14) for the multisymplectic formulation (6.6) of the Dirac equation (6.1), we obtain

$$\begin{aligned}
-(\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2}(A_t A_x p_j^n) + f(A_t u_{j+1}^n, A_t u_j^n, A_t v_{j+1}^n, A_t v_j^n) \\
-(\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2}(A_t A_x q_j^n) + f(A_t v_{j+1}^n, A_t v_j^n, A_t u_{j+1}^n, A_t u_j^n) \\
(\delta_t A_x u_j^n) + (\delta_x A_t p_j^n) &= 0 \\
(\delta_t A_x v_j^n) + (\delta_x A_t q_j^n) &= 0 \\
-(\delta_x A_t u_j^n) &= -(A_t A_x a_j^n) \\
-(\delta_x A_t v_j^n) &= -(A_t A_x b_j^n) \\
-(\delta_x A_t c_j^n) &= \frac{1}{2}(A_t A_x u_j^n) \\
-(\delta_x A_t f_j^n) &= \frac{1}{2}(A_t A_x v_j^n)
\end{aligned} \tag{6.19}$$

where $f(A, B, C, D) = -\frac{\alpha}{4}(A^3 + A^2 B + AB^2 + B^3) - \frac{\alpha}{12}(3AC^2 + AD^2 + C^2 B + 3BD^2 + 2ACD + 2CBD)$. Eliminating the auxiliary variables a, b, c, f, p, q , we obtain

$$\begin{aligned}
(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) - \delta_x A_x f(A_t u_{j+1}^n, A_t u_j^n, A_t v_{j+1}^n, A_t v_j^n) &= 0 \\
(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) - \delta_x A_x f(A_t v_{j+1}^n, A_t v_j^n, A_t u_{j+1}^n, A_t u_j^n) &= 0
\end{aligned} \tag{6.20}$$

6.4 Local Momentum-Preserving PAVF Methods for CMKDV Equation

In this section, we present a new local momentum-preserving algorithm (3.41) for the CMKDV equation (6.1) based on the multisymplectic formulation (6.6) in Sec. 3.4.

Now, we introduce our new local momentum-preserving PAVF method (3.41)

$$\begin{aligned}
-(\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2}(A_t p_j^n) + F(A_t u_{j+1}^n, A_t u_j^n, A_t A_x u_j^n, A_t v_j^n) \\
-(\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2}(A_t q_j^n) + F(A_t v_{j+1}^n, A_t v_j^n, A_t A_x v_j^n, A_t u_{j+1}^n) \\
(\delta_t A_x u_j^n) + (\delta_x A_t p_j^n) &= 0 \\
(\delta_t A_x v_j^n) + (\delta_x A_t q_j^n) &= 0 \\
-(\delta_x A_t u_j^n) &= -(A_t A_x a_j^n) \\
-(\delta_x A_t v_j^n) &= -(A_t A_x b_j^n) \\
-(\delta_x A_t c_j^n) &= \frac{1}{2}(A_x u_{j+1}^n) \\
-(\delta_x A_t f_j^n) &= \frac{1}{2}(A_x v_{j+1}^n)
\end{aligned} \tag{6.21}$$

where $F(A, B, C, D) = -\frac{\alpha}{4}(A^3 + A^2 B + AB^2 + B^3) - \alpha CD^2$. Eliminating the auxiliary

variables we obtain the compact form

$$\begin{aligned}(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) - \delta_x A_x F(A_t u_{j+1}^n, A_t u_j^n, A_t A_x u_j^n, A_t v_j^n) &= 0 \\(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) - \delta_x A_x F(A_t v_{j+1}^n, A_t v_j^n, A_t A_x v_j^n, A_t u_{j+1}^n) &= 0\end{aligned}\quad (6.22)$$

The adjoint-PAVF scheme for CMKDV system (6.21) is given by

$$\begin{aligned}- (\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{2} (A_t p_{j+1}^n) + F(A_t u_{j+1}^n, A_t u_j^n, A_t A_x u_j^n, A_t v_j^n) \\- (\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{2} (A_x q_{j+1}^n) + F(A_t v_{j+1}^n, A_t v_j^n, A_t A_x v_j^n, A_t u_j^n) \\(\delta_t A_x u_j^n) + (\delta_x A_t p_{j+1}^n) &= 0 \\(\delta_t A_x v_j^n) + (\delta_x A_t q_{j+1}^n) &= 0 \\-(\delta_x u_j^n) &= -(A_x a_j^n) \\-(\delta_x v_j^n) &= -(A_x b_j^n) \\-(\delta_x c_j^n) &= \frac{1}{2} (u_j^n) \\-(\delta_x f_j^n) &= \frac{1}{2} (v_j^n)\end{aligned}\quad (6.23)$$

where $f(A, B, C, D) = -\frac{\alpha}{4}(A^3 + A^2 B + AB^2 + B^3) - \alpha CD^2$. Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned}(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) - \delta_x A_x f(A_t u_{j+1}^n, A_t u_j^n, A_t A_x u_j^n, A_t v_j^n) &= 0 \\(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) - \delta_x A_x g(A_t v_{j+1}^n, A_t v_j^n, A_t A_x v_j^n, A_t u_j^n) &= 0.\end{aligned}\quad (6.24)$$

The PAVF-P scheme for the CMKDV system (6.21) is

$$\begin{aligned}- (\delta_t A_x c_j^n) + (\delta_x A_t a_j^n) &= \frac{1}{4} A_t (p_{j+1}^n + p_j^n) - f(A_t u_{j+1}^n, A_t u_j^n, A_t A_x u_j^n, A_t v_j^n) \\- (\delta_t A_x f_j^n) + (\delta_x A_t b_j^n) &= \frac{1}{4} A_t (q_{j+1}^n + q_j^n) - g(A_t v_{j+1}^n, A_t v_j^n, A_t A_x v_j^n, A_t u_j^n, A_x A_t v_j^n) \\\frac{1}{2} \delta_t A_x (u_{j+1}^n + u_j^n) + \frac{1}{2} \delta_x A_t (p_{j+1}^n + p_j^n) &= 0 \\\frac{1}{2} \delta_t A_x (v_{j+1}^n + v_j^n) + \frac{1}{2} \delta_x A_t (q_{j+1}^n + q_j^n) &= 0 \\-(\delta_x u_j^n) &= -(A_x a_j^n) \\-(\delta_x v_j^n) &= -(A_x b_j^n) \\-(\delta_x c_j^n) &= \frac{1}{2} (A_x u_j^n) \\-(\delta_x f_j^n) &= \frac{1}{2} (A_x v_j^n)\end{aligned}$$

where $f(A, B, C, D) = -\frac{\alpha}{4}(A^3 + A^2 B + AB^2 + B^3) - \alpha CD^2$ and $g(A, B, C, D, E) = -\frac{\alpha}{4}(A^3 + A^2 B + AB^2 + B^3) - \frac{\alpha}{2} E(C^2 + D^2)$. Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned}(\delta_t A_x^3 A_t u_j^n) + (\delta_x^3 A_t^2 u_j^n) - \delta_x A_x f(A_t u_{j+1}^n, A_t u_j^n, A_t A_x u_j^n, A_t v_j^n) &= 0 \\(\delta_t A_x^3 A_t v_j^n) + (\delta_x^3 A_t^2 v_j^n) - \delta_x A_x g(A_t v_{j+1}^n, A_t v_j^n, A_t u_{j+1}^n, A_t u_j^n, A_x A_t v_j^n) &= 0.\end{aligned}\quad (6.25)$$

6.5 Global Energy-Preserving AVF Method for CMKDV Equation

In this section, we descretize the ∂_x with an anti-symmetric differential matrix D and time with AVF method to obtain the full discrete system

$$\begin{aligned}
-(\delta_t c_j^n) + (A_t D a_j^n) &= \frac{1}{2}(A_t p_j^n) - \frac{\alpha}{4} [(u_j^{n+1})^3 (u_j^{n+1})^2 (u_j^n) + (u_j^{n+1})(u_j^n)^2 + (u_j^n)^3] \\
&\quad - \frac{\alpha}{12} [3(u_j^{n+1})(v_j^{n+1})^2 + (u_j^{n+1})(v_j^n)^2 + (v_j^{n+1})^2 (u_j^n) \\
&\quad + 3(u_j^n)(v_j^n)^2 + 2(u_j^{n+1})(v_j^{n+1})(v_j^n) + 2(v_j^{n+1})(u_j^n)(v_j^n)] \\
-(\delta_t f_j^n) + (A_t D b_j^n) &= \frac{1}{2}(A_t q_j^n) - \frac{\alpha}{4} [(v_j^{n+1})^3 (v_j^{n+1})^2 (v_j^n) + (v_j^{n+1})(v_j^n)^2 + (v_j^n)^3] \\
&\quad - \frac{\alpha}{12} [3(v_j^{n+1})(u_j^{n+1})^2 + (v_j^{n+1})(u_j^n)^2 + (u_j^{n+1})^2 (v_j^n) \\
&\quad + 3(v_j^n)(u_j^n)^2 + 2(v_j^{n+1})(u_j^{n+1})(u_j^n) + 2(u_j^{n+1})(v_j^n)(u_j^n)] \\
(\delta_t u_j^n) + (A_t D p_j^n) &= 0 \\
(\delta_t v_j^n) + (A_t D q_j^n) &= 0 \\
-(A_t D u_j^n) &= -(A_t a_j^n) \\
-(A_t D v_j^n) &= -(A_t b_j^n) \\
-(A_t D c_j^n) &= \frac{1}{2}(A_t u_j^n) \\
-(A_t D f_j^n) &= \frac{1}{2}(A_t v_j^n)
\end{aligned} \tag{6.26}$$

Eliminating the auxiliary variables a, b, c, f, p, q , we obtain

$$\begin{aligned}
(\delta_t A_t u_j^n) + (A_t^2 D^3 u_j^n) + D A_t F(u_j^{n+1}, u_j^n, v_j^{n+1}, v_j^n) &= 0 \\
(\delta_t A_t v_j^n) + (A_t^2 D^3 v_j^n) + D A_t F(v_j^{n+1}, v_j^n, u_j^{n+1}, u_j^n) &= 0
\end{aligned} \tag{6.27}$$

which is a three-time level scheme, requires two initial conditions. Since the last four equations of (6.26) contain no time derivative, we can omit the average vector A_t in the corresponding equations. Applying the same procedure for (6.26), thus, we get

$$\begin{aligned}
(\delta_t u_j^n) + (A_t D^3 u_j^n) + D F(u_j^{n+1}, u_j^n, v_j^{n+1}, v_j^n) &= 0 \\
(\delta_t v_j^n) + (A_t D^3 v_j^n) + D F(v_j^{n+1}, v_j^n, u_j^{n+1}, u_j^n) &= 0
\end{aligned} \tag{6.28}$$

which is a two time level scheme for CMKDV equation.

6.6 Global Energy-Preserving PAVF Methods for CMKDV Equation

The PAVF scheme for the CMKDV system (6.5) can be given as

$$\begin{aligned}
-(\delta_t c_j^n) + (DA_t a_j^n) &= \frac{1}{2}(p_j^n) - f(u_j^{n+1}, u_j^n, v_j^n, A_t u_j^n) \\
-(\delta_t f_j^n) + (DA_t b_j^n) &= \frac{1}{2}(q_j^n) - g(v_j^{n+1}, v_j^n, u_j^{n+1}, A_t v_j^n) \\
(\delta_t u_j^n) + (DA_t p_j^n) &= 0 \\
(\delta_t v_j^n) + (DA_t q_j^n) &= 0 \\
-(DA_t u_j^n) &= -(A_t a_j^n) \\
-(DA_t v_j^n) &= -(A_t b_j^n) \\
-(DA_t c_j^n) &= \frac{1}{2}(u_j^{n+1}) \\
-(DA_t f_j^n) &= \frac{1}{2}(v_j^{n+1})
\end{aligned} \tag{6.29}$$

where $f(\xi, \beta, \eta, \phi) = -\frac{\alpha}{4}(\xi^3 + \xi^2\beta + \xi\beta^2 + \beta^3) - \alpha\eta^2\phi = g(\xi, \beta, \eta, \phi)$. Eliminating the auxiliary variables, we obtain the compact form

$$\begin{aligned}
(\delta_t A_t u_j^n) + (D^3 A_t^2 u_j^n) + DA_t f(u_j^{n+1}, u_j^n, v_j^n, A_t u_j^n) &= 0 \\
(\delta_t A_t v_j^n) + (D^3 A_t^2 v_j^n) + DA_t g(v_j^{n+1}, v_j^n, u_j^{n+1}, A_t v_j^n) &= 0
\end{aligned} \tag{6.30}$$

The adjoint-PAVF scheme for CMKDV system (6.29) is given by

$$\begin{aligned}
-(\delta_t c_j^n) + (DA_t a_j^n) &= \frac{1}{2}(p_j^{n+1}) - f(u_j^{n+1}, u_j^n, v_j^{n+1}, A_t u_j^n) \\
-(\delta_t f_j^n) + (DA_t b_j^n) &= \frac{1}{2}(q_j^{n+1}) - g(v_j^{n+1}, v_j^n, u_j^{n+1}, A_t v_j^n) \\
(\delta_t u_j^n) + (DA_t p_j^{n+1}) &= 0 \\
(\delta_t v) + (DA_t q_j^{n+1}) &= 0 \\
-(DA_t u_j^n) &= -(A_t a_j^n) \\
-(DA_t v_j^n) &= -(A_t b_j^n) \\
-(DA_t c_j^n) &= \frac{1}{2}(u_j^n) \\
-(DA_t f_j^n) &= \frac{1}{2}(v_j^n)
\end{aligned} \tag{6.31}$$

where $f(\xi, \beta, \eta, \phi) = -\frac{\alpha}{4}(\xi^3 + \xi^2\beta + \xi\beta^2 + \beta^3) - \alpha\eta^2\phi = g(\xi, \beta, \eta, \phi)$. Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned}
(\delta_t A_t u_j^n) + (D^3 A_t^2 u_j^n) + DA_t f(u_j^{n+1}, u_j^n, v_j^{n+1}, A_t u_j^n) &= 0 \\
(\delta_t A_t v_j^n) + (D^3 A_t^2 v_j^n) + DA_t g(v_j^{n+1}, v_j^n, u_j^n, A_t v_j^n) &= 0
\end{aligned} \tag{6.32}$$

Using the adjoint scheme (6.32), we can directly write down the corresponding PAVF-C scheme (3.8). For this, we denote the GEP-PAVF scheme (6.30) by $\Phi_{GE,\tau}$ and the corresponding adjoint scheme (6.32) by $\Phi_{GE,\tau}^*$ and then write the PAVF-C scheme for CMKDV equation (6.1) as

$$\Psi_{GE,\tau} = \Phi_{GE,\frac{\tau}{2}} \circ \Phi_{GE,\frac{\tau}{2}}^*. \quad (6.33)$$

Analogously, the PAVF-P scheme for the CMKDV system (6.29) is

$$\begin{aligned} -(\delta_t c_j^n) + (DA_t a_j^n) &= \frac{1}{2}(A_t p_j^n) - f(u_j^{n+1}, u_j^n, v_j^n, v_j^{n+1}, A_t u_j^n) \\ -(\delta_t f_j^n) + (DA_t b_j^n) &= \frac{1}{2}(A_t q_j^n) - g(v_j^{n+1}, v_j^n, u_j^n, u_j^{n+1}, A_t v_j^n) \\ (\delta_t A_t u_j^n) + (DA_t^2 p_j^n) &= 0 \\ (\delta_t A_t v_j^n) + (DA_t^2 q_j^n) &= 0 \\ -(DA_t u_j^n) &= -(A_t a_j^n) \\ -(DA_t v_j^n) &= -(A_t b_j^n) \\ -(DA_t c_j^n) &= \frac{1}{2}(A_t u_j^n) \\ -(A_t f_j^n) &= \frac{1}{2}(A_t v_j^n) \end{aligned} \quad (6.34)$$

where $f(\xi, \beta, \eta, \phi, \zeta) = -\frac{\alpha}{4}(\xi^3 + \xi^2\beta + \xi\beta^2 + \beta^3) - \frac{1}{2}\alpha\zeta(\eta^2 + \phi^2) = g(\xi, \beta, \eta, \phi, \zeta)$.

Eliminating the auxiliary variables we obtain the compact form

$$\begin{aligned} (\delta_t A_t u_j^n) + (D^3 A_t^2 u_j^n) + DA_t f(u_j^{n+1}, u_j^n, v_j^n, v_j^{n+1}, A_t u_j^n) &= 0 \\ (\delta_t A_t v_j^n) + (D^3 A_t^2 v_j^n) + DA_t g(v_j^{n+1}, v_j^n, u_j^n, u_j^{n+1}, A_t v_j^n) &= 0. \end{aligned} \quad (6.35)$$

6.7 Numerical Results

In this section, we implement several local energy-preserving, global energy-preserving, and local momentum-preserving methods for the nonlinear CMKDV equation (6.1). We note that the discrete systems are nonlinear. They are solved by Newton-Raphson's method.

To evaluate the local conservation laws of energy (3.14) we use the residual (3.12)

$$(R_E)_{j+1/2}^{n+1/2} = \delta_t E_{j+1/2}^n + \delta_x F_j^{n+1/2} \quad (6.36)$$

where

$$\begin{aligned} E_{j+1/2}^n &= \frac{1}{2} [(\delta_x u_j^n)^2 + (\delta_x v_j^n)^2] - \frac{\alpha}{4} [(A_x u_j^n)^2 + (A_x v_j^n)^2]^2 \\ F_j^{n+1/2} &= -(\delta_t u_j^n)(A_t a_j^n) - (\delta_t v_j^n)(A_t b_j^n) - (\delta_t c_j^n)(A_t p_j^n) - (\delta_t f_j^n)(A_t q_j^n). \end{aligned} \quad (6.37)$$

Moreover, to evaluate the local conservation laws of momentum (3.15) we use the residual (3.13)

$$(R_M)_{j+1/2}^{n+1/2} = \delta_t I_{j+1/2}^n + \delta_x G_j^{n+1/2} \quad (6.38)$$

where

$$\begin{aligned} I_{j+1/2}^n &= (\delta_x u_j^n)(A_x c_j^n) + (\delta_x v_j^n)(A_x f_j^n) \\ G_j^{n+1/2} &= S(A_t z_j^n) - (\delta_t u_j^n)(A_t c_j^n) - (\delta_t v_j^n)(A_t f_j^n) \end{aligned} \quad (6.39)$$

Moreover, the corresponding discrete total energy is

$$\mathcal{E}^n = h \sum_{j=0}^{J-1} E_{j+1/2}^n \quad (6.40)$$

and the total momentum

$$\mathcal{I}^n = h \sum_{j=0}^{J-1} I_{j+1/2}^n \quad (6.41)$$

To justify the efficiency of the presents methods, we also report the relative errors of the total energy and total momentum defined by

$$\mathcal{E}_{\text{Relative error}} = \frac{\mathcal{E}^n - \mathcal{E}^0}{\mathcal{E}^0}, \quad \mathcal{I}_{\text{Relative error}} = \frac{\mathcal{I}^n - \mathcal{I}^0}{\mathcal{I}^0}. \quad (6.42)$$

The CMKDV equation (6.1) admits the following one-soliton solution [7]

$$\psi_1(x, t) = \sqrt{\frac{2c}{\alpha}} \operatorname{sech}(\sqrt{c}(x - x_0 - ct)) e^{i\theta} \quad (6.43)$$

which is a single solitary wave with velocity c and located at the spatial location x_0 .

The initial conditions (5.3) are taken form the exact solution (6.43)

$$\psi_1(x, 0) = \sqrt{\frac{2c}{\alpha}} \operatorname{sech}(\sqrt{c}(x - x_0)) e^{i\theta} \quad (6.44)$$

We take the constant $c = 1$, $\alpha = 2$ and $\theta = \pi$ in the CMKDV equation (6.44). All of the solutions are computed with the space and time step sizes $h = 0.2$, $k = 0.01$. Periodic boundary conditions are imposed in all simulations. We solve the problem in the spatial interval $-30 \leq x \leq 30$ for $0 \leq t \leq 10$. The spatial domain has been chosen large enough so that solitary wave propagation do not effect the propagation of wave.

6.7.1 Numerical Experiment for Local Energy-Preserving Schemes

Our objective in this section is to demonstrate the effectiveness of the local energy preserving AVF (LEP-AVF) method (6.11), local energy preserving PAVF (LEP-PAVF) method (6.13), local energy preserving PAVF composition (LEP-PAVF-C) method (6.16), and local energy preserving PAVF plus (LEP-PAVF-P) method (6.18). As stated in (2.7), and (3.23), these methods preserves the global energy under periodic boundary condition.

In all numerical simulation of local energy preserving algorithm, we represent the numerical solitary wave solutions $u(x, t)$ and $v(x, t)$, obtained by the LEP-PAVF scheme (6.13). The results of AVF method (6.11), the PAVF-C method (6.16) and the PAVF-P method (6.18) are similar. For this reason they are not shown. **Accuracy test:** First, the correctness of the numerical schemes are examined. Table 6.1 gives spatial accuracy of the four energy preserving schemes. We can find that methods are second-order accuracy in space. The accuracy test validates the correctness of the methods.

Figure 6.1 represents the behaviour of the single soliton for $0 \leq t \leq 10$. We can observe that the shape of the $|\psi(x, t)|$ is preserved accurately. Figure 6.2 shows relative errors in energy conservation $\mathcal{E}_{\text{Relative error}}$ (6.42). From the figure we can see that all methods conserve global energy up to round-off error except the composition method. We suspect that non-conservative behavior of the composition method is because it is a three-level scheme.

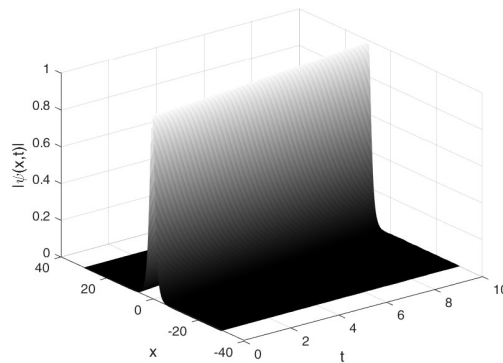


Figure 6.1: LEP scheme for CMKDV Equation. Propagation of wave by PAVF method

Table 6.1: The L_∞ and L_2 errors and convergence orders in space of the LEP methods with fixed time step $\tau = 0.001$, $-35 \leq x \leq 35$, at $t = 1$

	h		1/4	1/8	1/12
AVF	L_∞	error	2.01e-2	4.85e-3	1.89e-3
		order	—	2.1	2.4
	L_2	error	2.82e-2	6.7e-3	2.62e-3
		order	—	2.1	2.3
PAVF	L_∞	error	2.06e-2	5.33e-3	2.37e-3
		order	—	1.95	1.99
	L_2	error	2.89e-2	7.38e-3	3.29e-3
		order	—	1.97	1.99
PAVF -C	L_∞	error	2.06e-2	5.33e-3	2.37e-3
		order	—	1.95	1.99
	L_2	error	2.89e-2	7.38e-3	3.29e-3
		order	—	1.97	1.99
PAVF-P	L_∞	error	2.06e-2	5.32e-3	2.37e-3
		order	—	1.95	1.99
	L_2	error	2.89e-2	7.38e-3	3.29e-3
		order	—	1.96	1.99

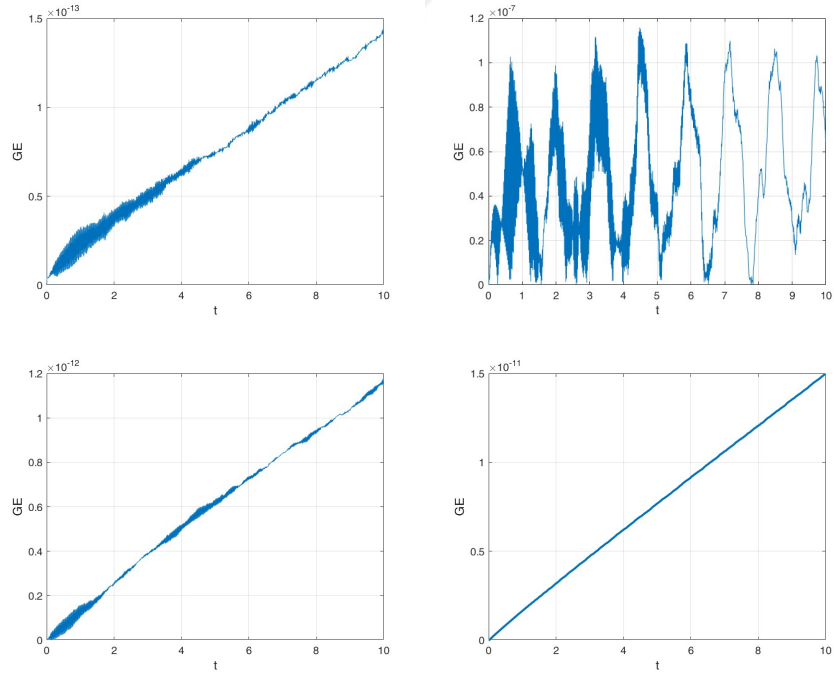


Figure 6.2: LEP scheme for CMKDV Equation. Relative Errors in Global Energy Conservation obtained by LEP schemes. The left-top one is PAVF method (5.15), the right-top is the PAVF-C method, the left-bottom is the PAVF-ADJ method, the right-bottom is the AVF method (5.14), respectively.

Table 6.2: The L_∞ and L_2 errors and convergence orders in space of the LMP methods with fixed time step $\tau = 0.001$, $-35 \leq x \leq 35$, at $t = 1$

		h	1/4	1/8	1/12
AVF	L_∞	error	1.91e-2	4.6e-3	1.77e-3
		order	–	2.05	2.4
	L_2	error	2.67e-2	6.33e-3	2.49e-3
		order	–	2.07	2.3
PAVF	L_∞	error	1.91e-2	4.6e-3	1.77e-3
		order	–	2.05	2.4
	L_2	error	2.67e-2	6.33e-3	2.49e-3
		order	–	2.07	2.3
PAVF-P	L_∞	error	1.91e-2	4.6e-3	1.77e-3
		order	–	2.05	2.4
	L_2	error	2.67e-2	6.33e-3	2.49e-3
		order	–	2.07	2.3

6.7.2 Numerical Simulation for the Local Momentum-Preserving Schemes

In this section, we conduct numerical simulation of local momentum preserving PAVF (LMP-PAVF) method (6.22), local momentum preserving adjoint (LMP-PAVF-ADJ) method (6.24) and local momentum preserving composition (LMP-PAVF-P) method (6.25) and local momentum preserving AVF (LMP-AVF) method (6.20). To demonstrate the accuracy of the present methods, we list the numerical results in terms of the L_∞ error and L_2 error and rates of convergence with $\tau = 0.001$ at time $T = 1$ in Table 6.2. From the table, we can see that convergence rate obtained from the present finite difference schemes are close to 2.0 which confirms theoretical order of convergence of the implicit mid-point rule.

Fig. 6.3 represents solitary wave solutions of the LMP-PAVF method (6.22). Solitary waves obtained from the other methods are similar. Therefore, they are not shown here. We notice from the Fig. 6.3 that the wave $|\psi(x, t)|$ moves to left direction without changing its shape. This shows that the present scheme well preserves the shape of the wave. Fig. 6.4 represents the relative errors $\mathcal{I}_{\text{Relative error}}$ (6.42) in momentum preservation. From the figure, we can see that all methods preserves the global momentum up to roundoff error.

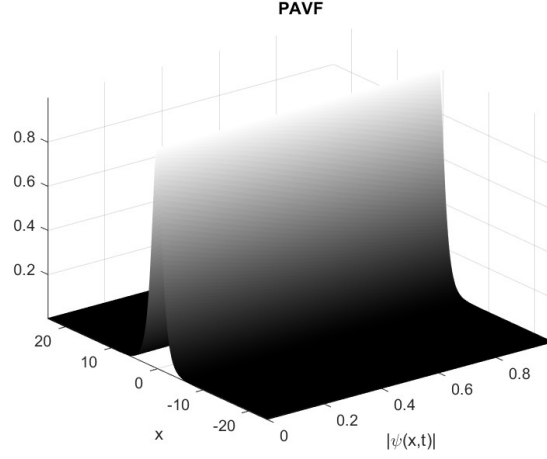


Figure 6.3: LMP scheme for CMKDV Equation. Propagation of wave by PAVF method (6.22)

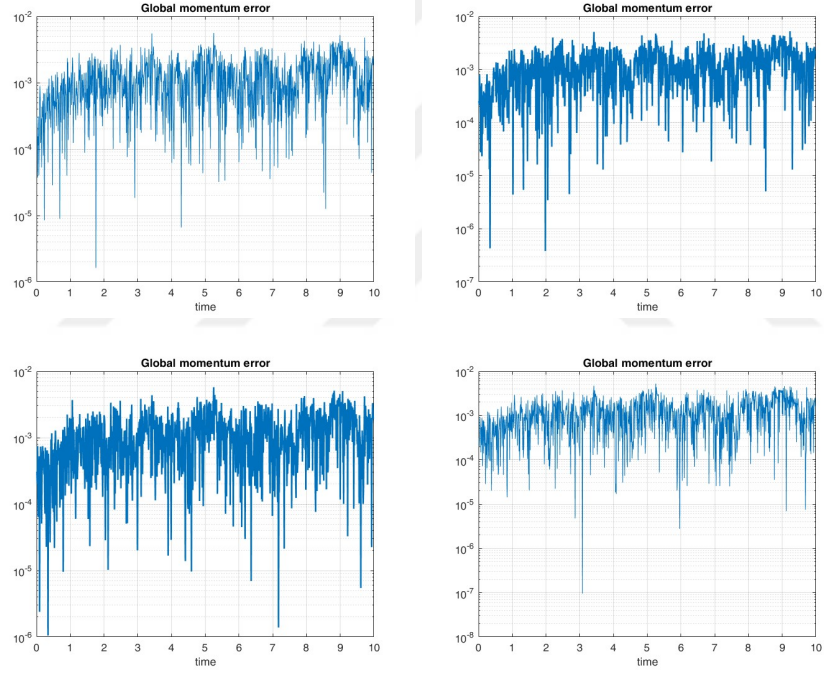


Figure 6.4: LMP scheme for CMKDV Equation. Relative Errors in Global momentum Conservation obtained by LMP schemes. The left-top one is PAVF method (6.22), the right-top is the PAVF-C method, the left-bottom is the PAVFP method (6.25), the right-bottom is the AVF method (6.20), respectively.

6.7.3 Numerical Simulation for the Global Energy-Preserving Schemes

In this section, numerical results are presented for global energy preserving PAVF (GEP-PAVF) method (6.30), global energy preserving PAVF composition (GEP-PAVF-

C) method (6.33), and global energy preserving PAVF plus (GEP-PAVF-P) method (6.33).

To show the correctness of the presents method, we list the L_∞ error and L_2 error including the convergence order in Table 6.3. Remember that the space derivative in all schemes were discretized by the second-orde implicit mid-point rule. From the Table 6.3 we can see that, the present scheme are second-order accurate in space which verifies theoretical second-order convergence of the implicit mid-point rule.

To demonstrate the effectiveness of the GEP schemes, we also represent the shape of the soliton solution in Fig. 6.5 at different time level. From the figure, we notice that the solitary eave moves to left direction with the same height without changing its shape. This shows that our presents scheme well simulates the solitary waves of the CMKDV equation. Fig. 6.6 represents the corresponding relative errors $\mathcal{E}_{\text{Relative error}}(6.42)$ in energy preservation.

For the numerical solutions of CMKDV equation, we see that among the LEP methods, the composition method did not yield good results. We think that this is because the composition method defined for one-step methods. However, the LEP methods for the CMKD equation are three-level methods. Neither local momentum nor global momentum results were obtained among the LMP algorithms. This is because momentum conservation, such as global momentum conservation, involves the term $\delta_x uc$. Here, the auxiliary variable used to convert the CMKDV equation into multi-symplectic form is $\delta_x c = 1/2u$, where δ_x is not invertible. For this reason, we cannot find the value c and therefore cannot provide local and global conservation values. However, we experimentally added a term like 10^{-12} to the last row and first column of the δ_x decomposition to make the decomposition matrix invertible, but we still found that conservation was not achieved. Among the GEP methods proposed for the numerical solutions of the CMKD equation, the composition method did not yield good results because the methods were three-level methods.

Table 6.3: The L_∞ and L_2 errors and convergence orders in space of the GEP methods with fixed time step $\tau = 0.001$, $-35 \leq x \leq 35$, at $t = 1$

		h	1/4	1/8	1/12
AVF	L_∞	error	2.37e-4	6.23e-5	2.91e-4
		order	–	1.93	1.93
	L_2	error	3.9e-4	1.03e-4	4.11e-4
		order	–	1.92	1.93
PAVF	L_∞	error	4.19e-2	9.57e-3	4.24e-3
		order	–	2.1	2.00
	L_2	error	5.63e-2	1.3e-2	5.76e-3
		order	–	2.1	2.00
PAVF-C	L_∞	error	4.19e-2	9.57e-3	4.24e-3
		order	–	2.1	2.01
	L_2	error	5.63e-2	1.3e-2	5.76e-3
		order	–	2.1	2.01
PAVF-P	L_∞	error	4.19e-2	9.57e-3	4.24e-3
		order	–	2.1	2.01
	L_2	error	5.63e-2	1.3e-2	5.76e-3
		order	–	2.1	2.01

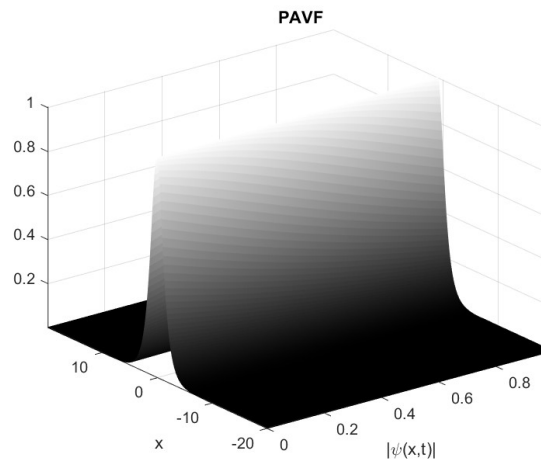


Figure 6.5: GEP scheme for CMKDV Equation. Propagation of wave by PAVF method

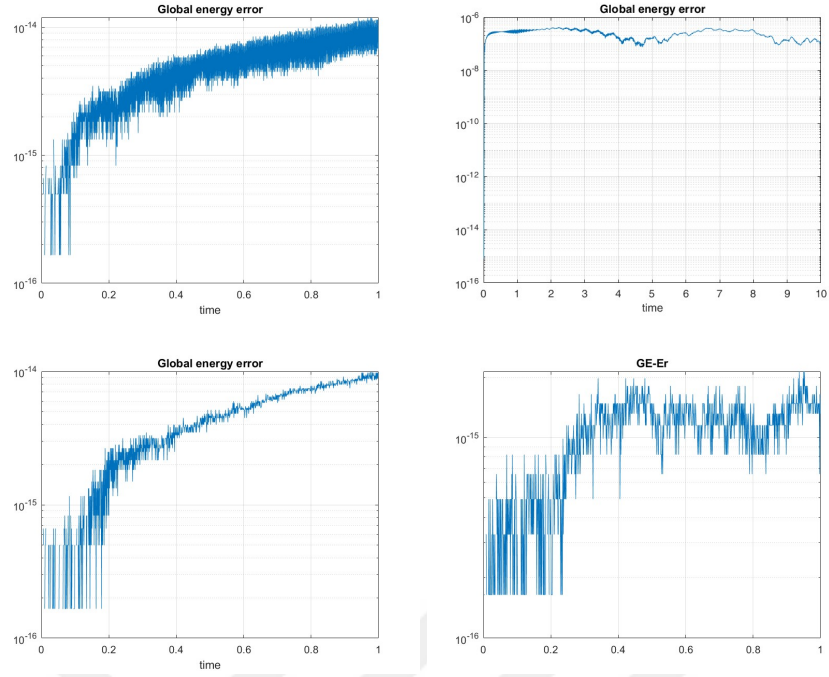


Figure 6.6: GEP scheme for CMKDV Equation. Relative Errors in Global energy Conservation obtained by GEP schemes. The left-top one is PAVF method (6.22), the right-top is the PAVF-C method, the left-bottom is the PAVFP method, the right-bottom is the AVF method (6.28), respectively.

CHAPTER 7

Conclusion

Multi-symplectic Hamiltonian PDEs are first-order PDEs that preserve the multi-symplectic structure of the underlying equation. In these equations, the multi-symplectic structure is the local structure and is independent of the boundary conditions. These equations have two other local conservations, called local energy and local momentum. These local conservations are also preserved globally under periodic or homogeneous boundary conditions. For a long time, many authors have focused on methods that preserve the discrete multisymplectic structure of multisymplectic PDEs, neglecting local conservation. While local conservations have sometimes been considered for a single equation, methods that preserve the local properties of a general multisymplectic PDEs have not been found until the last decade. Recently, Average Vector Field-based and Runge-Kutta-based methods have been developed that preserve the local energy and momentum of a general multisymplectic equation but they are not sufficient.

In this thesis, new and novel methods (algorithms) based on the Partitioned Average Vector Field (PAVF) method are developed that preserve the local energy and local momentum of a general multi-symplectic PDEs. It is also shown that these new locally conservative methods preserve the global energy and global momentum properties under periodic boundary conditions.

In addition to local energy conservation, a new and novel method based on the PAVF method is also developed that preserves the global energy of multi-symplectic PDEs.

These methods were applied to nonlinear Dirac equations and CMKDV equations.

The accuracy of the methods was verified with tables and numerical results. PAVF method is known to produce explicit methods, depending on the equation to which it is applied such as the Klein-Gordon-Schrödinger in Hamiltonian form. However, for the nonlinear Dirac equation and CMKDV equation discussed in this thesis, fully implicit methods were encountered, and the advantages of the PAVF method were not fully demonstrated. Numerical results show that discrete local conservation cannot be numerically demonstrated in local conservation equations that include the auxiliary variables required for the multi-symplectic formulation. This is clearly evident in the local energy and momentum conservation equations of the nonlinear Dirac equation and the CMKDV equation. We suspect this is due to the recalculation of the auxiliary variables required for the local conservation equations. This is because, while the local energy and momentum conservations are clearly depicted in the nonlinear Dirac equation, the CMKD equation fails to demonstrate these local conservations. Numerical results also show that no method is superior to other methods in every situation.

According to the results of the LEP schemes, LMP schemes and GEP schemes, it is not possible to say that there is a prominent method for the numerical solution of the nonlinear Dirac equation. Among the LEP schemes, the composition method preserves the local energy better than the other methods. PAVF method preserves the global energy and global momentum better than the other method. Among the LMP schemes, PAVF preserves the global momentum better than the other methods. Among the GEP methods PAVF and PAVF-P methods preserve the global energy better than the other methods.

For the numerical solutions of the CMKD equations, the following conclusions can be drawn between the LEP, LMP, and GEP methods: Among the LEP methods, the composition method did not yield good results. This is thought to be due to the composition method is a method defined for one-step methods. However, the LEP methods for the CMKD equation are three-level methods. Moreover, we see that neither local momentum nor global momentum results were obtained among the LMP algorithms. We suspect that this is because local conservations, such as global momentum conservation, involve the term $(\delta_x u_j^n)(A_t c_j^n)$. But, from the definition of the auxiliary variable $\delta_x c_j^n = 1/2u_j^n$ used to convert the equation into multi-symplectic form, the op-

erator δ_x is not invertible. For this reason, we can not find the value c_j^n . Therefore, we couldn't provide local and global conservation values. However, as a test, we added a term 10^{-12} to the last row and first column of the difference operator δ_x to make the difference matrix invertible, but we still found that conservation was not achieved. Among the GEP methods proposed for the numerical solutions of the CMKD equation, the composition method did not yield good results either, because the methods were three-level methods.

This thesis also addresses the one- and two-dimensional Schrödinger-Boussinesq equations in finite-dimensional Hamiltonian form, and proposes new numerical methods that conserve energy and mass based on PAVF method.



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APPENDIX

Proof of Lemma

In this Appendix, we give the proof of the Lemma 1.9.1.

$$A_t A_x f_j^n = A_x A_t f_j^n, \quad \delta_t A_x f_j^n = A_x \delta_t f_j^n, \quad A_t \delta_x f_j^n = \delta_x A_t f_j^n \quad (.1)$$

1. The equality $\delta_t \delta_x f_j^n = \delta_x \delta_t f_j^n$ holds.

Proof.

$$\begin{aligned} \delta_t(\delta_x f_j^n) &= \delta_t \left[\frac{f_{j+1}^n - f_j^n}{h} \right] = \frac{1}{h} [\delta_t f_{j+1}^n - \delta_t f_j^n] \\ &= \frac{1}{h} \left[\left(\frac{f_{j+1}^{n+1} - f_{j+1}^n}{\tau} \right) - \left(\frac{f_j^{n+1} - f_j^n}{\tau} \right) \right] = \frac{1}{h\tau} [f_{j+1}^{n+1} - f_j^{n+1} - f_{j+1}^n + f_j^n] \\ \delta_x(\delta_t f_j^n) &= \delta_x \left[\frac{f_j^{n+1} - f_j^n}{\tau} \right] = \frac{1}{\tau} [\delta_x f_j^{n+1} - \delta_x f_j^n] \\ &= \frac{1}{\tau} \left[\left(\frac{f_{j+1}^{n+1} - f_j^{n+1}}{h} \right) - \left(\frac{f_{j+1}^n - f_j^n}{h} \right) \right] = \frac{1}{h\tau} [f_{j+1}^{n+1} - f_j^{n+1} - f_{j+1}^n + f_j^n] \end{aligned}$$

Thus, we can conclude that $\delta_t \delta_x f_j^n = \delta_x \delta_t f_j^n$ is satisfied. □

2. The equality $A_t A_x f_j^n = A_x A_t f_j^n$ holds.

Proof.

$$\begin{aligned} A_t(A_x f_j^n) &= A_t \left[\frac{f_{j+1}^n + f_j^n}{2} \right] = \frac{1}{2} [A_t f_{j+1}^n + A_t f_j^n] \\ &= \frac{1}{2} \left[\left(\frac{f_{j+1}^{n+1} + f_{j+1}^n}{2} \right) + \left(\frac{f_j^{n+1} + f_j^n}{2} \right) \right] = \frac{1}{4} [f_{j+1}^{n+1} + f_j^{n+1} + f_{j+1}^n + f_j^n] \\ A_x(A_t f_j^n) &= A_x \left[\frac{f_j^{n+1} + f_j^n}{2} \right] = \frac{1}{2} [A_x f_j^{n+1} + A_x f_j^n] \\ &= \frac{1}{2} \left[\left(\frac{f_{j+1}^{n+1} + f_j^{n+1}}{2} \right) + \left(\frac{f_{j+1}^n + f_j^n}{2} \right) \right] = \frac{1}{4} [f_{j+1}^{n+1} + f_j^{n+1} + f_{j+1}^n + f_j^n] \end{aligned}$$

Thus, the equality $A_t A_x f_j^n = A_x A_t f_j^n$ is satisfied. $\square$

3. The equality $\delta_t A_x f_j^n = A_x \delta_t f_j^n$ holds.

Proof.

$$\begin{aligned}\delta_t(A_x f_j^n) &= \delta_t \left[\frac{f_{j+1}^n + f_j^n}{2} \right] = \frac{1}{2} [\delta_t f_{j+1}^n + \delta_t f_j^n] \\ &= \frac{1}{2} \left[\left(\frac{f_{j+1}^{n+1} - f_{j+1}^n}{\tau} \right) + \left(\frac{f_j^{n+1} - f_j^n}{\tau} \right) \right] = \frac{1}{2\tau} [f_{j+1}^{n+1} - f_{j+1}^n + f_j^{n+1} - f_j^n] \\ A_x(\delta_t f_j^n) &= A_x \left[\frac{f_j^{n+1} - f_j^n}{\tau} \right] = \frac{1}{\tau} [A_x f_j^{n+1} - A_x f_j^n] \\ &= \frac{1}{\tau} \left[\left(\frac{f_{j+1}^{n+1} + f_j^{n+1}}{2} \right) - \left(\frac{f_{j+1}^n + f_j^n}{2} \right) \right] = \frac{1}{2\tau} [f_{j+1}^{n+1} - f_{j+1}^n + f_j^{n+1} - f_j^n]\end{aligned}$$

Thus, the equality $\delta_t A_x f_j^n = A_x \delta_t f_j^n$ is satisfied. $\square$

4. The equality $A_t \delta_x f_j^n = \delta_x A_t f_j^n$ holds.

Proof.

$$\begin{aligned}A_t(\delta_x f_j^n) &= A_t \left[\frac{f_{j+1}^n - f_j^n}{h} \right] = \frac{1}{h} [A_t f_{j+1}^n - A_t f_j^n] \\ &= \frac{1}{h} \left[\left(\frac{f_{j+1}^{n+1} + f_{j+1}^n}{2} \right) - \left(\frac{f_j^{n+1} + f_j^n}{2} \right) \right] = \frac{1}{2h} [f_{j+1}^{n+1} - f_j^{n+1} + f_{j+1}^n - f_j^n] \\ \delta_x(A_t f_j^n) &= \delta_x \left[\frac{f_j^{n+1} - f_j^n}{2} \right] = \frac{1}{2} [\delta_x f_j^{n+1} - \delta_x f_j^n] \\ &= \frac{1}{2} \left[\left(\frac{f_{j+1}^{n+1} - f_j^{n+1}}{h} \right) - \left(\frac{f_{j+1}^n - f_j^n}{h} \right) \right] = \frac{1}{2h} [f_{j+1}^{n+1} - f_j^{n+1} + f_{j+1}^n - f_j^n]\end{aligned}$$

The equality $A_t \delta_x f_j^n = \delta_x A_t f_j^n$ is satisfied. $\square$

5. The difference operators (1.77) satisfy the *Discrete Leibnitz rule*

$$\delta_x(f \cdot g)_j^n = (\varepsilon f_{j+1}^n + (1 - \varepsilon) f_j^n) \cdot \delta_x g_j^n + \delta_x f_j^n \cdot ((1 - \varepsilon) g_{j+1}^n + \varepsilon g_j^n), \quad 0 \leq \varepsilon \leq 1. \quad (.2)$$

Proof. The left hand side of (.2) can be written as

$$\delta_x(f \cdot g)_j^n = \frac{f_{j+1}^n g_{j+1}^n - f_j^n g_j^n}{h}. \quad (.3)$$

Now, the right hand side of (.2) is

$$\begin{aligned}
& (\epsilon f_{j+1}^n + (1 - \epsilon) f_j^n) \cdot \delta_x g_j^n + \delta_x f_j^n \cdot ((1 - \epsilon) g_{j+1}^n + \epsilon g_j^n) \\
&= \epsilon f_{j+1}^n \cdot \delta_x g_j^n + f_j^n \cdot \delta_x g_j^n - \epsilon f_j^n \cdot \delta_x g_j^n + \delta_x f_j^n g_{j+1}^n - \epsilon \delta_x f_j^n g_{j+1}^n + \epsilon \delta_x f_j^n g_j^n.
\end{aligned} \tag{.4}$$

Claim:

$$\epsilon f_j^n \delta_x g_j^n = \epsilon \delta_x f_j^n g_j^n$$

so that,

$$\frac{f_j^n g_{j+1}^n - f_j^n g_j^n}{h} = \frac{f_{j+1}^n g_j^n - f_j^n g_j^n}{h}$$

hence,

$$f_j^n \cdot \delta_x g_j^n = \delta_x f_j^n \cdot g_j^n \tag{.5}$$

In addition, we have

$$\epsilon f_{j+1}^n \cdot \delta_x g_j^n = \epsilon \delta_x f_j^n \cdot g_{j+1}^n. \tag{.6}$$

put (.5) and (.6) in (.4), we get

$$\begin{aligned}
f_j^n \delta_x g_j^n + \delta_x f_j^n g_{j+1}^n &= \frac{f_j^n g_{j+1}^n}{h} - \frac{f_j^n g_j^n}{h} + \frac{f_{j+1}^n g_{j+1}^n}{h} - \frac{f_j^n g_{j+1}^n}{h} \\
&= \frac{f_{j+1}^n g_{j+1}^n - f_j^n g_j^n}{h}.
\end{aligned} \tag{.7}$$

□

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