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Local structure-preserving algorithms for partial differential equations

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Abstract In this paper, we discuss the concept of local structure-preserving algorithms (SPAs) for partial differential equations, which are the natural generalization of the corresponding global SPAs. Local SPAs for the problems with proper boundary conditions are global SPAs, but the inverse is not necessarily valid. The concept of the local SPAs can explain the difference between different SPAs and provide a basic theory for analyzing and constructing high performance SPAs. Furthermore, it enlarges the applicable scopes of SPAs. We also discuss the application and the construction of local SPAs and derive several new SPAs for the nonlinear Klein-Gordon equation.

Keywords: SPAs, local conservation law, construction method, discrete Leibnitz rule

MSC(2000): 65L06, 65M06, 65M12

1 Introduction

With the fast development of computer, numerical methods become more and more powerful in scientific research. However not all the problems can be solved by increasing the power of the computers because of a large amount of computation and long-time integration in some special fields such as molecular chemistry, weather forecasting and biology computing. The stability and effectiveness of the numerical algorithms are still the key problems, which motivates various numerical algorithms. As to difference schemes, the earlier attempts can date back to 1928 when Courant, Friedrichs, and Lewy constructed special algorithms that are not only consistent with the original equation, but also yield a global invariant form referred to as "energy". Although not all of these conserved quantities are truly energy in the physical sense, they are usually just some positive definite quantities. Thus a norm can be devised to guarantee the global stability of the algorithms. Because energy is the most important first integral of many evolutional equations, the energy-conserving algorithms are naturally interesting to researchers and therefore developed very fast[1−4].

Based on the basic rule that numerical algorithms should preserve the intrinsic properties

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of the original problems as much as possible, Feng[5] first presented the concept of symplectic schemes for Hamiltonian systems and further the structure-preserving algorithms (SPAs) for the general conservative dynamical systems. He and his research group obtained a series of results on construction and theory analysis of symplectic schemes[6−8], which triggered the interest of many researchers. Subsequently, many important results on symplectic schemes were obtained. It is proved by the practical computations that the symplectic schemes have very wide and important applications in many fields because of their excellent stability and accurate long-time numerical behavior[9, 10].

However, there is a principal difficulty that arises when generalizing the symplectic algorithms from Hamiltonian ODEs to Hamiltonian PDEs. A popular method to treat Hamiltonian PDEs is the so-called method of line which first discretes PDEs in space resulting in a large system of Hamiltonian ODEs. The resulting ODEs is then integrated by the symplectic algorithms. The disadvantage of this method is that no method is mature to guarantee the resulting ODEs to be Hamiltonian. Another method to apply symplectic algorithms to Hamiltonian PDEs is to rewrite the PDEs into the Hamiltonian form on Banach space and use the symplectic theory in the Banach space directly. This method has the disadvantage that only very few PDEs can be integrated by this method[11,12]. Recently, Marsden, Patrick, Shkoller[13] and Bridges, Reich[14] presented the concept of multi-symplectic structure and multi-symplectic algorithms for PDEs, which can be regarded as the direct generalization of Fen's symplectic algorithms. Treating PDEs with the space same as the time, multi-symplectic algorithms generalize the symplectic structure of PDEs on the global time level to any domain and even every point in the time-space region. This takes further insight into the applications of the symplectic schemes on the Hamiltonian PDEs and makes them facile. Actually, besides the geometric structure, the concept of Fen's SPAs also contains the other conservative properties of the PDEs such as the physically conservation law and the algebraic characters. In some fields, it is convenient sometimes to construct numerical algorithms to preserve other conservative laws rather than the symplectic one. For example, The square-conserving schemes were proposed and systematically developed in the weather forecasting. The square-conserving schemes which preserve the energy of the system have made a rapid progress in the numerical weather forecasting. Nowadays, we can find plenty of papers on the numerical methods for the conservative systems. All those numerical methods which can preserve some structures of original problems can be called SPAs generally. However, similar to the symplectic algorithms, those SPAs may bring the constrains and inconvenience when used to integrate the PDEs. Because the structures of PDEs are defined on the global time level, they will inevitably depend on the boundary conditions. That is to say, the necessary conditions for applying an SPA to a given PDEs are not only the conservative system itself but also the proper boundary conditions. We cannot apply an SPA to a conservative system without proper boundary conditions. Let us take the barotropic primitive equations in the study of numerical weather forecasting as an example. The square-conserving law is valid on the golbal time level and the square-conserving schemes can be applied to providing that the equations are under the homogeneous or periodic boundary conditions. However, such boundary conditions are impossible for the local model of studying the storms and thus there is no theoretical basis for application of square-conserving schemes. To our surprise,

numerical results show that the square-conserving schemes perform very well in the simulations of some local models. Why? The same problems will arise when other SPAs are applied to some PDEs. In this paper, we try to discuss this problem. We will propose the novel concept of local SPAs for the PDEs and present some elementary results on them. The local SPAs are still in the category of SPAs. The basic idea of them is generalize the preserved structures of the SPAs on the global time level to local area so that the structures can be preserved in any local areas or any points in time-space region. Therefore, the boundary conditions are not necessary any more. The concept of local SPAs gives a good explanation for the difference of the performance between the different SPAs. That is, some of them can preserve the local structure, and the others cannot. The concept of the local SPAs can also explain the above proposed problem. The reason is that those SPAs are local SPAs, thus the boundary conditions are not necessary. When the proper boundary conditions are imposed, those local SPAs can naturally preserve the structures on the global time level. Next, we will introduce the concept of local SPAs first.

2 The introduction of the local structure-preserving algorithms

To make it clear, we will take the nonlinear Klein-Gordon as an example to introduce the concept of local SPAs and show that the local SPAs are the natural generalization of the existing SPAs. All the discussions and results can be applied to the general conservative PDEs such as KdV equation, the nonlinear Schrödinger equation and the Z-K equation. Consider the nonlinear Klein-Gordon equation

$$\partial_{tt}u = \partial_{xx}u - F'(u), \qquad (x,t) \in \Omega \subset \mathbb{R}^2, \tag{1}$$

where, the subscript denotes differentiation and $F'(u) : \mathbb{R} \to \mathbb{R}$ is a smooth nonlinear function. The initial conditions are

$$u(x,0) = u_1(x), \quad u_t(x,0) = u_2(x), \tag{2}$$

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

Under some proper boundary conditions such as the homogeneous or periodic boundary conditions, we can rewrite the above equation in the form of the Hamiltonian

$$\frac{d\mathbf{z}}{dt} = J^{-1}\frac{\delta H(\mathbf{z})}{\delta \mathbf{z}}, \quad \mathbf{z} = \begin{bmatrix} v \\ u \end{bmatrix} = \begin{bmatrix} u_t \\ u \end{bmatrix}, \; J = \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \tag{3}$$

where, $H(\mathbf{z}) = \int v^2 + u_x^2 + F(u)$, $\frac{\delta H}{\delta \mathbf{z}}$ is the variational derivative and the variable $v = u_t$ is implied in (3).

Eq. (3) has the following symplectic conservation law:

$$\frac{\partial \omega}{\partial t} = 0; \quad \omega = \int du \wedge dv \; dx. \tag{4}$$

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

An algorithm is called the symplectic algorithm for (1) or (3) if it can preserve the discrete form of the symplectic conservation law (4), i.e., the discrete form of ω on the n-th time level equals it on the $(n+1)$-th time level. $\omega_D^n = \omega_D^{n+1}$, $\omega_D = \sum_i du_i \wedge dv_i$. The simplest symplectic algorithms for (1) is

$$D_t^2 u_i^j - D_x^2 u_i^j + F'(u_i^j) = 0, \tag{5}$$

where, $D_t^2 u_i^j = \frac{u_i^{j+1} - 2u_i^j + u_i^{j-1}}{\tau^2}$, $D_x^2 u_i^j = \frac{u_{i+1}^j - 2u_i^j + u_{i-1}^j}{h^2}$, $u_i^j \approx u(x_i, t_j)$, τ and h are the time the step and the space step respectively.

Again under the homogeneous or periodic boundary conditions, (1) has the energy conservation law as

$$\frac{dE}{dt} = 0; \quad E = \int \frac{1}{2}(v^2 + w^2) + F(u)\, dx, \quad w = u_x. \tag{6}$$

An algorithm is called a energy-conserving algorithm if it can preserve the discrete form of (6), i.e. the discrete energy is the same on all the time level. An example of the energy-conserving algorithms is

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

The corresponding discrete energy on the t_m 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 the homogeneous and periodic boundary conditions, (1) may have the momentum conservation law as

$$\frac{dM}{dt} = 0; \quad E = \int wv\, dx. \tag{8}$$

An algorithm is called a momentum-conserving algorithm if it can preserve the discrete form of (8). An example of the momentum-conserving algorithms for (1) is

$$D_t^2 u_i^j - D_x^2 u_i^j + \frac{F(u_{i+1}^j) - F(u_{i-1}^j)}{u_{i+1}^j - u_{i-1}^j} = 0 \tag{9}$$

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

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

All the symplectic, energy-conserving and momentum-conserving conservation laws are important properties of the PDE (1). In [5], Feng wrote "It is natural to look forward to those discrete systems which preserve as much as possible the intrinsic properties of the continuous system." He also pointed out that the ability to preserve the invariant properties of the continuous system is a criterion to judge the success of a numerical simulation. It has been proved by plenty of numerical results that the SPAs are more stable and accurate for long-time computations than other algorithms. However, the applications of the SPAs to the PDE (1) depend on the homogeneous and periodic boundary conditions. In the contrast, many practical problems are not necessary under the homogeneous or periodic boundary conditions.

Actually, (1) has the local conservation laws corresponding to the symplectic conservation law (4), the energy-conserving law (6) and momentum-conserving law (8) as

$$\partial_t[du \wedge dv] - \partial_x[du \wedge dw] = 0; \tag{10}$$

$$\partial_t\left[\frac{1}{2}(w^2 + v^2) + F(u)\right] - \partial_x(wv) = 0; \tag{11}$$

$$\partial_t(wv) - \partial_x\left[\frac{1}{2}(w^2+v^2) - F(u)\right] = 0. \tag{12}$$

(10), (11) and (12) are called the multi-symplectic conservation law, the local energy-conserving law and the local momentum-conserving law respectively. For clarification, we then call the conservation laws (4), (6) and (8) the global conservation law. The local conservation laws are valid in any area of the time-space region and do not depend on the boundary conditions. They are equivalent to the original PDE except for some trivial solutions. Integrating these local conservation laws over the spatial interval under the proper boundary conditions, which are the necessary conditions for the global conservation laws, we can derive the corresponding global conservation laws. In this sense, the local conservation laws are more intrinsic than the global ones. In the form of the conservation laws, the local ones hold the flux terms, thus containing much information of the PDE than the global ones. According to Fen's idea, those more intrinsic properties should be preserved in the numerical simulations. We call the numerical algorithms which can preserve the local conservations laws the local SPAs. Many basic problems then naturally arise to this new concept. For example, do the local SPAs exist? If they do, what are the relations between the original global SPAs and them? Are they definitely superior to the global SPAs? Can we derive some new robust numerical algorithms for PDEs based on the local SPAs? What kind of local SPAs are the best for some given PDEs? How to apply the local SPAs to the practice? and so on.

In fact, local SPAs which preserve the multi-symplectic conservation law (10) are the so-called multi-symplectic schemes. Marsden, Bridges, Reich, Qin and his group and Hong have had lots of contributions on this topic[15−18]. We can also prove that the scheme (7) preserves numerically the following discrete local conservation law:

$$D_t\left[\frac{1}{2}(v_i^j)^2 + \frac{1}{2}w_{i+1}^{j-1}w_{i+1}^j + A_tF_i^{j-1}\right] = D_x(w_i^jA_tv_i^j), \tag{13}$$

where, D_t and D_x are the first order forward difference operator on time and space respectively, A_t is the first order average operator on time. Please refer the detailed definition of those operators in Section 5. We will also prove some numerical algorithms to preserve the local momentum conservation law in the later discussions. In addition, the schemes proposed by Vu-Quoc and Li[19, 20] to preserve the invariant structures are essentially the local SPAs. Therefore, we should not doubt the existence of the local SPAs. Furthermore, we will use the concatenating method to construct a series of local SPAs for the nonlinear Klein-Gordon equation.

Under the homogeneous or periodic boundary conditions, the local SPAs are the correspondingly global SPAs spontaneously. If we sum a discrete local conservation law over the spatial grids, we can obtain the discrete global conservation laws by the boundary condition. For example, summing the local energy conservation law (13) over i, we can obtain a discrete analogue of the local conservation law (6) by the boundary condition. In the contrast, the global SPAs are not always the local SPAs because the conservation laws preserved on the global time level cannot avoid the distortion in local areas. Another advantage of the local SPAs is that they do not depend on the boundary condition any more. Thus they enlarge the applicable area of the SPAs.

3 Applications of local structure-preserving algorithms

By the definition of the local SPAs, they can be applied to any PDEs with local conservation laws. Thus the question we should answer is what kind of PDEs have the local conservation laws. Recently, the studies of multi-symplectic PDEs and multi-symplectic schemes are very hot. Nearly all the equations with the solitary solutions and some other important evolutionary equations can be rewritten into multi-symplectic PDEs. These equations include the KdV equation, the K-P equation, the nonlinear Schrödinger equation, the Maxwell's equation and so on. Please refer the recent survey article by Bridges and references therein for details[21].

The general form of the $1+1$ dimensional multi-symplectic PDEs is

$$M\mathbf{z}_t + K\mathbf{z}_x = \nabla_{\mathbf{z}} S(\mathbf{z}), \tag{14}$$

where, M and K are skew-symmetric, $\nabla_{\mathbf{z}}$ is the gradient operator based on the standard Euclidean inner product. For the nonlinear Klein-Gordon equation (1), we have

$$M = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad K = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix},$$

$\mathbf{z} = (u, v, w)^T$, $v = u_t$, $w = u_x$, $S(\mathbf{z}) = \frac{1}{2}(v^2 - w^2) + F(u)$.

The multi-symplectic PDEs (14) have the following three local conservation laws:

$$\partial_t \left[\frac{1}{2} d\mathbf{z} \wedge M d\mathbf{z}\right] - \partial_x [d\mathbf{z} \wedge K d\mathbf{z}] = 0; \tag{15}$$

$$\partial_t \left[S(\mathbf{z}) - \frac{1}{2}\mathbf{z}^T K \mathbf{z}_x\right] - \partial_x \left(\frac{1}{2}\mathbf{z}^T K \mathbf{z}_t\right) = 0; \tag{16}$$

$$\partial_z (\mathbf{z}^T M \mathbf{z}_x) - \partial_x \left[S(\mathbf{z}) - \frac{1}{2}\mathbf{z}^T M \mathbf{z}_t\right] = 0. \tag{17}$$

For the nonlinear equation (1), they are the multi-symplectic conservation law (10), the local energy conservation law (11) and the local momentum conservation law (12) respectively. Therefore, we conclude that any PDEs with the multi-symplectic structure can be integrated by the local SPAs.

Additionally, we can discuss the local properties of PDEs by tool of the total variational principle[22].

Let the Lagrangian action functional of a system be $\Phi(u) = \int_\Omega L(u(x,t), u_t, u_x) dx dt$. The variational principle states that the stationary curves of the action integral on the configuration manifold are the solutions of the corresponding Euler-Lagrange equation which can be derived by taking the variation of the action functional. The variational principle here only considers the variation of the u. In fact, we can consider the variations of the x and t, together with u. Such a variation is the so-called total variation. Let $\tilde{u} = u + \lambda\delta u$, $\tilde{t} = t + \lambda\delta t$, $\tilde{x} = x + \lambda\delta x$, then

$$\delta\Phi = \frac{d}{d\lambda}\bigg|_{\lambda=0} \Phi(\tilde{u}, \tilde{x}, \tilde{t}) = \frac{d}{d\lambda}\bigg|_{\lambda=0} \int_{\tilde{\Omega}} L(\tilde{u}(\tilde{x}, \tilde{t}), \tilde{u}_{\tilde{t}} \tilde{u}_{\tilde{x}}) d\tilde{x} d\tilde{t} = A + B, \tag{18}$$

where

$$A = \int_\Omega \left[\left(D_t\left(\frac{\partial L}{\partial u_t} u_t - L\right) + D_x\left(\frac{\partial L}{\partial u_x} u_t\right)\right)\delta t\right.$$

$$+\left(D_x\left(\frac{\partial L}{\partial u_x}u_x - L\right) + D_t\left(\frac{\partial L}{\partial u_t}u_x\right)\right)\delta x$$
$$+\left(\frac{\partial L}{\partial u} - D_x\frac{\partial L}{\partial u_x} - D_t\frac{\partial L}{\partial u_t}\right)\delta u\Bigg]dx\wedge dt \tag{19}$$

$$B = \int_{\partial\Omega}\left[\left(\left(\frac{\partial L}{\partial u_t}u_t - L\right)dx - \frac{\partial L}{\partial u_x}u_t dt\right)\delta t + \left(\left(L - \frac{\partial L}{\partial u_x}u_x\right)dt + \frac{\partial L}{\partial u_t}u_x dx\right)\delta x\right.$$
$$\left.+\left(\frac{\partial L}{\partial u_x}dt - \frac{\partial L}{\partial u_t}dx\right)\delta u\right]. \tag{20}$$

By the expression of A, we can obtain the local energy conservation law from the variation of time t, the local momentum conservation law from the variation of space x and the Euler-Lagrange equation from the variation of u. By the expression of B, we can derive the Cartan-form and subsequently the multi-symplectic form and multi-symplectic conservation law[13]. The total variation of the nonlinear Klein-Gordon equation (1) can be found in [23].

It is clear now that all the system with the conservative Lagrangian action functional can be applied by the local SPAs. This means that besides the hyperbolic PDEs, a large number of elliptic PDEs can be integrated by the local SPAs. For example,

$$u_{xx} + u_{yy} + f(u) = 0, \quad (x,t)\in\Omega. \tag{21}$$

It has the Lagrangian action functional $\int_\Omega[\frac{1}{2}u_x^2 + \frac{1}{2}u_y^2 + F(u)]dxdt$, $F'(u) = f(u)$, and can be rewritten into the multi-symplectic form (14) with the parameters as

$$M = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}, \qquad K = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{bmatrix},$$

$\mathbf{z} = (u, v, w)^T$, $v = u_y$, $w = u_x$, $H(\mathbf{z}) = \frac{1}{2}(w^2 + v^2) - F(u)$.

4 Some examples of the applications

4.1 Numerical simulation in geophysical fluid dynamics

Zen et al.[24] proposed and developed the energy-conserving scheme and applied the square-conserving schemes successful on lots of meteorological models. The square-conserving schemes are global SPAs, so the applications of them need the proper boundary conditions. Actually, the local square-conserving schemes can be fit perfectly on those models. Consider the system of two dimensional barotropic atmosphere equations

$$\begin{aligned} &\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial \phi}{\partial x} - fv = 0,\\ &\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial \phi}{\partial y} + fu = 0,\\ &\frac{\partial \phi}{\partial t} + \frac{\partial u\phi}{\partial x} + \frac{\partial v\phi}{\partial y} = 0, \end{aligned} \tag{22}$$

where u and v are wind filed, ϕ is potential height. This system has several local conservation laws and one of them is the local square conservation law

$$\frac{1}{2}\frac{\partial}{\partial t}(U^2 + V^2 + \phi^2) + \frac{1}{2}\frac{\partial}{\partial x}[(U^2 + V^2)u + 2U\Phi\phi] + \frac{1}{2}\frac{\partial}{\partial y}[(V^2 + U^2)v + 2V\Phi\phi] = 0, \tag{23}$$

where, $\Phi=\sqrt{\phi}$, $U=\Phi u$, $V=\Phi v$. We can construct the local square-conserving scheme as follows:

$$\begin{aligned} &U_{+t}+\mathcal{L}\overline{U}=-\overline{\Phi}\,\overline{\phi}_{-x}+f\overline{V},\\ &V_{+t}+\mathcal{L}V=-\overline{\Phi}\,\overline{\phi}_{-y}-f\overline{U},\\ &\phi_{+t}+(\overline{U}\,\overline{\Phi})_{+x}+(\overline{V}\,\overline{\Phi})_{+y}=0, \end{aligned} \tag{24}$$

where, $\mathcal{L}\overline{U}=\frac{1}{2}[(u\overline{U})_{+x}+u\overline{U}_{-x}]+\frac{1}{2}[(v\overline{U})_{+y}+v\overline{U}_{-y}]$. The corresponding discrete local square conservation law is

$$\begin{aligned} &(U^2+V^2+\phi^2)_{+t}+(u\overline{U}S_x^{-1}\overline{U}+u\overline{V}S_x^{-1}\overline{V}+2\overline{\Phi}\,\overline{U}S_x^{-1}\overline{\phi})_{+x}\\ &\quad+(v\overline{U}S_y^{-1}\overline{U}+v\overline{V}S_y^{-1}\overline{V}+2\overline{\Phi}\,\overline{V}S_y^{-1}\overline{\phi})_{+y}=0. \end{aligned} \tag{25}$$

Here the notations used in computation of geophysical fluid dynamics are adopted. For example, $U_{+t}=(U_i^{j+1}-U_i^j)/\Delta t$ is the forward difference on time, $\overline{U}=(U_i^{j+1}+U_i^j)/2$ is the average on time and $S_{+x}U_i^j=U_{i+1}^j$ denotes the forward shift on time.

4.2 Computations of the solitary wave equations

The theory of solitary waves is one of the most important part of developments of the applied mathematics and mathematical physics with applications in lots of fields such as the dynamical fluid, plasma physics, the nonlinear optics and the classical field theory. Numerical simulation is an effective method to study the solitary waves. An example is the computations of the Schrödinger equation in quantic mechanics[9]. Local SPAs provide a new viewpoint to study the solitary wave equations and produce some new robust numerical algorithms. Take the KdV equation as an example,

$$\frac{\partial u}{\partial t}+\eta u\frac{\partial u}{\partial x}+\mu^2\frac{\partial^3 u}{\partial x^3}=0,\quad t>0, \tag{26}$$

where,η and μ are two real constants. As we all know, for small μ explicit schemes can arise nonlinear oscillation when used to carry long-time computations. The most well-known example is the Zabusky-Kruskal (Z-K) scheme which was applied to discovering the solitons in 1960s. Based on the local property of the KdV equation, we construct an SPA as

$$\begin{aligned} &\frac{1}{2}\left(\frac{u_i^{j+1}-u_i^j}{\tau}+\frac{u_{i+1}^j-u_{i+1}^{j-1}}{\tau}\right)+\eta\frac{u_i^j+u_{i-1}^j}{2}\left(\frac{u_i^j-u_{i-1}^j}{h}\right)\\ &\quad+\mu^2\frac{u_{i+2}^j-3u_{i+1}^j+3u_i^j-u_{i-1}^j}{h^3}=0. \end{aligned} \tag{27}$$

It is a new explicit scheme and much better than the Zabusky-Kruskal scheme when used to compute the same problem. It removes the phenomenon of nonlinear oscillation and can preserve approximatively several first integrals[25].

4.3 Computations of the Maxwell's equations

Consider the Maxwell's equations

$$\frac{\partial \mathbf{B}}{\partial t}+\nabla\times\mathbf{E}=0,\quad \frac{\partial \mathbf{D}}{\partial t}-\nabla\times\mathbf{H}=0,\quad \mathbf{B}=\mu\mathbf{H},\quad \mathbf{D}=\varepsilon\mathbf{E}. \tag{28}$$

The equations admit the multi-symplectic structure and therefore have the multi-symplectic conservation law, local energy conservation law and local momentum conservation law[26].

We construct a new scheme which is not a multi-symplectic scheme but also a local energy-conserving scheme. For simplicity, we present here the scheme for the two dimensional equations (the scheme is denoted as MPS)

$$\begin{aligned} &D_x A_y^2 A_t A_x E_{zi,j}^k = D_t A_x^2 A_y^2(\mu H_{yi,j}^k),\\ &D_y A_x^2 A_t A_y E_{zi,j}^k = -D_t A_x^2 A_y^2(\mu H_{xi,j}^k),\\ &-D_y A_x^2 A_t A_y H_{xi,j}^k + D_x A_y^2 A_t A_x H_{yi,j}^k = D_t A_x^2 A_y^2(\varepsilon E_{zi,j}^k), \end{aligned} \tag{29}$$

where, E_z is the electric field component in z axis, H_x and H_y are the magnetic field components in x and y axes respectively, D_t, D_x and D_y are the first order forward difference operators in t, x and y directions respectively, A_t, A_x and A_y are the corresponding first order average operators. Numerical results show that the new scheme is better than the famous Yee's scheme[27].

We take the periodic boundary condition and the following initial values:

$$E_z(x,y,0)=0,\quad H_y(x,y,0)=-\frac{3}{\sqrt{5}}\cos(3\pi x)\sin(\pi y),\quad H_x(x,y,0)=\frac{1}{\sqrt{5}}\sin(3\pi x)\cos(\pi y)$$

to compare the MPS scheme with Yee's scheme. The computing area is $[0,2/3]\times[0,2]$ and the space step for both schemes is $\Delta x=\Delta y=h=1/123$. We find that the Yee's scheme cannot provide the reasonable numerical solutions for a long time when the time step is great than 0.0015, whereas the MPS scheme works very well all along. Moreover, the total errors of the MPS scheme is much less than that of the Yee's scheme even if we take time step 0.001 for the Yee's scheme and 0.01 for the MPS scheme. Figure 1 shows the total errors of the two schemes changing with time.

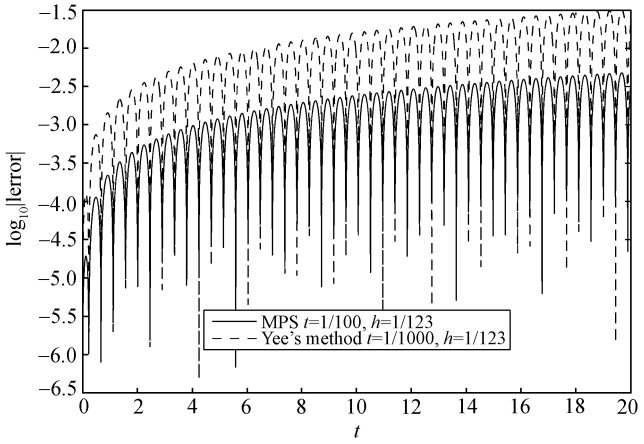

Figure 1 The total errors of the MPS scheme and the Yee's scheme changing along the time

In Figure 1, the total errors |error| on some time level is defined by the maximal normal of the difference between numerical solutions and the exact solutions. The detailed numerical results of the MPS scheme will be reported in another paper.

5 Construction of the local SPAs

In the section, we use the concatenating method to construct the local SPAs. This method to construct difference schemes for PDEs is different from the line method and the alternating

direction method. Its basic idea is from the Runge-Kutta method which deals with PDEs by space and time separately. In [28], Reich proved that concatenating the Runge-Kutta method in type Gauss collocation leads to multi-symplectic schemes for the nonlinear wave equation. In [29], the author used this method to construct a series of multi-symplectic schemes for the sine-Gordon equation. Here we take the nonlinear Klein-Gordon equation to illustrate this method. The equivalent equations of (1) are

$$v_t - w_x + F'(u) = 0, \quad u_t = v, \quad u_x = w. \tag{30}$$

Introduce a new variable $v_t = p$, we can rewrite the above equations into a combination of two ordinary differential equations (ODEs).

$$\frac{d}{dt}v = p, \quad \frac{d}{dt}u = v; \tag{31}$$

$$\frac{d}{dx}w = p + F'(u), \quad \frac{d}{dx}u = w. \tag{32}$$

Discreting the two ODEs (31) and (32), then we can obtain the numerical algorithms for the PDEs by combining the two discreted ODEs. This method is called the concatenating method in the sense that it concatenates different numerical algorithms for ODEs. In practical computations, all the introduced variables will be eliminated in order not to increase the computing costs. Thus the large number of resulting algorithms for ODEs can be used to construct algorithms for PDEs by this method. In this paper, we intend to use this method to construct local SPAs. In order to make the resulting algorithms constructed by the concatenating method preserve the local conservation laws, we first study the properties of some difference operators and some special algorithms for ODEs.

5.1 Properties of some difference operators

Let

$$D_t f^j = \frac{f^{j+1} - f^j}{\tau}, \quad D_x f_i = \frac{f_{i+1} - f_i}{h}, \quad A_t f^j = \frac{f^{j+1} + f^j}{2}, \quad A_x f_i = \frac{f_{i+1} + f_i}{2},$$

then we have the following properties:

(i) Commutative law

$$D_x D_t = D_t D_x, \quad A_x A_t = A_t A_x, \quad DA = AD.$$

(ii) Chain rule

$$D_t G(u^j) = D_u G(u^j) D_t u^j + o(\Delta t); \quad D_x G(u_i) = D_u G(u_i) D_x u_i + o(\Delta x).$$

(iii) Generalized discrete Leibnitz rule

$$D_x(f \cdot g)_i = (af_{i+1} + (1-a)f_i) \cdot D_x g_i + D_x f_i \cdot ((1-a)g_{i+1} + ag_i), \quad \forall\, 0 \leqslant a \leqslant 1.$$

Some special cases for the generalized discrete Leibnitz rule are

$$a = 0, \quad D_x(f \cdot g)_i = f_i \cdot D_x g_i + D_x f_i \cdot g_{i+1},$$

$$a = \frac{1}{2}, \quad D_x(f \cdot g)_i = A_x f_i \cdot D_x g_i + D_x f_i \cdot A_x g_i,$$

$$a = 1, \quad D_x(f \cdot g)_i = f_{i+1} \cdot D_x g_i + D_x f_i \cdot g_i.$$

Deduction 1 of the discrete Leibnitz rule $D_x(\frac{1}{2}f_i^2) = D_x f_i \cdot A_x f_i$.

Deduction 2 of the discrete Leibnitz rule $D_x(\frac{1}{2}f_{i-1} \cdot f_i) = f_i \cdot A_x D_x f_{i-1}$.

Proof. Take $f = g$ in the discrete Leibnitz rule and apply the rule with $a = 1$, then we have

$$D_x\left(\frac{1}{2}f_{i-1} \cdot f_i\right) = \frac{1}{2}[f_i \cdot D_x f_i + D_x f_{i-1} \cdot f_i] = f_i \cdot \frac{1}{2}(D_x f_i + D_x f_{i+1}) = f_i A_x D_x f_i.$$

Remark 1. In property (i), the law $AD = DA$ is valid for any combinations of the subscripts t and x.

Remark 2. The proof of the generalized discrete Leibnitz rule can be obtained by the extending its right terms. It is also valid, as well as are the deductions in the t direction. In fact, they are valid provided that the product "$\cdot$" is bilinear. For example, the product may be the wedge product and then f, g are the differential one-forms.

$$D_x(dv \wedge du)_i = (adv_{i+1} + (1-a)dv_i) \wedge D_x du_i + D_x dv_i \wedge ((1-a)du_{i+1} + adu_i). \tag{33}$$

Moreover, they are also valid for some other difference operators such as the central difference operator.

Remark 3. The importance of the Leibnitz rule is well known and it is a basic tool for principle mathematics, while the discrete one is ignored by most people. It is actually the key to study and derive the numerical schemes, especially the SPAs. We will see its key feature in the following discussions. Sometimes, it is the difference between the Leibnitz rule and the discrete one to bring troubles in derivation of SPAs.

Consider the canonical Hamiltonian equations

$$\frac{d}{dt}p = H_q(p,q), \quad \frac{d}{dt}q = -H_q(p,q).$$

and their discrete form

$$\begin{aligned} D_t p_i &= H_q((1-a)p_{i+1} + ap_i, aq^{i+1} + (1-a)q^i), \\ D_t q_i &= -H_p((1-a)p_{i+1} + ap_i, aq^{i+1} + (1-a)q^i), \end{aligned}$$

The corresponding discrete variation equations are

$$\begin{aligned} D_t dp_i &= H_{qp} \cdot ((1-a)dp_{i+1} + adp_i) + H_{qq} \cdot (adq^{i+1} + (1-a)dq^i), \\ D_t dq_i &= -H_{pp} \cdot ((1-a)dp_{i+1} + adp_i) + H_{pq} \cdot (adq^{i+1} + (1-a)dq^i). \end{aligned} \tag{34}$$

By the discrete Leibnitz rule, we have

$$D_t\omega_i = D_t(dp_i \wedge dq_i) = ((1-a)dp^{i+1} + adp^i) \wedge D_t q_i + D_t dp^i \wedge (adq^{i+1} + (1-a)dq^i),$$

and then the symplectic conservation law by the (34), $D_t\omega_i = 0$. Note that the discrete Leibnitz rule is a key point in this simplified prove of the symplectic scheme.

5.2 Some basic algorithms for ODEs

For the sake of later discussion, we here present two basic symplectic schemes and two energy-conserving schemes for ODEs. The detailed discussion of those schemes can be found in the

relative papers or textbooks. The separated Hamiltonian system whose Hamiltonian function is the sum of several depended functions is

$$\frac{d}{dt}p = f(q), \qquad \frac{d}{dt}q = g(p). \tag{35}$$

Its Leap-frog scheme is

$$D_t p_i = f(q_i), \qquad D_t q_i = g(p_{i+1}). \tag{36}$$

The general forms of this scheme are the multi-stage explicit symplectic schemes and the Partition-Runge-Kutta methods.

Its central point Euler scheme is

$$D_t p_i = f(A_t q_i), \qquad D_t q_i = g(A_t p_i). \tag{37}$$

The general forms of this scheme are the symplectic Runge-Kutta method in type of Gauss-collocation.

The first-order energy-conserving scheme for the canonical Hamiltonian system is

$$\begin{aligned} D_t p_i &= -D_q(p_i, q^i) = -\frac{H(p_i, q^{i+1}) - H(p_i, q^i)}{q^{i+1} - q^i}, \\ D_t q^i &= D_p(p_{i+1}, q^{i+1}) = \frac{H(p_{i+1}, q^{i+1}) - H(p_i, q^{i+1})}{p_{i+1} - p_i}, \end{aligned}$$

which was first proposed by Fen and the second order one is

$$\begin{aligned} D_t p_i &= -D_q A_p H(p_i, q^i) \\ &= -D_q \frac{1}{2}\big[H(p_{i+1}, q^i) + H(p_i, q^i)\big] \\ &= -\frac{1}{2}\Big[\frac{H(p_{i+1}, q^{i+1}) - H(p_{i+1}, q^i)}{q^{i+1} - q^i}\Big] - \frac{1}{2}\Big[\frac{H(p_i, q^{i+1}) - H(p_i, q^i)}{q^{i+1} - q^i}\Big] \\ D_t q^i &= D_p A_q H(p_i, q^i) \\ &= D_p \frac{1}{2}\big[H(p_i, q^{i+1}) + H(p_i, q^i)\big] \\ &= \frac{1}{2}\frac{H(p_{i+1}, q^{i+1}) - H(p_i, q^{i+1})}{p_{i+1} - p_i} + \frac{1}{2}\frac{H(p_{i+1}, q^i) - H(p_i, q^i)}{p_{i+1} - p_i}, \end{aligned}$$

which was first proposed by Qin in [30]. We will use the above algorithms to concatenate the local SPAs for the PDEs in the next discussion. The derived algorithms are in low order. How to get high order local SPAs, for example the third-order or fourth-order local energy-conserving algorithm is still open.

5.3 Construction of multisymplectic schemes

We first take insight of the process of the derivation of the multisymplectic conservation law. The variation equations for (30) are

$$dv_t - dw_x + F''(u)du = 0, \quad du_t = dv, \quad du_x = dw. \tag{38}$$

Take the wedge product of the first line of (38) by du, we have $dv_t \wedge du - dw_x \wedge du = 0$. By the Leibnitz rule and the second line of (38),

$$\frac{\partial}{\partial t}(dv \wedge du) = \frac{\partial}{\partial t}dv \wedge du + dv \wedge \frac{\partial}{\partial t}du = \frac{\partial}{\partial t}dv \wedge du + dv \wedge dv = \frac{\partial}{\partial t}dv \wedge du.$$

Similarly, $\frac{\partial}{\partial x}(dw \wedge du) = \frac{\partial}{\partial x} dw \wedge du$.

Thus we obtain the multisymplectic conservation law $\partial_t[du \wedge dv] - \partial_x[du \wedge dw] = 0$.

5.3.1 Multisymplectic scheme I

Discreting (31) and (32) by using the Leap-frog scheme, we have

$$D_t v_i^j = p_i^j, \quad D_t u_i^j = v_i^{j+1}, \tag{39}$$

and

$$D_x w_i^j = P_i^j + F'(u_i^j), \quad D_x u_i^j = w_{i+1}^j. \tag{40}$$

Combining (39) and (40) yields a multisymplectic scheme for the multisymplectic equations (30). If the auxiliary variable p_i^j is eliminated, we get its equivalent scheme as

$$D_t v_i^j - D_x w_i^j + F'(u_i^j) = 0, \quad D_t u_i^j = v_i^{j+1}, \quad D_x u_i^j = w_{i+1}^j. \tag{41}$$

Further eliminating the variables v and w leads to the classical five-point scheme,

$$D_t^2 u_i^{j-1} - D_x^2 u_{i-1}^j + F'(u_i^j) = 0. \tag{42}$$

Next we prove that the five-point scheme is a multisymplectic scheme. The proof of the process is nearly same as the one of derivation of the continuous conservation law.

By (41),

$$D_t dv_i^j - D_x dw_i^j + F''(u_i^j) du_i^j = 0, \quad D_t du_i^j = dv_i^{j+1}, \quad D_x du_i^j = dw_{i+1}^j. \tag{43}$$

Taking the wedge product of the first line of (43) by du_i^j, we have $D_t dv_i^j \wedge du_i^j - D_x dw_i^j \wedge du_i^j = 0$. By the discrete Leibnitz rule,

$$\begin{aligned} D_t(dv_i^j \wedge du_i^j) &= D_t dv_i^j \wedge du_i^j + dv_i^{j+1} \wedge D_t du_i^j \\ &= D_t dv_i^j \wedge du_i^j + dv_i^{j+1} \wedge dv_i^{j+1} \\ &= D_t dv_i^j \wedge du_i^j. \end{aligned}$$

Similarly, $D_x(dw_i^j \wedge du_i^j) = D_x dw_i^j \wedge du_i^j$, then we obtain the discrete multisymplectic conservation law $D_t(dv_i^j \wedge du_i^j) - D_x(dw_i^j \wedge du_i^j) = 0$.

5.3.2 Multisymplectic scheme II

Discreting (31) and (32) by the central point Euler scheme and eliminate the variable p in the combined scheme, we then get the Preissman scheme

$$D_t A_x v_i^j - D_x A_t w_i^j + F'(A_x A_t u_i^j) = 0, \quad D_t u_i^j = A_t v_i^j, \quad D_x u_i^j = A_x w_i^j. \tag{44}$$

Further eliminating the variables v and w, we obtain the nine-point scheme proposed in [23],

$$D_t^2 A_x^2 u_i^j - D_x^2 A_t^2 u_i^j + A_x A_t F'(A_x A_t u_i^j) = 0,$$

with the discrete multisymplectic conservation law

$$D_t(A_x dv_i^j \wedge A_t du_i^j) - D_x(A_t dw_i^j \wedge A_t du_i^j) = 0.$$

5.3.3 Multisymplectic scheme III

Discreting (31) by the Leap-frog scheme and (32) by the central point Euler scheme, we then have

$$D_t v_i^j = p_i^j, \quad D_t u_i^j = v_i^{j+1}, \tag{45}$$

$$D_x w_i^j = A_x p_i^j + F'(A_x u_i^j), \quad D_x u_i^j = A_x w_i^j. \tag{46}$$

Combining (45) and (46) yields a multisymplectic scheme. The equivalent scheme of the resulting scheme is as follows if the variable p is eliminated:

$$D_t A_x v_i^j - D_x w_i^j + F'(A_x u_i^j) = 0, \tag{47}$$

$$D_t u_i^j = v_i^{j+1}, \tag{48}$$

$$D_x u_i^j = A_x w_i^j. \tag{49}$$

Further eliminating v and w, we derive a explicit nine-point scheme

$$A_x^2 D_t^2 u_i^{j-1} - D_x^2 u_i^j + A_x F'(A_x u_i^j) = 0.$$

Taking the differential operator on (47), we get

$$D_t A_x dv_i^j - D_x dw_i^j + F''(A_x du_i^j) A_x du_i^j = 0,$$

which leads to, if taken wedge product by $A_x du_i^j$

$$D_t A_x dv_i^j \wedge A_x du_i^j - D_x dw_i^j \wedge A_x du_i^j = 0. \tag{50}$$

By the time t with $a = 1$ and (48),

$$\begin{aligned} D_t(A_x dv_i^j \wedge A_x du_i^j) &= D_t A_x dv_i^j \wedge A_x du_i^j + A_x dv_i^{j+1} \wedge D_t A_x du_i^j \\ &= D_t A_x dv_i^j \wedge A_x du_i^j + A_x dv_i^{j+1} \wedge A_x dv_i^{j+1} \\ &= D_t A_x dv_i^j \wedge A_x du_i^j, \end{aligned} \tag{51}$$

while by the discrete Leibnitz on space x with $a = \frac{1}{2}$ and (49), we have

$$\begin{aligned} D_t(dw_i^j \wedge du_i^j) &= A_x dw_i^j \wedge D_x du_i^j + D_x dw_i^j \wedge A_x du_i^j \\ &= D_x du_i^j \wedge D_x du_i^j + D_x dw_i^j \wedge A_x du_i^j \\ &= D_x dw_i^j \wedge A_x du_i^j. \end{aligned} \tag{52}$$

Substituting (51) and (52) into (50) yields the discrete multisymplectic conservation law

$$D_t(A_x dv_i^j \wedge A_x du_i^j) - D_x(dw_i^j \wedge du_i^j) = 0.$$

Thus we prove the explicit nine-point scheme and its equivalent scheme are multisymplectic.

5.3.4 Multisymplectic scheme IV

Discreting (31) by the central-point Euler scheme and (32) by the Leap-frog scheme, then we have

$$D_t v_i^j = A_t p_i^j, \quad D_t u_i^j = A_t v_i^j, \tag{53}$$

and

$$D_x A_t w_i^j = A_t p_i^j + F'(A_t u_i^j), \quad D_x u_i^j = w_{i+1}^j. \tag{54}$$

Eliminating the variable p_i^j yields a multisymplectic scheme

$$D_t v_i^j - D_x A_t w_i^j + F'(A_t u_i^j) = 0, \tag{55}$$

$$D_t u_i^j = A_t v_i^j, \tag{56}$$

$$D_x u_i^j = w_{i+1}^j. \tag{57}$$

Further eliminating v and w, we derive another nine-point scheme,

$$D_t^2 u_i^j - A_t^2 D_x^2 u_{i-1}^j + A_t F'(A_t u_i^j) = 0$$

with the discrete multisymplectic conservation law

$$D_t(dv_i^j \wedge du_i^j) - D_x(A_t dw_i^j \wedge A_t du_i^j) = 0.$$

5.4 Construction of the local energy-conserving algorithms

Again we see the detailed process of derivation of the local energy conservation law. By (30),

$$\begin{aligned}
&v_t - w_x + F'(u) = 0,\\
&\quad\Longrightarrow v_t - w_x + \frac{F_t}{u_t} = 0,\\
&\quad\Longrightarrow v_t u_t - w_x u_t + F_t = 0,\\
&\quad\Longrightarrow v_t v + F_t = w_x v,\\
&\quad\Longrightarrow \frac{\partial}{\partial t}\left[\frac{1}{2}v^2 + \frac{1}{2}w^2 + F\right] = w_x v + w w_t = w_x v + u_{xt} = w_x v + w v_x = \frac{\partial}{\partial x}(wv).
\end{aligned}$$

The chain rule, communicative law and the Leibnitz rule of the differential operator are used in the above process.

5.4.1 Local energy-conserving scheme I

Discreting both equations by using the Leap-frog scheme and the nonlinear term by using the discrete chain rule in time t and eliminating the auxiliary variable p, we then get a scheme

$$D_t v_i^j - D_x w_i^j + D_u(A_t F_i^{j-1}) = 0, \quad D_t u_i^j = v_i^{j+1}, \quad D_x u_i^j = w_{i+1}^j, \tag{58}$$

where $D_u(A_t F_i^{j-1}) = \frac{D_t(A_t F_i^{j-1})}{D_t(A_t u_i^{j-1})}$.

Further eliminating v and w yields the well-know energy-conserving scheme (7)

$$D_t^2 u_i^{j-1} - D_x^2 u_{i-1}^j + \frac{D_t(A_t F_i^{j-1})}{D_t(A_t u_i^{j-1})} = 0.$$

Multiply the first line of (58) by $D_t A_t u_i^{j-1}$,

$$D_t v_i^j D_t A_t u_i^{j-1} - D_x w_i^j D_t A_t u_i^{j-1} + D_t A_t F_i^{j-1} = 0, \tag{59}$$

$$D_t v_i^j A_t v_i^j + D_t A_t F_i^{j-1} = D_x w_i^j D_t A_t u_i^{j-1}, \tag{60}$$

$$D_t\left(\frac{1}{2}(v_i^j)^2 + A_t F_i^{j-1}\right) = D_x w_i^j A_t v_i^j, \tag{61}$$

$$D_t\left(\frac{1}{2}(v_i^j)^2 + A_t F_i^{j-1}\right) + w_{i+1}^j D_x A_t v_i^j = D_x w_i^j A_t v_i^j + w_{i+1}^j D_x A_t v_i^j, \tag{62}$$

$$D_t\left(\frac{1}{2}(v_i^j)^2 + A_t F_i^{j-1}\right) + w_{i+1}^j D_x A_t v_i^j = D_x(w_i^j A_t v_i^j), \tag{63}$$

$$D_t\left(\frac{1}{2}(v_i^j)^2 + A_t F_i^{j-1}\right) + w_{i+1}^j A_t D_t w_{i+1}^{j-1} = D_x(w_i^j A_t v_i^j), \tag{64}$$

$$D_t\left[\frac{1}{2}(v_i^j)^2 + \frac{1}{2}w_{i+1}^{j-1}w_{i+1}^j + A_t F_i^{j-1}\right] = D_x(w_i^j A_t v_i^j). \tag{65}$$

The last line is the discrete local energy conservation law. In the above derivations, we use (58) in (60) and Deduction 1 of discrete Leibnitz rule in (61), add the same term on both sides of (62), and use the discrete Leibnitz rule with $a = 0$ in (63), the communicative law of the difference operator and (58) in (64) and Deduction 2 of discrete Leibnitz rule in (65).

5.4.2 Local energy-conserving scheme II

Discreting (31) in time t direction by using central point scheme and (32) by the Leap-frog scheme, we then get

$$D_t v_i^j = A_t p_i^j, \quad D_t u_i^j = A_t v_i^j, \tag{66}$$

$$D_x A_t w_i^j = A_t p_i^j + D_u A_t F(u_i^j), \quad D_x u_i^j = w_{i+1}^j, \tag{67}$$

where, $D_u A_t F(u_i^j) = \frac{D_t F_i^j}{D_t u_i^j}$.

Combining (66) and (67) yields a scheme. Eliminating p leads to its equivalent scheme

$$D_t v_i^j - D_x A_t w_i^j + \frac{D_t F_i^j}{D_t u_i^j} = 0, \quad D_t u_i^j = A_t v_i^j, \quad D_x u_i^j = w_{i+1}^j.$$

Further eliminating v and w, we arrive at the scheme discussed by Lov Vu-quoc in [19],

$$A_t D_t^2 u_i^j - A_t^2 D_x^2 u_{i-1}^j + A_t \frac{D_t F_i^j}{D_t u_i^j} = 0$$

with the local energy conservation law

$$D_t\left[\frac{1}{2}(v_i^j)^2 + \frac{1}{2}(w_{i+1}^j)^2 + F_i^j\right] = D_x(A_t w_i^j A_t v_i^j).$$

5.4.3 Local energy-conserving scheme III

Discreting the two equations by the central point Euler scheme, we then have

$$D_t A_x v_i^j - D_x A_t w_i^j + \frac{D_t F(A_x u_i^j)}{D_t A_x u_i^j} = 0, \quad D_t u_i^j = A_t v_i^j, \quad D_x u_i^j = A_x w_i^j. \tag{68}$$

Eliminating v and w, we derive a new scheme

$$D_t^2 A_x^2 u_i^j - D_x^2 A_t^2 u_i^j + A_t A_x \frac{D_t F(A_x u_i^j)}{D_t A_x u_i^j} = 0 \tag{69}$$

with the local energy conservation law

$$D_t\left(\frac{1}{2}(A_x v_i^j)^2 + \frac{1}{2}(A_x w_i^j)^2 + F(A_x u_i^j)\right) = D_x(A_t v_i^j A_t w_i^j).$$

5.5 Construction of the local momentum-conserving algorithms

The process of the derivation of the local momentum conservation law is as follows. By (30) and the chain rule $F'(u)u_x = F_x$,

$$
\begin{aligned}
&v_t - w_x + \frac{F_x}{u_x} = 0, \quad v_t u_x - w_x u_x + F_x = 0, \quad v_t w = w_x w - F_x,\\
&v_t w + v w_t = w_x w - F_x + v w_t, \quad v_t w + v w_t = w_x w - F_x + v v_x,\\
&\frac{\partial}{\partial t}(vw) = \frac{\partial}{\partial x}\left(\frac{1}{2}w^2 + \frac{1}{2}v^2 - F(u)\right).
\end{aligned}
$$

Again we use the chain rule, communicative law and the Leibnitz rule of the differential operator in the derivation

5.5.1 Local momentum-conserving scheme I

Discreting the two equations by using the Leap-frog scheme, taking $D_u F(u_{i-1}^j) = \frac{A_x D_x F_{i-1}^j}{A_x D_x u_{i-1}^j}$ and eliminating the auxiliary variable p in the combined scheme, we then have

$$D_t v_i^j - D_x w_i^j + \frac{A_x D_x F_{i-1}^j}{A_x D_x u_{i-1}^j} = 0, \tag{70}$$

$$D_t u_i^j = v_i^{j+1}, \tag{71}$$

$$D_x u_i^j = w_{i+1}^j. \tag{72}$$

Further eliminating v and w leads to the well-known momentum-conserving scheme (9),

$$D_t^2 u_i^{j-1} - D_x^2 u_{i-1}^j + \frac{A_x D_x F_{i-1}^j}{A_x D_x u_{i-1}^j} = 0. \tag{73}$$

The proof of its local conservation property is as follows:

$$
\begin{aligned}
&(D_t v_i^j - D_x w_i^j) A_x D_x u_{i-1}^j + A_x D_x F_{i-1}^j = 0,\\
&(D_t v_i^j - D_x w_i^j) A_x w_i^j + A_x D_x F_{i-1}^j = 0,\\
&D_t v_i^j A_x w_i^j = D_x w_i^j A_x w_i^j - A_x D_x F_{i-1}^j,\\
&D_t v_i^j A_x w_i^j = D_x \left(\frac{1}{2} w_i^j\right)^2 - A_x D_x F_{i-1}^j,\\
&D_t v_i^j A_x w_i^j + v_i^{j+1} D_t A_x w_i^j = D_x \left(\frac{1}{2} w_i^j\right)^2 + v_i^{j+1} D_t A_x w_i^j - A_x D_x F_{i-1}^j,\\
&D_t (v_i^j A_x w_i^j) = D_x \left(\frac{1}{2} w_i^j\right)^2 + v_i^{j+1} D_t A_x w_i^j - A_x D_x F_{i-1}^j,\\
&D_t (v_i^j A_x w_i^j) = D_x \left(\frac{1}{2} w_i^j\right)^2 + v_i^{j+1} D_t A_x D_x u_{i-1}^j - A_x D_x F_{i-1}^j,\\
&D_t (v_i^j A_x w_i^j) = D_x \frac{1}{2} (w_i^j)^2 + v_i^{j+1} D_x A_x v_{i-1}^{j+1} - A_x D_x F_{i-1}^j,\\
&D_t (v_i^j A_x w_i^j) = D_x \left[\left(\frac{1}{2} w_i^j\right)^2 + \frac{1}{2} v_{i-1}^{j+1} v_i^{j+1} - A_x F_{i-1}^j\right].
\end{aligned}
$$

The last line is the discrete local momentum conservation law for the scheme (73).

5.5.2 Local momentum-conserving scheme II

Discreting (31) by the Leap-frog scheme and (32) by the central point scheme, and eliminating the auxiliary variable in the combined scheme, we then have

$$D_t A_x v_i^j - D_x w_i^j + \frac{D_x F_i^j}{D_x u_i^j} = 0, \tag{74}$$

$$D_t u_i^j = v_i^{j+1}, \tag{75}$$

$$D_x u_i^j = A_x w_i^j. \tag{76}$$

Further eliminating v and w yields a new scheme

$$D_t^2 A_x^2 u_i^{j-1} - D_x^2 u_i^j + A_x \frac{D_x F(u_i^j)}{D_x u_i^j} = 0. \tag{77}$$

We then prove that it is a local SPA. By (74),

$$\begin{aligned}
&D_t A_x v_i^j D_x u_i^j - D_x w_i^j D_x u_i^j + D_x F_i^j = 0,\\
&D_t A_x v_i^j A_x w_i^j - D_x w_i^j A_x w_i^j + D_x F_i^j = 0,\\
&D_t A_x v_i^j A_x w_i^j + A_x v_i^{j+1} D_t A_x w_i^j = D_x w_i^j A_x w_i^j + A_x v_i^{j+1} D_t A_x w_i^j - D_x F_i^j.
\end{aligned}$$

Using the deduction of the discrete Leibnitz rule, we can obtain the discrete local momentum conservation law with help of (75) and (76),

$$\begin{aligned}
D_t(A_x v_i^j A_x w_i^j) &= D_x \frac{1}{2}(w_i^j)^2 + A_x v_i^{j+1} D_t D_x u_i^j - D_x F_i^j\\
&= D_x \frac{1}{2}(w_i^j)^2 + A_x v_i^{j+1} D_x v_i^{j+1} - D_x F_i^j\\
&= D_x \left[\frac{1}{2}(w_i^j)^2 + \frac{1}{2}(v_i^{j+1})^2 - F(u_i^j)\right].
\end{aligned} \tag{78}$$

5.5.3 Local momentum-conserving scheme III

Discreting both equations with the central point scheme, we have

$$\begin{aligned}
&D_t v_i^j = A_t p_i^j, \quad D_t u_i^j = A_t v_i^j,\\
&D_x A_t w_i^j = A_t A_x p_i^j + \frac{D_x F(A_t u_i^j)}{D_x A_t u_i^j}, \quad D_x u_i^j = A_x w_i^j.
\end{aligned}$$

Combining the above two discretes and Eliminating p yield

$$D_t A_x v_i^j - D_x A_t w_i^j + \frac{D_x F(A_t u_i^j)}{D_x A_t u_i^j} = 0, \tag{79}$$

$$D_t u_i^j = A_t v_i^j, \tag{80}$$

$$D_x u_i^j = A_x w_i^j. \tag{81}$$

Further eliminating v and w, we obtain a new scheme

$$D_t^2 A_x^2 u_i^j - D_x^2 A_t^2 u_i^j + A_t A_x \frac{D_x F(A_t u_i^j)}{D_x A_t u_i^j} = 0.$$

The derivation of the its local property is as follows.

By (79)

$$D_t A_x v_i^j D_x A_t u_i^j - D_x A_t w_i^j D_x A_t u_i^j + D_x F(A_t u_i^j) = 0.$$

Substituted by (81), then

$$D_t A_x v_i^j A_t A_x w_i^j - D_x A_t w_i^j D_x A_t u_i^j + D_x F(A_t u_i^j) = 0. \tag{82}$$

By the discrete Leibnitz rule, we have

$$D_t(A_x v_i^j A_x w_i^j) = A_t A_x v_i^j D_t A_x w_i^j + D_t A_x v_i^j A_t A_x w_i^j.$$

By (80) and (81), we get $D_x A_t v_i^j = D_t A_x w_i^j$. Then (82) becomes

$$\begin{aligned} D_t(A_x v_i^j A_x w_i^j) &= A_t A_x v_i^j D_t A_x w_i^j + D_x A_t w_i^j A_t A_x w_i^j - D_x F(A_t u_i^j) \\ &= \frac{1}{2} D_x (A_t v_i^j)^2 + \frac{1}{2} D_x (A_t w_i^j)^2 - D_x F(A_t u_i^j) \\ &= D_x \left[\frac{1}{2} (A_t v_i^j)^2 + \frac{1}{2} (A_t w_i^j)^2 - F(A_t u_i^j) \right]. \end{aligned} \tag{83}$$

It means that this scheme is a local SPA.

Under the homogeneous or periodic boundary condition, we can get the corresponding discrete global conservation laws if we sum all the above discrete local conservation laws over the space grids. That is to say, all the local SPAs we constructed here are the global SPAs. For example, if we sum the local conservation law (83) over the space grids, we can obtain the original global discrete momentum conservation law $D_t M = D_t \sum_D A_x v_i^j \cdot A_x w_i^j = 0$.

Remark 4. For the limit of the paper, we just use some simple algorithms for the ODEs to illustrate the concatenating method. We did not present all the detail processes and prove some local SPAs, because they are similar to the other ones. We may get more local SPAs if some other algorithms are used to be concatenated.

6 An numerical example

For comparison, we use the line method to construct a symplectic algorithm for the Klein-Gordon equation. Using the fourth-order symmetric difference operator to discrete the differential operator on space to guarantee the resulting ODEs of a Hamiltonian system and then applying the first-order explicit symplectic to discrete the Hamiltonian system[30], we obtain a symplectic scheme

$$\delta_t^2 u_n^m - \frac{-u_{n+2}^m + 16u_{n+1}^m - 30u_n^m + 16u_{n-1}^m - u_{n-2}^m}{h^2} + f(u_n^m) = 0 \tag{84}$$

with the truncation error $O(\tau^2) + O(h^4)$. According to the construction theory of the multi-symplectic schemes, this scheme is not a multi-symplectic scheme because the space discrete is not symplectic. We use the symplectic scheme (84) and multisymplectic scheme (42) to simulate the oscillation wave of the nonlinear Klein-Gordon equation with the periodic boundary condition and initial values $u(x, 0) = A(1 + \cos(2\pi/L))$, $L = 1.28$. The time step and space step for both schemes are taken as $\tau = 0.005$ and $h = 1.28/99$ respectively. The amplitude is

taken as $A = 30$. Figure 2 shows the numerical results. As we can see from Figure 2, the multisymplectic scheme gives very reasonable numerical waves all the time, whereas the symplectic scheme shows the blow-up at time $t = 2.3$. It is worthy to mention that the accuracy order the multisymplectic five-point scheme is $O(\tau^2) + O(h^2)$ only.

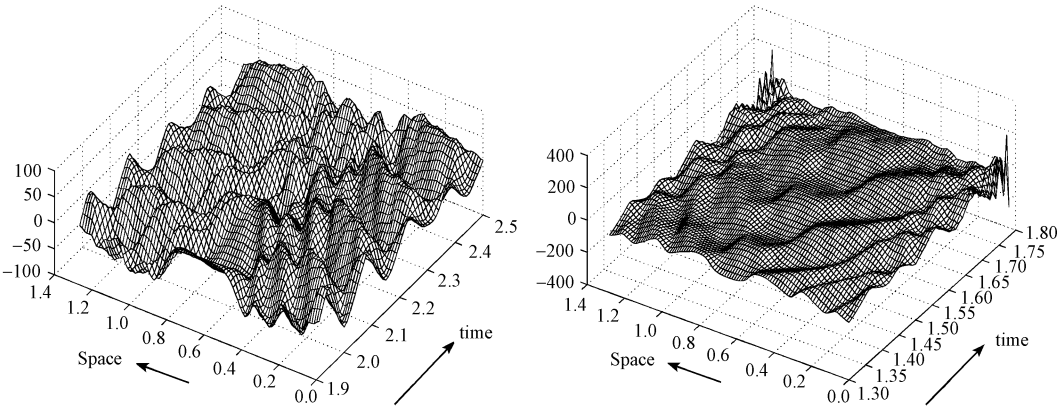

Figure 2 Numerical waves with a large amplitude for the Klein-Gordon equations. The left is obtained by the multisymplectic scheme and the right is by the symplectic one

The above numerical experiment is just an example, and from it we cannot draw the general conclusion that the local SPAs are superior to the global ones. More experiments should be carried on this topic.

7 Conclusion and discussion

Inspired by the idea of the SPAs, we propose the concept of the local SPAs for PDEs. The local SPAs are the natural generalization of the original global SPAs for PDEs. The concept of the local SPAs covers all kinds of the original global SPAs and can provide a basic theory to analyze, construct and classify the SPAs. For example, the energy-conserving algorithms for PDEs can be divided into two categories. One category has the local properties and the other has not. Thus the concept of the local SPAs also discovers some reasons for the difference between different SPAs. Another main advantage of local SPAs is to overcome the shortage of the SPAs on the boundary conditions. The local SPAs can be applied to any conservative systems with whatever kind of boundary conditions. It enlarges largely the application areas of the SPAs and gives a good interpretation on why some SPAs can perform very well without proper boundary conditions. We also show that a large number of elliptic equations, as well as the hyperbolic equations, can be integrated by the local SPAs. It inspires us to go back to define a symplectic algorithm for the non-evolutionary equations. The idea of the symplectic algorithms to preserve the structure statically on space regions accords just with the idea of [31].

At last, we would like to point out that some PDEs may have infinite local conservation laws, similar to the infinite first integrals. The nonlinear Klein-Gordon equation with homogeneous or periodic boundary condition also has the angular momentum first integral,

$$\frac{dA}{dt} = 0, \quad A = \int \frac{1}{2}(v^2 + w^2)x + wvt + F(u)x \, dx.$$

Equally, it has the local angular momentum conservation law which does not depend on any boundary condition,

$$\partial_t\left(\frac{1}{2}(v^2+w^2)x+wvt+F(u)x\right)+\partial_x\left(-vwx-\frac{1}{2}(v^2+w^2)t+F(u)t\right)=0.$$

How to construct local SPAs to preserve this local property is still unanswered.

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