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The Splitting Multisymplectic Numerical Methods for Hamiltonian Systems

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Abstract: For Hamiltonian systems, symplectic integrators or multisymplectic integrators are superior to traditional numerica methods for Hamiltonian systems. However, most of them are implicit and engender a coupled nonlinear algebraic system at every time step. It leads to reduce the computational efficiency directly. Splitting multisymplectic integrator which combines multisymplectic integrators with splitting technique can offset this flaw. The framework of this numerical method will be briefly reviewed. Some numerical examples are shown to illustrate the application of the methods in physics.

Key words: splitting method; multisymplectic integrator; computational efficiency; Hamiltonian system

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0 Introduction

Symplectic integrators have been applied to many contexts (such as quantum mechanics, astronomy) since they were first established systematically by Feng in 1984 [1]. For this kind of numerical methods, a lot of theoretical progresses and applications are made during the last three decades [2-3]. It was extended to multisymplectic background by Marsden, Reich & Bridges at the end of last century [4-6], in other words, we did not only consider symplectic structures in time, but also in space direction. Now, multisymplectic integrators (MIS) are widely used to solve mathematical models with multisymplectic structures [6,7-10].

However, to preserve the multisymplectic conservation law which is the naturalistic character of the original Hamiltonian system (HS), an undesirable and intrinsic feature of this kind of methods is their implicity for inseparable HS. This leads to solve a nonlinear algebraic system for nonlinear problems, and huge scale algebraic system for multidimensional problems. For example, to numerically solve 3D Gross Pitavskii equation in Bose-Einstein Condensates by MIs, we divide the spatial domain in each direction with 100 parallel lines. Then a 10^6 scale nonlinear algebraic system need be solved at every time step. It is very difficult to finish such a duty by general PC. This drawback will greatly narrow the application of MIs and reduce the computational efficiency [10-14].

To repair this deficiency and widen the applicable fields of MIs, we proposed a novel kind of MIs which is said to be splitting multisymplectic integrator (SMI) [11-13,15-20]. The main idea underlying this kind of methods is just to use splitting technique to resolve the difficulty. In other words, we split the original HS into several sub systems which are symplectic or multisymplectic. Each of the sub HS should be easier to solve than the original one. Then we approximate them by symplectic methods or MIs. For example, we can split a nonlinear PDE into one or more linear PDEs and nonlinear PDEs [11,15]. We can also decompose a multidimensional PDE into several local one-dimensional PDEs [12-13]. The splitting is very flexible.

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The multisymplectic Hamiltonian partial differential equation with m-dimensional spatial variables reads

$$\boldsymbol{M}z_t + \sum_{i=1}^{m} \boldsymbol{K}_i z_{x_i} = \nabla_z S(z), \quad (1)$$

where $\boldsymbol{M}$ and $\boldsymbol{K}_i$ are skew-symmetric matrices, and $S(z)$ is some smooth function which is called Hamiltonian function. Taking variational formulation of this form, we can get the following multisymplectic conservation law (MSCL)

$$\frac{\partial}{\partial t}\omega + \sum_{i=1}^{m} \frac{\partial}{\partial x_i}\kappa_i = 0,$$

with symplectic forms $\omega = \mathrm{d}z \wedge \boldsymbol{M}\mathrm{d}z, \kappa_i = \mathrm{d}z \wedge \boldsymbol{K}_i \mathrm{d}z$. Furthermore, for the multi-symplectic system, there is local energy conservation law

$$\frac{\partial}{\partial t}P(z) + \nabla \cdot Q(z) = 0,$$

if $S(z)$ is autonomous, with the energy density $P(z) = S(z) - \frac{1}{2}\sum_{i=1}^{m} z^{\mathrm{T}}\boldsymbol{K}_i z_{x_i}$, and energy flux $Q(z) = \frac{1}{2}(z^{\mathrm{T}}\boldsymbol{K}_1 z_t, z^{\mathrm{T}}\boldsymbol{K}_2 z_t, \cdots, z^{\mathrm{T}}\boldsymbol{K}_m z_t)^{\mathrm{T}}$.

Details about symplectic and multisymplectic background for (1), we refer to [1-4,6-10] and we will omit them to save the length of the paper. In this review, we will illustrate the SMIs for 1D case and multidimensional case.

This paper is organized as follows: In Section 1, brief overview on splitting method will be reported. Section 2 focuses on SMIs for 1D multisymplectic systems. In Section 3, the SMI for multidimensional multisymplectic system, that is, LOD-MI will be presented. Some conclusions and remarks will be drawn to end the paper.

1 Splitting Method

As is stated in the previous section, the main idea of splitting multisymplectic integrators (SMI) is to combine MIs with splitting technique, here a short retrospection of the splitting method will be performed. The starting point of splitting method is to decompose the original problem into several easier subproblems. Then the subproblems will be solved one by one exactly or numerically. The solver of one subproblem is employed as the initial data of the following one.

For the formal ordinary differential equation with initial data

$$\frac{\partial}{\partial t}u(x,t) = \mathscr{A}u(x,t) = (\mathscr{L} + \mathscr{N})u(x,t),$$
$$u(x,0) = u_0(x), \quad (2)$$

where $\mathscr{A}, \mathscr{L}$ and $\mathscr{N}$ are spatial operators, we have the formal solution

$$u(x,t) = \exp(t\mathscr{A})u_0(x) = \exp(t(\mathscr{L} + \mathscr{N}))u_0(x).$$

In practical computation, it is not easy to present the exponential operator $\exp(t(\mathscr{L} + \mathscr{N}))$ exactly or numerically. However, $\exp(t\mathscr{L})$ and $\exp(t\mathscr{N})$, which are formal solution operators of the simpler procedures

$$\frac{\partial}{\partial t}u(x,t) = \mathscr{L}u(x,t), \quad (3)$$

$$\frac{\partial}{\partial t}u(x,t) = \mathscr{N}u(x,t), \quad (4)$$

respectively, may be computed easier than problem (2). Unfortunately, $\exp(t(\mathscr{L} + \mathscr{N})) \neq \exp(t\mathscr{L})\exp(t\mathscr{N})$ except $\mathscr{L}$ and $\mathscr{N}$ are commutators. To find the approximate solution for the original problem, we can solve the simpler subproblems (3) and (4) one by one with an appropriate step sizes.

Suppose τ be the time step size, $t^n = n\tau$, the following two composition are often adopted.

• First-order splitting:

$$u(t^n) = \exp(t(\mathscr{L} + \mathscr{N}))u(t^{n-1}) \approx \exp(\tau\mathscr{L})\exp(\tau\mathscr{N})u(t^{n-1}) \approx [\exp(\tau\mathscr{L})\exp(\tau\mathscr{N})]^n u_0.$$

In this splitting, to get the solution u^{n+1}, we only need solve both subproblems (3) and (4) one time at every time step with full time step τ. It is suitable for parallel computing.

• Second-order splitting:

$$u(t^n) \approx \exp(\frac{\tau}{2}\mathscr{L})\exp(\tau\mathscr{L})u(t^{n-1}) \approx$$
$$\exp(\frac{\tau}{2}\mathscr{L})\exp(\tau\mathscr{N})\exp(\tau\mathscr{L})\exp(\tau\mathscr{N})\exp(\frac{\tau}{2}\mathscr{L}) \cdot u(t^{n-2}) \approx \exp(\frac{\tau}{2}\mathscr{L})[\exp(\tau\mathscr{N})\exp(\tau\mathscr{L})]^{n-1} \cdot \exp(\tau\mathscr{N})\exp(\frac{\tau}{2}\mathscr{L})u_0. \quad (5)$$

In the SMI context, it is required that the subproblems (3) and (4) be approximated by symplectic integrators or MIs. In this article, we consider nonlinear splitting [11,15-16] and local one-dimensional splitting [12-13,18,20].

2 Splitting MIs for 1D HS

To describe the main point SMIs for 1D HS, we consider the fourth-order nonlinear Schrödinger equation with a trapped term (FNSETT) [11]

$$\begin{aligned} &\mathrm{i}u_t + u_{xxxx} + 6|u|^2u - 150(\sin^2 x)u = 0,\\ &(x,t) \in (0,L) \times (0,T],\\ &u(x,0) = u_0(x), x \in [0,L],\\ &u(x,t) = u(x+L,t), t \in [0,T], \end{aligned} \tag{6}$$

where $u_0(x)$ is a prescribed complex-valued function.

We will only give a sketch of the method here, for detailed description we refer to [11,15].

Let $z = (p,q,\varphi,\alpha,\psi,\beta,\eta,\gamma)^{\mathrm{T}}$, we can get the multisymplectic Hamiltonian formulation of FNSETT (6) with Hamiltonian functional

$$S(z) = -\frac{3}{2}(p^2+q^2)^2 + 75\sin^2 x(p^2+q^2) + \frac{1}{2}(\psi^2+\beta^2) - \varphi\eta - \alpha\gamma,$$

and skew symmetric matrices

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

$$\boldsymbol{K} = \begin{bmatrix} 0 & -1 & 0 & 0 & 0 & 0 & 1 & 0\\ 1 & 0 & 0 & 0 & 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0\\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}. \tag{7}$$

We discretize the system by midpoint rules both in time and space,

$$\boldsymbol{M}\frac{z_{j+1/2}^{n+1} - z_{j+1/2}^{n}}{\tau} + \boldsymbol{K}\frac{z_{j+1}^{n+1/2} - z_{j}^{n+1/2}}{\tau} = \nabla_z S(z_{j+1/2}^{n+1/2}),$$

where $z_{j+1/2}^{n+1/2} = (z_{j+1/2}^{n+1} + z_{j+1/2}^{n})/2 = (z_{j+1}^{n+1/2} + z_{j}^{n+1/2})/2 = (z_{j+1}^{n+1} + z_{j+1}^{n} + z_{j}^{n+1} + z_{j}^{n})/4$. This scheme is of second-order both in time and space directions and can be coded in the following form

$$\frac{\mathrm{i}}{16}(\delta_t u_{j-2}^{n} + 4\delta_t u_{j-1}^{n} + 6\delta_t u_{j}^{n} + 4\delta_t u_{j+1}^{n} + \delta_t u_{j+2}^{n}) + \delta_x^4 u_j^{n+1/2} = -\frac{3}{4}(|u_{j-3/2}^{n+1/2}|^2 u_{j-3/2}^{n+1/2} + 3|u_{j-1/2}^{n+1/2}|^2 u_{j-1/2}^{n+1/2} + 3|u_{j+1/2}^{n+1/2}|^2 u_{j+1/2}^{n+1/2} + |u_{j+3/2}^{n+1/2}|^2 u_{j+3/2}^{n+1/2}) + \frac{75}{4}(\sin^2 x_{j-3/2} \cdot u_{j-3/2}^{n+1/2} + 3\sin^2 x_{j-1/2} u_{j-1/2}^{n+1/2} + 3\sin^2 x_{j+1/2} u_{j+1/2}^{n+1/2} + \sin^2 x_{j+3/2} u_{j+3/2}^{n+1/2}), \tag{8}$$

here δ_x^4 is the standard central difference quotient operator to ∂_{x^4}.

This scheme is very inefficient because a completely coupled nonlinear algebraic system needs to be solved at every time step. To improve the computational efficiency, we split the original FNSETT (6) into the linear subproblem and nonlinear subproblem

$$\mathrm{i}u_t = \mathscr{L}u = -u_{xxxx}, \tag{9}$$

$$\mathrm{i}u_t = \mathscr{N}u = 150(\sin^2 x)u - 6|u|^2u. \tag{10}$$

Then the linear subproblem (9) can be transferred into the multisymplectic form (1) with the same symplectic structure matrices (7), and different Hamiltonian function

$$S_1(z) = \frac{1}{2}(\psi^2+\beta^2) - \varphi\eta - \alpha\gamma.$$

The nonlinear subproblem (10) is Hamiltonian at every spatial point x with Hamiltonian function

$$S_2(z) = 75(\sin^2 x)(p^2+q^2) - \frac{3}{2}(p^2+q^2)^2.$$

With the midpoint rule used to subproblems (9) and (10), and adopting the second-order splitting (5), we have the following procedure:

$$u_j^n \Rightarrow u_j^*, \mathrm{i}\frac{u_j^* - u_j^n}{\tau/2} = \frac{1}{2}(150\sin^2 x_j - 1.5|u_j^n + u_j^*|^2)(u_j^n + u_j^*);$$

$$u_j^* \Rightarrow u_j^{**}, \frac{\mathrm{i}}{16}(\delta_t \hat{u}_{j-2} + 4\delta_t \hat{u}_{j-1} + 6\delta_t \hat{u}_j + 4\delta_t \hat{u}_{j+1} + \delta_t \hat{u}_{j+2}) + \delta_x^4 \hat{u}_j = 0;$$

$$u_j^{**} \Rightarrow u_j^{n+1}, \mathrm{i}\frac{u_j^{n+1} - u_j^{**}}{\tau/2} = \frac{1}{2}(150\sin^2 x_j - 1.5|u_j^{n+1} + u_j^{**}|^2)(u_j^{n+1} + u_j^{**}), \tag{11}$$

$j = 0,1,2,\cdots,N$, where $\hat{u}_j = (u_j^* + u_j^{**})/2$, $\delta_t \hat{u}_j = (u_j^{**} - u_j^*)/\tau$.

The scheme is of second order in time and space directions. Readers who are interested in this scheme can take an additional overview [11].

It is not hard to find that to code the procedure, one only need to solve a coupled linear algebraic system, and two uncoupled nonlinear algebraic systems. It will spend much less time than MI (8) which will be verified in the numerical example 1.

To compare the computational efficiency between the general MI (8) and SMI (11), we give a numerical example.

Example 1 We study the following 2π-periodic initial value problem

$$\begin{cases} \mathrm{i}u_t + u_{xxxx} - 150(\sin^2 x)\,u + 6|u|^2 u = 0, \\ u(x,0) = \dfrac{5}{\sqrt{2}}(1+\mathrm{i})\sin x, \\ u(x,t) = u(x+2\pi,t) = 0, \end{cases} \tag{12}$$

The problem (12) admits a theoretical solution

$$u(x,t) = 5\exp(\mathrm{i}(t+\pi/4))\sin x.$$

We simulate the problem by MI (8) and SMI (11). The time length is $T = 2$. The results including error in l_2 and l_∞ under various mesh partitions, consumed CPU time by these two schemes are listed in Table 1.

Table 1 Comparison between MI and SMI.

τ/h	scheme	$\|e^n\|_2$	$\|e^n\|_\infty$	CPU(sec)
$\tau = 0.001$	MSRK	5.552×10^{-3}	8.255×10^{-3}	14
$h = \pi/20$	SMI	9.903×10^{-14}	3.250×10^{-13}	2.8
$\tau = 0.002$	MSRK	5.922×10^{-4}	1.252×10^{-3}	41
$h = \pi/40$	SMI	1.084×10^{-13}	6.004×10^{-13}	3
$\tau = 0.001$	MSRK	1.845×10^{-5}	3.826×10^{-5}	58
$h = \pi/40$	SMI	3.973×10^{-13}	1.375×10^{-12}	5

From Table1, one can observe that the SMI (11) is much more efficient than MI (8).

3 LOD-MI for Multidimensional HS

In this section, we give an overview for local one-dimensional MI for multi-dimensional HS. To save the length of this paper, we only present the framework of the method, for more details about this method, we refer to [12-13].

The dimensionless Gross-Pitaevskii (GP) equation

$$\mathrm{i}u_t = -\frac{1}{2}\nabla^2 u + V_d(x)\,u + \beta_d|u|^2 u = (L_x + L_y + L_z)\,u + N(V,|u|^2)\,u \tag{13}$$

is used to explain the method. Here the operators $L_x = -\frac{1}{2}\partial_{xx}, L_y = -\frac{1}{2}\partial_{yy}, L_z = -\frac{1}{2}\partial_{zz}, N(V,|u|^2)\,u = V_d(x) + \beta_d|u|^2$.

Let $z = (p,q,\varphi,\alpha,\psi,\beta,\eta,\gamma)^{\mathrm{T}}$, we can reformulate the GP equation (13) into multisymplectic form (1) with

$$\boldsymbol{M} = \begin{bmatrix} \boldsymbol{J}_4 & \boldsymbol{0}_4 \\ \boldsymbol{0}_4 & \boldsymbol{0}_4 \end{bmatrix}, \boldsymbol{K}_1 = \frac{1}{2}\begin{bmatrix} \boldsymbol{J}_4 & \boldsymbol{0}_4 \\ \boldsymbol{0}_4 & \boldsymbol{0}_4 \end{bmatrix},$$

$$\boldsymbol{K}_2 = \frac{1}{2}\begin{bmatrix} \boldsymbol{0}_4 & \boldsymbol{C}_4 \\ -\boldsymbol{C}_4 & \boldsymbol{0}_4 \end{bmatrix}, \boldsymbol{K}_3 = \frac{1}{2}\begin{bmatrix} \boldsymbol{0}_4 & \boldsymbol{D}_4 \\ -\boldsymbol{D}_4 & \boldsymbol{0}_4 \end{bmatrix},$$

here $\boldsymbol{J}_4 = \begin{bmatrix} J_2 & \boldsymbol{0}_2 \\ \boldsymbol{0}_2 & \boldsymbol{0}_2 \end{bmatrix}, \boldsymbol{J}_2 = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix},$

$$\boldsymbol{L}_4 = \begin{bmatrix} \boldsymbol{0}_2 & \boldsymbol{I}_2 \\ \boldsymbol{I}_2 & \boldsymbol{0}_2 \end{bmatrix}, \boldsymbol{C}_4 = \begin{bmatrix} \boldsymbol{I}_2 & \boldsymbol{0}_2 \\ \boldsymbol{0}_2 & \boldsymbol{0}_2 \end{bmatrix}, \boldsymbol{D}_4 = \begin{bmatrix} \boldsymbol{0}_2 & \boldsymbol{I}_2 \\ \boldsymbol{0}_2 & \boldsymbol{0}_2 \end{bmatrix},$$

where $\boldsymbol{I}_n$ and $\boldsymbol{0}_n$ are $n\times n$ identity matrix and zeros matrix, respectively, and the Hamiltonian function

$$S(z) = \frac{1}{4}\int [2V(x,y,z)(p^2+q^2) + \beta(p^2+q^2)^2 - (v^2+\omega^2+\varphi^2+\psi^2+\zeta^2+\eta^2)]\,.$$

By direct calculation, one can find that the Cauchy problem of GP equation (13) with initial data $u_0(x)$ admits the following two conservation laws:

• Mass invariant

$$Q(t) = \int_{\mathbf{R}^d} |u(X,t)|^2 \mathrm{d}X = \int_{\mathbf{R}^d} |u_0(X)|^2 \mathrm{d}X = Q(0),$$

• Energy invariant

$$\varepsilon(t) = \int_{\mathbf{R}^d} \left[\frac{1}{2}|\nabla u(X,t)|^2 + V_d(X)|u|^2 + \frac{\beta_d}{2}|u|^4\right]\mathrm{d}X = \varepsilon(0).$$

For this Hamiltonian system, it is very difficult to

establish practical MIs because of its inseparability. To construct a practical numerical method with the characters of MIs, we use LOD technique to split the GP equation (13) into three locally one-dimensional Schrödinger equations and a nonlinear Schrödinger equation

$$\mathrm{i}u_t = -\frac{1}{2}u_{xx} = L_x u, \tag{14}$$

$$\mathrm{i}u_t = -\frac{1}{2}u_{yy} = L_y u, \tag{15}$$

$$\mathrm{i}u_t = -\frac{1}{2}u_{zz} = L_z u, \tag{16}$$

$$\mathrm{i}u_t = [V(x,y,z) + \beta|u|^2]u = N(V,|u|^2)u. \tag{17}$$

We can reformulate the LOD Schrödinger equations (14) ~ (16) into the form of HS (1)

$$\boldsymbol{J}_4 \frac{\partial}{\partial t}\bar{z}_j + \boldsymbol{L}_4 \frac{\partial}{\partial x_j}\bar{z}_j = \nabla_{\bar{z}_j} S_j(\bar{z}_j), j = 1,2,3,$$

where $x_1 = x, x_2 = y, x_3 = z$ and $\bar{z}_1 = (p,q,\nu,\omega)^{\mathrm{T}}$, $\bar{z}_2 = (p,q,\varphi,\psi)^{\mathrm{T}}, \bar{z}_3 = (p,q,\zeta,\eta)^{\mathrm{T}}$, with the Hamiltonian functions

$$S_1(\bar{z}_1) = -\frac{1}{4}(\nu^2 + \omega^2),$$

$$S_2(\bar{z}_2) = -\frac{1}{4}(\varphi^2 + \psi^2),$$

$$S_3(\bar{z}_3) = -\frac{1}{4}(\zeta^2 + \eta^2).$$

The nonlinear subproblem (17) degenerates to the Hamiltonian formulation

$$\frac{\mathrm{d}}{\mathrm{d}t}\hat{z} = J_2^{-1}\nabla_{\hat{z}} H(\hat{z}), \forall x,y,z,$$

where $\hat{z} = (p,q)^{\mathrm{T}}$, and the Hamiltonian function is

$$H(\hat{z}) = \frac{1}{4}[2V(x,y,z)(p^2+q^2) + \beta(p^2+q^2)^2].$$

As a matter of fact, the exact solution of this system is

$$u(x,y,z,t^{n+1}) = \exp(-\mathrm{i}(V(x,y,z) + \beta|u(x,y,z,t^n)|^2))u(x,y,z,t^n),$$

with the contribution of pointwise conservation law

$$|u(x,y,z,t)|^2 = |u(x,y,z,0)|^2, \forall x,y,z,t.$$

Therefore, we can get an LOD-MI in the form

$$\mathrm{i}\frac{(u^*_{j-1/2,kl} + u^*_{j+1/2,kl}) - (u^n_{j-1/2,kl} + u^n_{j+1/2,kl})}{\tau/2} + \delta_x^2 u^{n^*+1/2}_{jkl} = 0, \tag{18}$$

$$\mathrm{i}\frac{(u^{**}_{j,k-1/2,l} + u^{**}_{j,k+1/2,l}) - (u^*_{j,k-1/2,l} + u^*_{j,k+1/2,l})}{\tau/2} + \delta_y^2 u^{n^{**}+1/2}_{jkl} = 0, \tag{19}$$

$$\mathrm{i}\frac{(u^{***}_{j,k,l-1/2} + u^{***}_{j,k,l+1/2}) - (u^{**}_{j,k,l-1/2} + u^{**}_{j,k,l+1/2})}{\tau/2} + \delta_z^2 u^{n+1/2}_{jkl} = 0, \tag{20}$$

$$\bar{u}_{jkl} = \exp(-\mathrm{i}(V_{jkl} + \beta|u^{***}_{jkl}|^2)\tau)u^{***}_{jkl} = \exp(-\mathrm{i}\theta^{***}_{jkl})u^{***}_{jkl}, \tag{21}$$

$$\mathrm{i}\frac{(\bar{\bar{u}}_{jk,l-1/2} + \bar{\bar{u}}_{jk,l+1/2}) - (\bar{u}_{jk,l-1/2} + \bar{u}_{jk,l+1/2})}{\tau/2} + \delta_z^2 u^{n^\circ+1/2}_{jkl} = 0, \tag{22}$$

$$\mathrm{i}\frac{(\bar{\bar{u}}_{j,k-1/2,l} + \bar{\bar{u}}_{j,k+1/2,l}) - (\bar{\bar{u}}_{j,k-1/2,l} + \bar{\bar{u}}_{j,k+1/2,l})}{\tau/2} + \delta_y^2 u^{n^{\circ\circ}+1/2}_{jkl} = 0, \tag{23}$$

$$\mathrm{i}\frac{(u^{n+1}_{j-1/2,kl} + u^{n+1}_{j+1/2,kl}) - (\bar{\bar{u}}_{j-1/2,kl} + \bar{\bar{u}}_{j+1/2,kl})}{\tau/2} + \delta_x^2 u^{n^{\circ\circ\circ}+1/2}_{jkl} = 0, \tag{24}$$

where $u^{n^\circ+1/2} = \frac{1}{2}(\bar{u} + \bar{\bar{u}})$, $u^{n^{\circ\circ}+1/2} = \frac{1}{2}(\bar{\bar{u}} + \bar{\bar{\bar{u}}})$, $u^{n^{\circ\circ\circ}+1/2} = \frac{1}{2}(\bar{\bar{\bar{u}}} + u^{n+1})$.

This scheme is of second order both in space and time directions. Detailed numerical analysis of this scheme can be found in [13].

Next, we use an example to demonstrate the feasibility of our LOD-MI (18) ~ (24).

Example 2 In the example, we investigate the 3D anisotropic condensate problem with changing trapped frequency

$$\begin{cases} \mathrm{i}\psi_t = -\frac{1}{2}\nabla^2 u + V(x,y,z)u + \frac{1}{10}|\psi|^2\psi, \\ \psi(x,y,z,0) = \frac{2^{1/4}}{(\pi/4)^{3/8}}\exp(-2(x^2+2y^2+4z^2)), \end{cases}$$

where $V_3(x,y,z) = \frac{1}{2}(x^2 + 4y^2 + 16z^2)$.

It is a 3D nonlinear problem. We can imagine that one can not solve it by traditional MIs. We will not make any comparison between them. We only use LOD-MI (18) ~ (24) to solve the model under the mesh step size $h = 0.16, \tau = 0.01$. The profiles of the real part and imaginary part of the wave function at $z = 3.2, t = 3$ are shown in Fig. 1, and the residuals of mass and local energy are presented in Fig. 2.

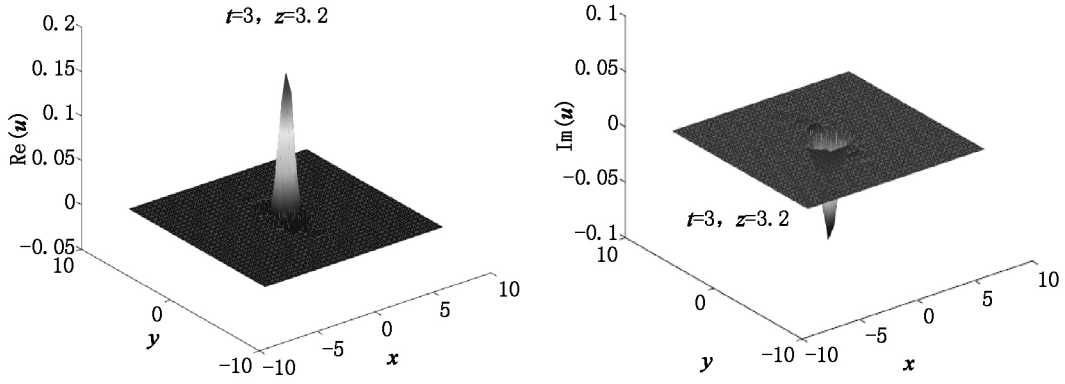

Figure 1 The real and imaginary parts of the wave function. Left: real; Right: imaginary.

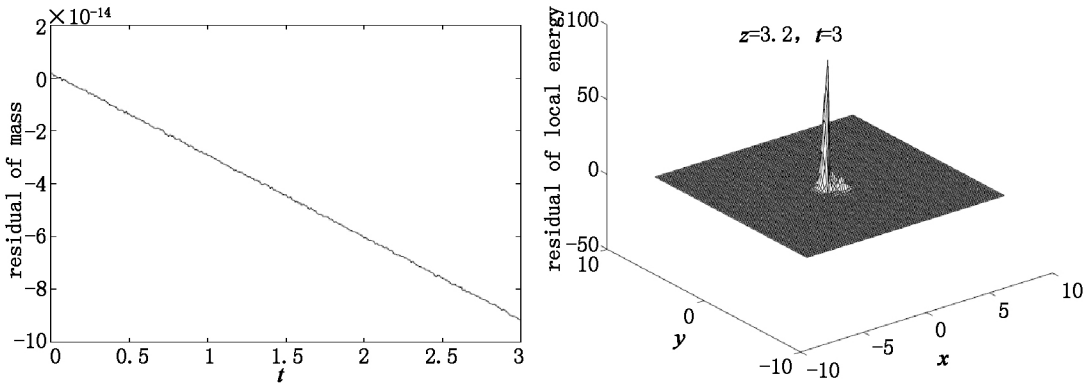

Figure 2 The residuals of mass and local energy. Left: mass; Right: local energy.

It is observed from these figures, we can find that the LOD-MI can simulate the original problem very well with the characters of traditional MIs. The mass is exactly preserved, but not the local energy. This is consistent with numerical analysis in [13].

4 Conclusions and Remarks

Traditional symplectic and multisymplectic integrators are inefficient in practical computing for complex and multidimensional Hamiltonian systems. Their application in these aspects is limited. Even though we can construct explicit MIs for separable HS, they are often constrained by CFL numbers. We consider a new kind of numerical integrators with the characters of MIs and very efficient. They are verified numerically and experimentally. However, there are still a lot of problems to be studied in this field, such as the detailed theoretical analysis of the multisymplectic conservation quantities of the MIs. The prior error estimation of the numerical solution of the MIs.

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哈密尔顿系统的分裂步多辛数值积分

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摘要: 对哈密尔顿系统而言,辛或多辛积分较传统的数值方法具有优越性. 然而,此类数值格式大部分都是隐式的,从而在每一个时间步需要求解一个非线性的代数方程组,这将直接导致计算效率不高. 在多辛积分中引进分裂步技巧,称之为分裂步多辛积分,可以弥补这一不足之处,这一数值方法的框架将在该文中简要地讨论,其中,数值例子给出了该方法在物理问题中的应用.

关键词: 分裂方法; 多辛积分; 计算效率; 哈密尔顿系统

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