SEMI-EXPLICIT MULTI-SYMPLECTIC INTEGRATION OF NONLINEAR SCHRÖDINGER EQUATION

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In this paper we apply Lobatto IIIA-IIIB type multi-symplectic discretization in space and time to the nonlinear Schrödinger equation. The resulting scheme is semi-explicit in time and therefore more efficient than implicit multi-symplectic schemes. Numerical results confirm excellent long time conservation of the local and global conserved quantities like the energy, momentum and norm.

Keywords: nonlinear Schrödinger equation, multi-symplectic integrators, Lobatto IIIA-IIIB methods

1. Introduction

Recently the field of numerical analysis experienced a growing interest in the numerical investigation of ordinary and partial differential equations (pde's) by using geometric integrators which preserve the essential features of the underlying system after discretization. Symplectic integrators for ordinary differential equations (ode's) have been thoroughly analyzed and the concept of symplectic time integration has also been extended to Hamiltonian pde's.[7,13] More recently nonlinear pde's were also studied numerically using multi-symplectic integrators (see for an overview[3] and[13]).

A multi-symplectic structure of a pde is generated by a pair of skew-symmetric matrices $\mathbf{M}, \mathbf{K} \in \mathbb{R}^{n\times n}$and a multi-symplectic Hamiltonian $S(z)$ which is a smooth function on $\mathbb{R}^n$:

$$\mathbf{M}z_t + \mathbf{K}z_x = \nabla_z S(z), \qquad z \in \mathbb{R}^n. \tag{1}$$

The Hamiltonian system (1) is multi-symplectic in the sense that associated with $\mathbf{M}$ and $\mathbf{K}$ are the two-forms

$$\omega = \frac{1}{2}(dz \wedge \mathbf{M}dz), \qquad \kappa = \frac{1}{2}(dz \wedge \mathbf{K}dz), \tag{2}$$

which define a space-time symplectic structure governed by the multi-symplectic conservation law (MSCL)

$$\partial_t \omega + \partial_x \kappa = 0. \tag{3}$$

This multi-symplecticity generalizes the symplectic conservation law of Hamiltonian ode's.

The multi-symplectic structure gives rise to local conservation laws which can be derived from a multi-symplectic form of Nöthers theorem. The invariance of the Hamiltonian $S(z)$ with respect to space-time shifts implies the following local energy and momentum conservation laws (LECL and LMCL), respectively

$$\begin{array}{l} \text{LECL: } E_t + F_x = 0,\ E = S - \frac{1}{2} z^T \mathbf{K} z_x,\ F = \frac{1}{2} z^T \mathbf{K} z_t \\ \text{LMCL: } I_t + G_x = 0,\ G = S - \frac{1}{2} z^T \mathbf{M} z_t,\ I = \frac{1}{2} z^T \mathbf{M} z_x. \end{array} \tag{4}$$

Additionally, norm preservation follows from the phase symmetry.

Multi-symplectic integrators based on simultaneous space-time discretization of the pde's preserve the MSCL (3) in the discrete sense. In contrast to the symplectic integrators; the multi-symplectic conservation law is not exactly preserved by the multi-symplectic integrators, different multi-symplectic integrators preserve different discretizations of the multi-symplectic conservation law. However, preservation of the multi-symplectic structure by a numerical scheme does not imply the exact preservation of the local conservation laws (4) or of global invariants of the pde's. Due to their local nature the multi-symplectic integrators preserve the conserved quantities locally better than the symplectic integrators. The word "local" here means that the conservation properties do not depend on the specific domain or the boundary conditions of the pde's.

The Runge-Kutta(RK) methods play an important role in the numerical solution of symplectic and multi-symplectic pde's. It was shown[17] that the scalar wave equation can be integrated using concatenation of Gauss-Legendre Runge-Kutta methods in space and time, which leads to a multi-symplectic integrator. It is known that the Preissmann scheme corresponds to the concatenation of mid-point methods in time and space. The main weakness of RK based multi-symplectic integrators is their implicit nature that causes theoretical and practical problems due to the solutions of

large nonlinear systems.[18,19] The nonlinear Schrödinger (NLS) equation is an often used example for testing the performance of multi-symplectic integrators like the Preissmann scheme or multi-symplerctic pseudospectral methods.[2,4,10–12,17]

The partitioned Runge-Kutta (PRK) methods are another useful class of symplectic integrators which are applied successfully to symplectic ode's yielding explicit methods. The approach for symplectic PRK methods was extended to Hamitonian pde's in multi-symplectic form and the conditions which have to be satisfied formally by the multi-symplectic PRK methods were given.[9] For higher order RK and PRK methods, the conditions for preserving the multi-symplecticity become very complicated and intractable. Different several multi-symplectic RK and PRK methods are considered based on different multi-symplectic formulations of the nonlinear wave equation.[15] Recently several PRK methods were applied to Hamiltonian pde's like nonlinear Schrödinger equation, nonlinear Dirac equation, Boussinesq equation and to the scalar wave equation.[1,8,9,14,15]

In this paper, we apply in Section 2 the 2-stage Lobatto IIIA-IIIB multi-symplectic integrator developed in[18,19] to the NLS equation. In Section 3 we present numerical results for the long term conservation of local and global invariants like energy, momentum and norm. The paper ends with some concluding remarks.

2. Multi-symplectic discretization of the nonlinear Schrödinger equation

The focusing one-dimensional nonlinear Schrdinger (NLS) equation,

$$i\psi_t + \psi_{xx} + 2|\psi|^2\psi = 0, \tag{5}$$

can be written in a multi-symplectic form by letting $\psi = p+iq$ and introducing the new variables $v = p_x$, $w = q_x$.[17] Separating into real and imaginary parts, the NLS equation (5) can be written in the multi-symplectic form (1) with

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

and Hamiltonian $S = \frac{1}{2}((p^2+q^2)^2 + v^2 + w^2)$.

Implementing the relations (4) for the NLS equation yields the local energy and momentum conservation laws (LECL and LMCL):

$$\begin{array}{l} E_t + F_x = 0,\ E = \frac{1}{2}((p^2+q^2)^2 - v^2 - w^2), F = vp_t + wq_t \\ I_t + G_x = 0,\ I = pw - qv, G = (p^2+q^2)^2 + v^2 + w^2 - (pq_t - p_t q). \end{array} \tag{6}$$

Additionally we have a norm conservation law for the NLS equation

$$N_t + M_x = 0, \quad N = \frac{1}{2}(p^2+q^2), \quad M = qv - pw.$$

For periodic boundary conditions, the local conservation laws can be integrated in x to obtain global conservation of energy, momentum and norm defined as

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

where $\mathcal{E}(z) = \int_0^L E(z)dx, \mathcal{I}(z) = \int_0^L \mathcal{I}(z)dx,\ \mathcal{N}(z) = \int_0^L N(z)dx.$

For the space and time discretization of the NLS equation we follow the formulation of PRK methods as multi-symplectic integrators in.[18,19] An s-stage time discretization of the differential equation $z_t = f(z)$ consists of a set of equations coupling the node values z_i to the stage vectors $Z_{i,n}$ is given by

$$\begin{aligned} Z_{i,j}^{(\gamma)} &= z_i^{(\gamma)} + \Delta t \sum_{k=1}^{s} a_{jk}^{(\gamma)} f(Z_{i,j}), \quad i = 1, \cdots, s \\ z_{i+1} &= z_i + \Delta t \sum_{j=1}^{s} b_j^{(\gamma)} f(Z_{i,j}). \end{aligned}$$

Here the vector of dependent variables z is partitioned in two parts, $z^{(\gamma)},\ \gamma = 1, 2$. The coefficients $b_j^{(\gamma)}$ and $a_{jk}^{(\gamma)}$ are chosen to satisfy certain order conditions. For the case of canonical Hamiltonian system the conditions for symplecticity for a two-partition PRK discretization are[7]

$$-a_{kj}^{(1)} b_k^{(2)} - b_j^{(1)} a_{jk}^{(2)} + b_j^{(1)} b_k^{(2)} = 0, \quad j, k = 1, \ldots s.$$

For a PRK discretization in space, the set of equations is given as

$$\begin{aligned} Z_{i,j}^{(\gamma)} &= z_i^{(\gamma)} + \Delta x \sum_{k=1}^{s} a_{jk}^{(\gamma)} \partial_x Z_{i,j}^{(\gamma)}, \quad i = 1, \cdots, s \\ z_{i+1} &= z_i + \Delta x \sum_{j=1}^{s} b_j^{(\gamma)} \partial_x Z_{i,j}^{(\gamma)} \end{aligned}$$

where the variables $\partial_x Z_{i,j}$ have to satisfy the multi-symplectic conservation law (3)

$$M\partial_t Z_{i,j} + K\partial_x Z_{i,j} = \nabla S(Z_{i,j}).$$

We use here the second order 2-stage symplectic Lobatto IIIA-IIIB method given by the RK table

$$\text{IIIA:}\quad \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1/2 & 1/2 \\ \hline & 1/2 & 1/2 \end{array}, \qquad \text{IIIB:}\quad \begin{array}{c|cc} 0 & 1/2 & 0 \\ 1 & 1/2 & 0 \\ \hline & 1/2 & 1/2. \end{array}$$

Grouping the dependent variables as $z^{(1)} = \{p, q\}$ and $z^{(2)} = \{v, w\}$, semi-discretization of NLS equation by the Lobatto IIIA-IIIB discretization results[18,19] in

$$\begin{aligned} \partial_t p_i &= -\frac{q_{i-1} - 2q_i + q_{i+1}}{\Delta x^2} - 2(p_i^2 + q_i^2)q_i, \\ \partial_t q_i &= \frac{p_{i-1} - 2p_i + p_{i+1}}{\Delta x^2} + 2(p_i^2 + q_i^2)p_i. \end{aligned} \tag{7}$$

These equations correspond precisely to second order finite difference approximation of the NLS equation in space. This implies that the 2-stage Lobatto IIIA-IIIB discretisation in space is equivalent to second order finite differences in space applied to such a pde.

Using the same partitioning of the variables in space and time yields implicit integrators.[18] Choosing the partitioning $z^{(3)} = (p, v), z^{(4)} = (q, w)$, it can be seen that the variables v and w do not appear in (7), so that 2-stage Lobatto IIIA-IIIB method in time can be applied to the partitioned ode (7) containing only the variables p and q. Second order Lobatto IIIA-IIIB in time in this form is commonly known as generalized leapfrog which is in general an implicit method. Applied to (7), we obtain the integrator that maps (p_i^n, q_i^n) to (p_i^{n+1}, q_i^{n+1}) in the following way:

$$\begin{aligned} q_i^{n+(1/2)} &= q_i^n + \frac{\Delta t}{2\Delta x^2}(p_{i-1}^n - 2p_i^n + p_{i+1}^n) + \Delta t((q_i^{n+(1/2)})^2 + (p_i^n)^2)p_i^n, \\ p_i^{n+1} &= p_i^n - \frac{\Delta t}{\Delta x^2}(q_{i-1}^{n+(1/2)} - 2q_i^{n+(1/2)} + q_{i+1}^{n+(1/2)}) \\ &\quad - \Delta t((p_i^n)^2 + (p_i^{n+1})^2 + 2(q_i^{n+(1/2)})^2)q_i^{n+(1/2)}, \\ q_i^{n+1} &= q_i^{n+(1/2)} + \frac{\Delta t}{\Delta x^2}(p_{i-1}^{n+1} - 2p_i^{n+1} + p_{i+1}^{n+1}) \\ &\quad + \Delta t((q_i^{n+(1/2)})^2 + (p_i^{n+1})^2)p_i^{n+1}. \end{aligned} \tag{8}$$

In this system the nonlinearities enter as scalar quadratic equations which can be solved explicitly. Applying one Newton iteration step to the first and second equation in (8), one can compute $q_i^{n+(1/2)}$ and p_i^{n+1}, $i = 1, \ldots, N$. The last equation is explicit in p_i^{n+1}, $i = 1, \ldots, N$. In contrast to this, the implicit multi-symplectic methods like the Preismann scheme require several Newton steps in order to find an approximate solution. The computational stencil for the 2-stage Lobatto IIIA-IIIB method in Fig.1 reveals that it can be interpreted as a method on staggered grids, because the values of the p_i's and q_i's are computed on different nodes.

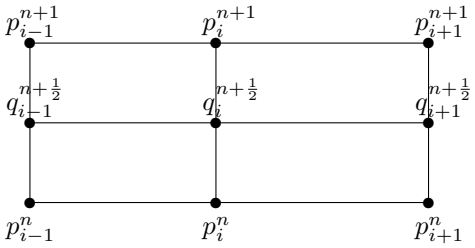

Fig. 1. Stencil for the Lobatto IIIA-IIIB method for the NLS equation

Similarly, the Volterra lattice equation which is an approximation of the Korteweg de Vries (KdV) equation as a Poisson system was discretized in time using the implicit and explicit Euler method[5] (first order Lobatto IIIA-IIIB method). Due to the quadratic terms appearing in the Volterra lattice, linear systems of equations have to be solved at each time step like in (8).

Higher order $s-$stage Lobatto IIIA-IIIB discretization in space and time can be constructed. But for Lobatto IIIA-IIIB methods, space-time discretizations with more than 2-stages lead to implicit integrators.[19] Only discretizations in space with higher order Lobatto IIIA-IIIB methods and applying composition methods in time lead to explicit integrators.

Another important feature of multi-symplectic integrators is the preservation of the linear dispersion relations of the pde's. The dispersion properties of the implicit multi-symplectic integrators like the Gauss-Legendre RK methods and including the Preissman scheme were investigated for the NLS equation and other multi-symplectic pde's.[6,15,16] These multi-symplectic integrators preserve the discrete dispersion relations for the linearized pde's and do not exhibit spurious solutions. Any symmetric and A-stable RK

methods like the Lobatto IIIA-IIIB method preserve the discrete dispersion relations too.[6] It was shown that, similarly, a space-time discretization of the Boussinesq equation by the 2-stage Lobatto IIIA-IIIB method preserves the numerical dispersion relation and there are no spurious solutions.[1]

3. Discretization of conserved quantities and numerical results

We can use the residual for the local energy conservation law as:[8,9]

$$RE = \frac{1}{\Delta t}\sum_{m=1}^{2} b_m^{(1)}\left(E(\mathbf{z}_{i,m}^{n+1}) - E(\mathbf{z}_{i,m}^{n})\right) + \frac{1}{\Delta x}\sum_{k=1}^{2} b_k^{(2)}\left(F(\mathbf{z}_{i+1}^{n,k} - F(\mathbf{z}_{i}^{n,k})\right) \tag{9}$$

where $\mathbf{z}_{i,m}^{n+1} \approx z(c_m\Delta x, (n+1)\Delta t)$, $\mathbf{z}_{i,m}^{n} \approx z(c_m\Delta x, n\Delta t)$ and $\mathbf{z}_{i+1}^{n,k} \approx z((i+1)\Delta x, \widetilde{c}_k\Delta t)$, $\mathbf{z}_{i}^{n,k} \approx z(i\Delta x, \widetilde{c}_k\Delta t)$. The residual in (9) does not mean the local error at the mesh point x_i, t_n, it was derived from the local integration over the rectangular domain $(x_i, t_n), (x_{i+1}, t_n), (x_{i+1}, t_n), (x_{i+1}, t_{n+1})$.[8]

Since $c_1 = 0, c_2 = 1$ and the weights $b_i^{(2)} = b_i^{(2)} = 1/2,\ i = 1, 2$ for the Lobatto IIIA-IIIB method, we can write the residual (9) as

$$RE = \frac{E_i^{n+1} - E_i^n + E_{i+1}^{n+1} - E_{i+1}^n}{2\Delta t} + \frac{F_{i+1}^n - F_i^n + F_{i+1}^{n+1} - F_{i+1}^{n+1}}{2\Delta x} \tag{10}$$

where

$$E_i^n = -\frac{1}{2}\left[\left((p_i^n)^2 + (q_i^n)^2\right)^2 - (v_i^n)^2 - (w_i^n)^2\right],$$
$$F_i^n = -v_i^n\left(\frac{p_i^{n+1} - p_i^n}{\Delta t}\right) - w_i^n\left(\frac{q_i^{n+1} - q_i^n}{\Delta t}\right).$$

We can use the residual for the momentum conservation law as[9]

$$RI = \frac{1}{\Delta t}\sum_{m=1}^{2} b_m\left(I(\mathbf{z}_m^{\mathbf{1}}) - I(\mathbf{z}_m^{\mathbf{0}})\right) + \frac{1}{\Delta x}\sum_{k=1}^{2}\widetilde{b}_k\left(G(\mathbf{z}_{\mathbf{1}}^k) - G(\mathbf{z}_{\mathbf{0}}^k)\right) \tag{11}$$

which can be rewritten as

$$RI = \frac{I_i^{n+1} - I_i^n + I_{i+1}^{n+1} - I_{i+1}^n}{2\Delta t} + \frac{G_{i+1}^n - G_i^n + G_{i+1}^{n+1} - G_{i+1}^{n+1}}{2\Delta x} \tag{12}$$

where

$$I_i^n = -\frac{1}{2}\left(p_i^n w_i^n - q_i^n v_i^n\right),$$
$$G_i^n = -\frac{1}{2}\left[\left((p_i^n)^2 + (p_i^n)^2\right)^2 + (v_i^n)^2 + (w_i^n)^2 - (p_i^n)\left(\frac{q_i^{m+1} - q_i^m}{\Delta t}\right) + (q_i^n)\left(\frac{p_i^{m+1} - p_i^m}{\Delta t}\right)\right]$$

The global energy GE and the global momentum GI for both integrators are given by

$$GE = \Delta x \sum_{j=1}^{N} (E_j^n - E^0), \qquad GI = \Delta x \sum_{j=1}^{N} (I_j^n - I^0)$$

where E^0 and I^0 are the initial energy and momentum respectively.

The local and global norm conservation laws can be defined analogously.

Time discretization by Lobatto IIIA-IIIB methods does not the preserve phase symmetry[19] and the quadratic invariants appearing in the norm conservation $N = (p^2 + q^2)/2$ can not be preserved exactly. But the Lobatto IIIA-IIIB methods preserve the quadratic invariants like $I = pw - qv$ in the momentum exactly.[20]

For a numerical experiment we consider the NLS equation (5) with the initial condition[10] $\psi_0(x) = 0.5(1 + 0.1\cos(\mu x)),\ \mu = 2\pi/L,\ L = 2\sqrt{2}\pi$. We set the spatial mesh-size to $\Delta x = L/64$ and the time step to $\Delta t = 5 \times 10^{-3}$.

In Fig. 2 the numerical results obtained by the Lobatto IIIA-IIIB multi-symplectic integrator are presented over the time domain $[0, 100]$. We see that the surface exhibits a quasi periodic behavior in time. We notice that the spatial period is $2\pi/\mu$ or L; within that length there is only one peak in space. The wave oscillates between the near uniform state and the one hump state. From Fig. 2 we see that the errors in local energy and momentum are concentrated in the region where there are peaks in the solution. The local errors are bounded and do not grow in time. The global conservation laws are preserved very well over the long time integration. Numerical results obtained for the preservation of the locally and globally conserved quantities confirm the theoretically predicted ones. The global momentum is preserved up to the machine accuracy. The errors for the global energy and momentum remain bounded as in the case of the implicit multi-symplectic integration of NLS equation.

4. Conclusions

Multi-symplectic Lobatto IIIA-IIIB space-time discretization of the NLS equation is second order accurate in time and space variables and requires less computation than the Preissman scheme. Local and global energy can be preserved more accurately using semi-discretization in space using a higher order Lobatto IIIA-IIIB pair and symmetric composition in time.

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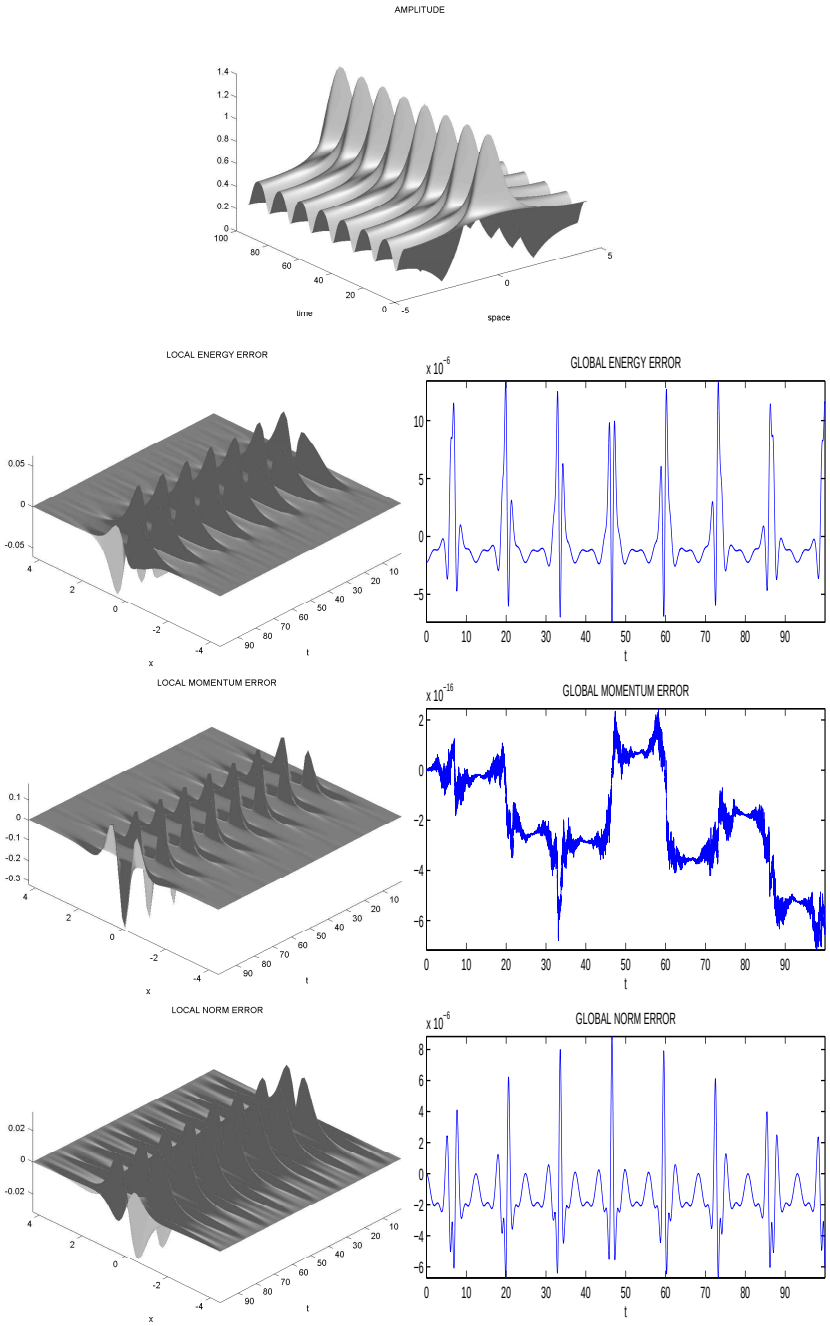

Fig. 2. Lobatto IIIA-IIIB integration of NLS