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Conservation properties of multisymplectic integrators

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Abstract

Recent results on the local and global properties of multisymplectic discretizations of Hamiltonian PDEs are discussed. We consider multisymplectic (MS) schemes based on Fourier spectral approximations and show that, in addition to a MS conservation law, conservation laws related to linear symmetries of the PDE are preserved exactly. We compare spectral integrators (MS versus non-symplectic) for the nonlinear Schrödinger (NLS) equation, focusing on their ability to preserve local conservation laws and global invariants, over long times. Using Lax-type nonlinear spectral diagnostics we find that the MS spectral method provides an improved resolution of complicated phase space structures.

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1. Introduction

Multisymplectic integrators are a new class of structure preserving algorithms for solving Hamiltonian PDEs. In this approach, a multisymplectic structure of a PDE is generated by a pair of skew-symmetric matrices $\boldsymbol{M}, \boldsymbol{K} \in \mathbb{R}^{n\times n}$ and a multisymplectic Hamiltonian $S(z)$ which is a smooth function on $\mathbb{R}^n$ [1,2]:

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

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

$$\omega = \tfrac{1}{2}(\mathrm{d}z \wedge \boldsymbol{M}\mathrm{d}z), \qquad \kappa = \tfrac{1}{2}(\mathrm{d}z \wedge \boldsymbol{K}\mathrm{d}z), \tag{2}$$

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

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

Eq. (3) is derived directly from (1) and generalizes the symplectic conservation law of Hamiltonian ODEs.

The multisymplectic structure naturally gives rise to local conservation laws typically associated with Nöthers theorem. In fact, in the presence of a MS structure, the invariance of the Hamiltonian $S(z)$ with re-

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spect to space-time shifts, implies the local energy and momentum conservation laws (LECL and LMCL, respectively)

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

Further, it can be shown that these conservation properties are equivalent to those obtained using Nöthers theorem from the Lagrangian density

$$\Lambda = \tfrac{1}{2} z^T \boldsymbol{M} z_t + \tfrac{1}{2} z^T \boldsymbol{K} z_x - S(z). \tag{5}$$

Multisymplectic integrators exactly preserve the MSCL (3) in the discrete sense [2]. However, preservation of the multisymplectic structure by a numerical scheme does not imply preservation of the local conservation laws (4) or of global invariants which determine the phase space structure. It has been shown that symplectic integration methods in time, as opposed to non-symplectic methods, can be superior for Hamiltonian PDEs provided the spatial structure of the PDE is judiciously discretized, see e.g. [7]. What is still an unresolved issue is the extent to which it is advantageous to preserve a local discrete multi-symplectic form. Spectral discretizations yield a class of multisymplectic integrators with associated spectral local conservation laws [3]. In addition, we show that conservation laws related to linear symmetries of the PDE are preserved exactly. In this paper we examine the local and global conservation properties of multisymplectic spectral methods focusing on their ability to resolve complicated phase space structures.

To address this issue we use the nonlinear Schrödinger (NLS) equation, with periodic boundary values, as our model equation. The phase space geometry of the NLS equation is specified in terms of the "nonlinear spectrum" of the spatial operator of an associated Lax pair (see Eq. (12)) [5]. In addition to using traditional phase space portraits, we use the nonlinear spectrum as a diagnostic to determine the ability of a scheme to capture phase space dynamics. Significantly, we find that conservation of multisymplecticity by a numerical scheme does result in an improved preservation of global phase space structure over long times. In particular, the MS spectral method is shown to provide an improved resolution of the LCLs, global invariants and of the nonlinear spectrum, when compared with a standard non-symplectic spectral integrator.

The rest of the paper is organized as follows. In Section 2 we present the multisymplectic formulation and integrable structure of the NLS equation. We provide the elements of the nonlinear spectral theory which are relevant for interpreting the ability of the numerical schemes to preserve the phase space structure. In Section 3 we demonstrate that spectral discretizations yield another class of multisymplectic integrators, discuss their conservation properties, and obtain a MS spectral discretization of the NLS equation. The numerical experiments, which illustrate the remarkable behavior of MS schemes, are discussed in Section 4 and Section 5 contains concluding remarks.

2. The model equation

2.1. Multisymplectic formulation of the nonlinear Schrödinger equation

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

$$\mathrm{i}u_t + u_{xx} + 2|u|^2 u = 0, \tag{6}$$

can be written in multisymplectic form by letting $u = p + \mathrm{i}q$ and introducing the new variables $v = p_x,\ w = q_x$ [12]. Separating into real and imaginary parts, the NLS Eq. (6) can be written in the multisymplectic form (1) with

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

$$
\boldsymbol{K} = \begin{pmatrix} 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}, \tag{7}
$$

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

Implementing relations (4) for the NLS equation yields the local energy and momentum conservation