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A LINEARLY-IMPLICIT STRUCTURE-PRESERVING EXPONENTIAL TIME DIFFERENCING SCHEME FOR HAMILTONIAN PDEs*

Yayun Fu
Henan Joint International Research Laboratory of High Performance Computation for Complex Systems, School of Science, Xuchang University, Xuchang 461000, China
Email: fyyly@xcu.edu.cn
Dongdong Hu
School of Mathematics and Statistics, Jiangxi Normal University, Jiangxi, Nanchang 330022, China
Email: hudongdong2021@gmail.com
Wenjun Cai
Jiangsu Key Laboratory for NSLSCS,
Jiangsu Collaborative Innovation Center of Biomedial Functional Materials,
School of Mathematical Sciences, Nanjing Normal University, Nanjing 210023, China
Email: caiwenjun@njnu.edu.cn
Yushun Wang[1)]
Jiangsu Key Laboratory for NSLSCS,
Jiangsu Collaborative Innovation Center of Biomedial Functional Materials,
School of Mathematical Sciences, Nanjing Normal University, Nanjing 210023, China
Email: wangyushun@njnu.edu.cn

Abstract

In the paper, we propose a novel linearly implicit structure-preserving algorithm, which is derived by combing the invariant energy quadratization approach with the exponential time differencing method, to construct efficient and accurate time discretization scheme for a large class of Hamiltonian partial differential equations (PDEs). The proposed scheme is a linear system, and can be solved more efficient than the original energy-preserving exponential integrator scheme which usually needs nonlinear iterations. Various experiments are performed to verify the conservation, efficiency and good performance at relatively large time step in long time computations.

Mathematics subject classification: 65M06, 65M70.
Key words: Structure-preserving algorithm, Hamiltonian PDE, Energy quadratization method, Exponential time differencing.

1. Introduction

It is well known that all real physical processes with negligible dissipation can be described by Hamiltonian form, so the latter is becoming one of the most useful tools in modeling many scientific and engineering problems. In the past few years, studies in this field have captured researchers' increasing attention and many significant achievements have been made [16, 17]. Many partial differential equations (PDEs) can be reformulated as Hamiltonian systems, and

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[1)] Correspondence author

these equations posses some conservation laws, such as multi-symplectic conservation law [12, 25, 43], momentum conservation law [6] and energy conservation law [8, 9, 21, 26]. Among them the conservation of energy is particularly important for proving the existence and uniqueness of solutions for PDEs [42]. Therefore, developing stable and accurate numerical algorithms to preserve energy of the systems becomes extremely important and this is becoming a norm for one to judge the effectiveness of numerical algorithms.

In this paper, our aim is to present and analyze an efficient linearly implicit scheme with energy-preserving property for a class of Hamiltonian PDEs, such as the sine-Gordon equation, the nonlinear Schrödinger equation and the Klein-Gordon-Schrödinger equation, etc., which can be rewritten as the following canonical Hamiltonian system:

$$\boldsymbol{z}_t = \mathcal{S}\frac{\delta \mathcal{H}}{\delta \boldsymbol{z}} \quad \text{with} \quad \mathcal{S} = \begin{pmatrix} \boldsymbol{O} & -\boldsymbol{I}_m \\ \boldsymbol{I}_m & \boldsymbol{O} \end{pmatrix}, \tag{1.1}$$

where $\boldsymbol{z}$ belongs to a Hilbert space $\mathcal{W}(\Omega)$ with values $\boldsymbol{z}(\boldsymbol{x}, t) = (z_1(\boldsymbol{x}, t), z_2(\boldsymbol{x}, t), \cdots, z_{2m}(\boldsymbol{x}, t))^T \in \mathbb{R}^{2m}$, $(\boldsymbol{x}, t) \in \Omega \times [0, T] \subset \mathbb{R}^d \times \mathbb{R}, d = 1, 2$, and $\delta\mathcal{H}/\delta\boldsymbol{z}$ is the variational derivative of the Hamiltonian energy functional $\mathcal{H}$ with respect to the variable $\boldsymbol{z}$.

Structure-preserving algorithms are achieved by constructing numerical methods which can preserve some properties of continuous systems [18, 28, 34]. The prior researches substantiated that numerical schemes inheriting such properties from the continuous dynamical system have been shown in many cases to be advantageous, especially when integration over long time intervals is considered. Over the years, developing structure-preserving numerical schemes to conserve the energy conservation law for Hamiltonian PDEs has gained increasing attention [7, 9, 31]. For instance, Furihata [23] presented the discrete variational derivative method for a large class of PDEs that inherit energy conservation or dissipation properties of the PDEs. Matsuo and Furihata [38] generalized the method to complex valued nonlinear PDEs and obtained a series of schemes [24]. Dahlby and Owren [14] clarified the concept of the discrete variational derivative and proposed a general framework for deriving integral-preserving numerical methods for PDEs. Celledoni *et al.* [11, 35] used the averaged vector field (AVF) method to construct a systematic energy-preserving or energy dissipation method for a class of PDEs. Brugnano *et al.* [3, 4] developed Hamiltonian boundary value methods (HBVM) which can be recast as a multistage Runge-Kutta (RK) method to construct energy-preserving scheme for polynomial Hamiltonian systems. There are many related researches, the readers can refer to [5, 7, 21, 22] and references therein for more details.

The exponential integrators scheme was systematically studied in [2] and then further developed by scholars [1, 15, 19, 30, 33, 47]. A distinctive feature of exponential integrators schemes is the exact evaluation of the contribution of the linear part, which provides satisfactory stability and accuracy even though the linear terms have strong stiffness. Such advantage leads some successful applications of the schemes on Hamiltonian PDEs. For instance, Celledoni *et al.* [10] constructed an implicit exponential integrators scheme for the cubic Schrödinger equation by using the symmetric projection approach, the proposed scheme can preserve symmetric and energy. Li and Wu [36] developed an energy-preserving scheme for conservative systems based on the exponential integrators and discrete gradient method. The resulted scheme permitted lager step sizes and achieved higher accuracy than non-exponential ones. However, most existing energy-preserving exponential integrators schemes for Hamiltonian PDEs are fully implicit, therefore, one needs to use iterations to solve a system of nonlinear algebraic equations at each time step, which brings a large number of calculations in long time numerical simulation.