Novel Symplectic Discrete Singular Convolution Method for Hamiltonian PDEs

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Abstract. This paper explores the discrete singular convolution method for Hamiltonian PDEs. The differential matrices corresponding to two delta type kernels of the discrete singular convolution are presented analytically, which have the properties of high-order accuracy, bandlimited structure and thus can be excellent candidates for the spatial discretizations for Hamiltonian PDEs. Taking the nonlinear Schrödinger equation and the coupled Schrödinger equations for example, we construct two symplectic integrators combining this kind of differential matrices and appropriate symplectic time integrations, which both have been proved to satisfy the square conservation laws. Comprehensive numerical experiments including comparisons with the central finite difference method, the Fourier pseudospectral method, the wavelet collocation method are given to show the advantages of the new type of symplectic integrators.

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Key words: Discrete singular convolution, differential matrix, symplectic integrator, Hamiltonian PDEs.

1 Introduction

Non-dissipative phenomena in quantum physics, fluid mechanics, oceanography, electromagnet field and other sciences are often modeled by the Hamiltonian systems of ordinary differential equations (ODEs) and partial differential equations (PDEs). Symplectic integrator is usually attached to a numerical scheme that intends to solve such a Hamiltonian system approximately, while preserving one or more intrinsic properties of the original system, such as the symplectic structure. There are various symplectic

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schemes for Hamiltonian ODEs, one can refer to [1-4] for details. The most obvious generalization of the concept of a symplectic integrator to Hamiltonian PDEs is a numerical scheme which is designed to preserve a semi-discretization of the symplectic form associated with the infinite-dimensional evolution equation. The crucial part is how to guarantee the semi-discretization in a finite-dimensional Hamiltonian system. A general approach is that, instead of discretizing the PDE directly, we discretize both the Hamiltonian functional and the Hamiltonian (Poisson) structure, then form the resulting ODEs. The Hamiltonian functional can be discretized in any suitable way, being careful to maintain the symmetry of any derivatives in the functional. For the Hamiltonian structure, replacing the differential operators with any appropriate matrix difference operator may discretize it. The conventional semi-discrete methods are based on the finite difference method (FDM) [5,6], the Fourier pseudospectral method (PSM) [7,8], the wavelet collocation method (WCM) [9–11] and they have been applied on sorts of applications like the nonlinear wave equation [12], the Schrödinger equation [13, 14], the Maxwell's equations [15,16], the KdV equation [5], the Gross-Pitaevskii equation [17,18] and so on. Numerical experiments show that the corresponding symplectic schemes are superior to other non-symplectic schemes.

This paper presents a new type of semi-discrete method which is the discrete singular convolution method. Such method can be constructed to preserve the symplecticity of the semi-discrete system. The discrete singular convolution (DSC) method was first proposed in [19, 20] for the Fokker-Planck equation and then widely applied on many other partial differential equations including the Fisher's equation [21], the heat equation, the wave equation, the Navier-Stokes equation [22], the sine-Gordon equation [23] and the KdV equation [24]. The first combination of the DSC method and the symplectic method is given by Li [25] for the elastic wave modeling in order to deal with the seismic wave propagation. In this paper, we give the analytical expression of the differential matrices corresponding to the DSC method and apply the DSC method to systematically construct symplectic integrators for general Hamiltonian PDEs.

Comparing with the FDM, PSM, WCM, the DSC algorithm has the following advantages:

- 1 The DSC method is a generalization of the standard FDM because one can adjust the free parameters in the DSC method to get the central difference scheme (i.e. $\frac{1}{2h}$, $0, -\frac{1}{2h}$) for the first order derivative and $\frac{1}{h^2}, -\frac{2}{h^2}, \frac{1}{h^2}$ for the second order derivative where *h* is the spatial grid step. However, the DSC method is usually much more accurate than the FDM.
- 2 Such method is as accurate as the PSM for the bandlimited periodic functions and can be even more accurate than the PSM for approximating non-bandlimited functions [22]. Since the DSC method is a local approach, it is more flexible than the PSM in dealing with complex geometry and boundary conditions.
- 3 The differential matrices for the DSC method can be given explicitly while a recurrence algorithm has to be imposed for deriving the differential matrices for the