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Development of an Explicit Symplectic Scheme that Optimizes the Dispersion-Relation Equation of the Maxwell's Equations

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Abstract. In this paper an explicit finite-difference time-domain scheme for solving the Maxwell's equations in non-staggered grids is presented. The proposed scheme for solving the Faraday's and Ampère's equations in a theoretical manner is aimed to preserve discrete zero-divergence for the electric and magnetic fields. The inherent local conservation laws in Maxwell's equations are also preserved discretely all the time using the explicit second-order accurate symplectic partitioned Runge-Kutta scheme. The remaining spatial derivative terms in the semi-discretized Faraday's and Ampère's equations are then discretized to provide an accurate mathematical dispersion relation equation that governs the numerical angular frequency and the wavenumbers in two space dimensions. To achieve the goal of getting the best dispersive characteristics, we propose a fourth-order accurate space centered scheme which minimizes the difference between the exact and numerical dispersion relation equations. Through the computational exercises, the proposed dual-preserving solver is computationally demonstrated to be efficient for use to predict the long-term accurate Maxwell's solutions.

AMS subject classifications: 52B10, 65D18, 68U05, 68U07
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1 Introduction

In Maxwell's equations, two field variables $\underline{B}$ (magnetic flux density) and $\underline{D}$ (electric flux density) are theoretically constrained by the solenoidal conditions given by $\nabla\cdot\underline{B}=0$ and

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$\nabla\cdot\underline{D}=0$. Provided that these two zero-divergence constraint equations are imposed initially, the field variables $\underline{B}$ and $\underline{D}$ governed by the coupled Faraday's and Ampère's equations can remain divergence free within the continuous context. In many numerical calculations of Maxwell's equations, the divergence-free conditions for the magnetism and electricity are unfortunately not satisfied due to some inevitably introduced discretization errors. The inability to retain the zero-divergence constraint conditions (or the Gauss's law) may result in a numerical instability problem when simulating the electromagnetic wave propagation. How to resolve this non-divergence problem becomes one of the major research themes in the development of a proper Maxwell's equation solver [1]. One can enforce these divergence-free constraint conditions all the time in the well known Yee's staggered grids [2]. The generalized Lagrange multiplier formulation of Munz et al. [3] belongs to the other class of numerical methods that can be applied to retain also the divergence-free condition in the Maxwell's equations. One can get a local divergence-free Maxwell's solution as well using the discontinuous Galerkin finite element method introduced in [4].

When approximating the derivative terms, dissipation error can smear the solution and at the same time dispersion error can cause an erroneously predicted phase speed or group velocity. Since Maxwell's equations contain only the first-order spatial derivative terms, the indispensable dispersion error can more or less destabilize the scheme. It is therefore essential to reduce the dispersion error when approximating the first-order spatial derivative terms. How to get an accurately predicted propagation characteristics during the simulation of Maxwell's equations becomes the second objective of the present study.

Discretization error is always cumulative. After solving the electromagnetic wave equations for a long time, the computed time-evolving solution will be gradually deteriorated by the non-symplectic temporal schemes. Failure to preserve the symplectic geometric structure can very often lead to numerical instability problem after a long time simulation. How to preserve symplecticity embedded in the Maxwell's equations for a long-term computation poses another difficulty, thus motivating us to properly approximate the time derivative terms shown in the Faraday's and Ampère's equations.

The rest of this paper will be organized as follows. In Section 2, the Maxwell's equations, which include the Faraday's law for the time-evolving magnetic flux density, Ampère's law for the propagation of electric flux density, and the Gauss' laws for ensuring the solenoidal nature of the magnetism and electricity, will be presented. In Section 3 two divergence-free constraints are imposed on the electric and magnetic vector fields. In Section 4, the first-order spatial derivative terms in the coupled Faraday's and Ampère's equations will be approximated in a way that the computed difference between the exact and numerical dispersion relation equations is minimized. Since Maxwell's equations are classified to be Hamiltonian (Eq. (2.8)), we will apply a symplectic structure-preserving time integrator to conserve its symplecticity numerically using the explicit symplectic partitioned Runge-Kutta scheme. We will also present in the same section a detailed analysis of the scheme in Fourier space. In Section 5, one problem with the exact solution