INTERNATIONAL JOURNAL OF NUMERICAL ANALYSIS AND MODELING Volume 15, Number 6, Pages 747-784

CONSTRUCTION AND ANALYSIS OF WEIGHTED SEQUENTIAL SPLITTING FDTD METHODS FOR THE 3D MAXWELL'S EQUATIONS

VRUSHALI A. BOKIL AND PUTTHA SAKKAPLANGKUL

Abstract. In this paper, we present a one parameter family of fully discrete Weighted Sequential Splitting (WSS)-finite difference time-domain (FDTD) methods for Maxwell's equations in three dimensions. In one time step, the Maxwell WSS-FDTD schemes consist of two substages each involving the solution of several 1D discrete Maxwell systems. At the end of a time step we take a weighted average of solutions of the substages with a weight parameter θ , $0 \le \theta \le 1$. Similar to the Yee-FDTD method, the Maxwell WSS-FDTD schemes stagger the electric and magnetic fields in space in the discrete mesh. However, the Crank-Nicolson method is used for the time discretization of all 1D Maxwell systems in our splitting schemes. We prove that for all values of θ , the Maxwell WSS-FDTD schemes are unconditionally stable, and the order of accuracy is of first order in time when $\theta \neq 0.5$, and of second order when $\theta = 0.5$. The Maxwell WSS-FDTD schemes are of second order accuracy in space for all values of θ . We prove the convergence of the Maxwell WSS-FDTD methods for all values of the weight parameter θ and provide error estimates. We also analyze the discrete divergence of solutions to the Maxwell WSS-FDTD schemes for all values of θ and prove that for $\theta \neq 0.5$ the discrete divergence of electric and magnetic field solutions is approximated to first order, while for $\theta = 0.5$ we obtain a third order approximation to the exact divergence. Numerical experiments and examples are given that illustrate our theoretical results.

Key words. Maxwell's equations, Yee scheme, Crank-Nicolson method, operator splitting, weighted sequential splitting.

1. Introduction

The electric and magnetic fields inside a material are governed by the macroscopic Maxwell's equations along with constitutive laws that account for the response of the material to the incident electromagnetic (EM) field. The computational simulation of electromagnetic interrogation problems, for the determination of the dielectric properties of materials (such as permittivities and permeabilities), requires the use of highly efficient forward simulations of the propagation of transient electromagnetic waves in these media. Thus, a lot of research has concentrated on the development of fully discrete forward solvers of Maxwell's equations that are accurate, consistent, stable, and computationally efficient.

The Yee scheme is a simple and efficient finite difference time domain (FDT-D) method [28], and one of the most important numerical techniques for solving Maxwell's equations in the time domain. The Yee-FDTD method, first proposed by Yee in 1966 [28], is an explicit scheme that employs staggered (uniform) grids in both space and time for the electric and magnetic field components. On the staggered grids, central difference approximations in space and time are constructed for each component of the electric and magnetic fields in Maxwell's equations which gives second order accuracy in both space and time. The scheme is non-dissipative for EM wave propagation in vacuum. The Yee scheme along with other discrete methods have been extended to numerically solve Maxwell's equations for EM wave propagation in a variety of linear and nonlinear materials [1, 2, 3, 27], and applied

Received by the editors April 26, 2017 and, in revised form, October 20, 2017. 2000 Mathematics Subject Classification. 65M06, 65M12, 65Z05.

to a wide variety of applications in nondestructive evaluation, optical simulations, bioelectromagnetic simulations among others [11, 21, 25]. The Yee scheme has also been extended to nonuniform meshes for EM propagation in a variety of materials [15, 19, 20].

The most limiting aspect of the Yee scheme is the fact that the time step Δt and the spatial step sizes Δx , Δy and Δz must satisfy a Courant-Friedrichs-Lewy (CFL) stability condition [26, 27]. The conditionally stable Yee scheme has a stability condition that is determined by the smallest cell size in the domain. For geometries which include features that are smaller than the wavelengths of typical interrogating pulses, fine scale spatial resolution is required to resolve small features. For example, to study the effect of microwaves on brain cells, the size of geometrical features can be five orders of magnitude smaller than a typical wave length [14]. In this case, the conditionally stable Yee scheme requires a very small time step in the *entire* domain to resolve the smallest spatial scales. Thus, the FDTD analysis of very fine geometric structures via the Yee scheme can require a large number of time iterations and long computation times.

The Crank-Nicolson (CN) FDTD method for the numerical simulation of the time domain Maxwell's equations is an implicit FDTD technique and is unconditionally stable [22, 23, 24]. Unconditionally stable schemes are well suited for problems involving geometries needing different details of discretization such as narrow slots [13]. For geometries requiring fine scale spatial resolution, non-uniform meshing techniques can be created by using locally small spatial increments which do not require extremely small time steps in the entire domain in an unconditionally stable scheme [9]. The implicit nature of the CN-FDTD method allows the time step to be chosen based on just accuracy requirements and not stability, and is thus a well suited scheme for the simulation of EM wave propagation in geometries with fine details. However, the CN method is computationally more intensive than the Yee scheme as it requires the solution of a large linear (3D spatial) system at every time step rather than a matrix vector multiplication as in the explicit Yee scheme [22, 23, 24].

The operator splitting method [10] is a powerful tool to solve multi-dimensional and multi-physics problems. In this approach, we replace the original problem involving a complicated operator into a sequence of sub-problems each involving a single operator that models a single physical process. The sub-problems communicate via their initial conditions and an approximation to the solution of the original problem is obtained by combining the solutions of sub-problems. Operator splitting methods are classified based on how the sequence of sub-problems are solved and how these sub or intermediate solutions are combined to approximate the solution of the original problem, which also determines the accuracy of the splitting technique. The classical operator splittings, which include sequential splitting, the Strang-Marchuk splitting, the alternating direction implicit (ADI-FDTD) scheme [13], among others, are popular splitting methods for solving complex time-dependent problems. These splitting techniques can offer additional reductions in computational time over fully implicit methods like the CN scheme while preserving the property of unconditional stability. By using the sequential and symmetrized splitting methods, Chen, Li, and Liang presented the energy-conserved splitting FDTD methods for the free space Maxwell's equations in two- [6] and three-dimensions [7]. The sequential splitting method gives low accuracy in time although its algorithm has a simple structure. As shown in [6, 7], the order of accuracy of a sequential splitting FDTD method for Maxwell's equations is of the first order in time and