Journal of Computational Physics 325 (2016) 98–115

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Time-filtered leapfrog integration of Maxwell equations using unstaggered temporal grids

A. Mahalov, M. Moustaoui *

School of Mathematical and Statistical Sciences, Arizona State University, Tempe, AZ 85287-1804, United States

ARTICLE INFO

Article history:
Received 6 January 2016
Received in revised form 10 August 2016
Accepted 11 August 2016
Available online 16 August 2016

Keywords:
Maxwell's equations
FDTD schemes
Unstaggered leapfrog
Time-filtered integration
Reduction of dispersion errors

ABSTRACT

A finite-difference time-domain method for integration of Maxwell equations is presented. The computational algorithm is based on the leapfrog time stepping scheme with unstaggered temporal grids. It uses a fourth-order implicit time filter that reduces computational modes and fourth-order finite difference approximations for spatial derivatives. The method can be applied within both staggered and collocated spatial grids. It has the advantage of allowing explicit treatment of terms involving electric current density and application of selective numerical smoothing which can be used to smooth out errors generated by finite differencing. In addition, the method does not require iteration of the electric constitutive relation in nonlinear electromagnetic propagation problems. The numerical method is shown to be effective and stable when employed within Perfectly Matched Layers (PML). Stability analysis demonstrates that the proposed method is effective in stabilizing and controlling numerical instabilities of computational modes arising in wave propagation problems with physical damping and artificial smoothing terms while maintaining higher accuracy for the physical modes. Comparison of simulation results obtained from the proposed method and those computed by the classical time filtered leapfrog, where Maxwell equations are integrated for a lossy medium, within PML regions and for Kerr-nonlinear media show that the proposed method is robust and accurate. The performance of the computational algorithm is also verified by analyzing parametric four wave mixing in an optical nonlinear Kerr medium. The algorithm is found to accurately predict frequencies and amplitudes of nonlinearly converted waves under realistic conditions proposed in the literature.

1. Introduction

There are several numerical methods that are used to integrate Maxwell equations. The Finite-Difference Time-Domain (FDTD) technique refers to a finite difference approximation of Faraday's and Ampere's laws using a leapfrog scheme combined with centered finite difference approximations for spatial derivatives. This method was introduced for the first time by Yee [1]. It is the most common time-domain method used to numerically solve Maxwell's equations [2]. The FDTD method is an explicit leapfrog finite difference scheme. It employs central differences on a staggered grid in both time and space. The Yee scheme has the advantage of low complexity, generality, and simplicity for parallel computing. It is a flexible and simple method to implement for solving complex electromagnetic problems. The method requires one function evaluation

* Corresponding author.
E-mail addresses: mahalov@asu.edu (A. Mahalov), mohamed.moustaoui@asu.edu (M. Moustaoui).

http://dx.doi.org/10.1016/j.jcp.2016.08.016

per time step and can model electromagnetic responses of inhomogeneous materials with curved geometry [3,4]. However, the standard Yee method can introduce errors due to significant numerical dispersion induced by poor representation of spatial finite differences. Other FDTD schemes utilizing the same time stepping as in the Yee's method have been proposed. These schemes use a fourth-order approximations of spatial differences [5–12]. The fourth-order staggered difference achieves much lower numerical dispersion compared to the second-order spatial differencing.

A comparison of the accuracy of several low-dispersion FDTD schemes was analyzed by Shlager and Schneider [13]. They showed that almost all the schemes using high-order finite difference provide substantial improvement in the dispersion errors compared with the classical Yee algorithm. Finkelstein and Kastner [17] presented a methodology for deriving a dispersion reduction scheme based on modifications of the characteristic equation for electromagnetic wave propagation problems.

The schemes described above use different finite difference approximations, but they all use the same leapfrog time stepping method as in the Yee scheme. In these schemes, the temporal grid is staggered in that, the electric field (E) is defined at $t_n = n\Delta t$ and $t_{n+1} = (n+1)\Delta t$ while the magnetic field (H) is defined half time step away from E at $t_{n-1/2} = (n-1/2)\Delta t$ and $t_{n+1/2} = (n+1/2)\Delta t$. Although temporal staggering is more accurate and suitable for the terms $\nabla \times \mathbf{H}$ and $\nabla \times \mathbf{E}$, it is incompatible with the time-differencing needed to integrate other physical and artificial terms in the governing equations such as Perfectly Matched Layers (PML) [14,15] and selective numerical smoothing terms. For instance, since the electric field E is not defined at $t_{n+1/2} = (n+1/2)\Delta t$, the time-staggered leapfrog formulation is usually combined with a semi-implicit trapezoidal scheme, which is employed to stably integrate terms representing current density $J = \sigma E$ and PML layers. In addition, applications of staggered temporal grids to Maxwell equations require solving a constitutive relation for the electric field at each time step in nonlinear electromagnetic propagation problems [16]. For similar reasons, the temporal staggered leapfrog method cannot be applied to electric and magnetic numerical smoothing terms. These artificial terms are traditionally introduced in the governing equations to reduce short oscillations generated by poor representation of spatial differencing.

In this paper we present a FDTD numerical algorithm for Maxwell equations using unstaggered temporal grids. It is based on a time-filtered leapfrog scheme using a fourth-order implicit time filter recently proposed in [20]. In this method, the electric and the magnetic fields are defined at the same temporal location ($t_n = n\Delta t$). We will show that this method allows explicit integration of current density terms. It can be applied for numerical smoothers to control short oscillations inherent in the numerical solutions when centered differencing is used; and can also be employed to effectively and stably integrate PML terms. We will also demonstrate that this method does not require solving the electric constitutive relation in nonlinear electromagnetic propagation problems.

The time-unstaggered leapfrog is very simple to implement. This method is suitable for numerical integration of wave propagation problems. However, it suffers from a serious defect related to the development of spurious modes ($2\Delta t$ waves). These modes are neutral and do not interact with the physical solution in linear wave propagation. Nevertheless, they may become unstable for nonlinear problems and are unconditionally unstable when numerical smoothing, physical or artificial damping are employed.

The unphysical modes can be reduced by applying the standard Robert–Asselin filtered leapfrog method [21,22], which uses a second-order time filter. However, the method introduces errors in the amplitude of the physical modes and degrades the accuracy of the solution to first order [26]. Alternative time stepping methods, such as high-order Runge–Kutta schemes, that do not have this defect have been described in the literature. These have been used in computational fluid dynamics (e.g., [23–28]) and Maxwell equations (e.g., [18,19]). The advantage of the third-order Runge–Kutta scheme (RK3) is its conditional stability for both advection and diffusion equations. It is also stable for both even and odd-order finite difference approximations for the first derivative in advection problems [24]. RK3 has higher accuracy but it requires three function evaluations per time step. Traditionally, poorly resolved waves generated by finite differencing can be reduced by applying selective numerical smoothers. The unfiltered leapfrog is unconditionally unstable when these smoothers are added to the equations.

The scheme proposed by Moustaoui et al. [20] produces third-order accuracy for the amplitude of the physical solution. It is superior compared with those based on second-order time filtering. Stability analysis of this scheme using the oscillation equation demonstrated that it is effective in reducing the computational modes. However, the behavior of this scheme and its stability when it is combined with spatial differencing and applied to Maxwell equations were not studied. In this paper, we propose a method based on a filtered leapfrog scheme using a staggered temporal grid, which can be employed to integrate Maxwell equations. The scheme can be applied in combination with both staggered and collocated spatial grids. We show that this method can be used explicitly to integrate terms representing current density, numerical smoothing and PML layers, without having the need to combine it with other time-stepping schemes. We also show that the method is effective for nonlinear electromagnetic propagation problems. The paper is organized as follows. The formulation of the scheme is presented in Section 2. Tests and stability analysis are shown in section 3. Applications for lossy material, PML layers and parametric four wave mixing in an optical nonlinear Kerr medium are demonstrated in Section 4. Finally a summary is given in section 5.