



Discrete exterior calculus approach for discretizing Maxwell's equations on face-centered cubic grids for FDTD

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ABSTRACT

Maxwell's equations are discretized on a Face-Centered Cubic (FCC) lattice instead of a simple cubic as an alternative to the standard Yee method for improvements in numerical dispersion characteristics and grid isotropy of the method. Explicit update equations and numerical dispersion expressions, and the stability criteria are derived. Also, several tools available to the standard Yee method such as PEC/PMC boundary conditions, absorbing boundary conditions, and scattered field formulation are extended to this method as well. A comparison between the FCC and the Yee formulations is made, showing that the FCC method exhibits better dispersion compared to its Yee counterpart. Simulations are provided to demonstrate both the accuracy and grid isotropy improvement of the method.

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1. Introduction

The Finite-Difference Time-Domain (FDTD) [1] is an elegant yet simple numerical method for electromagnetics which has been around for many decades and is a component of many in-house codes and commercial software. In this method, the computational region is discretized into a cubic lattice so that it can be modeled on a computer. In the standard Yee grid, electric and magnetic field components are staggered in both space and time. Discretization inevitably introduces some error. One of the sources of error is numerical dispersion, which causes the phase velocity of propagating waves to be dependent on the frequency as well as the angle of propagation [2]. Consequently, a spherical wavefront is deformed after traveling some distance. This grid anisotropy error, unfortunately, is cumulative and can be troublesome in large scale simulations.

There have been several methods proposed for improving numerical dispersion characteristics and grid anisotropy. One approach is to utilize higher order methods [3–9] where additional neighboring fields – often from further away in the cardinal directions – are used in the update equations for more accuracy. A comprehensive overview and comparison of the higher order methods may be found in [10]. Although the absolute dispersion error can be significantly reduced, the grid anisotropy is not necessarily improved as the relative phase velocity difference at different propagation angles remains the same. One of the major drawbacks of such methods is that the implementation at material interfaces becomes much more complicated, as the computational stencil is no longer strictly local.

Another approach is to modify the coefficients in the update equations in a way that the dispersion error is optimized for particular propagation angles and/or ranges of frequencies [11–17]. These provide some flexibility to the user, and the

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concept can be applied to both higher order methods and to alternative grids, but their efficacy is more difficult to extend to applications requiring broadband and/or wide-angled simulation results.

In another approach, Forgy and Chew [18] used a superposition of two different Finite-Difference methods on an overlapped lattice which complement each other's dispersion anisotropy to create a more isotropic algorithm. Another way of modifying the dispersion characteristics is discretizing Maxwell's equation on a lattice other than the cubic grid. It has been reported [2] that a staggered scheme on a hexagonal grid in two dimensions leads to reduced errors and better isotropy compared to Cartesian grid. Keranen et al. in Reference [19] provide mathematical arguments on various space-filling dual grids upon which Yee-like schemes can be constructed. Using the perspective of cochains and covectors, they then go on to show how the choice of space-filling shapes can allow one to predict the error bounds on such a Yee-like scheme, and how shapes that better fill a circle (in 2D) or sphere (in 3D) will provide better error control. However, they only demonstrate this with examples in 2D.

In three dimensions, using a lattice that more closely resembles a sphere, for example, could potentially alleviate the grid anisotropy problem. In [2] and [20] the suggestion is made to use a body-centered cubic lattice, also known as Somerville mesh, for this purpose. Reference [21] also used a type of face-centered cubic (FCC) lattice to perform simulations for scalar wave equation in 3D, and reported improvements in grid isotropy. In an attempt to extend this to Maxwell's equation, a nodal-based method was developed in [22] with collocated fields of the same kind, but staggered magnetic and electric fields in space with respect to each other. However, nodal-based schemes are known to be prone to spurious solutions [23]. A step by step iteration of the fields, for example produced by two electric dipoles close to each other but opposite in sign, reveals that the method in [22] produces wrong fields even though the method is stable.

Recently Rabina et al. [24] developed an FDTD scheme on FCC lattice as well as on body-centered cubic and a number of other natural crystals using Discrete Exterior Calculus (DEC) [25]. They report that the average numerical wavelength error is the least for different propagation angles on FCC lattice compared to a number of other structured lattices, but the body-centered cubic lattice maintained the same order of error for a wider range of propagation angles, meaning better grid isotropy.

In this work, we utilize discrete exterior calculus, similar to [24], to discretize Maxwell's equations on FCC lattice. However, instead of using incidence matrices and taking an unstructured mesh approach, we derive Yee-like explicit update equations. The analytical numerical dispersion expression will also be derived. Several tools available to the Yee method will be extended to FCC grid such as absorbing boundary conditions, perfect electric conductors (PEC)/perfect magnetic conductors (PMC), and scattered field formulation, in a manner similar to [26]. Numerical examples will be provided to demonstrate the accuracy, stability and improvement in grid isotropy of the method. Preliminary results of this work were previously published in [27]. This paper will go much further into the details of the derivation of the method, as well as added analysis.

In what follows, we first briefly discuss Discrete Exterior Calculus, followed by derivation of the update equations, and the dispersion relationship. Next, implementation of PEC/PMC boundary conditions and absorbing boundary conditions are presented, and then scattered field formulation, interpolation rule, near-field to far-field transformation, and finally, the numerical results.

2. Discrete exterior calculus

Discrete Exterior Calculus is an elegant mathematical tool which aims to discretize differential forms rather than vector fields. It is closely related to the FDTD method in its integral form [28] and the "generalized FDTD" [29] and the work of Teixeira et al. [30]. Writing out Maxwell's equations in vector form shows no explicit difference between the flux densities and field intensities. However, in the differential forms formulation this difference is more pronounced, and in the discrete case is actually visible.

A good review of differential forms can be found in [31]. Although a space-time formulation can be derived [32], in this work because of simplicity we focus only on the space forms in a manner similar to [26]. Maxwell's equations in the differential forms formulation are written as

$$\partial_t B = -dE - J^* \quad (1)$$

$$\partial_t D = +dH + J \quad (2)$$

$$dB = \rho^* \quad (3)$$

$$dD = \rho \quad (4)$$

$$D = \star \epsilon E \quad (5)$$

$$B = \star \mu H \quad (6)$$

where ∂_t is the time derivative, and d is the exterior derivative, which is a generalization of gradient, divergence, and curl into one operator. Exterior derivative converts an (n) -form to $(n+1)$ -form. The field intensities E and H are considered 1-forms whereas the fluxes D and B and current densities J and J^* are 2-forms, and the charge densities ρ and ρ^* are 3-forms. A 0-form could for example be the static voltage V .

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