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Optimized three-dimensional FDTD discretizations of Maxwell's equations on Cartesian grids

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Abstract

In this paper, novel finite-difference time-domain (FDTD) schemes are introduced for the numerical solution of Maxwell's equations on dual staggered Cartesian three-dimensional lattices. The proposed techniques are designed to accomplish optimized performance according to certain features and requirements dictated by the investigated problems, thus making efficient use of the available computational resources. Starting from only few initial assumptions, a construction process based on the minimization of specific error formulae is developed, which is later exploited to derive the final form of the finite-difference operators. Previously, an elaborate analysis of the proposed indicators is provided, targeting at global error control over all propagation angles. Our methodology guarantees upgraded flexibility, as accuracy can be maximized within either narrow or wider frequency bands, without practically inducing significant computational overhead. Attractive qualities such as high convergence rates are now the natural consequence of the effective design process, rather than the minimization of the truncation errors of the difference expressions. In fact, the proposed FDTD approaches verify the possibility to attain improved levels of accuracy, without resorting to the traditional – Taylor based – forms of the individual operators. A theoretical analysis of the inherent dispersion artifacts reveals the full potential of the new algorithms, while numerical tests and comparisons unveil their unquestionable merits in practical applications.

Keywords: Finite differences; Time-domain methods; Higher-order schemes; Numerical dispersion; Optimization

1. Introduction

The continuous scientific research in the computational electromagnetics area, stimulated and motivated by various engineering applications, has led to the development of diverse numerical techniques for the simulation of wave-interaction phenomena. Among them, the finite-difference time-domain (FDTD) method has been established as a relatively simple, efficient and adequately accurate – in several instances – numerical tool [1,2]. Through extensive testing during the previous years, the FDTD algorithm has been proven to be

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especially suited for problems incorporating domains of small or moderate at most electrical size. Unfortunately, its accuracy is rendered questionable when studying electrically large structures. Moreover, poor performance may be observed even in small-scale simulations, if stringent accuracy requirements must be fulfilled for elongated time periods. Such undesirable situations are the natural consequences of the adopted second-order space–time approximations, and can undoubtedly constitute limiting factors when investigating electromagnetic problems of contemporary interest.

In essence, the FDTD-related inaccuracies do not manifest themselves as randomly distributed or generated errors, but appear with the form of numerical dispersion and anisotropy artifacts. The latter are recognized as one of the most significant sources of error (others may be related to the rather limited geometric flexibility of the structured Cartesian grids), whose detrimental consequences are further aggravated by their accumulative nature. As a result, fundamental properties of electromagnetic waves may not be always preserved to a reliable degree in simulations entailing energy propagation, thereby producing misleading numerical conclusions.

Unfortunately, within the rather limited framework of Yee's algorithm, the available choices for accuracy upgrade are directly related to the adoption of finer grid resolutions (which, due to stability limitations, also imply smaller time-steps). This kind of solutions is rarely attractive, as the low order of the classic FDTD method renders mesh refining quite costly (and often prohibitive). On the other hand, notable accuracy improvement can be ensured if the second-order approximations are replaced by higher-order counterparts, which are capable of accomplishing reduced error levels under the same computational cost. The relevant bibliography comprises various FDTD techniques that adopt high-order alternatives, such as explicit [3,4] or implicit [5–7] spatial approximations, combined with enhanced time-integration processes, including leapfrog and Runge–Kutta schemes [8], backward approximations [9], symplectic integrators [10], etc.

Since the best compromise between accuracy and computational cost remains an open matter for FDTD methodologies, the fundamental question that needs to be answered is concerned with the characterization of the adequacy or suitability of a finite-difference scheme for a given electromagnetic problem. In plain words, how the approximations to space–time derivatives should be designed (given e.g. the stencil size), in order to guarantee a solution with the highest degree of accuracy. On the other hand, it is generally recognized that maximizing the formal order in finite-difference expressions is not the optimum way to treat numerical simulations. Such an allegation simply implies that problems with different characteristics or accuracy requirements must not be dealt with in a unified manner. In accordance with this practice, there have been reported some instances – not only in computational electromagnetics – toward the design of problem-optimized finite differences. For example, modified compact schemes were derived in [11] by requiring the vanishing of an error formula at preselected frequency points, aiming for improvement at small wavelengths. Similarly, new approximate expressions were obtained in [12] through the solution of properly defined minimization problems, while control of both phase and amplitude errors was performed in [13]. Minimization of dispersion errors was also carried out in [14], where a $(2,4)$-like FDTD technique with high phase accuracy was developed, to deal with electrically large structures. A collection of finite-difference approaches that are capable of providing "flexible local approximations" was recently demonstrated in [15], referring to a wide variety of problems. As shown, these discretization strategies exploit the fact that specific features of the exact solutions are known a priori (the non-standard FDTD method [16,17], based on a single-frequency tuning, can be included in this category as well). Other higher-order FDTD algorithms [18,19] were optimized within specific frequency bands and/or angular sectors, based on the minimization of special error functionals. Modified schemes based on the $(2,4)$ stencil were constructed in [20], by minimizing errors along selected angles of propagation. A more generalized design methodology was presented in [21], which enabled the development of various algorithms through systematic modifications of their characteristic equations. We could also refer to some approaches that improve conventional FDTD methods by altering the constitutive parameters of the background media [22,23]. Apparently, they too can be considered equivalent to applying modified operators in conjunction with the physical materials.

It becomes clear that contemporary computational challenges dictate the establishment of a general design framework, founded on a solid theoretical basis, to enable flawless capturing and reproduction of electromagnetic properties in discrete spaces, without at the same time sacrificing the inherent simplicity of traditional FDTD methodologies. Towards this perspective, the present paper discusses the development of novel three-dimensional (3D) FDTD schemes with optimum discretization properties, suitable for solving demand-