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The element level time domain (ELTD) method for the analysis of nano-optical systems: I. Nondispersive media

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Abstract

We study a 3-dimensional, dual-field, fully explicit method for the solution of Maxwell's equations in the time domain on unstructured, tetrahedral grids. The algorithm uses the element level time domain (ELTD) discretization of the electric and magnetic vector wave equations. In particular, the suitability of the method for the numerical analysis of nanometer structured systems in the optical region of the electromagnetic spectrum is investigated. The details of the theory and its implementation as a computer code are introduced and its convergence behavior as well as conditions for stable time domain integration is examined. Here, we restrict ourselves to non-dispersive dielectric material properties since dielectric dispersion will be treated in a subsequent paper. Analytically solvable problems are analyzed in order to benchmark the method. Eventually, a dielectric microlens is considered to demonstrate the potential of the method. A flexible method of 2nd order accuracy is obtained that is applicable to a wide range of nano-optical configurations and can be a serious competitor to more conventional finite difference time domain schemes which operate only on hexahedral grids. The ELTD scheme can resolve geometries with a wide span of characteristic length scales and with the appropriate level of detail, using small tetrahedra where delicate, physically relevant details must be modeled.

Keywords: Maxwell's equations; Nano-optics; Computational electromagnetics; Unstructured tetrahedral grid; Time domain finite element method; Element-level decomposition

1. Introduction

Numerical algorithms in computational electromagnetics are generally subdivided in two main categories: time [1,2] and frequency domain methods [3]. The dielectric and magnetic material properties that appear in the constitutive relations, associated with Maxwell's equations, are generally frequency dependent. In the frequency domain, these relations take on simple algebraic shapes for any material property. In contrary, their formulation for dispersive materials in the time domain contains a convolution operation, which necessitates more elaborate solution methods. This fact, together with the simplicity of the involved differential equations, has favored the study of frequency domain methods for a considerable period [4]. As a Consequence, researchers have developed a myriad of methods in the frequency domain for solving general electromagnetic problems. Some of the more prominent ones are method of moments (MoM) [5], finite element method (FEM) [6,7], generalized multipole technique (GMT) [8], finite difference

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frequency domain (FDFD) [4], and the boundary element method (BEM) [9]. In the frequency domain, the problem is solved for one discrete frequency, which is itself a parameter in the analyzed system of equations. To obtain the system response for a range of frequencies, the solution process needs to be repeated for every frequency point. If reduced accuracy is acceptable, then fast-frequency sweep methods can be employed which in turn extrapolate the frequency response over a wide bandwidth [7]. By the emergence of new research areas, such as biomedical applications for health monitoring [10] and, specifically, optical engineering using nanometer sized structures [11] full-wave analysis of complex and large-scale problems became strongly required. The encountered problems have definitely challenged the established frequency domain methods. The large dimensions of the geometries not only render the repeated solution of the problem immensely time consuming but also prevent the frequency extrapolation methods to produce appropriate results. Moreover, there is often a need to know the response of the system over a wide frequency bandwidth through a single computation. To remedy these difficulties and for development of flexible and fast routines, time domain methods have been studied.

In time domain, once the problem has been analyzed for an excitation with broad frequency content, the spectral response of the system is retrieved via the Fourier transform of the time domain results. Therefore, time domain techniques are usually methods of choice for problems with broadband variations and large dimensions. Moreover, studying nonlinear phenomena, such as *Raman* response and *Kerr* media [1], is feasible in the time domain. In contrast to the wide variety of frequency domain methods, there is only a rather limited number of general purpose methods in the time domain [2]: complexity of the differential equations and the constitutive relations being preeminent reasons. For several decades, based on the pioneering work by Taflove, the finite difference time domain (FDTD) method has dominated time domain electromagnetics [1]. Although the method is robust, simple and fast, it has suffered from the severe limitation that it discretizes the considered geometries based on a uniform cartesian grid. Remedies, such as subgridding or split-material voxels [1], have been studied over the years without fully resolving the issue. Thus, FDTD has somewhat lost its competitive advantage for modeling photonic nano-structures, where multi-scale geometries are involved and surface effects, such as plasmonic resonances, are frequently encountered.

One can tackle the addressed problem with cartesian grids by taking advantage from unstructured, tetrahedral grids. Thus, the finite element time domain method (FETD) has been developed. In FETD, the electromagnetic fields are expanded, on an unstructured tetrahedral grid as a superposition of spatial basis functions scaled with a time dependent coefficient. Then, various finite difference schemes are used for temporal discretization leading to either *implicit* or *explicit* time marching processes [7]. We comment that *explicit* and *implicit* here refer to the temporal discretization of the differential operators. Both variants require the solution of a large linear system of equations at every time step for time update [7,12–15], leading to extremely high computation costs. Even parallelization on distributed memory cluster computers only partially resolves this issue. Hence, despite the capability of using unstructured grids, this method is only applicable for relatively small nano-optical problems [13–15].

In recent years, the discontinuous Galerkin (DG) time domain methods, an inherently different group of methods, have received substantial attention. DG algorithms provide explicit schemes on unstructured, tetrahedral grid but can be used on hexahedral grids as well. They are high order methods and are conceptually based on expanding the electromagnetic fields into a separate set of basis functions for each element. Then, the electromagnetic continuity conditions are enforced between the elements by coupling the fields over the common faces with the adjacent elements. The specific nature of this coupling condition, denoted as *numerical flux*, significantly influences the results [16]. Among these methods the interior penalty (IP) methods and variants based on central and upwinding flux were extensively investigated for two- and three dimensional problems in electromagnetics for the whole frequency range [17–21]. An alternative in this category is the finite volume time domain (FVTD) method. FVTD is a 1st order accurate method where each element is coupled to the adjacent ones based on conservation laws [2, chap. 9], [22–24]. The fully explicit nature of these methods considerably simplifies the computation of large problems, because just simple multiply-and-add style operations for marching in time are required. Additionally, the computational requirements, e.g. memory and calculation time, scale linearly with the number of tetrahedral elements.

Among the computational methods roughly classified as DG methods, a specific method was recently developed for unstructured tetrahedral grids by Lou and Jin [25], denoted as the element level time domain (ELTD) method. The original idea of this method is presented in a previous paper [26], where the concept of domain decomposition is employed for coarse-grained