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A topologically consistent class of 3-D higher order curvilinear FDTD schemes for dispersion-optimized EMC and material modeling

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Abstract

An enhanced higher order finite-difference time-domain (FDTD) algorithm for the precise analysis of complex 3-D electromagnetic compatibility (EMC) structures and arbitrary interface material distributions in general curvilinear, skewed and stretching lattices is presented in this paper. Introducing a systematic topological tessellation, the novel methodology develops a family of robust higher order non-standard forms, which exactly represent the material properties and significantly suppress the artificial dispersion errors. To handle inherent mesh deficiencies an enhanced low-pass filtering procedure is implemented, while a consistent class of self-adaptive compact operators ensures the correct evaluation of electromagnetic components near boundary walls. Moreover, for more involved media interfaces that do not follow the lines of the grid, a convergent transformation around these discontinuities leads to precise simulations. Therefore, this optimal field-preserving technique along with suitably tuned perfectly matched layers (PMLs), achieve high levels of accuracy, decrease the required number of points per wavelength and provide considerable computational savings, as indicated by extensive numerical results addressing 3-D EMC and hard-to-model material applications.

Keywords: Material modeling; Computational electromagnetics; Finite-difference time-domain methods; Higher order schemes; General curvilinear coordinates; Numerical solution of partial differential equations

1. Introduction

The progressively increasing demands for advanced simulations of electromagnetic compatibility (EMC) devices and the reliable materials processing of their complicated components have lately mandated strict stipulations on modeling and design tools [1–3]. Among existing numerical techniques, the finite-difference time-domain (FDTD) method has a wide applicability in many areas of research [4]. The original algorithm is relatively simple in the construction of the computational lattice, since no mathematically involved formulae are required. However, when solving an arbitrarily-curved problem via a second-order staircase discipline like the FDTD one, the artificial dispersion mechanisms place a major restraint to its usage. Also, several strenuous subwavelength geometries and multi-dimensional material compositions often prohibit the reliable interpretation of the underlying physics. Not to mention that when a field component is discontinuous along a curvilinear interface, the FDTD scheme may exhibit loss of global convergence and stability. Actually, the prior drawbacks have been the subject of an ongoing research [5–10], aiming at approaches that offer acceptable stability.

In this paper, a multi-space 3-D higher order FDTD methodology—based on generalized non-standard curvilinear operators—is presented for the systematic investigation of EMC and complex media structures. Using the language of algebraic topology, the unified framework hosts a covariant/contravariant flux theory which along with an appropriately established dual-grid formulation enables the correct mapping of acutely deformed meshes. This strategy, by means of a low-pass filtering process, optimizes the overall performance and subdues dispersion errors. Moreover, the resulting higher order FDTD expressions take into account a sufficiently larger amount of points for spatial derivatives, instead of the two points employed by the traditional counterparts. To overcome the inevitably widened spatial stencils

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near absorbing or perfectly electric conducting (PEC) boundaries, we develop a family of curvilinear compact differencing schemes, while all infinite spaces are terminated by a modified version of the efficient perfectly matched layer (PML) [11,12]. For the important case of dissimilar materials, whose interface does not coincide with any of the grid axes, the algorithm introduces a special transformation combining additional degrees of freedom. This perspective guarantees the fulfilment of the proper jump-conditions and the calculation of precise values for the corresponding constitutive parameters. Numerical results, studying a variety of 3-D curvilinear EMC applications and problems with diverse materials, depict the merits of the proposed method, even in coarse FDTD resolutions or geometric singularities.

2. The generalized higher order curvilinear FDTD algorithm

When objects of arbitrary curvature and multiple materials are to be modeled, the FDTD technique exhibits an ill-suited behavior, mainly, due to the incomplete imposition of continuity conditions at the interfaces. Unfortunately, to these errors one must add the lattice dispersion discrepancies intrinsic in the low-order schemes. A possible solution could be the averaging of constitutive parameters at the interfaces. However, in the case of ambiguous regions such a procedure is not at all exact or convergent. Actually, the above serious defects have been the primary motive for the development of our method, especially in curvilinear grids.

2.1. Construction of the consistent non-standard forms

The essential premise of the higher order (HO) algorithm resides in the representation of electromagnetic fields via a new class of 3-D non-standard concepts. Their form is given by

$$\mathbf{W}^{M}_{q,L}\left[f|^{t}_{u,v,w}\right] = \frac{g(u,v,w)}{C_S(kL\delta q)} \sum_{m=1}^{M} R^q_m \times \left\{ \sum_{l=1}^{L} P^q_{m,l} \mathbf{D}^{(m)}_{q,l\delta q}[f|^t_{u,v,w}] \right\}, \tag{1}$$

where M is the order of accuracy and q is a variable of the general coordinate system (u, v, w) described by its respective g metrics. Such a differencing rationale ensures that dispersion error mechanisms, having the potential to spoil the final outcomes, are drastically subdued or even completely eliminated. On the other hand, parameters R^q_m and $P^q_{m,l}$ achieve an inherent robustness both in the handling of geometric details and the right assignment of field quantities to space-time entities by satisfying the following gauges

$$\sum_{m=1}^{M} R^q_m = 1, \tag{2}$$

$$\sum_{l=1}^{L} P^q_{m,l} = \frac{1}{2} \quad \forall m. \tag{3}$$

Factor L defines the number of stencils, $l\delta q$, along each axis, which are needed for the accomplishment of a specific accuracy with a typical value of $L = 3$. The correction function $C_S(kl\delta q)$ ensures the smooth transition from the continuous to the discrete state. Its argument, depending on wavenumber k, is selected to handle broadband electromagnetic excitations with the non-standard concepts. This is conducted by employing the Fourier transform of the already computed electric or magnetic vectors at predetermined lattice positions. The process does not affect the total overhead, whereas its efficacy increases with the number of prefixed nodes. A possible choice of C_S could be

$$C_S(kl\delta q) = \frac{16}{k^2} \sin\left(\frac{kl\delta q}{3}\right) \cos\left(\frac{kl\delta q}{9}\right). \tag{4}$$

Operators $\mathbf{D}^{(m)}_{q,l\delta q}[.]$, in (1), cover all optimal node arrangements – irrespective of cell shape – leading to very coarse grids and mutual cancellation of material discrepancies. Therefore, unlike the common FDTD technique which involves only two mesh points for the calculation of spatial derivatives, the proposed method concerns a whole set of nodes. This remark is crucial for body-fitted tessellations with abrupt geometric attributes like slope discontinuities, skewness or stretching. An indicative v-directed $\mathbf{D}^{(m)}_{v,l\delta v}[.]$ is

$$\mathbf{D}^{(m)}_{v,l\delta v}[f|^t_{u,v,w}] = \frac{(\delta v)^m}{3m-2} \left(\sum_{r_A=\pm 1} f|^t_{r_A\delta u, -l\delta v/2, r_A\delta w} - m \times \sum_{r_B=\pm 1} f|^t_{-r_B\delta u, l\delta v/2, -r_B\delta w} \right). \tag{5}$$

Analogous expressions can be extracted towards the remaining u and w directions in the domain.

The aforementioned HO non-standard operators are now applied to the discretization of spatial and temporal derivatives appearing in Maxwell's curl equations. In this framework, the generalized forms are established via a series of parametric relations, depending on the approximation level. Hence,

spatial differentiator:

$$\mathbf{L}_q[f|^t_{u,v,w}] = \frac{b_1}{4\delta q} \left\{ \mathbf{W}^M_{q,L}[f|^t_{u,v,w}] + \sum_{s=1}^{3} f|^t_{q\pm s\delta q/2} \right\}, \tag{6}$$

temporal differentiator:

$$\mathbf{T}[f|^t_{u,v,w}] = \frac{1}{C_T(\delta t)} (f|^{t+\delta t/2}_{u,v,w} - f|^{t-\delta t/2}_{u,v,w}) - b_2 \partial_m f|^t_{u,v,w}, \tag{7}$$

with b_1 and b_2 being specific tuning parameters and $C_T(\delta t)$ the correction function of $\mathbf{T}[.]$. It stressed that (6) is applied everywhere in the domain except absorbing or PEC walls,