Enhanced Analysis of Multiconductor Nanostructured Devices via a Compact Block FDTD/VFETD Method

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Abstract—A reduced-order modeling FDTD/VFETD technique is presented in this paper, for the accurate and cost-effective study of multiconductor nanoscale structures. The novel algorithm blends a compact stencil-optimized discretization process with general vector finite elements and partitions the domain into tightly-coupled blocks. A key asset is that both approaches are time-advanced independently while their space-state variables are derived via a Krylov-based scheme with scaled Laguerre functions, which drastically decreases the order of the transfer matrix. Numerical results from various nanocomposite devices validate the hybrid method and reveal its applicability.

Index Terms—Carbon nanotubes (CNT), FDTD methods, FETD schemes, model-order reduction, nanostructured devices.

I. INTRODUCTION

The accurate evaluation of the electromagnetic response of nanostructured components and carbon nanotube (CNT) systems is strongly associated to the consistent representation of their size by the pertinent sampling rates [1], [2]. In particular, when multiconductor setups are involved, it is critical to quantify any intermodulation issues, as ever-increasing switching speeds drive signal bandwidths to tens of gigahertz at all levels of high-density packaging. Considering that many of these devices must be continually reconfigured, it is apparent that computational models can significantly restrict unduly construction expenses. However, their application is not always undemanding, because of the convoluted features and the nonlinear character of the preceding systems. To this objective, an assortment of robust schemes has been hitherto developed to mitigate the analysis’ total complexity [3]-[6].

In this paper, a hybrid 3-D algorithm for the comprehensive macromodeling of multiconductor nanocomposite applications is introduced. The new method combines a compact-stencil finite-difference time-domain (FDTD) technique with a modified vector finite-element time-domain (VFETD) formulation, which are updated independently and separate the domain into flexible local blocks coupled by the proper continuity conditions. The decrease of the discrete model is achieved via a Laguerre-oriented Krylov-subspace model-order reduction scheme that splits all subspace vectors into their electric field intensity and magnetic flux density parts at a stage prior to any simulation. Thus, the number of unknown variables is seriously confined and high levels of accuracy as well as resources economy are attained, even when sub-wavelength details are to be considered. These advantages are successfully certified by diverse nanostructured setups with complex geometries, large electrical sizes, and arbitrarily-curved interfaces.

II. REDUCED-ORDER-MODEL FDTD/VFETD TECHNIQUE

Starting from the first part of the 3-D hybrid method, the principal aim is to construct an efficient FDTD discretization, based on a generalized curvilinear dual-lattice regime. Hence, a family of compact spatial and temporal approximators is introduced as

\[ L^e \left[ f^e_p \right] = \sum_{r=1}^{K} \frac{(\Delta t)^{r-1}}{2!} \sum_{s=1}^{S+r-1} f^e_{p-r,s} + \frac{(\Delta t)^{r-3}}{3!} \sum_{s=r+2}^{S+r-1} f^e_{p-r,s}, \quad (1) \]

\[ T^m \left[ f^e_p \right] = \Xi(\Delta t) \left( f^{m+1/2}_p - f^{m-1/2}_p \right) + \sum_{s=r+2}^{M} \bar{v}_{s}^e f^e_{p}, \quad (2) \]

where $\Xi(\eta) = (2\eta + 5)(\Delta t)^{\eta-1} - 3(q+4)(\Delta t)^{\eta}$ for $q \in [0, 1/2]$,

(a) a log-spiral antenna with a multiconductor nanostructured superstrate

(b) a hemi-ellipsoidal cavity-backed antenna with a nanocomposite substrate.

Fig. 1. (a) A log-spiral antenna with a multiconductor nanostructured superstrate and (b) a hemi-ellipsoidal cavity-backed antenna with a nanocomposite substrate.

Concerning the modified VFETD algorithm, we define

\[ G_1 = \sum_j g_j^1 w_j^{(1)} \quad \text{and} \quad G_2 = \sum_j g_j^2 w_j^{(2)}, \]

with $G_1 = \{E, H\}$, $G_2 = \{D, B, J\}$ the electric/magnetic intensities, fluxes, and external source vectors, and $w^{(1)}$, $w^{(2)}$ the basis functions [7]. Also, $g_j^1 = \{E, H\}$ denotes the circulation of $G_1$ along edge $\ell_l$ and $g_j^2 = \{D, B, J\}$ the $G_2$ flux through facet $f_j$. Plugging (4) in Ampere’s and Faraday’s law, one gets

\[ \sum_j \mathcal{H} \nabla \times w_j^{(2)} = \sum_j \left( \hat{\partial}_j \mathcal{D}^e + j \mathcal{E}^j \right) w_j^{(2)}, \quad (5a) \]

\[ \sum_j \mathcal{E} \nabla \times w_j^{(1)} = - \sum_j \hat{\partial}_j \mathcal{B}^e w_j^{(2)}. \quad (5b) \]

To simplify the above formulas, one may employ the properties of differential forms. So, in matrix notation, (5a) and (5b) become

\[ \hat{\partial}_j \Phi = \mathcal{Y} \mathcal{H} - \mathcal{J} \quad \text{and} \quad \hat{\partial}_j \mathcal{B} = - \mathcal{E} \mathcal{E}, \]

for $\mathcal{Y}$ the circulation matrix occupied either by unity or zero elements. The system of (6) is completed by the correct association of fluxes with fields and the following constitutive relations

\[ \sum_j \mathcal{D}_j w_j^{(2)} = \mathcal{E} \sum_j \mathcal{E}^j w_j^{(1)}, \quad (7a) \]

\[ \sum_j \mathcal{B}_j w_j^{(2)} = \mathcal{H} \sum_j \mathcal{H}^j w_j^{(1)}. \quad (7b) \]

Time advancing in (6) is conducted via a leapfrog-like scheme and is completely independent of the time-update procedure in the compact FDTD approach, on condition that the minimum Courant limit is considered for the selection of both temporal increments.
Next, the domain is divided into simple FDTD or VETD blocks, related to the problem details, and coupled by the suitable media information, and Q, P matrices containing the coupling coefficients for the domain’s neighboring blocks. To lessen the size of $x$ in (8), without actually affecting the overall accuracy, a model-order reduction approach is developed. The principal concept is to construct another linear system with the same transfer function between $h$ and $s$, but with a different vector $x$. In particular, the state-space model (8), with $A$ inputs yields the $A \times A$ impulse response transfer matrix $h(t)$, that is expanded as

$$h(t) = \sum_{l=0}^{\infty} A_l \beta_l(t),$$

and an 80% higher arithmetic complexity. Also, Fig. 4 shows the serious directivity improvement. The second structure is the hemi-ellipsoidal antenna of Fig. 1(b) with a multi-conductor Nanotex™ CNT substrate. For $\alpha = 4$, $m = 6$, the grid comprises $78 \times 65 \times 20$ FDTD cells and $4.98 \times 10^7$ degrees of freedom. Results for the radiation pattern and $E_z$ magnitude snapshot are presented in Fig. 5(a), while Fig. 5(b) shows the significant decrease of the system memory needs (likewise for CPU time) in terms of $\alpha$ factor.

**REFERENCES**


