New Concepts for the Multiresolution Time Domain (MRTD) Analysis of Microwave Structures

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Abstract—The Multiresolution Time Domain (MRTD) technique presents a natural framework for the implementation of spatio-temporal adaptive gridding. This feature can lead to significant reductions in the simulation time for large-scale problems of practical interest to the microwave community. With the exception of the Haar-based MRTD scheme, all the other methods presented in the literature employ high-order finite difference operators for the numerical approximation of the spatial partial derivatives of Maxwell’s equations. However, little attention has been devoted to the study of the convergence properties of these schemes, which are typically associated with significantly increased numerical work and stability limits that are small fractions of the FDTD Courant stability limit. In this paper, it is first noted that high-order spatial finite differences still produce second-order error convergence for the method, as long as they are coupled with the second-order accurate leap-frog time integration. This prompts us to investigate other possibilities for the formulation of MRTD schemes, revisiting the choice of the leap-frog scheme for time-integration, with the purpose of improving the convergence properties of MRTD, employing high-order time integrators.

I. INTRODUCTION

In a seminal paper, Krumpholz et al. [1] showed that the Finite Difference Time Domain (FDTD) technique can be rigorously derived via the well-known Method of Moments, assuming an orthogonal expansion of electromagnetic field components in pulse basis functions, in both space and time. Based on this observation, Krumpholz and Katehi [2] proposed the derivation of a dispersion-wise improved numerical method, using the Battle-Lemarie cubic spline basis scaling functions, instead of pulses, for field expansion in space. Despite the fact that the field expansion in spline functions does not imply any type of multiresolution analysis by itself, it will be henceforth referred to as Scaling Multiresolution Time Domain (S-MRTD) method, following the terminology of [2], that alludes to the possibility of building up a multiresolution field expansion in space, by means of wavelet functions, orthogonal to the scaling ones. Yet, S-MRTD does use pulse functions as field basis functions in time, effectively retaining a leap-frog based time integration. Along the same lines, several other authors derived and applied similar schemes, based on Daubechies [3] and the Cohen-Daubechies-Feauveau bi-orthogonal [4] scaling functions. More recently, MRTD schemes using basis functions of the Coifman family were studied [5], [6].

All aforementioned contributions contain dispersion studies of S-MRTD schemes, explicitly demonstrating their superiority compared to Yee’s scheme, in terms of dispersion errors for certain choices of the cell size. Nevertheless, this result is expected, since MRTD employs high-order spatial finite differences, with the exception of the Haar-based MRTD. A well-known relevant drawback is the decay of the MRTD Courant stability limit, which typically reduces to nearly 0.6 of the corresponding FDTD Courant limit [7]. By inspection of the dispersion curves presented in [3]-[6], one can also observe an apparent contradiction. As one increases the order of S-MRTD spatial finite differences (for example, using Daubechies functions with an increasing number of vanishing moments [8]), the associated dispersion curve does not change from one point on. That is, increased numerical work does not pay-off in terms of observed accuracy. This question is readily resolved in this paper, by considering the global error convergence [9] of MRTD schemes and taking into account the fact that S-MRTD still uses a leap-frog time-integration approach.

Subsequently, emphasis is given in the role of time-integration for the formulation of efficient MRTD techniques. The possibility to formulate linear multi-step methods stemming from the temporal field expansion in scaling functions is pointed out. Preliminary dispersion investigations indicate the clear superiority of this approach, compared to the existing MRTD techniques.

II. CONVERGENCE OF THE MRTD TECHNIQUE

A. Importance of error convergence in MRTD

Despite its individual importance, S-MRTD is primarily studied as a first stage for the development of the so-called W-MRTD [2], in which fields are expanded in a multiresolution basis, including multiple wavelet levels. By basic multiresolution analysis (MRA) principles, the introduction of one wavelet level for the field expansion in a certain grid direction, effectively refines the grid in this direction by a factor of two (let us restrict our interest to dyadic multiresolution analyses). Hence, if the dispersion of S-MRTD is characterized by a homogeneous system of equations of the form:

$$\mathcal{J}(k_x \Delta x, k_y \Delta y, k_z \Delta z, \omega \Delta t) = 0,$$

a W-MRTD with one wavelet level in x, y, z, is characterized by the system:

$$\mathcal{J}(k_x \Delta x/2, k_y \Delta y/2, k_z \Delta z/2, \omega \Delta t) = 0.$$  

As discussed in [10], this behavior is achieved under the condition that the offset between electric and magnetic field nodes in space is modified to one quarter of a cell (as opposed to half-a-cell in FDTD). The use of wavelets introduces a significant volume of additional operations. Therefore, the rate at which the global error of the method is reduced, presents
a measure of the efficiency of the use of wavelets and the impact of mesh refinement (and the operations related to its implementation) to the accuracy of MRTD. This, in fact, motivates the following study.

B. Study of MRTD convergence ; order of accuracy

For simplicity, consider a uniform mesh of Yee’s cells \( \Delta x \times \Delta y \times \Delta z \), with \( \Delta x = \Delta y = \Delta z = h \), for wave propagation in a homogeneous space, with \( \Delta t = sh/u_p \) being the time step, if the phase velocity in the medium is \( u_p \). Then, the asymptotic form of the error of the FDTD technique is \( C_1 h^2 + C_2 \Delta t^2 \) or \( \hat{C} h^2 \), if the ratio of the cell size to the time step is kept constant. Then, \( p = 2 \) is the order of accuracy of the FDTD method. On the other hand, let us consider the S-MRTD technique, applied to the one-dimensional system of Maxwell’s equations:

\[
\frac{\partial E_x}{\partial t} = \frac{\partial H_z}{\partial y}, \quad \mu \frac{\partial H_z}{\partial t} = \frac{\partial E_x}{\partial y}.
\] (3)

To do so, \( E_x \) and \( H_z \) are expanded in space in terms of scaling functions (let us not specify their type for the moment) \( \phi_i(y) = \phi(y/\Delta y - i) \) and \( \phi_{i+1/2}(y) = \phi(y/\Delta y - i - 1/2) \), respectively:

\[
E_x(y, t) = \sum E_i^x(t) \phi_i(y)
\]

(4)

\[
H_z(y, t) = \sum H_{i+1/2}(t) \phi_{i+1/2}(y)
\]

(5)

Compared to the field expansions of [2], the expansions in (4), (5) are strictly spatial, allowing for the explicit investigation of multiple time-integration techniques. Applying the Method of Moments, in the sense of [2], the following system is derived:

\[
\frac{\partial E_i^x(t)}{\partial t} = \frac{1}{\epsilon \Delta y} \sum_{p=-L_z+1}^{L_z} \alpha(p) H_{i+1/2}(t)
\]

(6)

\[
\frac{\partial H_{i+1/2}(t)}{\partial t} = \frac{1}{\mu \Delta y} \sum_{p=-L_z+1}^{L_z} \alpha(p) E_i^x(t),
\]

(7)

where:

\[
\alpha(p) = \int_{-\infty}^{+\infty} \phi_i(x) \frac{d}{dx} \phi_{i+p}(x) dx
\]

(8)

\[
= \frac{1}{\pi} \int_{0}^{+\infty} \lambda |\phi(\lambda)|^2 \sin (\lambda(p - 1/2))
\]

(9)

Two observations are now in order. First, since \( \alpha(-p) = -\alpha(p+1) \), the number of multiplications needed for each spatial finite difference operator is equal to the stencil \( L_z \); not 2\( L_z \). Second, the order of accuracy of these operators is \( 2L_z \). Note, that in the literature, fourth-to-sixth order schemes have been shown to provide satisfactory dispersion performance for wave-propagation problems [11]. This observation provides a guideline for the choice of basis functions in MRTD schemes. For example, the Battle-Lemarie scheme of [2] has typical stencil values of 9-12, while MRTD of Daubechies functions with 2, 3 vanishing moments (D2, D3) use stencils 3, 5 respectively [3]. Practically, the accuracy offered by Battle-Lemarie finite differences is extraordinary, but un-necessary, while Daubechies functions with more than three vanishing moments are also of limited practical interest.

In addition, inspection of the dispersion curves in [3-6] shows that increasing the order of finite difference operators does not pay-off dispersion-wise. For example, the phase errors associated with the use of CDF(2,2) and CDF(2,6) in [4] are hardly distinguishable, despite the fact that their stencils are largely different (3 and 7 respectively), hence the latter employs more than twice as many operations as the former. This trend is more evident in Fig. 1, that presents phase velocity errors, numerically determined from the MRTD dispersion relation for one-dimensional wave propagation in an unbounded domain, using leap-frog time integration and Coifman scaling functions in space, with stencils varying from 7 to 19. The log-log scale used in the Figure displays that FDTD and MRTD have the same order of convergence, namely quadratic. This is explained as follows: Indeed, MRTD has a global error of the form \( C h^P + C_i \Delta t^2 \), where \( P \) is the typically (extremely) high order of the spatial finite difference. Evidently, as \( h \to 0 \) and \( \Delta t \to 0 \) (from the Courant stability condition), the asymptotic behavior of the time integrator becomes dominant. Hence, the global error asymptotically decays as \( \hat{C} h^2 \), independently of the order of the finite difference in space. Also, a log-log plot of the error as a function of the cell size is expected to be linear, with a slope equal to two.

This study provides the following conclusion: Relatively low order S-MRTD methods of moderate stencils are preferable. It only makes sense to employ even higher order finite differences in space, if high order time integration is also used. As a consequence the formulation and study of MRTD techniques coupled with high-order time integrators is motivated.

III. LINEAR MULTI-STEP METHODS (LMM) FOR S-MRTD

In this section, new possibilities for high-order S-MRTD schemes are investigated. Obviously, another alternative can be the use of high-order Runge-Kutta or Adams-Bashforth methods for time integration. The methods that are considered here, belong to the class of Linear Multi-step Methods (LMMs) [9]. The general form of an LMM for an initial value problem \( u_t = f(u) \) is:

\[
\sum_{j=0}^{r} \beta_j u(t_{n+j}) = \Delta t \sum_{j=0}^{r} \gamma_j f(u(t_{n+j})).
\]

(10)
Typically, the coefficients of an LMM are chosen so that higher order error terms in a Taylor expansion of the method cancel out. However, multi-stepping implies the existence of multiple modes (corresponding to multiple frequencies that one can extract from the polynomial dispersion relationship), whose excitation can be avoided via an appropriate choice of the initial conditions.

We pose the question if the systematic formulation of a linear multi-step method is possible by the expansion of fields in scaling functions in both space and time. Let us consider a staggered scheme, implied by the following expansions:

\[
E_x(y, t) = \sum_{p-L_x}^{L_x} \frac{\Delta t}{\epsilon \Delta y} \alpha(p) n + 1/2 H^{\epsilon}_{i+p-1/2} \phi_{n+1/2}(y) \phi_{n+1/2}(t)
\]

An implicit assumption embedded in these expressions (made only for convenience) is that the same basis is used in space and time, while \( \phi_n(t) = \phi(t/\Delta t - n) \). The resulting expression of (3) can be solved by several methods, including point-matching. The method followed in this work is again the Method of Moments. Then, explicit update equations are derived and the dispersion properties of the physical mode they provide are investigated. To facilitate the direct comparison of this approach and the conventional MRTD, in terms of mathematical formalism, the electric field update equations under leap-frog-based MRTD and under this space-time MRTD approach are provided in the following two equations, respectively:

\[
n + 1/2 E^\epsilon_i = n + 1/2 E^\epsilon_i + \frac{\Delta t}{\epsilon \Delta y} \sum_{p=-L_x}^{L_x} \alpha(p) n + 1/2 H^{\epsilon}_{i+p-1/2} (13)
\]

where the stencil coefficients \( \alpha(p) \) are as in (9). If we had used pulse functions as a temporal basis, equations (13),(14) would be the same. In this sense, the conventional MRTD is a special case of the space-time MRTD.

Finally, the dispersion properties of spatio-temporal schemes formulated with various scaling functions of the Coifman family (Fig. 2) are studied. Analytically, the dispersion equation of a three-dimensional space-time MRTD is given by the expression:

\[
D^2_x = \left( \frac{u_p \Delta t}{\Delta x} \right)^2 D^2_x + \left( \frac{u_p \Delta t}{\Delta y} \right)^2 D^2_y + \left( \frac{u_p \Delta t}{\Delta z} \right)^2 D^2_z
\]

with:

\[
D_\xi = \sum_{p=1}^{L_x} \alpha(p) \sin (k_\xi (p-1/2) \Delta \xi)
\]

\[
\xi = x, y, z \text{ and:}
\]

\[
D_\tau = \sum_{p=1}^{L_x} \alpha(p) \sin (\omega (p-1/2) \Delta \tau)
\]

Selective results for one-dimensional wave propagation along a mesh of cell size \( h \), are presented in Figs. 3-5. In all cases, the dispersion of the FDFTD and the space-time MRTD are calculated for \( s = u_p \Delta t/h = 0.1 \), while the conventional S-MRTD scheme for \( s = u_p \Delta t/h = 0.065 \). These values approximately correspond to 1/10 of their Courant stability limit. The plots confirm that the space-time MRTD schemes demonstrate higher order of accuracy as the order of the finite difference operator used increases. Thus, there is an obvious improvement from the Coifman of order 3 to Coifman of orders 6,8-based MRTD. Overall, the new schemes have superior performance compared to their conventional counterparts. Two notes need to be made: First, the space-time schemes meet the floor of the accuracy of our computations, which is compromised by the calculation of the stencil coefficients (integration routines). In fact, the Coifman functions are determined in the Fourier domain, via a well-known recursive procedure [8]. These calculations are responsible for the almost flat part of the dispersion curve, encountered at high discretization rates \( (h/\lambda, \rightarrow 0) \). Second, the slope with which the dispersion curve emerges from this numerical ‘floor’ indicates the order of accuracy of the scheme. Indeed, this becomes steeper as the order of the finite difference operator increases, contrary to our previous observations regarding the asymptotic behavior of the conventional MRTD.

IV. CONCLUSION

Previous MRTD studies tend to combine extremely high-order spatial finite difference operators with leap-frog time-integration. A simple convergence argument shows that this choice accumulates numerical operations without achieving tangible gains in accuracy, since the second-order time integration imposes a limitation in the overall accuracy of MRTD. This motivates the coupling of high-order time integration schemes with MRTD finite differences. One way to achieve this, is presented in this paper: Fields are expanded in scaling functions in both space and time. Sampling the resulting equations with the Method of Moment approach of [2] gives rise to explicit linear multi-step methods. The dispersion properties of the latter are clearly superior compared to the conventional MRTD, while they suffer from the disadvantages of LMM’s, namely the excitation of non-physical modes. This issue is under study, along with the effects of staggering to the stability properties of space-time MRTD. Finally, implicit space-time
MRTD formulations, stemming from point-matching in time are also of significant interest.

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