Numerical Error Analysis and Control in a Dynamically Adaptive Mesh Refinement (AMR) - FDTD Technique

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Abstract—A recently proposed Dynamically Adaptive Mesh Refinement (AMR) Finite-Difference Time-Domain (FDTD) technique has been shown to achieve up to two orders of magnitude execution time savings compared to the conventional FDTD, when applied to practical microwave design and analysis problems. Yet, its performance depends on several a priori defined parameters, in a way similar to frequency domain mesh adaptive techniques. The estimation of this dependence, as well as the derivation of related error bounds, is contributed by this paper, being achieved via numerical studies and confirmed through specific applications.

I. INTRODUCTION

A dynamically Adaptive Mesh Refinement (AMR) - Finite-Difference Time-Domain (FDTD) technique was recently introduced and applied to microwave integrated circuit and optical waveguide problems [1]-[4], demonstrating simulation time savings of up to two orders of magnitude, compared to the conventional FDTD. The method can be considered as a dynamic implementation of the static subgridding techniques, previously discussed in the time-domain modeling literature [5]-[6]. Instead of applying local mesh refinement in a priori defined regions of a computational domain, AMR-FDTD uses subgrids, which are adaptively defined according to the spatio-temporal evolution of field distributions. The concept of the technique is demonstrated in Fig. 1 that depicts the evolution of a dense mesh inside a coarse one, following the propagation and multiple reflections of a vertical electric field (excited by a Gaussian pulse) in a microstrip spiral inductor.

Throughout an AMR-FDTD simulation the computational domain consists of a “mesh tree” of hierarchically defined meshes. Each level-$m$ + 1 mesh is created by refining a subset of the cells of a level-$m$ mesh in a rectangular region by a factor of 2 (in each direction). There is only one level-1 mesh, the “root” mesh, which covers the entire computational domain (also shown in Fig. 1). The mesh tree is re-generated every $N_{AMR}$ time steps. The criteria for mesh refinement, performed every $N_{AMR}$ time steps, are briefly outlined. Assuming a current time step $n$, the electromagnetic energy $W_{i,j,k}^n$ of each $(i,j,k)$ cell of a mesh is approximated via the expression:

$$W_{i,j,k}^n \approx \frac{1}{2} \left\{ \epsilon_{i,j,k} |\vec{E}_{i,j,k}^n|^2 + \mu_{i,j,k} |\vec{H}_{i,j,k}^n|^2 \right\} V_{i,j,k},$$

where: $V_{i,j,k}$ is the volume of cell $(i,j,k)$, and $\vec{E}_{i,j,k}^n$, $\vec{H}_{i,j,k}^n$ are vector electric and magnetic field values at the center of the cell at time step $n$ (approximated by space/time averaging). Then, the gradient of the energy $\nabla W_{i,j,k}^n$ at each cell can be approximated by a second order finite-difference expression. Defining thresholds $\theta_g$ and $\theta_q$, a cell $(i,j,k)$ is marked for refinement if both of the following criteria are met:

$$|\nabla W_{i,j,k}^n| > \theta_g G^n, \quad W_{i,j,k}^n > \theta_q Q^n,$$  \hspace{1cm} (1)

where $G^n = \max_{i,j,k} |\nabla W_{i,j,k}^n|$ and $Q^n = \max_{0 \leq m \leq n} W_{av}^m$, and $W_{av}^m = (1/(N_x N_y N_z)) \sum_{i,j,k} W_{i,j,k}^m$. The first criterion tracks energy gradient peaks, while the second prevents numerical noise, at the late stages of the simulation, from triggering spurious mesh refinements. If a cell is marked for refinement, cells at a distance $\sigma_{AMR} N_{AMR} \Delta t$ around it (where $\Delta t$ is the time step of the root mesh and $c$ is the speed of light) are also marked, to account for arbitrary wave propagation during the time interval between two mesh refinements. As discussed in [3], marked cells of a level $m$ mesh are grouped together...
and enclosed in a rectangular level \( m + 1 \) mesh, in a way that ensures that the volume of the marked cells to the total volume of the new mesh surpasses a threshold \( \theta_c \). Once the mesh refinement algorithm is set and recursively performed, the non-uniform FDTD mesh, that its application produces, can be handled according to any static subgridding technique [5]-[6]. Although static subgridding is associated with late-time instability problems, the AMR-FDTD is not, since at late times the number of meshes reduces to one (namely the root mesh), while at early times the dense meshes enclose evolving pulses, ensuring that they never encounter a dense-to-coarse mesh interface, which would be responsible for gradually accumulating spurious reflections.

On the other hand, in order to elevate AMR-FDTD to the level of a microwave CAD technique, a clear set of guidelines for the choice of its aforementioned five parameters is needed. The main objective of this paper is to produce such guidelines, that would allow a user to determine the AMR-FDTD parameters for a given error tolerance.

II. NUMERICAL ERROR ESTIMATION: METHODOLOGY

The numerical error whose dependence on the AMR-FDTD parameters is sought for is defined as follows, for a 2-D TE case with field components(\( E_z, H_x, H_y \)). Given a computational domain, an array of probes is considered, where field values are recorded at each time step. The reference solution, that AMR-FDTD is compared to, is provided by applying the FDTD method in a uniform mesh, at a Yee cell resolution equal to the maximum achievable resolution of the AMR-FDTD. This is chosen to be dense enough to guarantee convergence. Then, if a field component recorded by the \( m \)-th probe at time \( t_k \) is denoted by \( f_m(t_k) \) and \( f_m^{ref}(t_k) \) the corresponding reference field value, the error is defined as:

\[
E = \sqrt{ \sum_{k,m} |f_m(t_k) - f_m^{ref}(t_k)|^2 / \sum_{k,m} |f_m^{ref}(t_k)|^2 }
\]

Note that different probes encounter different field waveforms, but also mesh configurations, due to the dynamic nature of mesh evolution in AMR-FDTD. Therefore, this metric is much more effective in capturing generic error effects, than a norm that would be based on field sampling at a port of a device, or the error in a frequency domain quantity (such as characteristic impedance or propagation constant). This approach is analogous to a Monte-Carlo type simulation and is aimed at rendering the obtained error less dependent on the device under test. Furthermore, such an approach is the only feasible, given the nature of the problem at hand. Contrary to static subgridding methods, the extraction of analytical error bounds seems

![Fig. 2](image-url)

Fig. 2. Error versus simulation time for variable (a) \( N_{AMR} \) (b) \( \sigma_{AMR} \) (c) \( \theta_c \).

to be impossible, due to the arbitrary distribution of submeshes in a domain. Finally, the same methodology can be easily extended to 2-D TM cases and 3-D cases.

III. NUMERICAL RESULTS AND ERROR BOUNDS

While the AMR-FDTD error performance on a number of structures was studied, results obtained from simulating three dielectric waveguide ones are shown. These are the power splitter and corrugated permittivity profile waveguide of [7] and the Y-junction of [8].

First, the effect of \( N_{AMR}, \sigma_{AMR} \) and \( \theta_c \) on the accuracy and simulation time is investigated. Fig. 2 includes error-simulation time curves, deduced by changing one of these three parameters and fixing the rest. All figures refer to 4-level AMR-FDTD simulations, but 2-and 3-level simulation results exhibit a similar behavior. The general pattern of these curves suggests that although increasing \( N_{AMR} \) and \( \sigma_{AMR} \) or decreasing \( \theta_c \) may improve accuracy (for example, as \( N_{AMR} \) is increased the AMR-FDTD tends to become equivalent to the reference FDTD technique), this improvement reaches a plateau beyond which, any change in the parameters merely increases the execution time. In a number of versatile situations, the choice of \( N_{AMR} = 10, \sigma_{AMR} = 2 \) and \( \theta_c = 0.7 \) balances accuracy and efficiency well. This conclusion is also supported
by Fig. 2. Essentially, these parameters do not explicitly control the mesh refinement procedure, which is why their choice is rather straightforward. This is not the case for $\theta_c$, $\theta_g$ that are studied next.

Fig. 3 shows the dependence of the error $E$ on $\theta_c$ and $\theta_g$ for all the cases studied. As expected, the error decreases as $\theta_c$ or $\theta_g$ decreases. For very small values of $\theta_g$, the error is mainly a function of $\theta_c$ and vice versa, since marking a cell for refinement depends on both thresholds. Based on this data $E(\theta_c, \theta_g)$ can be approximated, by linear interpolation around $\theta_c = \theta_g$. To a first order, this approximation requires $E(\theta_c, 0)$ and $E(0, \theta_g)$.

Figs. 4, 5 indicate these error functions for AMR-FDTD simulations of the same maximum resolution, but different number of levels. It is noted that $E(\theta_c, 0)$ and $E(0, \theta_g)$ follow similar trends for different devices. This also indicates the effectiveness of the error metric (2). The following curve-fitted bounds are thus deduced:

$$E_{bc}(\theta_c, \theta_g = 0) = 0.15 \theta_c^{0.37}$$

$$E_{bg}(\theta_g, \theta_c = 0) = 0.40 \theta_g^{0.35}$$

The asymptotic behavior of these functions as $\theta_c$ and $\theta_g$ tend to zero is correct; in this case, the refinement criteria are always satisfied and therefore the whole AMR-FDTD domain is covered by a uniform mesh of the maximum level of resolution, coinciding with the mesh used by the reference simulation. Moreover, a previous study [4] has shown that a number of more than four levels, leads to a compromise between the advantages of mesh adaptivity and the overhead of the operations needed for its implementation. Therefore, Figs. 4, 5 included up to 4 levels.

While the validity of these bounds can be confirmed through all previously published examples of AMR-FDTD, the case of a dielectric waveguide directional coupler (Fig. 6), similar to that of [8], is also discussed here. In this example, letting $N_{AMR} = 10$, $\sigma_{AMR} = 2$, $\theta_c = 0.7$ and $\theta_g = 0$, $\theta_e$ was chosen requiring that the error be less than 3%. Then, from (3), $\theta_e$ should be less than 0.013. A value of $\theta_e = 0.01$ satisfied this criterion. The excitation was a sine-wave modulated Gaussian pulse with a center frequency of 230 THz and a pulse width of 20 fs. The excitation was imposed at 1.2 $\mu$m from port 1. For AMR-FDTD, four levels of mesh resolution were used; the size of the coarsest mesh was 320 $\times$ 120. The time step for each mesh was determined by letting all mesh Courant numbers be equal to 0.7. Fields and errors were recorded over 3, 200 time steps of the root mesh. An array of 14 x 8 probes was used to record the $E_z$ field throughout the computation domain. The reference result was obtained by applying FDTD in a 2560 $\times$ 960 uniform mesh. The actual error was 0.37%, which satisfied the requirement, although it indicated that the deduced bound was rather conservative. Finally, Fig. 7 compares the fields obtained by AMR-FDTD and FDTD in ports 3 and 4 of the coupler. Evidently, AMR-FDTD cannot be distinguished from the reference solution, even for the weak field at port 4. For that waveform, the coarse mesh FDTD result suffers from a significant numerical dispersion induced error. The AMR-FDTD simulation last 6.2 hours, whereas the reference FDTD simulation 19.3 hours.
IV. CONCLUSIONS

The numerical error associated with the application of the AMR-FDTD technique was studied, and its dependence on the parameters controlling the accuracy and performance of this technique was outlined. Guidelines for the a priori choice of these parameters were provided, thus fulfilling an important condition for AMR-FDTD to be considered as a CAD oriented tool for electromagnetic applications.

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REFERENCES