Fast Time-Domain Simulation of Optical Waveguide Structures with a Multilevel Dynamically Adaptive Mesh Refinement FDTD Approach

Yaxun Liu and Costas D. Sarris

Abstract—The Finite-Difference Time-Domain (FDTD) technique has been widely employed for the modeling of both linear and nonlinear optical structures. Its main advantages though, namely simplicity and versatility, are offered at the expense of significant computational resources needed for the simulation of realistic geometries. In this paper, a recent approach that incorporated an adaptively refined moving mesh into the FDTD technique for microwave circuit design is applied to two-dimensional optical waveguide problems, resulting in dramatic simulation time savings, compared to FDTD, while maintaining its accuracy. To complement the applicability of the proposed technique as a novel photonics design tool, numerical error studies that facilitate the educated a priori choice of the simulation parameters are provided.

Index Terms—FDTD, dielectric waveguide, adaptive mesh refinement.

I. INTRODUCTION

The Finite-Difference Time-Domain technique (FDTD, [1], [2]) has been recognized as an effective simulation method for wave propagation in linear and nonlinear media, providing for the wideband characterization of a broad range of optical devices [3], [4], [5]. However, the FDTD advantage of being simple and versatile to apply comes with the drawback of requiring dense discretization rates (cell sizes of $\lambda/10$ or less) to guard against its pronounced numerical dispersion and small time steps in conformity with the Courant stability condition [2]. Both of these limitations translate into the formulation of computationally expensive problems. As a result, the application of FDTD to several practical geometries of interest is associated with excessively large simulation times.

Through the years, a number of alternative formulations have been presented for FDTD, aimed at reducing its computational cost. Most notably, hierarchical meshes, offering the possibility to resolve small geometrical features or localized field distributions in a simulated structure through one or multiple dense meshes, embedded within a coarser one, have been proposed for both microwave and optical applications [6]-[10]. The arrangement of these meshes can be decided a priori and remains fixed throughout the simulation. While this approach has been successful in achieving computational savings within the context of FDTD, it disregards the dynamic evolution of field waveforms tracked by time-domain solvers. For example, a high-dielectric inclusion in a photonic band-gap device would be permanently enclosed in a dense mesh under the static mesh refinement approach, while it would actually be illuminated by a wideband FDTD pulse excitation only within a fraction of the total computation time, when it would contribute to the response of the device. Therefore, static subgridding is only a sub-optimal solution to the inherently dynamic mesh refinement problem in FDTD.

In the area of computational fluid dynamics, the so-called Adaptive Mesh Refinement (AMR) technique was introduced for the solution of hyperbolic partial differential equations [11]. The application of AMR is based on the use of a hierarchical mesh, recursively developed through the refinement of a coarse root mesh, which covers the entire computational domain. The regions of the computational domain that need further mesh refinement are detected via certain indicators, as the simulation evolves. On the other hand, wherever a dense mesh is not needed anymore, it can be detected and replaced by a coarser one. In contrast to static mesh refinement, this method establishes a dynamically adaptive moving mesh, which is optimally suited to the nature of time-domain wave propagation simulations.

Recently, the AMR technique of [11] was combined with FDTD for the purpose of microwave integrated circuit modeling [12]-[14]. The feasibility of this approach was clearly demonstrated through realistic numerical examples, where speed-up factors as large as 20, compared to the conventional FDTD, were achieved. These savings increase with the size of the problem at hand, since then the overhead stemming from mesh adaptation related operations becomes small relative to the total number of operations. Therefore, electrically large optical waveguide structures present a class of problems where the dynamically adaptive technique of [12]-[14] can be the method of choice.

This paper develops a dynamic AMR-FDTD algorithm for optical waveguide topologies, extending previously reported static mesh refinement approaches employed in photonic applications, such as the one of [10], and demonstrates that dramatic execution time savings, compared to FDTD, are achievable by the technique, when applied to practical structures known to be solvable by FDTD in several hours or days of simulation time. Furthermore, while static subgridding techniques have been associated with the unstable growth of field solutions at a late stage of the simulation (the so-called late-time instability), it is shown that the dynamic AMR-FDTD inherently solves this
problem by eliminating its sources, namely static dense-to-coarse grid interfaces that propagating field solutions impinge upon generating spurious reflections that build up over time.

The proposed algorithm is a "multi-level" one, in the sense that it can support multiple levels of mesh resolution, by refining the Yee cells of an underlying root mesh by a predefined factor. In the terminology of this work, a two-level scheme would enclose Yee cells of size $\Delta x \times \Delta y \times \Delta z$ and $\Delta x/N_s \times \Delta y/N_s \times \Delta z/N_s$, while a $N$-level scheme would enclose Yee cells of size $\Delta x/N_s^i \times \Delta y/N_s^i \times \Delta z/N_s^i$, for $i = 0, 1, \cdots N - 1$, where the factor $N_s$ (here taken equal to 2) is the mesh refinement factor.

The paper is organized as follows: The multilevel dynamic AMR-FDTD algorithm is summarized in Section II; then, the generation and update procedure of the multiple meshes, and the handling of junctions between them is negotiated. This aspect of the algorithm is particularly important of inhomogeneous dielectric. Section III shows four numerical examples: a dielectric waveguide with corrugated permittivity profile, a dielectric waveguide power splitter, a Y-junction and a dielectric ring resonator. The results of these examples illuminate the outstanding efficiency of the proposed technique both in terms of speed and accuracy. Finally, numerical error estimates are provided as a function of the parameters of the algorithm involved, in order to provide guidelines for their choice by potential users of the method.

II. IMPLEMENTATION OF MULTILEVEL DYNAMIC MESH REFINEMENT

A. Overview of the dynamic AMR-FDTD

In the following, a brief overview of the dynamic AMR-FDTD algorithm is provided. For simplicity, the case of a two-dimensional system of TE Maxwell’s equations, involving the $E_z$, $H_y$, $H_y$ field components, is discussed.

Throughout an AMR-FDTD simulation the computational domain is comprised of hierarchically defined meshes, which form the structure of a “mesh tree”. The mesh tree is regenerated every $N_{\text{AMR}}$ time steps through a recursive mesh refinement procedure. An example is shown in Fig. 1. There is only one level-1 mesh, which is also called the root mesh and covers the entire computational domain. 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 $N_s$ (in each direction). Thus, the two meshes form a child-parent relation. The child meshes of the same parent may share an edge, but they may not overlap otherwise. In Fig. 1(b) a solid line corresponds to a child-parent relation, while a dashed line corresponds to a boundary shared by meshes of the same level. Each mesh includes Yee’s cells, where discrete field components are sampled. According to a standard convention, $E_z$ is sampled at the vertices, whereas $H_y$ and $H_y$ are sampled at the center of the cell faces along the $y-$ and $x-$direction, respectively.

B. Dynamic Generation of the AMR-FDTD Multilevel Mesh Tree

The criteria that the dynamic AMR-FDTD approach applies (every $N_{\text{AMR}}$ time steps) in order to decide whether to refine a Yee cell of the root mesh, are presented in section IV of [14]. For completeness, they are briefly outlined here. Assuming a current time step $n$, the electromagnetic energy $W^{n}_{i,j,k}$ of each $(i,j,k)$ cell of the root mesh is approximated via the expression:

$$W^{n}_{i,j,k} = \frac{1}{2} \int_{V_{i,j,k}} \left\{ \varepsilon \left[ (\mathbf{E}, n \Delta t) \right]^2 + \mu \left[ (\mathbf{H}, n \Delta t) \right]^2 \right\} dv \approx \frac{1}{2} \left\{ \varepsilon_{i,j,k} \left[ \mathbf{E}^{n}_{i,j,k} \right]^2 + \mu_{i,j,k} \left[ \mathbf{H}^{n}_{i,j,k} \right]^2 \right\} V_{i,j,k},$$  \hspace{1cm} (1)$$

where: $V_{i,j,k}$ is the volume of cell $(i,j,k)$, and $\mathbf{E}^{n}_{i,j,k}$, $\mathbf{H}^{n}_{i,j,k}$ 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 is approximated by a second order finite-difference expression, as:

$$\nabla W^{n}_{i,j,k} = \frac{W^{n}_{i+1,j,k} - W^{n}_{i-1,j,k}}{2\Delta x} \hat{x} + \frac{W^{n}_{i,j+1,k} - W^{n}_{i,j-1,k}}{2\Delta y} \hat{y} + \frac{W^{n}_{i,j,k+1} - W^{n}_{i,j,k-1}}{2\Delta z} \hat{z}. \hspace{1cm} (2)$$

Defining thresholds $\theta_e$ and $\theta_h$, a cell $(i,j,k)$ is marked for refinement if both of the following criteria are met:

$$\nabla W^{n}_{i,j,k} > \theta_e Q^n,$$

$$W^{n}_{i,j,k} > \theta_h G^n,$$  \hspace{1cm} (3)$$

where:

$$G^n = \max_{i,j,k} |\nabla W^{n}_{i,j,k}|,$$  \hspace{1cm} (4)$$

$$Q^n = \max_{0 \leq m \leq n} W^{m}_{i,j,k},$$  \hspace{1cm} (5)$$

$$W^{\text{av}}_{i,j,k} = \frac{1}{N_x N_y N_z} \sum_{i,j,k} W^{m}_{i,j,k}. \hspace{1cm} (6)$$

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 [6]-[9]. This paper follows the methodology outlined in [12]-[14].

For the multilevel case, the same algorithm is recursively applied at each mesh level. Assuming that $N_L$ is the maximum number of levels, the mesh re-generation (and, subsequently, the update of the mesh tree) is pursued as follows:

1) For $L$ from 1 to $N_L$, 

![Fig. 1. (a) Geometry and (b) data structure of a 3-level mesh tree.](image-url)
a) The maximum average energy $Q_L^n$ and maximum gradient of energy $G_L^n$ for level-$L$ is calculated.

b) For each mesh of level-$L$, the cells whose energy is greater than $\theta E Q_L^n$ and gradient of energy is greater than $\theta G_L^n$ are marked. If no cells are marked, we return to the previous step. Otherwise, the marked cells are clustered into rectangular regions, and for each rectangle, a level-$(L+1)$ mesh is created and added to the new mesh tree.

2) For $L$ varying from 2 to the number of levels of the new mesh tree, each level-$L$ mesh is initialized as follows: if it overlaps with any level-$L$ mesh of the old mesh tree, the electric and magnetic field components are obtained from the overlapping region. For the remainder of the mesh (which does not overlap with any other previous mesh) the electric and magnetic field components are calculated by interpolating their values from the corresponding parent mesh.

3) The previous mesh tree is then removed from memory. The only mesh that is not subject to regeneration every $N_{AMR}$ time steps is the root mesh.

C. Update equations for the multiple meshes

For simplicity, all meshes use the same Courant number $s$ to determine their time steps. For the root mesh:

$$\Delta t = s \frac{1}{u_p^{max}} \sqrt{\frac{1}{\Delta x^2} + \frac{1}{\Delta y^2} + \frac{1}{\Delta z^2}}. \quad (7)$$

Therefore, if $N_s$ is the mesh refinement factor, assuming that the level-1 (root) mesh uses a time step $\Delta t$, the level-$L$ meshes use a time step $\Delta t / N_s^{(L-1)}$. For level-$L$ meshes to advance one time step of theirs, level-$(L+1)$ meshes need to advance $N_s$ of their time steps to be synchronized with the former. It should be noted that all meshes of the same level need to be updated for a certain time step before advancing to the next time step, because their values are invoked in the update equations of neighboring meshes.

Letting again $N_L$ denote the total number of levels of the mesh tree, the following operations are recursively performed:

1) For each mesh of level-$L$, the magnetic field components are updated.

2) For each mesh of level-$L$, the electric field components are updated.

3) If $L+1 \leq N_L$, for each mesh of level-$L$, for $k$ from 0 to $N_s-1$, the previous two sets of updates are performed.

4) For all the meshes except the root mesh, one can define a “local” time step variable $S$, which enumerates the time steps executed within one time step of its parent mesh. Hence, this counter will take on values from 0 to $N_s-1$.

a) If $S = \lfloor N_s/2 \rfloor$, the magnetic field components of each mesh of level-$L$, are transferred to its parent mesh. Since the node points of parent and child meshes are not necessarily collocated (they are evidently offset if $N_s = 2$ [14]), the former are interpolated from the latter.

b) If $S = Ns - 1$, the electric field components of each mesh of level-$L$ are transferred to its parent mesh.

The aforementioned steps can be implemented in a function updateLevel($L$, $S$), which is recursively called to update all meshes with level greater or equal to $L$ and a local time step $S$. The main program just needs to call updateLevel($1$, 0) for the update of the entire mesh tree for one time step.

In the computational implementation that is used in the following results, a medium with inhomogeneous dielectric permittivity and permeability, as well as electric and magnetic conductivity is assumed. Hence, the incorporation of a matched absorber is straightforward. For example, the interior $E_z (i,j)$-nodes are updated through the equation:

$$E_{z,i,j}^{n+1} = C_1 E_{z,i,j}^n - C_y \left( H_{y,i,j+1/2}^{n+1/2} - H_{y,i,j-1/2}^{n+1/2} \right) + C_x \left( H_{y,j+1/2,i}^{n+1/2} - H_{y,j-1/2,i}^{n+1/2} \right), \quad (8)$$

where:

$$C_1 = \frac{\epsilon / \Delta t - \sigma e / 2}{\epsilon / \Delta t + \sigma e / 2},$$

$$C_{x,y} = \frac{1 / \Delta x y - \sigma e / 2}{\epsilon / \Delta t + \sigma e / 2},$$

with $\Delta x y = \Delta x$ and $\Delta y$, respectively, and $\sigma e$ being the electric conductivity of the medium. Updating electric field nodes on the boundary of a mesh requires four neighboring magnetic field values, at least one of which is obviously unavailable. In order to ensure that the updates can be performed, the following cases are considered and addressed [14].

1) The electric field is located on a perfect electric conductor or an absorbing boundary condition, therefore it can be updated otherwise than (8). In this case, the boundary is termed as a $PB$-type boundary (physical boundary).

2) The missing magnetic field component(s) can be obtained from neighboring meshes of the same level, which share a boundary with the mesh to be updated. In this case, the boundary is called an $SB$-type boundary (sibling boundary).

3) The missing magnetic field component(s) cannot be obtained from neighboring meshes of the same level, but the electric field can still be obtained by interpolating electric field values of the parent mesh. This type of boundary is called a $CPB$-type boundary (child-parent boundary).

It should be noted that an $SB$-type boundary is not limited to siblings of the same parent. Meshes of the same level having different parents may still share common edges, creating $SB$-type boundaries.

The treatment of the aforementioned types of boundaries in AMR-FDTD has been discussed in [14]. However, junctions of $SB$-type boundaries were treated as $CPB$-type boundaries in [14]. While this approach yields acceptable results for integrated circuit geometries, it causes significant spurious reflections, when applied to optical waveguides of inhomogeneous dielectric profile, such as the corrugated structure analyzed in the next section. The approach followed in this paper is explained next.
D. Handling of Junctions of SB-type Boundary in the dynamic AMR-FDTD Modeling of Dielectric Structures

Ideally, an SB-type boundary should be transparent and meshes linked by SB-type boundaries (connecting meshes of the same resolution) should behave like one larger mesh. Fig. 2 shows some typical SB-type boundaries, including junctions a, b, c, d and e.

As shown in the figures, the update of an electric field node (E-node) requires four neighboring magnetic field nodes (H-nodes), some of which may not belong to the same mesh. Let us call those external H-nodes. It should be noted that an E-node on a boundary may be shared by 2, 3 or 4 neighboring meshes of the same level. It only needs to be updated in one mesh and then copied to all the other meshes. To avoid double updates, the following three situations are considered:

1) If an E-node on a SB-type boundary is not at a corner of at least one neighboring mesh, it should be updated in that mesh by using one external H-node from the other mesh, then copied to all other meshes. For example, in Fig. 2, the E-node a should be updated in A then copied to B, b should be updated in B then copied to A, and d should be updated in E then copied to A and D.

2) If an E-node on a SB-type boundary is at a corner of all the neighboring meshes, the situation can be further divided in two sub-cases:

a) There is at least one pair of meshes forming a cross-junction around the E-node. For example, since meshes A and C form a cross-junction at the E-node c, c can be updated in A by using two external H-nodes from C, or vice versa. Then, c is copied to all the un-updated neighboring meshes.

b) There is no pair of meshes forming a cross-junction around the E-node, for example, E-node e. None of the neighboring meshes can obtain two external H-nodes, therefore this E-node has to be treated as a CPB-type boundary and updated accordingly [14].

III. NUMERICAL EXAMPLES

A. Dielectric Waveguide With a Corrugated Permittivity Profile

A dielectric waveguide with a corrugated permittivity profile, similar to the one presented in [15], is simulated by FDTD and a multilevel dynamic AMR-FDTD. This geometry is a good benchmark application for the proposed technique, since the multiple reflections created by the dielectric corrugations enforce strong numerical interactions between spatially distributed meshes, testing the stability and accuracy of the mesh refinement scheme. All interpolations employed are first order polynomial ones.

The geometry of the waveguide is shown in Fig. 3. Its width is 2µm and the dielectric constant of the host medium is 9. The dielectric constant of the corrugations is 7.9976. The computational domain is 12µm × 8µm and is truncated by a 1µm thick matched absorber. The excitation is imposed 1µm from the left edge of the waveguide and the electric field is recorded at the center of waveguide and 1.2µm from the right edge. The excitation is a modulated pulse of the form:

\[ (u(t) - u(t - T)) \sin^2 \left( \frac{\pi t}{T} \right) \sin \left( 2\pi f t e^{-\left( (y-y_0)^2 \right)} \right), \quad (9) \]

where \( u(t) \) is the unit step function, \( f = 193 THz, T = 5/f, W = 0.7\mu m \) and \( h = 2y_0 \) is the height of the waveguide (hence, the pulse is centered in the middle of the guide, along the \( y \)-direction). Table I compares the accuracy and computation time of AMR-FDTD using a root mesh of 240 × 160 and 2-4 mesh levels, to a reference FDTD simulation using a 3840 × 2560 mesh and several coarser FDTD schemes. The simulated time-window in all methods remains constant. Therefore, if one method has a time step \( \Delta t \) and another \( \Delta t/2 \), the latter will be run for twice the total number of time steps of the former. The accuracy is quantified by employing the following time-domain waveform error metric:

\[ E_t = \sqrt{\sum_k \frac{\| f(t_k) - f^{ref}(t_k) \|^2}{\sum_k \| f^{ref}(t_k) \|^2}}, \quad (10) \]

where, \( t_k \) is a discrete time within the modeled time range (up to 16.5 ps), \( f \) is the sampled electric field as determined by AMR-FDTD or the coarse mesh FDTD techniques and \( f^{ref} \) is the sampled electric field determined by the reference FDTD simulation. All AMR-FDTD simulations use a refinement factor \( N_\delta \) of 2 for successive levels, and \( \theta_\epsilon = 0.01, \theta_\eta = 0, \theta_\sigma = 0.8, N_{AMR} = 10, \sigma_{AMR} = 2 \) [14]. Table I shows that the dynamic AMR-FDTD can reach the accuracy of the reference FDTD method in a greatly reduced computation time. It should be noted that the error no longer decreases once the number of levels of the mesh tree reaches 5, while the execution time also starts increasing then. This trend continues as the number of levels increases and reflects a saturation point beyond which the benefits of the AMR algorithm are compensated for by the errors accumulated through the interpolating operations, as well as the time for their execution. These two problems are interconnected, since the reduction of interpolation errors can be achieved by applying a higher
order polynomial interpolation [9], which in turn increases the operations needed. Therefore, the conclusion of this study is that four levels, combined with first order interpolations can achieve an impressive reduction in the execution time (by a factor of 1/160), with less than 1% error in the time-domain.

Fig. 4 compares the time-domain waveforms of AMR and conventional FDTD schemes, while Fig. 5 demonstrates the late-time stability of the multi-level dynamic AMR-FDTD. In both figures, the AMR-FDTD uses 4 levels and a 240 × 160 mesh. The result of Fig. 5 can be explained by the following note regarding the stability of the dynamic AMR-FDTD, which is also its fundamental difference from static subgridding schemes. Assume a pulse propagating through a static interface between a coarse and a dense grid. Then, the interpolating operations needed for the update equations would involve large field values. As a result, the associated errors are large, contributing to the well-known late-time instability effects in static subgridding schemes. On the other hand, such an interface would not exist under the dynamic AMR scheme, the reason being that this algorithm tracks the propagating wavefronts. Therefore, the pulse of this thought example would be enclosed in a moving dense mesh.

### B. Dielectric Waveguide Power Splitter

To demonstrate the efficiency of the multi-level AMR-FDTD for the simulation of structures with non-conformal dielectric constant distribution, a dielectric waveguide power splitter, shown in Fig. 6 [15] is simulated. The dielectric constant of the cross-shaped waveguide is 9, whereas the dielectric constant of the slanted splitter (lens) is 4. It should be noted that due to the slanted orientation of the lens, its dielectric constant profile does not conform to a rectangular mesh. In FDTD simulations using different meshes, the dielectric constant distribution is discretized independently, according to an optimal staircase approximation. The multilevel AMR-FDTD similarly re-discretizes the dielectric constant distribution at different levels. The simulations use the same excitation as (9), which is imposed at (1.2µm, 9µm), and the electric field is recorded at 1µm from each port. All AMR-FDTD simulations use a refinement factor of 2 for successive levels, and \( \theta_e = 0.01, \theta_g = 0, \theta_c = 0.8, N_{AMR} = 10, \sigma_{AMR} = 2 \). Table II shows that AMR-FDTD can reach the accuracy of the reference FDTD method, in a much smaller execution time. In addition, the time-domain results of Figs. 7-9 demonstrate the late-time stability and accuracy of the method.

Figs. 10-12 show the evolution of the field and the mesh tree, which uses a 60 × 60 root mesh and a maximum number of three levels. The level-1 and level-2 meshes are drawn in red and blue, respectively, and the level-3 mesh is drawn in black. The dielectric constant is discretized in a staircase approximation at different levels. The mesh tree switches from level-3 to level-2 at 1000 time steps, and then to level-1 at 2000 time steps. The pulse of this thought example would be enclosed in a moving dense mesh.
C. Dielectric Waveguide Y-Junction

A dielectric waveguide Y-junction, shown in Fig. 13 is simulated. The dielectric constant of the waveguide is 9 and the dielectric constant of the surrounding medium is 1. The computational domain is 25µm x 10µm and a 1µm thick matched absorber is used to truncate it. The excitation is imposed at 1.2µm from the edge of Port 1 and the electric field is recorded at the center of the waveguide, 2µm from the edge of Port 2. The excitation is a modulated pulse of the form:

\[ e^{-\frac{(y-y_0)^2}{w^2}-(t-t_0)^2}{T^2} \sin(2\pi ft) \],

where \( f = 200THz \), \( T = 0.02ps \), \( t_0 = 3T \), \( W = 1\mu m \) and \( y_0 \) corresponds to the center of the waveguide. Table III compares the accuracy and computation time of AMR-FDTD using a root mesh of 250 x 100 and 2-4 mesh levels, to a reference FDTD simulation using a 2000 x 800 mesh and several coarser FDTD schemes. The AMR parameters are: \( \theta_x = 0.001 \), \( \theta_y = 0 \), \( \theta_z = 0.8 \), \( N_{AMR} = 10 \), \( \sigma_{AMR} = 2 \). All AMR-FDTD simulations use a refinement factor of 2 for their successive mesh levels. Table III shows that AMR-FDTD can achieve the accuracy of the reference FDTD method in a dramatically reduced computation time.

Field waveforms in time, extracted by an a 4-level AMR-FDTD, employing a 250 x 100 root mesh, and the reference FDTD simulation are shown and compared in Fig. 14, demonstrating the excellent agreement of the proposed approach to the reference data, despite its reduced numerical cost. A waveform extracted by a conventional FDTD run on the root mesh of the AMR-FDTD domain is appended, to indicate the amount of accuracy improvement, brought about by the mesh refinement. Fig. 15 shows that the multi-level AMR-FDTD is free from the late instability problems that characterize static subgridding techniques.

Figs. 16-19 show the evolution of the field and mesh tree, which uses a 125 x 50 root mesh and maximum level of 3. The level-1 mesh is drawn in the figures and the regions without
Fig. 10. Electric field magnitude distribution across the power splitter of Fig. 6, at $t = 100\Delta t$.

Fig. 11. Electric field magnitude distribution across the power splitter of Fig. 6, at $t = 300\Delta t$.

Fig. 12. Electric field magnitude distribution across the power splitter of Fig. 6, at $t = 400\Delta t$.

Fig. 13. Geometry of the dielectric waveguide Y-junction. The dielectric constant of the waveguide is 9 and the dielectric constant of the surrounding medium is 1. Dimensions are given in units of $\mu$m. P1 and P2 and P3 denote ports 1, 2 and 3, respectively.

Table III

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grid lines are covered by level-2 and level-3 meshes, which are not drawn because they are too dense. The rectangular boxes embedded in the solid gray regions indicate the boundaries of level-3 meshes. These figures indicate the wavefront tracking achieved by the dynamic AMR-FDTD.

D. Dielectric Ring Resonator

A highly resonant THz structure of a dielectric ring resonator coupled to two dielectric waveguides, previously modeled in [16] and shown in Fig. 20, is simulated. The width of the waveguide and the ring is $0.3\mu$m, and their dielectric constant is 10.24. The external radius of the ring is $2.5\mu$m. The edge-to-edge distance between the ring and the waveguide is $0.232\mu$m. The computational domain is $12\mu$m $\times 12\mu$m and it is truncated by a $1\mu$m thick matched absorber. The excitation
Fig. 15. Electric field at the center of the dielectric waveguide Y-junction of Fig. 13, 2 µm from the edge of port 2, obtained with the dynamic AMR-FDTD, for 25,000 time steps, indicating the absence of late-time instability.

Fig. 16. Electric field magnitude distribution across the Y-junction of Fig. 13, at \( t = 100\Delta t \).

Fig. 17. Electric field magnitude distribution across the Y-junction of Fig. 13, at \( t = 400\Delta t \).

Fig. 18. Electric field magnitude distribution across the Y-junction of Fig. 13, at \( t = 600\Delta t \).

is a modulated pulse of the form:

\[
e^{-\left(y-y_0\right)^2/W^2-(t-t_0)^2/T^2}\sin\left(2\pi ft\right),
\]

(12)

where \( f = 200 \text{ THz} \), \( T = 0.02\text{ps} \), \( t_0 = 3T \), \( W = 0.7\mu m \) and \( y_0 \) corresponds to the midsection of the waveguide. The excitation is imposed 1.1µm from the end of the lower left waveguide port, and the electric field is recorded at 2µm from each port. All AMR-FDTD simulations use a refinement factor of 2 for successive levels, and \( \theta_e = 0 \), \( \theta_g = 0 \), \( \theta_c = 0.8 \), \( N_{AMR} = 10 \), and \( \sigma_{AMR} = 2 \).

Table IV compares accuracy and execution times of AMR-FDTD and conventional FDTD for this large-scale computational problem. Again, a four level scheme can reproduce the results of the reference FDTD simulation within a smaller execution time (by a factor of 33), at a relative time-domain error of 1.56%.

The time domain results of Figs. 21-23 demonstrate the late-time stability and accuracy of the method. It should be noted that the first Gaussian pulse arrives at port 3 at about 0.2 ps. Before that, the field at port 3 is due to the disturbance caused by the excitation, which propagates through free space. Since this disturbance is very small compared with the main pulse propagating along the waveguide, it is not tracked by the finest mesh and therefore it induces a relatively large error. However, the pulses circulating the ring resonator and coupled to the waveguides are tracked by the finest mesh and therefore their amplitude and group velocity are very accurately resolved even at very late stages of the simulation.

Finally, the \( S_{21} \) obtained by using AMR-FDTD is shown in Fig. 24, which agrees quite well with the results of [16].
Fig. 20. Geometry of the dielectric ring resonator coupled to two dielectric waveguides. Dimensions are in units of μm. P1, P2, P3 and P4 denote ports 1, 2, 3 and 4, respectively.

Fig. 21. Electric field at 2μm from port 2 of the ring resonator of Fig. 20.

### TABLE V

<table>
<thead>
<tr>
<th>Order</th>
<th>AMR-FDTD</th>
<th>FDTD [16]</th>
</tr>
</thead>
<tbody>
<tr>
<td>25</td>
<td>186.01</td>
<td>185.85</td>
</tr>
<tr>
<td>26</td>
<td>192.03</td>
<td>191.88</td>
</tr>
<tr>
<td>27</td>
<td>198.06</td>
<td>197.90</td>
</tr>
<tr>
<td>28</td>
<td>204.08</td>
<td>203.92</td>
</tr>
<tr>
<td>29</td>
<td>210.11</td>
<td>209.94</td>
</tr>
</tbody>
</table>

Fig. 22. Electric field at 2μm from port 2 of the ring resonator of Fig. 20, obtained with the dynamic AMR-FDTD, for 100,000 time steps, indicating the absence of late-time instability.
extracted by FDTD. The AMR-FDTD uses a $120 \times 120$ root mesh and 4 levels. Since the structure is highly resonant, 100,000 time steps are executed. The resonant frequencies of the present method and [16] are compared in Table V, showing a very good agreement.

IV. NUMERICAL ERROR ESTIMATION

There are five parameters controlling the accuracy and computation time of AMR-FDTD, as described by the previous sections and Ref. [14]. To use AMR-FDTD as a CAD technique, a clear set of guidelines for the choice of the five parameters is needed. The main objective of this section is to produce such guidelines, that would allow a user to determine the AMR-FDTD parameters for a given error tolerance.

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:

$$\mathcal{E} = \sqrt{\frac{\sum_{k,m} |f_m(t_k) - f_m^{ref}(t_k)|^2}{\sum_{k,m} |f_m^{ref}(t_k)|^2}}$$

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

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, corrugated permittivity profile waveguide and the Y-junction, presented and simulated in the previous section.

First, the effect of $N_{AMR}$, $\sigma_{AMR}$ and $\theta_c$ on the accuracy and simulation time is investigated. Fig. 25 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. 25. 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. 26. Dependence of $-\log_{10} E$ on $\theta_c$ and $\theta_g$.

Fig. 27. Curve-fitted dependence of $-\log_{10} \tilde{E}$ on $\theta_c$ and $\theta_g$ based on (14).

Fig. 28. Curve-fitted dependence of error bound $-\log_{10} \mathcal{E}_b$ on $\theta_c$ and $\theta_g$ based on (14).

Following (14), we define a general error bound as

$$
\mathcal{E}_b(\theta_c, \theta_g) = C_1 \mathcal{E}_b(0, \theta_g) \arctan \left( \frac{\theta_g}{\theta_c} \right)^{C_2} + C_3 \mathcal{E}_b(\theta_c, 0) \arctan \left( \frac{\theta_c}{\theta_g} \right)^{C_4},
$$

where $C_1$, $C_2$, $C_3$ and $C_4$ are fine tuned to minimize the difference between $\tilde{E}$ and $\mathcal{E}$. As an example, Fig. 27 shows the curve-fitted error obtained by (14), where $C_1 = C_3 = 1.02$, $C_2 = 0.05$, $C_4 = 0.01$, which depicts a very good agreement with Fig. 26. Therefore, this approximation, requiring only $\mathcal{E}(\theta_c, 0)$ and $\mathcal{E}(0, \theta_g)$, is useful as sufficiently accurate.

By simulating typical optical waveguide structures, two empirical error bound functions are obtained for the special cases $\theta_c = 0$ and $\theta_g = 0$, respectively,

$$
\mathcal{E}_{b0}(\theta_c = 0, \theta_g) = 0.4 \theta_g^{0.35},
\mathcal{E}_{b0}(\theta_c, \theta_g = 0) = 0.15 \theta_c^{0.37}.
$$

V. CONCLUSION

This paper presented a multilevel, dynamic AMR-FDTD technique applied to optical waveguide structures. Numerical
examples demonstrated the efficiency and late-time stability of the proposed technique. Large speed-up factors (ranging from 30 to 100) compared to the conventional FDTD were achieved, while all errors involved remained small, typically of the order of 1% or less. This method can be utilized in several problems including plasmonic nanoparticle studies [20].

REFERENCES


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