FDTD Lattice Termination with Periodic Boundary Conditions

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Abstract—The potential of periodic boundary conditions to provide an alternative method for terminating Finite-Difference Time-Domain lattices, instead of absorbing boundary conditions or perfectly matched layers, is examined in this paper. Employing a recent combination of the sine-cosine technique with the array-scanning method, a large number of problems of interest can be efficiently terminated at periodic boundaries, which effectively act as absorbers. Hence, a unified treatment of inhomogeneous, dispersive and conductive media, each of which requires a reformulation of the perfectly matched layer, is attained, with an excellent performance that is not compromised by the close proximity of a source to the boundary. In addition, while the reflectivity of perfectly matched layers increases when the refractive index of the working volume is a non-analytic function, the proposed approach is not affected. The presence of non-periodic boundary conditions can still be accounted for by hybrid periodic/absorbing terminations.

Index Terms—Finite-difference time-domain, periodic boundary conditions, absorbing boundary conditions, perfectly matched layers.

I. INTRODUCTION

Over the years, several approaches have been developed for the termination of finite-difference time-domain (FDTD) lattices, modeling open boundary problems. Yet, two major categories can be identified, namely absorbing boundary conditions [1] and absorbing layers, including the perfectly matched layer (PML, [2]). Depending on the problem at hand, these approaches have certain strengths and limitations, invariably trading computational complexity with accuracy. First and second order absorbing boundary conditions are simple to implement, but they are based on paraxial approximations of wave propagation, hence being inadequate for fringe fields and non-normally incident waves. The PML is more efficient with obliquely incident waves, although its reflectivity does grow for near-grazing incidence, placing a lower bound to the distance of a source to the PML boundary. Yet, it requires an extension of the computational domain by several cells, additional auxiliary field variables and update operations for those. Non-trivial reformulations of the standard PML, through the use of additional field variables, are also needed for the termination of dispersive and conductive media, as well as backward wave media (to avoid instability [3]). Finally, a recent study has illustrated, by analytical and numerical means, a significant degradation in the performance of PMLs terminating a working volume with a refractive index that is a non-analytic function of space [4].

Such limitations render the problem of FDTD lattice termination still timely and motivate research into alternative techniques that may strike a better balance between accuracy, complexity and versatility. In the applied mathematics literature, the simple one-dimensional periodic boundary condition is a widely used absorbing boundary condition. In computational electromagnetics though, this option has not been explored, as it is incompatible with multi-dimensional wave propagation and the presence of complex source and boundary conditions. However, recent work that allows for the combination of localized sources and boundary conditions with periodic boundaries in FDTD [5], [6], enables the reconsideration of the role of the latter as an alternative lattice truncation method.

This paper presents a feasibility study of the aforementioned idea and reports numerical results that are clearly supportive of its viability. Based on a unified formulation for any linear medium, the proposed approach performs just as well as PML in most cases and better than PML when the source is close to the terminating boundary and for the types of media discussed in [4]. An obvious pre-requisite for the applicability of this method is that the working volume be periodic in the direction of termination. Still, if only part of the domain fulfills that condition, composite periodic/absorbing boundaries can be employed. The relevant methodology is shown through the example of a printed microstrip line.

II. THE SINE-COSINE ARRAY-SCANNING FDTD METHOD AS AN ABSORBING BOUNDARY CONDITION

A. Overview of the sine-cosine array-scanning FDTD

The sine-cosine based array-scanning FDTD method is briefly reviewed in this section. Consider a two-dimensional periodic structure with a lattice vector \( \mathbf{d} = d_x \mathbf{x} + d_y \mathbf{y} \), which is excited by a non-periodic broadband source. By modeling the computational domain within a single unit cell terminated in periodic boundary conditions, the electric field at any position can be obtained using the array-scanning method [7], as a weighted superposition of Floquet mode fields. In particular, let \( E_{array}(\mathbf{r}_0, \mathbf{k}_p, t) \) be the time domain electric field obtained by the sine-cosine method for a Floquet wave number \( \mathbf{k}_p \) (which belongs to the irreducible Brillouin zone of the structure) at a point \( \mathbf{r}_0 \) within the unit cell. Then, the electric field at a position \( \mathbf{r} = \mathbf{r}_0 + \mathbf{p}_{h,t} \), where \( \mathbf{p}_{h,t} = x h d_x + y l d_y \), due to the original source is given as:

\[
E_0(\mathbf{r}_0 + \mathbf{p}_{h,t}, t) \approx \left( \frac{1}{NM} \right) \sum_{n=-N/2}^{N/2} \sum_{m=-M/2}^{M/2} E_{array}(\mathbf{r}_0, \mathbf{k}_p, t) \exp(-j\mathbf{k}_p \cdot \mathbf{p}_{h,t})
\]

When this method is applied, the unit cell is effectively extended to infinity in the directions of periodicity, while this equivalent unbounded structure is driven by the original localized source. Hence, when an open structure is periodic in a certain direction, as in planar multi-layer circuits and antennas, the same formulation can act as a lattice termination scheme. Note that the application of (1) is not limited by the presence of dispersion or conductivity, nor does the actual complexity and computational work involved grow in these cases. On the other hand, no obvious extension of this approach to nonlinear media exists.

The array-scanning is an analytical method, whose implementation in discrete space suffers primarily from the sampling error in the \( \mathcal{H}_p \)-space. The following estimate of this error is provided by the sampling theorem:

\[
\epsilon(n\Delta t) = \frac{\sum_{h,l\neq0} |E_{ref}(\mathbf{r}_0 + hM\mathbf{d}_z, lN\mathbf{d}_y, t)|}{|E_{ref}(\mathbf{r}_0, t)|} \tag{2}
\]

where \( E_{ref} \) is the analytical solution of the problem. Accordingly, as a mesh truncation method, the sine-cosine based array-scanning’s accuracy depends on the number of the sampled Floquet vectors, rather than the proximity of the source and the angle of incident waves. The numerical results discussed next further illuminate this aspect.

**B. Numerical evaluation**

![Diagram](image.png)

**Fig. 1.** (a) The computational domain of a two-dimensional free space with a \( z \)-directional current source placed far from or near the boundary. (b) The computational domain of a structure with one-dimensionally periodic permittivities excited by an infinite line source.

The following two examples provide a comparative study of the sine-cosine array-scanning FDTD and PMLs, focusing on the potential of the former to provide an alternative to the latter, in some cases. Figure 1(a) shows the computational domain of the first example, consisting of a current source within a two-dimensional unbounded free space (a benchmark example included in [2]). The size of the computational domain is \( 10 \times 10 \text{ cm}^2 \), and is modeled in FDTD by \( 100 \times 100 \) Yee cells. A modulated Gaussian current source \( \mathcal{J}_z \) covering 0.5 GHz to 10 GHz is placed inside the domain. Periodic boundary conditions or PMLs are used to terminate the domain in \( x \)- and \( y \)-directions. The time step is set to 5.869 ps and 2048 time steps are run.

For the array-scanning method, 16-32 \( \mathcal{H}_p \)'s are sampled uniformly within the Brillouin zone in both the \( x \)- and the \( y \)-directions. The simulation is run on a grid server and takes 32 seconds. For comparison, an identical domain is set up and is terminated in 10-layer uniaxial PMLs with polynomial grading \( m = 4 \) and corresponding optimal parameters, which takes 41 seconds to execute. In all the cases, the maximum relative errors within the computational domain at the \( n \)-th time step are obtained by the norm:

\[
\epsilon(n\Delta t) = \max_{i,j} \left( \frac{|E_{z,i,j}^{ref} - E_{z,\text{ref}}|_{i,j}^{n}}{E_{z,\text{ref},\text{max}}|_{i,j}^{n}} \right) \tag{3}
\]

where \( E_{z,i,j}^{ref} \) is the electric field at Yee-cell location \((i,j)\) and time step \( n \). Here, the reference fields are obtained using a large computational domain of \( 2000 \times 2000 \) Yee cells, so that no reflections from the boundary can reach the positions of interest during the complete simulation time span. Two cases are simulated in which the excitation is located at point A, at the center of the computational domain, and at point B, just 1 mm from the boundary.

![Graph](image.png)

**Fig. 2.** The numerical error with respect to time of the array-scanning method with different sampling densities, compared with 10-layer PMLs, when the source is placed at point A or B in the geometry of Fig. 1(a).

Figure 2 shows the relative error of the array-scanning method and the PML with respect to time. It is shown that the numerical error of the PML increases dramatically when the source is near the boundary, while the error of the array-scanning FDTD remains at almost the same level.

The effect of the sampling density of \( \mathcal{H} \) on the accuracy of the sine-cosine based array-scanning FDTD method is also shown in the figure. The results indicate that the numerical error tends to decrease as the sampling density increases (note that the improvement is understated by the logarithmic scale of the plot).

The second example, also studied in [4], is shown in Fig. 1(b). The computational domain is \( 10 \times 10 \text{ cm}^2 \), with a periodic dielectric permittivity of the form \( \epsilon_r(y) = 6 + 5 \sin(2\pi y/a) \)
in the $y$-direction, where $a = 1$ cm. A uniform line source $J_z$, of a 5-25 GHz modulated Gaussian waveform in time, is applied at $y = 5$ cm. The domain is terminated in perfect magnetic conductors in the $x$-direction and in periodic boundary conditions/10-layer PMLs in the $y$-direction. The time step is set to 5.869 ps and 2048 steps are run. The numerical error with respect to time is evaluated using (3), with the reference solution obtained by a long domain with 2000 Yee cells in the $y$-direction.

The results of this simulation are shown in Fig. 3, which corroborates the significantly increased reflections from the PML reported in [4]. On the other hand, the sine-cosine based array-scanning FDTD delivers again a relative error of about 0.1%, with 16 and 32 $k_y$ samples. Note that all execution times of the array-scanning FDTD have been given for a single Floquet wavevector. Hence, for a serial environment, the total simulation time is derived by multiplying this time by the number of wavevectors used. This number can be reduced, using field interpolation in the $k$-domain (a subject of ongoing work). However, it is worth noting that the proposed method is optimally suited for parallel environments, as the Floquet wavevector simulations are totally independent from each other, and perfectly scalable as such. Thus, a readily realizable, memory reducing, FDTD parallelization paradigm based on "spectral decomposition", as opposed to domain decomposition that requires specialized parallel programming, is provided.

III. LATTICE TERMINATION FOR FDTD DOMAINS WITH NON-PERIODIC BOUNDARY CONDITIONS

A. Methodology

Periodic boundary conditions by themselves cannot terminate domains such as that of the microstrip line geometry of Fig. 4, which is also used as a benchmark example for evaluation of the PML in [2]. However, a hybrid periodic/absorbing boundary, with periodic boundary conditions terminating the alumina substrate and absorbers enclosing the space above the air/substrate interface (including the plane of the microstrip) can be alternatively employed. This type of mixed boundaries was successfully implemented in [6], [8] for the modeling of microstrip-based microwave circuit geometries and integrated antennas, respectively. As discussed in [6], the periodic boundary has to be discontinued at the plane of the metallic strip, or else it will produce artificial zeros in the tangential to the interface field for $-\infty < x, y < +\infty$, thus changing the simulated fields.

In this work, periodic/absorbing boundaries are compared to PMLs, as a means for FDTD lattice truncation. Note that this hybrid approach facilitates the modeling of antennas on dispersive or conductive substrates, bypassing the need for the introduction of new auxiliary field variables for the PML region. To that end, the following numerical experiment is performed with the microstrip line of Fig. 4. In the $x$-direction, the structure is terminated in periodic boundary conditions within the substrate and in 10-layer uniaxial PMLs onwards.

The $y$-direction is terminated in 10-layer uniaxial PMLs. The Yee cell size is $42.33 \times 120 \times 42.33 \, \mu m^3$. The whole computational domain is discretized with $16 \times 40 \times 11$ Yee cells. A 2-10 GHz modulated Gaussian excitation is applied at the 8th Yee cell in the propagation direction. The time step is $\Delta t = 0.28$ ps and 16384 time steps are run. For the array-scanning method, 16 $k_x$'s are sampled within the irreducible Brillouin zone. It takes 246 seconds to simulate the structure on the grid server. A finite structure terminated in 10-layer uniaxial PMLs is also simulated in 302 seconds. A large finite structure with 1000 Yee cells in the $x$-direction and terminated in PMLs is simulated to serve as a reference solution for the error estimation.

Figure 5 shows a contour plot of the relative numerical error norm (3) in the composite boundary domain, computed against the reference solution, at the cross section defined by the 20-th cell in the $y$-direction. The same contour plot is produced for the PML domain. Inspection of the error curves shows that the two methods have comparable performance, although the composite periodic/absorbing boundary has slightly smaller errors.

B. Discussion

The underlying mechanism that makes the hybrid periodic/absorbing boundary work is further investigated. Note
that by specifying a certain $k_p$ within the substrate region, the tangential to interface components of the wavevector are fixed. If the fields excited by the source are expanded in the complete basis of $\exp(-j k_p \cdot \tau)$, the periodic boundary condition ensures that within the substrate, only the component corresponding to the specified $k_p$ is excited. Then, boundary conditions at the interface, applied through the regular FDTD update equations, carry this spectral component to the upper space where it propagates and is eventually absorbed by the PMLs. Finally, the array-scanning step of the algorithm reconstructs the total field from its spectral components. Hence, this process is nothing else but the FDTD counterpart of spectral-domain techniques, based on a periodic Green’s function in the substrate and one satisfying the radiation boundary condition above it. Figure 6 confirms this point of view. In Figs. 6(a) and (b), the $E_z$ field distribution at the cross section is shown at the 10000-th time step, with $k_x = \pi/4$ and $k_y = \pi/2$. In both cases, a distinct Floquet mode can be clearly observed in the area terminated in periodic boundaries and in the area terminated in PMLs. Figure 6(c) shows the total field at the same cross section by applying the array-scanning method, and Fig. 6(d) shows the reference field distribution from the reference simulation. The two field patterns are identical, as expected.

IV. CONCLUSIONS

A feasibility study for the use of periodic boundaries, effected by the sine-cosine FDTD method, as absorbers has been presented. The performance of either pure periodic or hybrid periodic/absorbing boundaries was compared to PMLs for three benchmark examples. It was found that as long as periodic boundary conditions are applicable, they can deliver at least comparable and potentially better absorptivity than the PML, overcoming well-known constraints of conventional absorbers. Several potential applications can be identified, with dielectric waveguide and planar microwave circuit structures printed on dispersive, meta-material substrates being among the most important ones.

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REFERENCES