A Unified Treatment of FDTD Lattice Truncation for Dispersive Media via Periodic Boundary Conditions

Dongying Li and Costas D. Sarris
The Edward S. Rogers Sr. Department of Electrical and Computer Engineering,
University of Toronto, Toronto, ON, Canada

Introduction

Since the emergence of the finite-difference time-domain (FDTD) method, the development of stable and easy-to-implement boundary conditions to terminate unbounded structures has always been an interesting and timely topic. Various methods have been proposed to minimize reflections from absorbing boundaries, yet each of them exhibits certain intrinsic limitations. Analytical absorbing boundary conditions suffer from serious reflections away from normal incidence. On the other hand, perfectly matched layers (PMLs) are numerically cumbersome to implement, and additional auxiliary variables are needed when dealing with dispersive or conductive media [1]. Moreover, recent research on synthesized media has posed new challenges to existing absorbing boundary conditions. For example, it was reported in [2] that conventional dispersive PMLs fail to perform stably when terminating negative refractive index (NRI) materials, which support backward waves (with contra-directional phase and group velocities). Such limitations motivate the continuation of research on stable and versatile absorbing boundary conditions.

Recently, the possibility of using periodic boundary conditions to terminate FDTD lattices was studied. It was shown in [3, 4] that combined with the array-scanning method, periodic structures driven by localized sources can be terminated in periodic boundary conditions. This makes periodic boundary conditions an alternative candidate for FDTD lattice truncation, with the pre-requisite that the structure is periodic in the direction of mesh truncation.

In this paper, we validate the aforementioned technique as a means for lattice truncation of different types of media. It is shown through two numerical examples that the method is applicable to both conductive and dispersive media, presenting numerical errors comparable to those of PMLs. Also, it maintains stable performance in cases where conventional absorbers fail to function satisfactorily.

Theory

Consider a typical two-dimensional periodic structure with a lattice vector \( \vec{d} = d_x \hat{x} + d_y \hat{y} \) excited by a non-periodic broadband source. By applying the array-scanning sine-cosine FDTD [5]:

\[
\overline{E}_0 (\vec{r}_0 + \vec{p}_{h,t}, t) \approx \frac{1}{NM} \sum_{n=-N/2}^{N/2} \sum_{m=-M/2}^{M/2} \overline{E}_{array} (\vec{r}_0, \vec{x} \frac{2\pi n}{Nd_x} + \vec{y} \frac{2\pi m}{Md_y}, t) e^{-j \vec{k}_p \vec{p}_{h,t}}
\]

we effectively simulate an infinitely periodic structure with the same isolated non-periodic source. Here \( \overline{E}_{array}(\vec{r}_0, \vec{k}_p, t) \) is the time-domain electric field at \( \vec{r}_0 \) for a Floquet wave vector \( \vec{k}_p \) in the sine-cosine method applied to a single unit cell, and \( \vec{p}_{h,t} = hdx \hat{x} + ldy \hat{y} \).

Thus, the method behaves as an ideal boundary condition to terminate the FDTD lattice of
Figure 1: a) Current source in a conductive half-space medium, and b) a dispersive negative refractive index slab in free space illuminated by a harmonic current source.

an unbounded structure as well, provided that it is periodic along the direction of termination. Also, although not discussed in this paper, it is valuable to note that non-periodic boundary conditions, confined in parts of the computational domain, can be accounted for by introducing a combination of periodic and absorbing boundary conditions [4].

It is important to notice that unlike conventional absorbing boundary conditions, the complexity of the numerical implementation of the array-scanning method is not subject to any changes with conductivity or dispersion of the media enclosed. Furthermore, it is shown in [4] that the accuracy of the sine-cosine array-scanning FDTD is determined by the sampling density of the Floquet wave vectors, rather than impinging wave angles as in conventional absorbers. The following numerical examples are aimed at demonstrating this point.

**Numerical results**

A benchmark problem mentioned in [1] is considered to validate the method with conductive media. The geometry under study is shown in Fig. 1(a). The geometry consists of two half-space regions of free space and a conductive medium with $\varepsilon_r = 10$ and $\sigma = 0.3$ S/m, respectively, and excited by a modulated Gaussian current source covering $0.5 - 10$ GHz. The 24 mm wide computational domain is discretized into 40 Yee cells in the $x-$direction, and 2000 Yee cells in the $y-$direction to prevent any reflections. For the array-scanning method, the domain is terminated in periodic boundary conditions in the $x-$direction, with 16 or 32 $k_x$ sampled uniformly within the Brillouin zone. The time step is set to 0.925 ps and 4096 time steps are run. The program is simulated in parallel on a grid server, taking 533 seconds. For error comparison, an identical domain terminated in 10-layer uniaxial PMLs in the $x-$directions is also simulated, taking 712 seconds.

The time domain error of both termination methods in the complete computational domain is evaluated by

$$e(n\Delta t) = \max_{i,j} \left( \frac{|E_{z,n}^{i,j} - E_{z(ref)}^{n}||_{i,j}|}{|E_{z(ref)}^{max}||_{i,j}|} \right)$$

(2)

where $E_{z(ref)}$ is the reference field obtained by simulating a large domain with 2000 Yee
cells in both directions. Two cases are simulated where the source is placed at point A at the center of the interface between two half spaces, and at point B in the upper half space and one Yee cell from the boundary. Figure 2 shows the time-domain error of the array-scanning method, compared to the PML termination, and Fig. 3 shows the corresponding error in the frequency domain. It is clear that the change of the accuracy level of the sine-cosine array-scanning FDTD caused by the proximity of the source to the boundaries is much smaller than that of the PML. In the case of 32 sample points with source A, the accuracy level of the method is comparable to that of the PML. With a source close to the boundary, the performance of the proposed method clearly surpassed that of the PML.

![Figure 2](image1.png)

**Figure 2:** The time-domain relative error of the structure in Fig. 1(b) using the array-scanning method with 16 and 32 $k_x$ samples, compared with the relative error of 10-layer uniaxial PMLs.

![Figure 3](image2.png)

**Figure 3:** The frequency-domain relative error of the structure in Fig. 1(b) using the array-scanning method with 16 and 32 $k_x$ samples, compared with the relative error of 10-layer uniaxial PMLs.

![Figure 4](image3.png)

**Figure 4:** The electric fields at the first and second interfaces of the dispersive slab in Fig. 1(b), using the array-scanning method.

![Figure 5](image4.png)

**Figure 5:** The electric field distribution in the computational domain of Fig. 1(b) at the 2000-th time step.

A second example, which has been studied in [2], is simulated to validate the ability of the method to terminate doubly dispersive media. Figure 1(b) shows the two-dimensional computational domain. A 2 cm dispersive slab is placed in free space, with both magnetic and electric plasma response following the Drude model: $\mu_r = \varepsilon_r = 1 - \omega_p^2 / [\omega(\omega - j\Gamma_0)]$
with $\omega_p = 2\pi \times 22.6$ GHz and $\Gamma_0 = 2\pi \times 100$ MHz. A time-harmonic current source is placed 1 cm from the first interface between the free space and the slab. The frequency of the source is 16 GHz, which yields a meta-material lens of negative refraction index $n_N = -1$, with small loss introduced by the $\Gamma_0$ term. It has been shown in [2] that the conventional dispersive PML is unstable.

The computational domain is discretized with $118 \times 120$ Yee cells in FDTD. The dispersive slab is modeled using the auxiliary update with the Z-transform method [6]. The time step is set to 0.83 ps and 2048 time steps are run. For the array-scanning method, the computational domain is terminated in 10-layer uniaxial PMLs in the $y-$direction, and in periodic boundary conditions in the $x-$direction. Again, 16 $k_x$ are uniformly sampled and the program is run on a grid server, taking 105 seconds. Figure 4 shows the time domain electric field at at the first and the second interfaces of the slab, and Fig. 5 shows the electric field intensity at the 2000-th time step. The well-known behavior of the perfect NRI lens, i.e. the growth of the evanescent wave within the slab and the reversed phase velocity, is clearly observed. The method performs stably during the complete time span of the simulation. Figure 4 also shows the field in the first 1300 time steps at the first interface when the domain is terminated with the conventional PML, which is unstable.

Conclusions

The sine-cosine array-scanning FDTD is an alternative technique for the termination of FDTD lattices. It was shown that the method is applicable to a wide range of problems, including dispersive and conductive media, with the ability to overcome limitations of conventional absorbers. Two benchmark examples were presented, indicating that whenever applicable, the array-scanning method is able to match, if not exceed, the accuracy level of PML absorbers.

Acknowledgement

This work has been supported by the Natural Sciences and Engineering Research Council of Canada and Nortel Networks through a Strategic Grant.

References