Off-Grid Perfect BCs for the FDTD Method

Yotka S. Rickard, Natalia K. Nikolova
McMaster University
Hamilton, Ontario L8S 4K1, Canada
yotka@ece.mcmaster.ca, talia@mcmaster.ca

Abstract: This paper presents a method for implementing off-grid boundary conditions (BCs) within Yee's Finite-Difference Time-Domain (FDTD) method, without disturbing the existing uniform mesh or changing the standard FDTD code. Both perfect electric conductor (PEC) and perfect magnetic conductor (PMC) walls are considered. The field values at off-grid virtual boundaries are obtained by extrapolation of adjacent field values. The method greatly enhances the flexibility of the FDTD method with respect to its ability to represent complex geometrical domains without reducing the spatial step.

Keywords: Finite-Difference Time-Domain (FDTD) methods, Off-grid boundary conditions

1. Introduction

In the Finite-Difference Time-Domain (FDTD) method [1], for good spatial resolution, the spatial step is usually chosen to be between 5 % and 12.5 % of the minimal wavelength of interest. However, in many structures the positions of the boundaries may not be possible to represent by integer multiples of the chosen spatial step. The usual way to handle such structures is to reduce the spatial step or to use a non-uniform grid [2]. The first option leads to an increase in the computational load. The second option lowers the computational accuracy, requires reduction of the time step and may even lead to late-time instabilities.

Offset planar or curved metal boundaries have been treated also by few FDTD modifications. These include locally-conformal methods (compared in [3]) such as the conformal FDTD (C-FDTD) method [4] and the contour-path FDTD (CP-FDTD) method [5], as well as methods using new FDTD formulations [6] or sub-cell models [7]. All these methods require changes in the existing FDTD code as well as changes in the grid and the time step.

Here we propose an alternative to the above options, whereby the boundaries may be described without disturbing the original (coarse, uniform) spatial grid. The method employs off-grid virtual boundaries by extrapolation of adjacent field values. This enhances significantly the flexibility of the FDTD method with respect to complex geometrical shapes. In the approach proposed here, the modifications concern only the outer boundary values of the tangential electric field components. Moreover, the existing conventional FDTD code and the grid remain unchanged. Time step reduction is unnecessary, thus the high speed of the computations is preserved.

In the FDTD method, metal walls are usually considered to be perfect electric conductors (PEC). In general, PEC walls can be described mathematically in two ways: either (1) as vanishing tangential electric field components, which is Dirichlet boundary condition (BC); or (2) as vanishing normal derivatives of the tangential magnetic field components, which is Neumann BC. Similarly, when symmetry is present, a perfect magnetic conductor (PMC) wall may be employed to reduce the computational load. PMC is mathematically represented by either (1) vanishing normal derivatives of the tangential electric field components, Neumann BC, or (2) vanishing tangential magnetic field components, Dirichlet BC. Therefore, theoretically we may describe all on-grid or off-grid virtual perfect BCs in terms of Dirichlet and Neumann BC.

The FDTD method based on Yee's discretization of Maxwell's equations [1] assumes that the field variation between cells is linear. Therefore, a linear extrapolation of the field values is used in the derivation of off-grid Dirichlet BC. Correspondingly, a quadratic extrapolation of the field values for off-grid Neumann BC is used (the latter being linear with respect to the field derivatives).

To validate the proposed method, the resonant frequency for the dominant mode of a rectangular resonator is compared to its analytical value when it is slid with respect to and in parallel with the existing grid by non-integer number of cells. Displacements of PEC walls and of PMC (symmetry) walls are considered. Excellent accuracy is obtained. Beside the accuracy, we also investigate the stability with off-grid BC and give recommendations for their use.

2. Off-Grid Dirichlet BC

Firstly, the modelling of off-grid Dirichlet BC that are in parallel with the existing grid but do not coincide with the grid layers is explored. Without loss of generality, we can think of the PEC boundary walls when modelled with vanishing tangential electric field components. Consider a rectangular resonator, modelled by the FDTD method on a uniform grid of a spatial step $\triangle x = \triangle y = \triangle z$. While the original grid is kept stationary, the structure of size $(m\triangle x,\ n\triangle y,\ k\triangle z)$ is moved in the positive y-direction by $\xi \triangle y$, $\xi \in (0,1)$, as shown in Fig. 1.

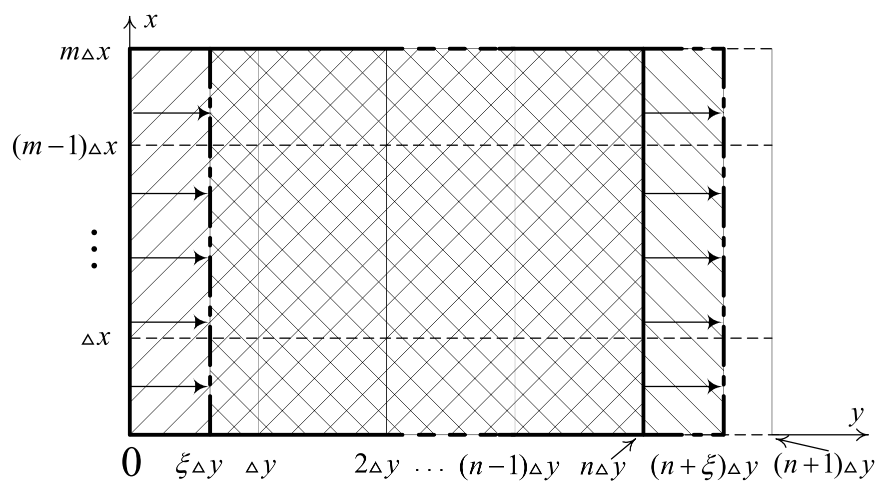

Fig. 1. Geometry of the cross section of the original rectangular cavity and its modified version displaced in the positive y-direction by $\xi \triangle y$.

As ξ is not an integer, the PEC walls perpendicular to the y-direction now have off-grid locations. Using the original grid, a virtual PEC wall at $\xi \triangle y$ can be modelled as follows. For brevity, denote any electric field component tangential to the PEC wall by $E_{\text{tang}}(x,y,z) = f(y)$ and its grid values by $f(k\triangle y) = f_k$, $k = 0,...,n+1$. Assuming a linear variation between adjacent layers and using the function values:

$$\begin{aligned} &\text{at } \triangle y, \quad f(\triangle y) = f_1 = a\triangle y + b \\ &\text{at } \xi\triangle y, \ f(\xi\triangle y) = 0 = a\xi\triangle y + b \end{aligned} \tag{1}$$

we arrive at

$$f(y) = \frac{f_1}{(1-\xi)}\left(\frac{y}{\triangle y} - \xi\right). \tag{2}$$

In particular, the values assigned to the leftmost layer at $y = 0$ ensure a virtual off-grid PEC wall at $\xi \triangle y$:

$$f_0 = f_1\left(\frac{\xi}{\xi - 1}\right). \tag{3}$$

Similarly, at the right end, the virtual off-grid PEC wall is at $(n+\xi)\triangle y$ and the field values of an auxiliary (additional) layer at $(n+1)\triangle y$, can be expressed in terms of the known field values from the layer at $n\triangle y$ as

$$f_{n+1} = f_n \left(\frac{\xi - 1}{\xi} \right). \tag{4}$$

3. Off-Grid Neumann BC

When modelling Neumann BC, without restricting ourselves we can think of a PMC wall modelled as vanishing normal derivatives of the tangential electric field components. Similarly to the PEC wall case, off-grid PMC walls can also be modelled without disturbing the existing mesh. Keeping the grid stationary, when a PMC wall is moved in the positive *y*-direction by $\xi \triangle y$, $\xi \in (0,1)$, Neumann BC is to be applied at $\xi \triangle y$:

$$\frac{\partial f(\xi \triangle y)}{\partial y} = 0 . \tag{5}$$

A linear variation with respect to this derivative requires the use of a quadratic variation of the tangential field values between adjacent layers. Thus,

$$\begin{aligned} &\text{at } \triangle y, && f(\triangle y) = f_1 = a(\triangle y)^2 + b\triangle y + c \\ &\text{at } 2\triangle y, && f(2\triangle y) = f_2 = a(2\triangle y)^2 + b(2\triangle y) + c \\ &\text{at } \xi\triangle y, && \frac{\partial f(\xi \triangle y)}{\partial y} = 0 = 2a(\xi \triangle y) + b . \end{aligned} \tag{6}$$

Eliminating *a*, *b* and *c* from (6), for a virtual PMC wall at $\xi \triangle y$ we obtain:

$$f(y) = \frac{1}{(3-2\xi)} \left[(f_2 - f_1)\left(\frac{y}{\triangle y}\right)^2 + 2\xi(f_2 - f_1)\left(\frac{y}{\triangle y}\right) + (2\xi - 1)f_2 + 4(1-\xi)f_1 \right]. \tag{7}$$

In particular, we assign for the leftmost layer at $y = 0$:

$$f_0 = f_1 + (f_2 - f_1)\left(\frac{2\xi - 1}{3 - 2\xi}\right) \tag{8}$$

Similarly, for virtual PMC wall at the right end, at $(n+\xi)\triangle y$, the tangential electric field values of the additional layer $(n+1)\triangle y$, are expressed as

$$f_{n+1} = f_n + (f_n - f_{n-1})\left(\frac{2\xi - 1}{2\xi + 1}\right). \tag{9}$$

4. Validation and Discussion

4.1. Modelling of off-grid Dirichlet BC

To validate the proposed method, we have implemented it in a standard FDTD code and computed the lowest resonant frequency of a rectangular cavity of dimensions $10\ \text{mm} \times 20\ \text{mm} \times 30\ \text{mm}$, shown in Fig. 2. The relative error is calculated as

$$\delta = \left| \frac{f_{reference} - f_{approx}}{f_{reference}} \right| \tag{10}$$

The excitation is a sine wave of 9 GHz modulated by Blackman-Harris window (BHW) function [8]. The results for the dominant resonant mode TE_{011} are compared with the analytical value $f_{TE_{011}} = 9.00764232763654$ GHz. Firstly, the resonator has been modelled by the standard FDTD algorithm on a uniform grid of $\triangle x = \triangle y = \triangle z = 1$ mm. The result of $f_{TE_{011}} = 9.00310039520264$ GHz represents a relative error

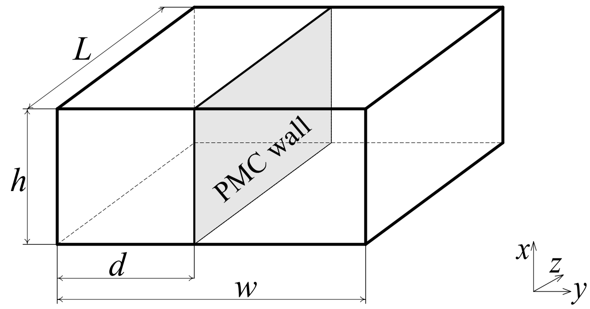

Fig. 2. Geometry of the rectangular resonator. All outer walls are PEC walls. Dimensions: $h = 10$ mm, $w = 20$ mm, $L = 30$ mm. For the off-grid Dirichlet BC experiment, the whole structure is simulated. For the off-grid Neumann BC experiment, half of the structure terminated by a PMC wall at $d = 0.5w$ is simulated.

of 5.04×10^{-4}. Then, keeping the grid stationary, the resonator has been slid in the positive *y*-direction by $\xi\Delta y$, for ξ from 0.15 to 0.85 with increments of 0.05. The off-grid (left and right) PEC boundaries have been modelled by the off-grid Dirichlet BC as described in Section 2. The results for the dominant resonant mode TE_{011} are undistinguishable from those obtained from the structure with on-grid PEC walls. The accuracy of calculating the frequency from the time-domain response is 3×10^{-4} GHz.

If the distance of the offset is less than 15 % of the spatial step, the method breaks down due to the division by too small number. Here it is important to note that the time step has not been changed from its original value of $\Delta t = 0.5\Delta x / c$, where c is the speed of light.

Next, the resonator is slid in the positive *x*-direction, and finally, in both *x*- and *y*-directions at the same time. In all cases the resultant frequency is exactly the same as for the initial structure with on-grid PEC walls. Using a coarser mesh of $\Delta x = \Delta y = \Delta z = 2$ mm, the relative error for TE_{011} with on-grid PEC walls is 1.8×10^{-3}. The application of off-grid Dirichlet BC again gives exactly the same value for the resonant frequency as when on-grid PEC BC are used. Although 30 000 time steps are more than enough to obtain the resonant frequency with sufficient accuracy from the time-domain response, simulations with 200 000 time steps have been performed. No late-time instabilities have been observed in the range $\xi \in [0.15, 0.85]$. When $\xi < 0.15$ or $\xi > 0.85$, the instabilities start after a few hundred time steps.

4.2. Modelling of off-grid Neumann BC

To explore the accuracy when implementing off-grid Neumann BC, the same resonator as above has been modelled using its symmetry with respect to the plane $y = 0.5w$, as half-structure in the *y*-direction and terminated with a PMC wall as shown in Fig. 2. Initially, the on-grid PMC wall at $n\Delta y$ has been modelled by applying Neumann BC to the tangential electric field components. This is implemented numerically either as:

$$f_{n+1} = f_{n-1} \tag{11}$$

or as

$$f_n = (4f_{n-1} - f_{n-2})/3 \tag{12}$$

Both approximations are of second-order accuracy.

With a spatial step of 1 mm and the on-grid Neumann BC (12), the relative error for the dominant resonant mode TE_{011} is 7.52×10^{-5}; with (11) it is 4.75×10^{-4}. Next, again leaving the grid stationary, the half-resonator terminated by the PMC wall has been slid in the positive *y*-direction by $\xi\Delta y$, $\xi \in [0.15, 0.85]$. The off-grid Neumann BC is applied for the right PMC wall, and off-grid Dirichlet BC is applied for the left PEC wall. The frequency of the dominant resonant mode TE_{011} is calculated with the offset boundaries. Its relative errors with respect to: (1) the analytical $f_{TE_{011}}$ value – δ_{analyt}, (2) the on-grid Neumann BC (11) – $\delta_{N(11)}$, and (3) the on-grid Neumann BC (12) – $\delta_{N(12)}$, are plotted versus the normalized displacement ξ in Fig. 3.

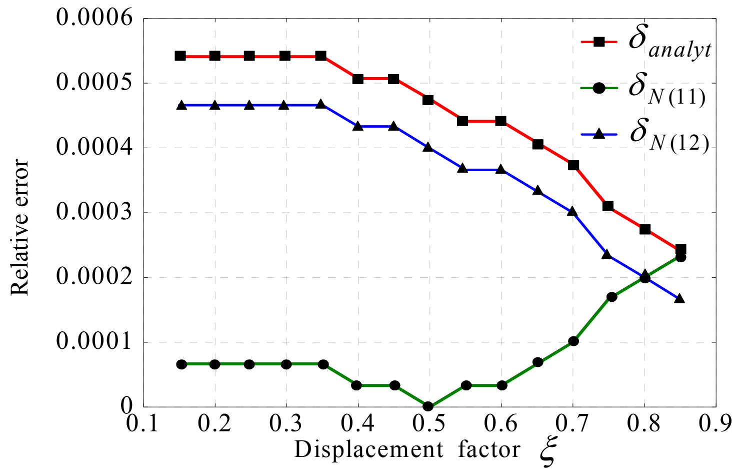

Fig. 3. Relative error in the dominant resonant mode TE_{011} for the rectangular resonator simulated as half of the structure terminated by a PMC wall at the symmetry plane. The off-grid Dirichlet and off-grid Neumann BCs are applied at a distance $\xi\Delta y$ with respect to their initial (on-grid) positions.

5. Conclusion

A simple novel method to implement off-grid PEC and PMC walls within the FDTD method is proposed. The method is very easy to incorporate into existing standard FDTD codes. It features very high accuracy and has a negligible programming and computational impact. Moreover, it has the potential to significantly improve the flexibility of FDTD method with respect to describing complex geometries without change in the code, or in the spatial and time steps. Further applications of the method in structures containing off-grid metal details and slanted walls are being performed and will be described in a future publication.

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