### Slanted Walls in the FDTD Method

Yotka S. Rickard<sup>(1)</sup>, and Natalia K. Nikolova\* <sup>(1)</sup>
(1) McMaster University, Hamilton, Canada, http://www.mcmaster.ca

### Introduction

In the Finite-Difference Time-Domain (FDTD) method [1], the spatial step is usually chosen to be between 5 % and 12.5 % of the minimal wavelength of interest. If the boundaries cannot be positioned at integer multiples of the chosen spatial step, one usually reduces the spatial step or uses a nonuniform grid. The former increases the computational load; the latter lowers the computational accuracy, and requires reduction of the time step. Offset metal boundaries have been treated by locally conformal methods (compared in [2]) such as the conformal FDTD (C-FDTD) method [3] and the contour-path FDTD (CP-FDTD) method [4], as well as methods using new FDTD formulations [5] or sub-cell models [6]. All these methods require substantial changes in the FDTD code, as well as changes in the grid and the time step. Recently, an alternative to the above options was proposed [7]-[8], whereby off-grid perfect electric conductor (PEC) and magnetic boundaries may be modeled without disturbing the original grid. The method employs extrapolation of adjacent field values from the internal computational domain to obtain exterior field values ensuring off-grid virtual boundaries in-between. As only the outer boundary values are modified, the conventional FDTD code, and the grid remain unchanged. Time step reduction is unnecessary, thus the high computation speed is preserved.

To validate the method, we compare the calculated frequencies of the first few resonant modes of a rectangular resonator to their analytical values when the resonator has off-grid wall(s) in parallel and slanted with respect to the existing grid. The off-grid BC are used to modify the conventional staircase approximation to the slanted boundary walls and to significantly improve its accuracy. Beside the accuracy, we also investigate the stability with off-grid BCs and give recommendations for their use.

# **Off-Grid PEC Boundaries**

Consider a rectangular resonator (Fig. 1) modeled on a uniform grid with an off-grid PEC wall at  $y^* = (j + \xi) \triangle y$ , where  $\xi \in (0,1)$ . To model the off-grid wall without disturbing the stationary grid, one can use linear extrapolation [7]: the tangential field values  $E_{\tau(i,j,k)}$  at an exterior layer  $y = j \triangle y$ , can be expressed through the field values  $E_{\tau(i,j\pm s,k)}$  of the adjacent interior layer  $(j\pm s) \triangle y$  as

$$E_{\tau(i,j,k)} = E_{\tau(i,j\pm s,k)} \left[ \xi / (\xi - s) \right]. \tag{1}$$

Here s = 1 for offsets  $\xi \le 0.85$  and s = 2 otherwise; the plus/minus sign refers to left/right off-grid boundary and the offset  $\xi$  is always measured from the exterior layer to the off-grid boundary.

Slanted PEC walls can be modeled in two ways [8] using the above extrapolation:

- (a) by single-plane off-grid BC when the off-grid wall within a cell consists of one plane in parallel to one of the cell faces, as shown in Fig. 2, and
- (b) by double-plane off-grid BC when the off-grid wall within a cell consists of two intersecting planes in parallel to two adjacent cell faces, as in Fig. 3.

When the single-plane BC is applied, as in Fig. 2, the components outside the off-grid wall are expressed through the closest internal components. In case the nearest neighbour has a zero value, s=2 is used in (1). Assigning non-zero values to the two (external) components parallel to the off-grid PEC wall is necessary as they participate in the calculations of the magnetic field components.

When the double-plane off-grid BC is applied, as in the examples in Fig. 3, for the  $E_y$ -component  $\xi = \xi_x$  is used; for the  $E_x$ -component  $\xi = \xi_y$  is used. Note that the components  $E_x(i,j,k)$ ,  $E_y(i+1,j,k)$ , and  $E_z(i+1,j,k)$  should all remain external to the off-grid staircase. Therefore, looking from the exterior cell corner, the off-grid boundaries within a given cell can be either:

- (a) both at a distance greater than one-half grid step [ $\xi_x > 0.5$  and  $\xi_y > 0.5$ ], or
- (b) both at a distance smaller than one-half grid step [ $\xi_x < 0.5$  and  $\xi_y < 0.5$ ].

The position of the off-grid boundaries is chosen as follows. Denote the normalized internal volume of a boundary cell as  $V_{in}$ ,  $0 \le V_{in} \le 1$ . The replacement of the actual slanted boundary with the off-grid boundary should preserve the original  $V_{in}$  in the modified staircase approximation. In the case of double-plane off-grid BC, this leads to the constraint (see Fig. 3)

$$1 - V_{in} = \xi_x \times \xi_y \qquad \text{for } \xi_x > 0.5, \ \xi_y > 0.5$$

$$V_{in} = (1 - \xi_x) \times (1 - \xi_y) \quad \text{for } \xi_x < 0.5, \ \xi_y < 0.5$$
(1)

One straightforward choice for the offsets is:

$$\xi_x = \xi_y = 1 - \sqrt{V_{in}} \quad \text{for } 0.25 < V_{in} < 0.4375$$
  
$$\xi_x = \xi_y = \sqrt{1 - V_{in}} \quad \text{for } 0.4375 \le V_{in} < 0.75$$
 (2)

This is the preferred choice because it is: (a) easy to program in a subroutine before the time stepping begins; (b) insensitive to rounding errors in the calculation of  $V_{in}$ ; (c) leading to very accurate and stable results.

The same reasoning applied to the offset with single-plane off-grid BCs gives:

$$\xi = 1 - V_{in}, \quad 0 < V_{in} < 1.$$
 (3)

The latter is not recommended for slanted walls, as it is not robust: the accuracy depends on the choice of the off-grid boundary direction and offset. However, it is very well suited for corner cells at the intersection of slanted walls.

The stability range of the single-plane off-grid BC is  $0 < V_{in} < 1$  and that of the double-plane off-grid BC is  $0.25 \le V_{in} < 1$ . To keep the relative error below 0.1% (-60 dB), it is enough to modify the staircase using the double-plane off-grid BC at all boundary cells of  $V_{in} = 0.50 \pm 0.25$ . Cells of  $V_{in} > 0.75$  are entirely included in, while cells of  $V_{in} < 0.25$  are entirely excluded from the computational domain.

The double-plane off-grid BC is used where possible; and the single-plane off-grid BC at those locations where the double-plane off-grid BC cannot be applied. The latter can happen (a) if there is only one non-zero internal field component in the cell, or (b) because the assigned field values at external nodes should not be used for calculations in two adjacent boundary cells. Then, a combination of single-plane and double-plane off-grid BCs in neighbouring cells is used, as follows. Let the internal volume of two adjacent boundary cells be  $0.25 < V_{in}^{(1)} < V_{in}^{(2)} < 0.75$ . Then, in order the assigned external field values in each cell *not to interfere with each other*, the double-plane off-grid BC must be applied in the cell of the lesser volume  $V_{in}^{(1)}$  and the single-plane off-grid BC must be applied in the cell of the greater volume  $V_{in}^{(2)}$ .

To validate the method in the case of straight walls, instead of sliding the whole resonator as in [7], we slide only its left wall (see Fig. 1) for  $0 < \xi < 1$  and compare the calculated resonant frequency with its analytical value in Fig. 4. The slopes of the next few (calculated and analytical) resonant frequencies are exactly the same, as well. The relative errors for the first two resonant frequencies are plotted in Fig. 5. Then, the conventional and modified staircase approximations of slanted walls are compared. At  $30^{0}$  rotation, the relative error is 1.88% with the conventional staircase – including the boundary cells of  $V_{in} \ge 0.5$ . The modified staircase using off-grid BCs when  $0.25 \le V_{in} \le 0.75$ , leads to relative error of 0.014%. Simulations with 200,000 time steps have been performed and no late time instabilities have been observed. Next, the error dependence on the angle of rotation is observed. For all angles between  $20^{0}$  and  $45^{0}$ , the relative error in the calculated first resonant frequency with respect to the analytical value is not more than 0.13%, which is the accuracy of the calculations with on-grid boundaries (before the rotation).

## Conclusion

A simple method to model off-grid PEC walls is proposed, which is easy to incorporate into standard FDTD codes. To apply the method to slanted walls, only the internal volume of the boundary cells is to be known. The accuracy of subgridding is achieved without its complexity and computational cost. For slanted walls combinations of single-plane and double-plane off-grid BCs are used, and a robust algorithm for the choice of the offsets is given.

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