An Unsplit Step 3-D PML for Use with the FDTD Method

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***Abstract*— An important advance in the use of the finite-difference time-domain (FDTD) method has been the introduction of the perfectly matched layer (PML) to act as the absorbing boundary condition. The initial implementation required the $\mathbf{E}$ and $\mathbf{H}$ fields to be split. Recent advances have suggested a new unsplit step PML. This paper describes an FDTD implementation of this new unsplit PML in three dimensions, but implements them in the $\mathbf{D}$ and $\mathbf{H}$ fields. This has the advantage of isolating the PML from the rest of the FDTD computation, but, unlike the split step formulation, requires almost no additional computational resources.**

I. Introduction

ONE OF THE most important developments in the use of the finite-difference time-domain (FDTD) method was Berenger's perfectly matched layer (PML) [1]. In a recent paper, Sacks *et al.* [2] suggested a PML which did not require that the computation of the individual E and H fields be split into two components. This was demonstrated on a finite-element code. Zhao and Cangellaris [3] formulated this into the FDTD method and demonstrated it in a two-dimensional FDTD code. This paper implements a three-dimensional (3-D) unsplit step PML following the theory of Sacks in a formulation similar to Zhao and Cangellaris. However, it varies in one important aspect: the PML is implemented using the magnetic field $\mathbf{H}$ and the electrical displacement $\mathbf{D}$ instead of the electric field $\mathbf{E}$, which makes the PML completely impervious to the background medium and completely separate from any "real" conductivity of the medium. Its accuracy and robustness are demonstrated in three-dimensional (3-D) problems with different background media. Furthermore, this PML is implemented with no additional computational resources.

II. Formulation

The normalized Maxwell's equations can be written as

$$j\omega\mathbf{D} = c_0 \cdot \nabla \times \mathbf{H} \tag{1a}$$

$$\mathbf{D}(\omega) = \varepsilon_r^*(\omega) \cdot \mathbf{E}(\omega) \tag{1b}$$

$$j\omega\mathbf{H} = -c_0 \nabla \times \mathbf{E}. \tag{1c}$$

Fictitious anisotropic constants comparable to the relative dielectric constant and relative permeability will be added to $\mathbf{D}$ and $\mathbf{H}$ [4], respectively. The x direction equations are

$$j\omega D_x \cdot \varepsilon_{FX}^*(x) = c_0 \cdot \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) \tag{2a}$$

$$j\omega H_x \cdot \mu_{FX}^*(x) = c_0 \cdot \left(\frac{\partial \tilde{E}_y}{\partial z} - \frac{\partial \tilde{E}_z}{\partial z}\right) \tag{2b}$$

where

$$\varepsilon_{FX}^*(x) = \left(\varepsilon_{Dx}(x) + \frac{\sigma_{Dx}(x)}{j\omega\varepsilon_0}\right) \tag{3a}$$

$$\mu_{FX}^*(x) = \left(\mu_{Hx}(x) + \frac{\sigma_{Hx}(x)}{j\omega\mu_0}\right). \tag{3b}$$

The definitions are similar in the Y and Z directions.

Sacks *et al.* showed that there are two conditions to form a PML.

1) The impedance going from the background medium to the PML must be constant,

$$Z_0 = Z_m = \sqrt{\frac{\mu_{Fm}^*}{\varepsilon_{Fm}^*}} \quad m = x, y, \text{ and } z \tag{4}$$

where Z_0 is the impedance of the background medium and Z_m is the impedance of the PML.

2) In the direction perpendicular to the Boundary (x, for instance), the relative dielectric constant and relative permeability must be the inverse of those in the other directions, i.e.,

$$\frac{1}{\varepsilon_{FX}^*(x)} = \varepsilon_{FY}^*(x) = \varepsilon_{FZ}^*(x) \tag{5a}$$

$$\frac{1}{\mu_{FX}^*(x)} = \mu_{FY}^*(x) = \mu_{FZ}^*(x). \tag{5b}$$

The following selection of parameters satisfies (5):

$$\varepsilon_{Dm} = \mu_{Hm} = 1, \qquad \text{all } m \tag{6a}$$

$$\frac{\sigma_{Dm}}{\varepsilon_0} = \frac{\sigma_{Hm}}{\mu_0} = \frac{\sigma_D}{\varepsilon_0}, \qquad \text{all } m. \tag{6b}$$

Substituting (6) into (4) gives

$$Z_0 = Z_m = \sqrt{\frac{\mu_{Fm}^*}{\varepsilon_{Fm}^*}} = \sqrt{\frac{1+\sigma(x)/j\omega\varepsilon_0}{1+\sigma(x)/j\omega\varepsilon_0}} = 1. \tag{7}$$

The value of $\sigma(x)$ is gradually increased as it goes into the PML.

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Implementing (5) in the x direction gives

$$j\omega D_x \cdot \left(1+\frac{\sigma_D(x)}{j\omega\varepsilon_0}\right)^{-1} = c_0 \cdot \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) \quad (8a)$$

$$j\omega \cdot \left(1+\frac{\sigma_D(x)}{j\omega\varepsilon_0}\right) D_y = c_0 \cdot \left(\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x}\right) \quad (8b)$$

$$j\omega \cdot \left(1+\frac{\sigma_D(x)}{j\omega\varepsilon_0}\right) D_z = c_0 \cdot \left(\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y}\right) \quad (8c)$$

$$j\omega H_x \left(1+\frac{\sigma_D(x)}{j\omega\varepsilon_0}\right)^{-1} = c_0 \cdot \left(\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y}\right) \quad (8d)$$

$$j\omega \left(1+\frac{\sigma_D(x)}{j\omega\varepsilon_0}\right) H_y = c_0 \cdot \left(\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z}\right) \quad (8e)$$

$$j\omega \left(1+\frac{\sigma_D(x)}{j\omega\varepsilon_0}\right) H_z = c_0 \cdot \left(\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x}\right). \quad (8f)$$

Now, the task is to put these in the FDTD formulation. Starting with (8c), going to the sampled time domain using time step $T = \Delta x/2 \cdot c_0$, and using the usual first-order difference approximations in time and space, the following difference equation is obtained:

$$\begin{aligned} D_z^n(i,j,k+1/2) &= gi3(i) \cdot D_z^{n-1}(i,j,k+1/2) + gi2(i) \\ &\quad \cdot (0.5) \cdot \big[H_y^{n-1/2}(i+1/2,j,k+1/2) \\ &\quad - H_y^{n-1/2}(i-1/2,j,k+1/2) \\ &\quad - H_x^{n-1/2}(i,j+1/2,k+1/2) \\ &\quad + H_x^{n-1/2}(i,j-1/2,k+1/2)\big]. \end{aligned} \quad (9)$$

The new parameters $gi2$ and $gi3$ are given by

$$gi2(i) = \frac{1}{1+\sigma(i)\cdot T/(2\varepsilon_0)}. \quad (10a)$$

$$gi3(i) = \frac{1-\sigma(i)\cdot T/(2\varepsilon_0)}{1+\sigma(i)\cdot T/(2\varepsilon_0)}. \quad (10b)$$

An almost identical treatment of (8f) gives

$$\begin{aligned} &H_z^{n+1/2}(i+1/2,j+1/2,k) \\ &\quad = fi3(i+1/2) \cdot H_z^{n-1/2}(i+1/2,j+1/2,k) \\ &\quad - fi2(i+1/2) \cdot 0.5 \cdot \big[E_y^n(i,j+1/2,k) \\ &\quad - E_y^n(i,j-1/2,k) - E_x^n(i+1/2,j,k) \\ &\quad + E_x^n(i-1/2,j,k)\big] \end{aligned} \quad (12)$$

and $fi2(i+1/2)$ and $fi3(i+1/2)$ are

$$fi2(i+1/2) = \frac{1}{1+\sigma(i+1/2)\cdot T/(2\varepsilon_0)} \quad (13a)$$

$$fi3(i+1/2) = \frac{1-\sigma(i+1/2)\cdot T/(2\varepsilon_0)}{1+\sigma(i+1/2)\cdot T/(2\varepsilon_0)}. \quad (13b)$$

Note that they are calculated at $i+1/2$ because of the position in the Yee cell for H_z, moving in the X direction.

Obviously, (8b) and (8e) will be similar. Equation (8a), however, will require a different treatment. Start by rewriting it as

$$j\omega D_x = c_0 \cdot \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) + c_0 \frac{\sigma}{j\omega\varepsilon_0}\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right). \quad (14)$$

The $(1/j\omega)$ may be regarded as an integrator operator. Implementing this into an FDTD formulation gives

$$\begin{aligned} curl\_h = \big[&H_z^{n-1/2}(i+1/2,j+1/2,k) \\ &- H_z^{n-1/2}(i+1/2,j-1/2,k) \\ &- H_y^{n-1/2}(i+1/2,j,k+1/2) \\ &+ H_y^{n-1/2}(i+1/2,j,k-1/2)\big] \end{aligned} \quad (15a)$$

$$\begin{aligned} I_{Dx}^n(i+1/2,j,k) &= I_{Dx}^{n-1}(i+1/2,j,k) \\ &\quad + .5 gi1(i+1/2) \cdot \text{curl\_}h \end{aligned} \quad (15b)$$

$$\begin{aligned} D_x^n(i+1/2,j,k) &= D_x^{n-1}(i+1/2,j,k) + 0.5 \cdot \text{curl\_}h \\ &\quad + .5 \cdot I_{Dx}^n(i+1/2,j,k) \end{aligned} \quad (15c)$$

where

$$gi1(i+1/2) = \frac{\sigma(i+1/2)\cdot T}{2\varepsilon_0}. \quad (16)$$

A similar treatment of (8d) gives

$$\begin{aligned} \text{curl\_}e = \big[&E_y^n(i,j+1/2,k+1) - E_y^n(i,j+1/2,k) \\ &- E_z^n(i,j+1,k+1/2) - E_z^n(i,j,k+1/2)\big] \end{aligned} \quad (17a)$$

$$\begin{aligned} &I_{Hx}^{n+1/2}(i,j+1/2,k+1/2) \\ &\quad = I_{Hx}^{n-1/2}(i,j+1/2,k+1/2) + .5 \cdot fi1(i) \cdot \text{curl\_}e \end{aligned} \quad (17b)$$

$$\begin{aligned} &H_x^{n+1/2}(i,j+1/2,k+1/2) \\ &\quad = H_x^{n-1/2}(i,j+1/2,k+1/2) + 0.5 \cdot \text{curl\_}e \\ &\quad + .5 \cdot I_{Hx}^{n+1/2}(i,j+1/2,k+1/2) \end{aligned} \quad (17c)$$

with

$$fi1(i) = \frac{\sigma(i)\cdot T}{2\varepsilon_0}. \quad (18)$$

In calculating the parameters, it is not necessary to actually vary conductivties. Instead, an auxiliary parameter, xn, is calculated so as to increase as it goes into the PML and the f and g parameters are calculated from xn

$$xn(i) = .333 * \left(\frac{i}{\text{length\_pml}}\right)^3, \qquad i = 1,2,\ldots,\text{length\_pml} \quad (19)$$

$$fi1(i) = xn(i) \quad (20a)$$

$$gi2(i) = \left(\frac{1}{1+xn(i)}\right) \quad (20b)$$

$$gi3(i) = \left(\frac{1-xn(i)}{1+xn(i)}\right). \quad (20c)$$

Notice that the quantity in paretheses ranges between zero and one. The factor .333 was found to be the largest number that still always guarenteed stability. $gi1$, $fi2$, and $fi3$ are different, only in that they are computed at the half intervals, $i+1/2$. The parameters vary in the following manner:

$fi1(i)$ and $gi1(i)$	from 0 to .333	
$fi2(i)$ and $gi2(i)$	from 1 to .75	
$fi3(i)$ and $gi3(i)$	from 1 to .5.	

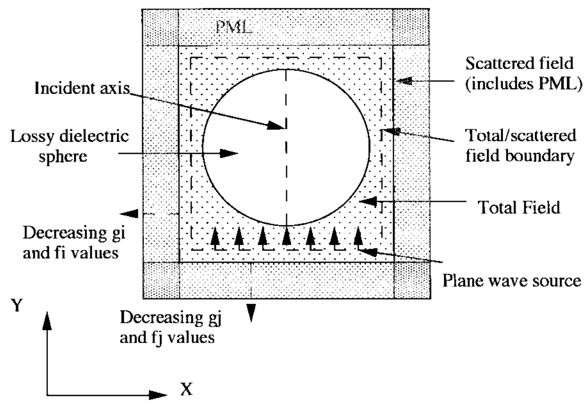

Fig. 1. Description of the problem space used to evaluate the accuracy of the FDTD calculations with Bessel function expansion results. The dielectric sphere is 20 cm in diameter, with $\varepsilon_r = 30$, $\sigma = .3$. The cells are 1 cm^3. The entire space is 40^3 cells.

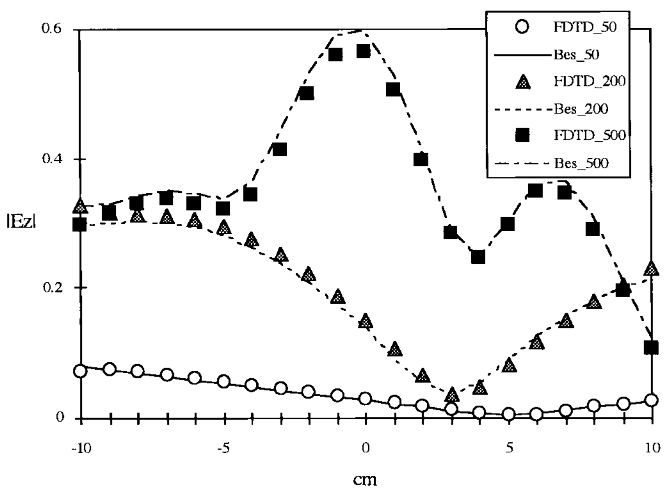

Fig. 2. FDTD versus Bessel function expansion along the incident axis at 50, 200, and 500 MHz for the problem described in Fig. 1. Background medium is air.

Throughout the main problem space, $gi1$ and $fi1$ are zero, while $fi2$, $gi2$, $fi3$, and $gi3$ are one. Therefore, there is a "seamless" transition from the main part of the program to the PML.

III. Demonstration

The ability of the PML to absorb outgoing waves has been demonstrated [2], [3], and the one described in this letter displays the same robust characteristics. Instead of reporting on such tests, an example will be shown to demonstrate the flexibility of this PML in varying the background medium. Fig. 1 is an illustration of the problem space of a 3-D FDTD program. A dielectric sphere is illuminated by a plane wave, and the resulting E-field calculation is compared with a solution from Bessel function expansions. The plane wave is a gaussian impulse, and the E fields are determined by a running Fourier transform [5]. Any number of frequencies can be calculated with one run, requiring only two additional words of core memory.

Fig. 2 shows a comparison along the main incident axis in the dielectric sphere ($\varepsilon_r = 30$, $\sigma = .3$) for a problem run using an air background medium. Fig. 3 shows a similar result for a water background. The same program was used for these two calculations, and no modification to the PML was needed. Remember, the PML was implemented by artificial conductivities associated with the calculation of $\mathbf{D}$ and $\mathbf{H}$; both the dielectric sphere and the background medium are specified by ε_r and σ, which are used in the calculation of $\mathbf{E}$ from $\mathbf{D}$ [see (1b)]. Note that there is very good agreement between Bessel values and FDTD values. At 500 MHz, some error starts to show in the water background problem, because the wavelength in water is 6.67 cm, and the FDTD code is using 1-cm cells.

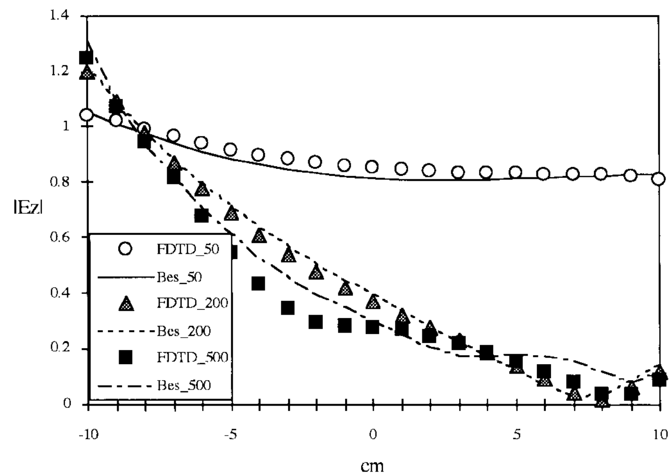

Fig. 3. FDTD versus Bessel function expansion along the incident axis at 50, 200, and 500 MHz for the problem described in Fig. 1. Background medium is water.

IV. Resources to Implement the PML

One final note on the resources needed to implement the PML: recall that a parameter was needed to implement the integrating term [I_{Hx} in (17b)]. This is only needed in the PML, which is in the scattered field of the problem space (Fig. 1). The running Fourier transform, which needs two words per cell per frequency, is only needed in the total field (Fig. 1). Therefore, the matrices used to implement the Fourier transform are also used for the PML, i.e., the implementation of this PML requires no new resources.

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