Improved PML formulation for the unconditionally stable D-H ADI-FDTD method

Stefan Schmidt* and Gianluca Lazzi

Department of Electrical and Computer Engineering,
North Carolina State University, Raleigh, NC 27695-7914, USA

1. Introduction

In a large number of electromagnetic problems, the spatial discretization is dominated by very fine geometric details rather than the smallest wavelength of interest. These fine details dictate a small time-step due to the Courant-Friedrichs-Lewy stability bound [1], when an explicit finite-difference time-domain (FDTD) scheme is used, which in turn leads to a large number of computational steps. The use of the alternating direction implicit (ADI) method was introduced for the time-domain analysis of electromagnetic problems to eliminate the Courant stability bound of the explicit FDTD method [2,3]. The ADI method appears to be of particular interest for large bio-electromagnetic problems and problems in which the larger dispersion and phase error of the ADI method [4,5] is tolerable. In this class of problems, it is often necessary to truncate the model and therefore extend a dielectric material into the absorbing boundary conditions. Use of the D-H formulation allows an easy implementation of unsplit field components PML absorbing boundary conditions, independent of the materials modeled in the FDTD space [6]. An unconditionally stable finite-difference time-domain (FDTD) method based on a D-H formulation and the alternating-direction-implicit (ADI) marching scheme was previously proposed [7]. Here we present an extension to the previous PML implementation of the unconditionally stable method with reduced reflection error.

2. D-H ADI FDTD Formulation

The modified Maxwell's equations for the D-H FDTD formulation with PML absorbing boundary conditions was given in [7] as

$$j\omega D_x\left(1+\frac{\sigma_x^{PML}(x)}{j\omega\varepsilon_0}\right)^{-1}\left(1+\frac{\sigma_y^{PML}(y)}{j\omega\varepsilon_0}\right)\left(1+\frac{\sigma_z^{PML}(z)}{j\omega\varepsilon_0}\right)=c_0\left(\frac{\partial H_z}{\partial y}-\frac{\partial H_y}{\partial z}\right). \quad (1)$$

The $\sigma_i^{PML}(i)$ denote the PML conductivity profile in the x, y, and z directions. For the sake of brevity, we show the derivation of the D-H ADI FDTD scheme for the x-component only. The other components follow similarly. In the previous formulation [7], the FDTD equations were derived as uniaxial PML layers in x, y, and z, respectively, and then superimposed in the corners. Here, equation (1) is discretized directly in one step. To this end, the modified Maxwell's Equation (1) is transformed into the time domain as:

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$$D_x\left(j\omega+\frac{\sigma_y+\sigma_z}{\varepsilon_0}+\frac{\sigma_y\sigma_z}{j\omega\varepsilon_0^{\,2}}\right)=c_0\left(1+\frac{\sigma_x}{j\omega\varepsilon_0}\right)\left(\frac{\partial H_z}{\partial y}-\frac{\partial H_y}{\partial z}\right) \tag{2}$$

$$\rightarrow\frac{\partial D_x}{\partial t}+\frac{\sigma_y+\sigma_z}{\varepsilon_0}D_x+\frac{\sigma_y\sigma_z}{\varepsilon_0^{\,2}}\int_0^t D_x\,dt=c_0\left(\frac{\partial H_z}{\partial y}-\frac{\partial H_y}{\partial z}\right)+c_0\frac{\sigma_x}{\varepsilon_0}\int_0^t\left(\frac{\partial H_z}{\partial y}-\frac{\partial H_y}{\partial z}\right). \tag{3}$$

As indicated by the ADI scheme [2,3], the discretized equation for the first-half time step for D_x follows as

$$\begin{aligned}D_x^{n+\frac{1}{2}}&=\frac{P_y^{N1}P_z^{N1}}{P_y^D P_z^D}D_x^n-4\frac{P_y^{N2}P_z^{N2}}{P_y^D P_z^D}\sum_{s=\frac{1}{2}}^{n}D_x^s\\&+c_0\Delta t\left[\frac{P_x^{N3}}{P_y^D P_z^D}\frac{\partial H_z^{n+\frac{1}{2}}}{\partial y}-\frac{P_x^{N4}}{P_y^D P_z^D}\frac{\partial H_y^n}{\partial z}+\frac{2P_x^{N5}}{P_y^D P_z^D}\sum_{s=\frac{1}{2}}^{n}\left(\frac{\partial H_z^s}{\partial y}-\frac{\partial H_y^s}{\partial z}\right)\right],\end{aligned} \tag{4}$$

and the second-half time step as

$$\begin{aligned}D_x^{n+1}&=\frac{P_y^{N1}P_z^{N1}}{P_y^D P_z^D}D_x^{n+\frac{1}{2}}-4\frac{P_y^{N2}P_z^{N2}}{P_y^D P_z^D}\sum_{s=\frac{1}{2}}^{n+\frac{1}{2}}D_x^s\\&+c_0\Delta t\left[\frac{P_x^{N4}}{P_y^D P_z^D}\frac{\partial H_z^{n+\frac{1}{2}}}{\partial y}-\frac{P_x^{N3}}{P_y^D P_z^D}\frac{\partial H_y^{n+1}}{\partial z}+\frac{2P_x^{N5}}{P_y^D P_z^D}\sum_{s=\frac{1}{2}}^{n+\frac{1}{2}}\left(\frac{\partial H_z^s}{\partial y}-\frac{\partial H_y^s}{\partial z}\right)\right].\end{aligned} \tag{5}$$

The PML coefficients P_i are functions of the conductivity profiles σ_i^{PML} of the ABC layers and given by:

$$\begin{aligned}P_x^D=P_x^{N3}&=1+\left(\sigma_x^{PML}\Delta t\right)/(2\varepsilon_0)=1+X_n(i)\\P_x^{N1}=P_x^{N4}&=1-\left(\sigma_x^{PML}\Delta t\right)/(2\varepsilon_0)=1-X_n(i)\,.\\P_x^{N2}=P_x^{N5}&=\left(\sigma_x^{PML}\Delta t\right)/(2\varepsilon_0)=X_n(i)\end{aligned} \tag{6}$$

The equations for the magnetic field are derived dually. The second-half time step for H_z would be:

$$\begin{aligned}H_z^{n+1}&=\frac{P_x^{N1}P_y^{N1}}{P_y^D P_x^D}H_z^{n+\frac{1}{2}}-4\frac{P_x^{N2}P_y^{N2}}{P_x^D P_y^D}\sum_{s=\frac{1}{2}}^{n+\frac{1}{2}}D_z^s\\&+c_0\Delta t\left[\frac{P_z^{N4}}{P_x^D P_y^D}\frac{\partial E_x^{n+\frac{1}{2}}}{\partial y}-\frac{P_z^{N3}}{P_x^D P_y^D}\frac{\partial E_y^{n+1}}{\partial x}+\frac{2P_z^{N5}}{P_x^D P_y^D}\sum_{s=\frac{1}{2}}^{n+\frac{1}{2}}\left(\frac{\partial E_x^s}{\partial y}-\frac{\partial E_y^s}{\partial x}\right)\right]\end{aligned} \tag{7}$$

The finite difference equation that is used to calculate the y-component of electric field E from D for a given lossy dielectric material is given by

$$E_y^{n+1}=\left(D_y^{n+1}-\frac{\sigma_y\Delta t}{\varepsilon_0}\sum_{s=\frac{1}{2}}^{n+\frac{1}{2}}E_y^s\right)\cdot\left(\varepsilon_{r,y}+\frac{\sigma_y\Delta t}{2\varepsilon_0}\right)^{-1}, \tag{8}$$

where ε_r is the relative permittivity and σ is conductivity. To obtain the tridiagonal system of equations implicitly relating the $D_x^{n+\frac{1}{2}}$ along the y-axis to the fields D, E, and H at time step n, equation (8) is substituted into (7) and then into (5). The ADI algorithm is completed by deriving the equations for the second-half time step and the other field components in a similar fashion [7].

3. Numerical Results and Conclusions

To validate the PML termination of the D-H ADI FDTD space, a single-cell electric current source radiating in free space was used [1]. A compact pulse source was placed in the center of a uniform grid with dimensions of 95x95x95 cells and a uniform discretization $\Delta x=\Delta y=\Delta z=0.4\text{mm}$. A 10-layer PML with polynomial grading of the PML conductivity-profile was used. The fields co-polarized to the source were compared to the reference solution in a sufficiently large grid (241x241x241). The observation points were placed two cells diagonally from the corner of the PML and two cells from the face center of the PML. Fig. 1 illustrates the respective relative reflection error using the proposed new formulation and the previous formulation for the case where the time step was twice that of the Courant stability bound. Fig. 2 is a similar plot for when the time step was four times that of the Courant stability bound. The figure shows that the reflection error from the new PML formulation lies well below that of the previous formulation. In both cases, the large error observed with the previous PML formulation appears to originate from the trihedral corner cells of the PML, as the observed error appears earlier at the corner observation cell and then propagates to the face center. The new formulation does not exhibit such a large error originating from the corners.

We present an improved anisotropic PML for the unconditionally stable D-H ADI FDTD method. The relative reflection error observed from numerical experiments is reduced by 15 to 20 dB as compared to the formulation in [7]. The error is bound in late time, even for time step lengths that are larger than the Courant stability limit, which implies that the method is unconditionally stable for late time.

4. Acknowledgment

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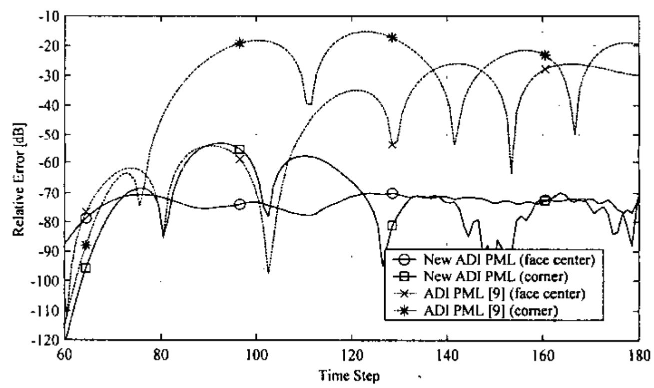

Fig. 1. Maximum reflection error. CFL#=2.

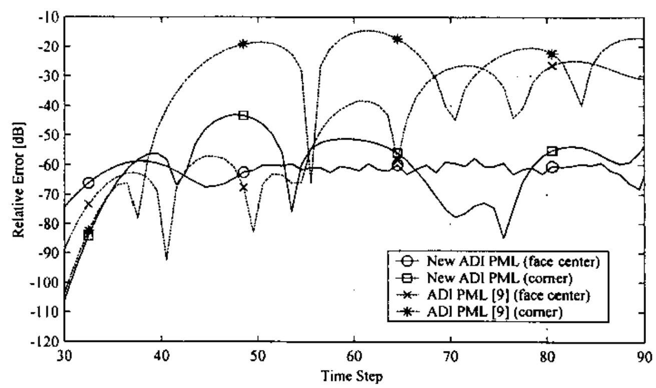

Fig. 2. Maximum reflection error. CFL#=4.