Extension and Validation of a Perfectly Matched Layer Formulation for the Unconditionally Stable D-H FDTD Method

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***Abstract*—In this letter, a modification to the recently proposed unconditionally stable D-H ADI FDTD method is presented that considerably reduces the late-time error induced by the corner cells. The PML boundary is derived from the direct discretization of the modified D-H Maxwell's equations rather than the superposition of uniaxial PML boundaries. An optimal choice of the PML conductivity profile coefficients is proposed. Results show that the reflection error of the PML is limited for increased time step size beyond the Courant-Friedrichs-Lewy stability bound, and maximum reflection errors are 15 to 20 dB lower than the original formulation.**

***Index Terms*—ADI, FDTD methods, PML ABC.**

I. INTRODUCTION

IN A LARGE number of electromagnetic problems, including bioelectromagnetic problems, the spatial discretization is dominated by very fine geometric details rather than the smallest wavelength of interest. When a traditional explicit finite-difference time-domain (FDTD) scheme is used, fine geometric details dictate a small time step due to the Courant-Friedrichs-Lewy stability bound [1], which in turn could require an excessively large number of computation steps.

The use of the alternating-direction-implicit (ADI) scheme was introduced for the time-domain analysis of electromagnetic problems to eliminate the courant stability bound of the FDTD method [2]–[5]. 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 [6], [7] is acceptable. In this class of problems, it is often necessary to truncate the model and therefore extend a dielectric material into the absorbing boundary conditions.

Using the $D-H$ formulation allows an easy implementation of an unsplit field components PML absorbing boundary condition that is independent of the materials modeled in the FDTD space [8].

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 [9]. Numerical experiments with this PML implementation, however, showed that reflection errors originating from the corner cells of the absorbing boundary conditions were not negligible and were increasing with the ADI factor. In this letter, we present an extension to the previous PML implementation of the unconditionally stable method with reduced reflection error.

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II. DERIVATION OF THE D-H ADI FDTD FORMULATION

For the $D-H$ formulation of the finite-difference time-domain method, the normalized Maxwell's equations are written as [8]

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

$$\vec{D}(\omega) = \varepsilon_r(\omega) \cdot \vec{E}(\omega) \tag{2}$$

$$j\omega\vec{H} = -c_0 \cdot \nabla \times \vec{E}. \tag{3}$$

The initial equation for the $D-H$ ADI FDTD formulation with PML absorbing boundary conditions was given as [9]

$$j\omega D_x \left(1 + \frac{\sigma_x^{PML}(x)}{j\omega\varepsilon_0}\right)^{-1} \left(1 + \frac{\sigma_y^{PML}(y)}{j\omega\varepsilon_0}\right) \times \left(1 + \frac{\sigma_z^{PML}(z)}{j\omega\varepsilon_0}\right) = c_0\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) \tag{4}$$

where 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 x-component for the $D-H$ ADI FDTD only. All other components follow similarly. Different from the previous formulation [9], where the FDTD equations where derived as uniaxial PML layers in x, y, and z, respectively, and then superimposed in the corners, (4) is discretized directly, without further simplification. First, the modified Maxwell's (4) transformed into the time domain [10] leads to

$$\begin{aligned} D_x &\left(j\omega + \frac{\sigma_y + \sigma_z}{\varepsilon_0} + \frac{\sigma_y\sigma_z}{j\omega\varepsilon_0^2}\right) \\ &= c_0\left(1 + \frac{\sigma_x}{j\omega\varepsilon_0}\right)\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) \end{aligned} \tag{5}$$

$$\begin{aligned} \rightarrow &\frac{\partial D_x}{\partial t} + \frac{\sigma_y + \sigma_z}{\varepsilon_0} D_x + \frac{\sigma_y\sigma_z}{\varepsilon_0^2}\int_0^t D_x\,dt \\ &= c_0\left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right) + c_0\frac{\sigma_x}{\varepsilon_0}\int_0^t \left(\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z}\right). \end{aligned} \tag{6}$$

Thus, the discretized equations for D_x using the ADI scheme [2]–[5] for the first half time-step reduces to

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

and for the second half time-step to

$$\begin{aligned} D_x^{n+1} =& \frac{P_y^{N1}P_z^{N1}}{P_y^D P_z^D} D_x^{n+1/2} - 4\frac{P_y^{N2}P_z^{N2}}{P_y^D P_z^D}\sum_{s=1/2}^{n+1/2} D_x^s \\ &+ c_0\Delta t\left[\frac{P_x^{N4}}{P_y^D P_z^D}\frac{\partial H_z^{n+1/2}}{\partial y} - \frac{P_x^{N3}}{P_y^D P_z^D}\frac{\partial H_y^{n+1}}{\partial z}\right. \\ &\left.+\frac{2P_x^{N5}}{P_y^D P_z^D}\sum_{s=1/2}^{n+1/2}\left(\frac{\partial H_z^s}{\partial y} - \frac{\partial H_y^s}{\partial z}\right)\right] \end{aligned} \tag{8}$$

where PML coefficients P_i are a functions of the conductivity profiles σ_i^{PML} of the ABC layers

$$\begin{aligned} P_x^D =& P_x^{N3} = 1 + \frac{(\sigma_x^{PML}\Delta t)}{(2\varepsilon_0)} = 1 + X_n(i) \\ P_x^{N1} =& P_x^{N4} = 1 - \frac{(\sigma_x^{PML}\Delta t)}{(2\varepsilon_0)} = 1 - X_n(i) \\ P_x^{N2} =& P_x^{N5} = \frac{(\sigma_x^{PML}\Delta t)}{(2\varepsilon_0)} = X_n(i). \end{aligned} \tag{9}$$

The finite difference equations for the magnetic field can be derived similarly. For example, the second half time-step for H_z would be

$$\begin{aligned} H_z^{n+1} =& \frac{P_x^{N1}P_y^{N1}}{P_y^D P_x^D} H_z^{n+1/2} - 4\frac{P_x^{N2}P_y^{N2}}{P_x^D P_y^D}\sum_{s=1/2}^{n+1/2} H_z^s \\ &+ c_0\Delta t\left[\frac{P_z^{N4}}{P_x^D P_y^D}\frac{\partial E_x^{n+1/2}}{\partial y} - \frac{P_z^{N3}}{P_x^D P_y^D}\frac{\partial E_y^{n+1}}{\partial x}\right. \\ &\left.+\frac{2P_z^{N5}}{P_x^D P_y^D}\sum_{s=1/2}^{n+1/2}\left(\frac{\partial E_x^s}{\partial y} - \frac{\partial E_y^s}{\partial x}\right)\right]. \end{aligned} \tag{10}$$

Further, a finite difference equation is used to calculate the electric field E from D for a given lossy dielectric material with relative permittivity ε_r and conductivity σ, which is given here for the y-component

$$E_y^{n+1} = \frac{\left(D_y^{n+1} - \frac{\sigma_y\Delta t}{\varepsilon_0}\sum_{s=1/2}^{n+1/2} E_y^s\right)}{\left(\varepsilon_{r,y} + \frac{\sigma_y\Delta t}{2\varepsilon_0}\right)}. \tag{11}$$

Equation (11) is substituted into (10) and then into (7), which yields the tridiagonal system of equations that implicitly relates the $D_x^{n+1/2}$ along the y-axis to the fields D, E, and H at time step n. To complete the ADI algorithm, the equations for the second half time-step and the remaining field components of D are derived in a similar fashion [9].

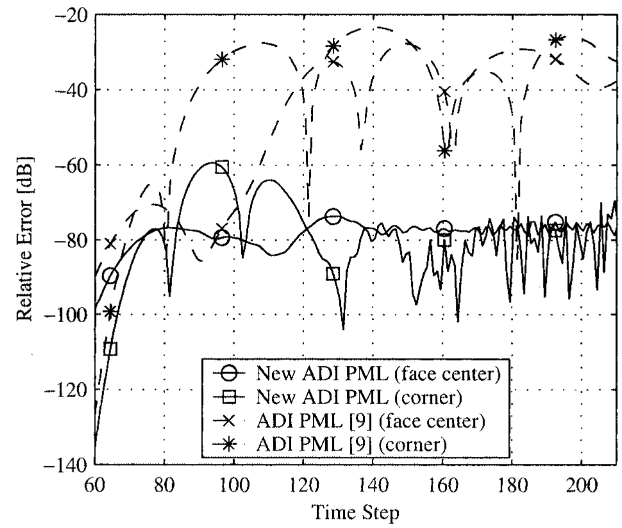

Fig. 1. Maximum reflection error for the two PML formulations close to the corner and the face center of the PML. $\mathrm{CFL}\# = 2$, $X_{n,\max} = 0.33$.

In this formulation, additional computations and memory are necessary for the field sum terms of D and H, given in (8) and (10). However, these terms are only required on the dihedral corners inside the PML since the products of the coefficients P_i^{N2} are zero elsewhere. The added complexity is small compared to the summation of the curl terms associated with P_i^{N5}, which is already required for the original formulation.

III. Numerical Results

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]. The compact pulse source [11] was placed in the center of uniform grid with dimensions of $107 \times 107 \times 107$ cells and a uniform discretization $\Delta x = \Delta y = \Delta z = 0.4$ mm. A 16-layer PML was used. For the PML conductivity-profile, a polynomial grading with

$$X_n(i) = X_{n,\max}\left(\frac{i}{npml}\right)^p, \quad i = 1, 2, \ldots, npml \tag{12}$$

and $p = 3$ was used, where $npml = 16$ is the number of PML layers. The fields co-polarized to the source were compared to the reference solution with a sufficiently large grid ($289 \times 289 \times 289$).

Fig. 1 illustrates the relative reflection error from the PML using the proposed new formulation and the previous formulation for the case where the time step was twice that of the Courant stability bound $dt = 1.54$ ps. The observation points were placed two cells diagonally from the corner of the PML ($89 \times 89 \times 89$) and two cells from the face center of the PML ($54 \times 54 \times 89$). The figure shows that the reflection error from the new PML formulation lies well below that of the previous formulation.

Fig. 2 is a similar plot for the case where the time step was four times that of the Courant stability bound $dt = 3.08$ ps.

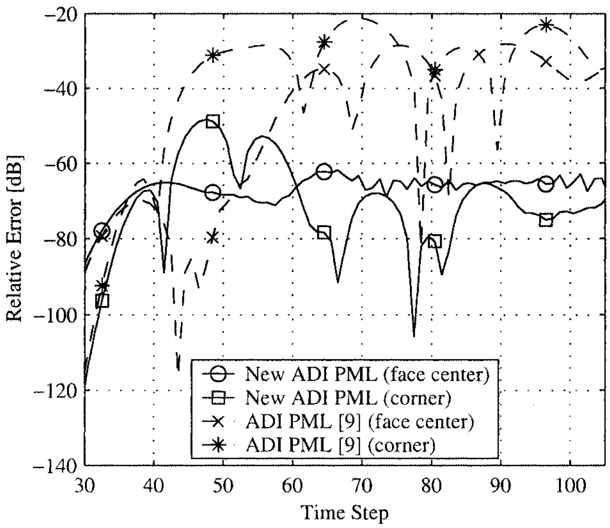

Fig. 2. Maximum reflection error for the two PML formulations close to the corner and the face center of the PML. $\mathrm{CFL\#} = 4, X_{n,\max} = 0.65$.

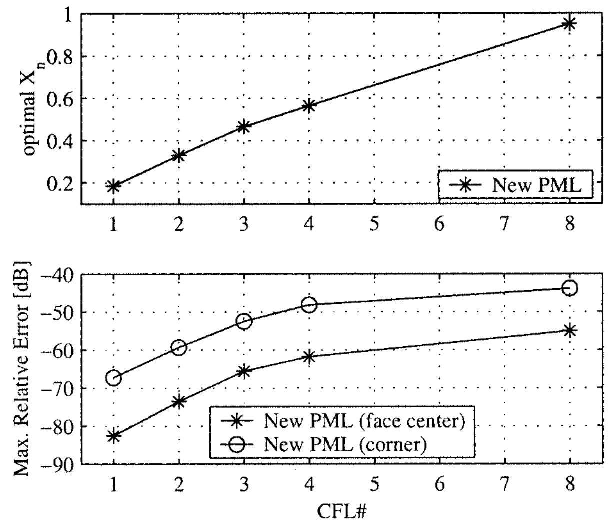

Fig. 4. Optimal X_n and maximum reflection error at the face center of the new PML formulation as a function of the time step length CFL#.

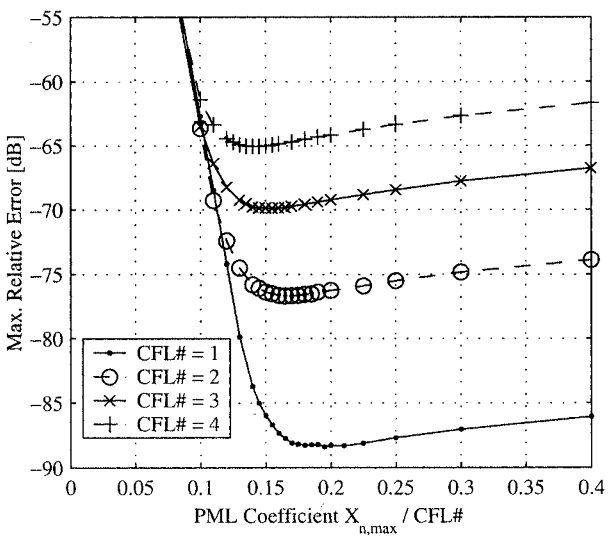

Fig. 3. Maximum reflection error for the new PML formulation as a function of the largest PML conductivity coefficient X_n and the time step length CFL# close to the face center of the PML.

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. The largest occurring error is 15 to 20 dB lower than that of the old formulation, even for large time step lengths beyond the Courant stability bound.

Fig. 3 shows the maximum reflection error of the new PML for different time step lengths as a function of the PML conductivity normalized by CFL#, while Fig. 4 shows the maximum reflection error formulation and optimal X_n as a function of the time step length CFL#. A choice of $X_{n,\max} = 0.175 \cdot CFL\#$ is nearly optimal.

IV. Conclusions and Final Remarks

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 [9]. 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.

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