Accuracy Considerations in Using the PML ABC with FDFD Helmholtz Equation Computation

Carey M. Rappaport, Misha Kilmer and Eric Miller
Center for Electromagnetics Research, Northeastern University, Boston, MA

Abstract—A careful analysis of discretization error in various implementations of Berenger's PML absorbing boundary condition for the FDFD method applied to the Helmholtz equation is presented. Analytic and numerical formulations indicates the clear superiority of specifying the material characteristics in terms of the coupled Ampere's and Faraday's laws first, and then combining the first order differential equations into a discrete Helmholtz-like difference equation.

Index terms—FDFD, PML, Absorbing Boundary Conditions

I. INTRODUCTION

The introduction of Berenger's perfectly matched layer (PML) absorbing boundary condition (ABC) [1] has significantly increased the performance and popularity of the finite difference methods of electromagnetic field computation. The time domain version (FDTD) [2-4] has seen explosive acceptance of the PML lattice termination in the past three years, while its use in the finite difference frequency domain (FDFD) [5,6] as well as finite element methods [7-9] are considerably less popular.

One reason why FDFD is avoided is the perception that it is computationally expensive, requiring solutions of thousands or millions of simultaneous equations. Another flaw with this method is its reliance on highly non-reflective ABCs in preventing reflection from any point on the grid perimeter. In the frequency domain, small imperfections in the ABC can lead to the dominant field solution in the propagation domain. The first concern is overcome by combining the complementary sampled Faraday's and Ampere's Laws into the Helmholtz Equation (thus reducing the number of unknowns by 67% in two dimensional problems), and by using preconditioned iterative methods [10]. The latter issue is successfully addressed with the PML ABC, but only with careful considerations. In particular, when using the Helmholtz equation, it is no longer possible to assume that the PML layer conductivity profile is piecewise constant. It is the intention of this study to demonstrate the subtleties required in applying the FDTD PML procedure to the Helmholtz Equation while preventing significant numerical errors.

II. FDFD PML FORMULATION

The essential aspect of the PML is the additional loss factor $S(n)$—which depends on the direction n normal to a boundary. This unitless quantity alters the wave number in the PML according to the relation:

$$k_{\text{PML}n} = k^{\text{rel}}(n)k_{0n} \quad (1)$$
$$k^{\text{rel}}(n) = 1 - \mathrm{j}S(n)$$

(where n is the direction normal to the layer boundary, $k_{n\text{PML}}$ and k_{n0} are the normal components of the PML and propagation space wave numbers) which multiplies the differential element of the direction normal to the layer boundary [6]. This PML factor can be considered a complex anisotropic mapping of the normal coordinate, or a stretching of the coordinate system in the normal direction [11,12], and follows from Maxwell's equations with the assignment $S(n) = \sigma(n)/\omega\epsilon_0$, where $\sigma(n)$ is the spatially dependent PML conductivity. With this choice, using the inverse dependence on frequency ω, the time domain transforms have frequency independent exponential decay with distance into the PML. However, in most lossy layer ABCs, the conductivity $\sigma(n)$ is profiled from small values closest to the propagation space interface to a maximum value at the PML termination. Both power and geometric series profiling have been studied for optimal absorption of incident signal [13-15].

In the frequency domain, the equations for a two-dimensional transverse electric (relative to the longitudinal direction z into the paper) PML region terminating a lattice at $x = x_{max}$ (assume, without loss of generality that $x_{max} = 0$) have the form:

$$\frac{\partial H_z}{\partial y} = \mathrm{j}\omega\epsilon_0 E_x \quad (2a)$$

$$-\frac{\partial H_z}{\partial x}\left(\frac{1}{1 - \mathrm{j}\sigma_e(x)/\omega\epsilon_0}\right) = \mathrm{j}\omega\epsilon_0 E_y \quad (2b)$$

$$\frac{\partial E_y}{\partial x}\left(\frac{1}{1 - \mathrm{j}\sigma_m(x)/\omega\epsilon_0}\right) - \frac{\partial E_x}{\partial y} = -\mathrm{j}\omega\mu_0 H_z \quad (2c)$$

For the continuous case, $\sigma_e(x) = \sigma_m(x)$. Since the PML conductivity changes with distance, so does the loss factor $S(x)$ and the normal wave number $k_{\text{PML}\,x}$, and therefore the propagation behavior of the wave in the PML will not have a simple linear phase dependence. For continuously varying conductivity, the normal wave number for the boundary $x = x_{max}$ is given by:

$$k_{\text{PML}\,x} = \int^x k_{0\,x}k^{\text{rel}}(x)dx \quad (3)$$

1

where the conductivity $\sigma(x)$ is labeled differently for Ampere's and Faraday's laws. For the both the coupled first-order FDFD and FDTD formulations, in which the electric and magnetic fields are sampled on interlocking grid points [16], the values of PML conductivity can be thought of as piecewise constant, changing every one-half grid cell: $\sigma_m(x) = \sigma_i, |x - i\Delta| < \Delta/4$ and $\sigma_e(x) = \sigma_{i+\frac{1}{2}}, |x - (i + \frac{1}{2})\Delta| < \Delta/4$. Although a parabolic variation of conductivity with distance $\sigma_i = \sigma_f(i/N)^2$ for an N sublayer PML gives acceptable absorption [1], it has been determined empirically that for wide angle absorption, an excellent choice of profile for wide-incidence angle matching to free space using an eight grid cell PML layer in both the time and frequency domains is [13, 5]:

$$\sigma_i = \left(\frac{2i-1}{16}\right)^{3.7}\frac{0.02}{\Delta}, \quad i = 1, ..., 8 \qquad (4a)$$

$$\sigma_{i+\frac{1}{2}} = \left(\frac{2i}{16}\right)^{3.7}\frac{0.02}{\Delta}, \qquad i = 0, ..., 8 \qquad (4b)$$

Using the Helmholtz equation with dependent variable H_z, instead of separate Ampere's and Faraday's laws with additional dependent variables E_x, E_y, leads to a three-fold reduction in the number of unknown discretized field values. Even using fast solvers for the sparse FDFD matrix equations, this reduction leads to great improvements in computation time. It is important to maintain the distance dependencies when combining the three first order TE equations (1) into the Helmholtz equation:

$$\frac{1}{k^{\mathrm{rel}}(x)}\frac{\partial}{\partial x}\frac{1}{k^{\mathrm{rel}}(x)}\frac{\partial H_z}{\partial x} + \frac{\partial^2 H_z}{\partial y^2} + k_0^2 H_z = 0 \qquad (5)$$

for the continuous case. Note that if $\sigma(x)$ (and hence $k^{\mathrm{rel}}(x)$) is treated as piecewise constant, an important first derivative term would be absent.

Discretizing Equation (5) for FDFD computation can be done in three ways:

(1.) Analytically expand the second partial derivative term to give:

$$-\left(\frac{1}{k_i^{\mathrm{rel}}}\right)^3 \frac{\partial k^{\mathrm{rel}}}{\partial x}\Big|_{x=i\Delta}\left(\frac{H_{i+1,j} - H_{i-1,j}}{2\Delta}\right) +$$

$$\left(\frac{1}{k_i^{\mathrm{rel}}}\right)^2\left(\frac{H_{i+1,j} - 2H_{i,j} + H_{i-1,j}}{\Delta^2}\right) + \qquad (6)$$

$$\left(\frac{H_{i,j+1} - 2H_{i,j} + H_{i,j-1}}{\Delta^2}\right) + k_0^2 H_{i,j} \approx 0$$

where $H_{i,j} = H_z(i\Delta, j\Delta)$ and $k_i^{\mathrm{rel}} = 1 - \mathrm{j}S(i\Delta)$

(2.) Expand as in (1.), but use the discretized values of conductivity. The first term becomes:

$$-\frac{k_{i+1}^{\mathrm{rel}} - k_{i-1}^{\mathrm{rel}}}{2(k_i^{\mathrm{rel}})^3\Delta}\left(\frac{H_{i+1,j} - H_{i-1,j}}{2\Delta}\right) \qquad (7)$$

(3.) Discretize the first-order equations (2) on one-half grid cell increments first, then combine them into the discrete Helmholtz equation:

$$\frac{1}{k_i^{\mathrm{rel}}\Delta}\left(\frac{H_{i+1,j} - H_{i,j}}{k_{i+\frac{1}{2}}^{\mathrm{rel}}\Delta} - \frac{H_{i,j} - H_{i-1,j}}{k_{i-\frac{1}{2}}^{\mathrm{rel}}\Delta}\right)$$
$$+ \left(\frac{H_{i,j+1} - 2H_{i,j} + H_{i,j-1}}{\Delta^2}\right) + k_0^2 H_{i,j} \approx 0$$

which combines to give:

$$\left(\frac{H_{i+1,j}k_{i-\frac{1}{2}}^{\mathrm{rel}} - H_{i,j}(k_{i+\frac{1}{2}}^{\mathrm{rel}} + k_{i-\frac{1}{2}}^{\mathrm{rel}}) + H_{i-1,j}k_{i+\frac{1}{2}}^{\mathrm{rel}}}{k_i^{\mathrm{rel}}k_{i+\frac{1}{2}}^{\mathrm{rel}}k_{i-\frac{1}{2}}^{\mathrm{rel}}\Delta^2}\right) \quad (8)$$
$$+ \left(\frac{H_{i,j+1} - 2_{i,j} + H_{i,j-1}}{\Delta^2}\right) + k_0^2 H_{i,j} \approx 0$$

Although each method is accurate to order $(k_0\Delta)^2$ for function which have Taylor series representations, the first method would appear to be the most exact, since it delays the discretization step to last, requiring the material parameters only at the central point of the three-point stencil. However, the third method incorporates three material parameters instead of just two (as with the other two methods), and will be shown to have the greatest accuracy.

III. Error Analysis for FDFD Difference Equations

To quantify the accuracy of the three discretization methods above, assume the continuous version of the power conductivity profile given in (4) $S(x) = S_0 x^p$, where S_0 is constant. With this loss factor form, the corresponding exact plane wave solution to Equation (5) is readily computed using Equations (1) and (3):

$$H_z(x, y) = H_0 e^{-jk_{0x}x - jk_{0y}y - \frac{k_{0x}S_0}{1+p}x^{1+p}} \qquad (9)$$

where the incident wave propagation vector is $\mathbf{k} = k_{0x}\hat{x} + k_{0y}\hat{y}$.

Applying this exact solution to each of the discretized Helmholtz equations (6-8) gives a measure of the discretization error. Care must be used in deriving the expansion of the exponential power functions for non-integer values of p. First, it must be understood that the small argument $\Delta << 1/k_0$ expansion relative to the central position (say x_i) in the stencil must take into account that the central position is itself an integer multiple of that small argument: $x_i = i\Delta$. Next, it is important to expand in terms which include both Δ and Δ^p. For *constant* S_0 and non-integer p, the resulting lowest order error for $H(x, y)$ for Equations (6-8)

2

are respectively:

$$\frac{(k_{0x}^4 + k_{0y}^4)\Delta^2}{12k_0^2} + \frac{k_{0x}S_0\Delta^{p-1}}{k_0^2}\left(i^{p-1}p\right.$$

$$\left. - \frac{(i-1)^{p+1} - 2i^{p+1} + (i+1)^{p+1}}{p+1}\right) \quad (10)$$

$$\frac{(k_{0x}^4 + k_{0y}^4)\Delta^2}{12k_0^2} + \frac{k_{0x}S_0\Delta^{p-1}}{k_0^2}\left(\frac{(i+1)^p - (i-1)^p}{2}\right.$$

$$\left. - \frac{(i-1)^{p+1} - 2i^{p+1} + (i+1)^{p+1}}{p+1}\right) \quad (11)$$

$$\frac{(k_{0x}^4 + k_{0y}^4)\Delta^2}{12k_0^2} + \frac{k_{0x}S_0\Delta^{p-1}}{k_0^2}\left((i+\tfrac{1}{2})^p - (i-\tfrac{1}{2})^p\right.$$

$$\left. - \frac{(i-1)^{p+1} - 2i^{p+1} + (i+1)^{p+1}}{p+1}\right) \quad (12)$$

Note that in each of these expressions the leading term constitutes the standard FDFD error:

$$\frac{k_0^2\Delta^2(\sin^4\theta + \cos^4\theta)}{12} \quad (13)$$

for incidence angle θ. For subsequent terms, the error is of higher order for $p > 3$. For non-integer p, no Taylor series exists for $H_z(x,y)$ as $x \to 0$, so the dependence on Δ can be lower order than $(k_0\Delta)^2$.

However, for predefined, frequency-independent loss of the form of Equation (4), $S_0 = \sigma_f/(N\Delta)^p\omega\epsilon_0 = \sigma_f\eta_0/k_0(N\Delta)^p$, a different expansion is needed. In this case, the dependence on Δ must be evaluated before the exponential function of Equation (9) is approximated. The first term of each error expression of Equations (10-12) remain the same, the lowest order dependence on Δ at the first layer ($n = 1$), for three cases now becomes:

$$\frac{U(\lambda/\Delta)}{2\pi}\left(f_1(p) + V f_2(p)\right) \quad (14)$$

$$f_1(p) = \begin{cases} p + \frac{2(1-2^p)}{1+p} & \text{method 1} \\ 2^{p-1} + \frac{2(1-2^p)}{1+p} & \text{method 2} \\ 2^{-p}(3^p - 1) + \frac{2(1-2^p)}{1+p} & \text{method 3} \end{cases}$$

$$f_2(p) = \begin{cases} p\left(1 - \frac{2^p}{(1+p)}\right) & \text{method 1} \\ 2^{p-1}\left(1 - \frac{2^p}{(1+p)}\right) & \text{method 2} \\ 2^{-p}\left(\frac{p(3^p-1)-2(1-2^p)^2}{1+p}\right) & \text{method 3} \end{cases}$$

$$U = \frac{\sigma_f\Delta\eta_0(\lambda/\Delta)}{2\pi N^p}$$

$$V = \frac{\text{j}U}{\cos\theta - \text{j}U}$$

with dependence only on the conductivity-grid product $\sigma_f\Delta$, the number of grid points per wavelength (λ/Δ), number of PML sublayers N, and incidence angle θ.

Note that the error is not proportional to $\cos\theta$, indicating that although the error is greatest for normal incidence, predicting the wide-angle absorption of a PML with given parameters is non-trivial.

Figure 1 shows the magnitude of the error at normal incidence, for each of the three Equations (6-8), as a function of depth into the PML region, for the power parameter given in Equation (4), $p = 3.7$. The value of S_0 is chosen using $\sigma_f = .02/\Delta$, as in Equation (4) to provide a two-way absorption of 223 dB, corresponding to an eight-layer loss of 2.67×10^{-6}. From Equation (9), $S_0 = -\ln(2.67 \times 10^{-6})(1 + p)/(k_0(8\Delta)^{1+p})$. In this figure, $\Delta = \lambda/40$, implying $S_0 = 18511$. The solid curve represents the first discretization method, Equation (6), the dotted curve represents Equation (7), and the dashed line corresponds to Equation (8). Clearly, the third method is superior. It is noted that if the conductivity variation is not included in the Helmholtz equation, the error are more than an order of magnitude greater than these presented in Figure 1.

For integer power $p \geq 2$ and constant S_0, the error for all three methods is $O(\Delta^2)$, but depends on the particular value of p. For the parabolic variation $p = 2$, the error for each of the first two methods is given by:

$$\frac{(k_{0x}^4 + k_{0y}^4)\Delta^2}{12k_0^2} + \text{j}\frac{8k_{0x}^2S_0\Delta^2}{k_0^2} + \frac{2k_{0x}\Delta^3S_0i(k_{0x}^2 - \text{j}S_0)}{3k_0^2}$$

$$(15)$$

while for the third method, it is:

$$\frac{(k_{0x}^4 + k_{0y}^4)\Delta^2}{12k_0^2} + \text{j}\frac{5k_{0x}^2S_0\Delta^2}{k_0^2} + \frac{k_{0x}\Delta^3S_0i(4k_{0x}^2 - \text{j}S_0)}{6k_0^2}$$

$$(16)$$

Using the loss parameter for 120 dB two-way loss, PML(p, 8, 0.0001) as in [1], with the loss dependence specified in Equation (9): $S_0 = -\ln(10^{-3})\,3/(k_0(8\Delta)^3)$. When $\Delta = \lambda/40$, $S_0 = 412$. In terms of conductivity,

$$\sigma_i = \sigma_f\left(\frac{2i-1}{16}\right)^2, \quad i = 1, ..., 8 \quad (17a)$$

$$\sigma_{i+\frac{1}{2}} = \sigma_f\left(\frac{2i}{16}\right)^2, \quad i = 0, ..., 8 \quad (17b)$$

with $\sigma_f = -3\ln 10^{-6}/16\eta_0\Delta$

Figure 2 shows this error dependence with sublayer number. The error for the third method is lowest for both the $p = 2$ and $p = 3.7$ cases.

IV. Two Dimensional Simulation Results for PML ABCs

The results of the previous section have been tested with a specific two dimensional FDFD scattering problem. The solution to the Helmholtz equation with a two dimensional point source:

$$(\nabla^2 + k_0^2)H_z = \delta(x - x_0, y - y_0) \quad (18)$$

3

(where δ is the 2D Dirac delta function) is given by the Hankel function $H_0^{(2)}(k_0\sqrt{(x-x_0)^2 + (y-y_0)^2})$. To approximate the solution to Equation (18) a 3λ by 2λ space is discretized with an $121\Delta \times 81\Delta$ grid. The grid is surrounded by a PML layer of width 8Δ (that is, $N = 8$). The origin of the point source is $x_0 = 14\Delta, y_0 = -6\Delta$, where the origin $(0,0)$ is assumed to be at row 21 and column 61 of the grid. The PML is terminated with a perfect magnetic conductor.

Discretization of Equation (18) together with either Equations (6) or (8) and lexicographical ordering of the unknowns leads to a system of linear equations $Ax = b$. The resulting matrix is sparse, complex, non-symmetric and non-hermitian. For this particular problem, A has dimension 13,192 but only 65,494 non-zero elements and was reasonably well conditioned; thus it was feasible to solve the system naively by Gaussian elimination. We note that a stable and fast approach effective at solving large systems of this type is given in [10].

Two separate experiments were performed, one in which we set the conductivity profile as in Equation (4) and then calculated solutions using Equations (6) and (8), respectively, and one in which we set the parabolic conductivity profiles as in Equation (18). All experiments were performed in Matlab in double precision floating point arithmetic. We used the Matlab command `besselh` to compute the analytic solution at our grid-points. For each of the two experiments, we compare our computed solutions with the analytic in terms of relative error at each grid-point. That is, Figures 3 and 4 show values of $|H_{i,j} - H_0^{(2)}(i,j)|/|H_0^{(2)}(i,j)|$ corresponding to the two discretizations of the PML given in (6) and (8), respectively, where the profile is as given in Equation [4]. Here, $H_0^{(2)}(i,j)$ is the value of the analytical solution at (x_i, y_j) and $H_{i,j}$ is our computed estimate of H_z at the same point. Figures 5 and 6 show the relative errors when the profile is given by $p = 2$ and equations (6) and (8) are used for the PML, respectively.

Note that in both Figures 4 and 6 the symmetry of the error patterns indicates almost no appreciable reflections from any of the grid edges. In addition, the pattern of error is consistent with the standard angle dependent free-space FDFD sampling error, given by Equation (13); in other words, the PML is absorbing the wave as it should. However, the error in Figures 3 and 5 is noticeably larger and the patterns seem to indicate reflection from the four side boundaries. These results are consistent with the asymptotic PML error results of the previous section.

V. Conclusions

The Perfectly Matched Layer can be efficiently implemented as the absorbing boundary condition for the Helmholtz equation FDFD method as long as the profiling of PML conductivities is incorporated into the computational stencil. A comparison of three methods of discretizing the Helmholtz equation with non-linearly increasing loss has shown that the numerical errors are smallest when the loss values are discretized first, at the first-order Maxwell's equations level, before combination into the Helmholtz equation. The error analysis is more difficult when the conductivity profile dependence has non-integer powers p of distance into the PML.

References

[1] J. Berenger, "A perfectly matched layer for the absorption of electromagnetic waves", *J. Math. Phys.*, Vol. 114, pp. 185-200, 1994.

[2] L. Zhao and A. Cangellaris, "GT-PML: Generalized Theory of Perfectly Matched Layers and Its Application to the Reflectiveness Truncation of Finite Difference Time-Domain Grids", *IEEE Transactions on Microwave Theory and Techniques*, Vol. 44, pp. 2555-2563, 1996.

[3] S. Gedney, "An Anisotropic Perfectly Matched Layer-Absorbing Medium for the Truncation of FDTD Lattices", *IEEE Transactions on Antennas and Propagation*, Vol. 44, pp. 1630-1639, 1996.

[4] Z. Sacks, D. Kingsland, R. Lee, and J. Lee, "A Perfectly Matched Anisotropic Absorber for Use as an Absorbing Boundary Condition", *IEEE Transactions on Antenna and Propagation*, Vol. 43, pp. 1460-1463, 1995.

[5] E. Marengo and C. Rappaport and E. Miller, "Optimum PML ABC Conductivity Profile in FDFD", in review 1998.

[6] C. Rappaport, "Interpreting and improving the PML absorbing boundary condition using anisotropic lossy mapping of space", *IEEE Trans. Magn.*, Vol. 32, pp. 968-974, 1996.

[7] M. Kuzuoglu, R. Mittra, "Investigation of Nonplanar Perfectly Matched Absorbers for Finite-Element Mesh Truncation", *IEEE Trans. Ant. Prop.*, Vol. 45, pp. 474-486, 1997.

[8] J. Tang, K. Paulson, S. Haider, "Perfectly Matched Layer Mesh Terminations for Nodal-Based Finite-Element Methods in Electromagnetic Scattering", *IEEE Trans. Ant. Prop.*, Vol. 46, pp. 507-516, 1998.

[9] J. Wu, R. Lee, and J. Lee, "The Use of Higher Order Edge-Based Finite Elements to Improve the Accuracy of the Anisotropic Perfectly Matched Layer", *URSI Symposium Digest*, pp. 364, 1996.

[10] Kilmer, Miller, and Rappaport, "Preconditioners for structured matrices rising in subsurface object detection", *SIAM Journal on Scientific Computation*, in review

[11] Rappaport, "Perfectly Matched Absorbing Boundary Conditions Based on Anisotropic Lossy mapping of Space", *IEEE*

Microwave and Guided Wave Letters, Vol. 5, pp. 90-92, 1995.

[12]   W. Chew and W. Weedon, "A 3-D Perfectly Matched Medium of Modified Maxwell's Equations with Stretched Coordinates", *Microwave and Optical Technology Letters*, Vol. 7, pp. 559-604, 1994.

[13]   S. Winton and C. Rappaport, "Profiling the Perfectly Matched Layer to Improve Large Angle Performance", *IEEE Transactions on Antennas and Propagation*, in review

[14]   J-P. Berenger, "Improved PML for the FDTD Solution of Wave Structure Interaction Problems", *IEEE Transactions on Antenna and Propagation*, Vol. 45, pp. 466-473, 1997.

[15]   Z. Wu and J. Fang, "High-Performance PML Algorithms", *IEEE Transactions on Microwave Theory and Techniques*, Vol. 6, pp. 2676-2683, 1995.

[16]   Yee, K.S., "Numerical Solution of Initial Boundary Value Problems Involving Maxwell's Equations in Isotropic Media", *IEEE Transactions on Antennas and Propagation*, Vol. AP-14, pp. 302–307, 1966.

FIGURE CAPTIONS

Figure 1. Numerical error in the discretized Helmholtz equation for eight sublayer PML with loss factor $S_0 x^{3.7}$, $S_0 = 18511$ ($\sigma_f \Delta = 0.02$), for continuously varying conductivity (solid curve), conductivity discretized at the second-order equation level (dotted curve), and conductivity discretized at the first order equation level (dashed curve). $\Delta = \lambda/40$.

Figure 2. Numerical error in the discretized Helmholtz equation for eight sublayer PML with loss factor $S_0 x^2$, $S_0 = 412$ ($\sigma_f \Delta = 0.00687$), for continuously varying conductivity (solid curve), conductivity discretized at the second-order equation level (dotted curve coincident with solid curve), and conductivity discretized at the first order equation level (dashed curve). $\Delta = \lambda/40$.

Figure 3: Relative error when FDFD computed solution has PML discretized as in Equation (6), wide-angle conductivity profile as in Equation (4).

Figure 4: Relative error when FDFD computed solution has PML discretized as in Equation (8), wide-angle conductivity profile as in Equation (4).

Figure 5: Relative error when FDFD computed solution has PML discretized as in Equation (6) with Berenger type parabolic conductivity profile in Equation (15).

Figure 6: Relative error when FDFD computed solution has PML discretized as in Equation (7) with Berenger type parabolic conductivity profile in Equation (15).