Stability Considerations in the Application of PML Absorbing Boundary Condition to FDTD Simulation of Microwave Circuits

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Abstract: Berenger introduced the concept of a terminating boundary known as *perfectly matched layer* (PML), in which electromagnetic waves are absorbed without reflection, irrespective of frequency and angle of incidence of the incoming wave. This absorbing boundary condition promises to be very attractive for microwave CAD applications involving complex geometries such as high-density microwave integrated circuits and electronic packages, because the computational domain can be significantly reduced. This paper presents, for the first time, a rigorous analysis of the stability of the PML boundary condition applied to finite-difference time-domain (FDTD) simulation. We discuss the FDTD simulation of a high-Q microstrip filter to show improvement in computational efficiency without any manifestation of instability.

1. Introduction

Berenger [1] introduced the concept of a perfectly matched layer (PML) to absorb without reflection incident electromagnetic (EM) waves of arbitrary polarization, incidence angle and frequency, at the walls of a computational mesh. Berenger showed that such a layer can be designed for a specified bound on the reflection coefficient at the boundary, and applied the PML boundary condition to the finite-difference time-domain (FDTD) simulation of two-dimensional EM wave interaction in an open region. The PML concept has been discussed further in [2], and applied to the FDTD analysis of microstrip circuits in [3]. Mittra and Pekel [2] consider the time-harmonic representation of the fields in a PML medium and show that these fields involve distributed dependent sources. This observation raises the question of temporal stability of the difference approximations of these fields, particularly in view of the non-Maxwellian nature of the split-field representation in Berenger's original formulation.

Berenger's PML absorbing boundary condition (ABC) promises to be very attractive for EM simulations involving complex geometries such as high-density microwave integrated circuits and electronic packages, because the computational domain can be significantly reduced. This paper discusses, for the first time, the stability of the finite difference approximations for the EM field in a computational mesh terminated by Berenger's PML ABC, and thus, provides valuable insight into its application to microwave circuit analysis. In recent years, the FDTD method is being used competitively with other EM simulation methods, partly because of the advances in computer technology and the improvement in accuracy caused by ABCs such as superabsorption [4]. However, all the ABCs prior to Berenger's had limitations such as numerical dispersion and restriction to normal incidence, which precluded their general applicability toward enhancement in accuracy of the FDTD algorithm. The advent of an ABC with residual reflection of the order of -80 dB or less indicates that a comprehensive, yet accurate, full-wave CAD tool, with practically no limitation on the complexity of geometry and physical description of the circuit or scatterer, is at hand.

The stability analysis presented in this paper follows the classical von Neumann method for the stability of partial differential equations. The eigenmode structure of the difference approximations of Berenger's split-field representation in a PML is utilized to derive a transcendental equation for the stability (or amplification) factor. The transcendental equation is solved numerically and stability of the *time-domain* difference equations for the EM field in a PML medium is established rigorously in terms of the computational parameters such as angle of incidence, frequency and layer conductivity. The stability of the EM field approximations at a boundary between a PML medium and free space is also investigated. The PML ABC is applied to the FDTD analysis of a microstrip filter which involves fairly long simulation times, and it is shown that an accurate (in comparison with measurements), stable solution can be obtained by placing the PML boundary only a few cells away from the element. Thus, the filter simulation also demonstrates the computational savings made possible by Berenger's PML.

2. Stability Analysis

2.1. PML Medium

The transverse electric (TE) field in a two-dimensional PML medium can be obtained from [1]

$$\epsilon_0 \frac{\partial E_x}{\partial t} + \sigma_y E_x = \frac{\partial (H_{zx} + H_{zy})}{\partial y} \tag{1}$$

$$\epsilon_0 \frac{\partial E_y}{\partial t} + \sigma_x E_y = -\frac{\partial (H_{zx} + H_{zy})}{\partial x} \tag{2}$$

$$\mu_0 \frac{\partial H_{zx}}{\partial t} + \sigma_x^* H_{zx} = -\frac{\partial E_y}{\partial x} \tag{3}$$

$$\mu_0 \frac{\partial H_{zy}}{\partial t} + \sigma_y^* H_{zy} = \frac{\partial E_x}{\partial y} \tag{4}$$

where the couples $(\sigma_x,\ \sigma_y)$ and $(\sigma_x^*,\ \sigma_y^*)$ denote anisotropic electric and magnetic conductivities, respectively, of the PML medium. The splitting of the longitudinal magnetic field into two components as embodied in (1) – (4) is an important starting point of Berenger's formulation. The stability of this system of equations is addressed next.

The equations above are central differenced in space and exponentially differenced in time [5] to obtain the set of difference equations given by

$$\begin{aligned} E_x^{n+1}(i,j) &= e^{-\sigma_y(j)\Delta t/\epsilon_0} E_x^n(i,j) + \frac{1-e^{-\sigma_y(j)\Delta t/\epsilon_0}}{\sigma_y(j)\Delta y} \\ &\times \Big[H_{zx}^{n+1/2}(i,j+1) - H_{zx}^{n+1/2}(i,j) \\ &+ H_{zy}^{n+1/2}(i,j+1) - H_{zy}^{n+1/2}(i,j) \Big] \end{aligned} \tag{5}$$

$$\begin{aligned} E_y^{n+1}(i,j) &= e^{-\sigma_x(i)\Delta t/\epsilon_0} E_y^n(i,j) - \frac{1-e^{-\sigma_x(i)\Delta t/\epsilon_0}}{\sigma_x(i)\Delta x} \\ &\times \Big[H_{zx}^{n+1/2}(i+1,j) - H_{zx}^{n+1/2}(i,j) \\ &+ H_{zy}^{n+1/2}(i+1,j) - H_{zy}^{n+1/2}(i,j) \Big] \end{aligned} \tag{6}$$

$$\begin{aligned} H_{zx}^{n+1/2}(i,j) &= e^{-\sigma_x^*(i+1/2)\Delta t/\mu_0} H_{zx}^{n-1/2}(i,j) \\ &- \frac{1-e^{-\sigma_x^*(i+1/2)\Delta t/\mu_0}}{\sigma_x^*(i+1/2)\Delta x} \\ &\times \left[E_y^n(i+1,j) - E_y^n(i,j) \right] \end{aligned} \tag{7}$$

$$\begin{aligned} H_{zy}^{n+1/2}(i,j) &= e^{-\sigma_y^*(j+1/2)\Delta t/\mu_0} H_{zy}^{n-1/2}(i,j) \\ &+ \frac{1-e^{-\sigma_y^*(j+1/2)\Delta t/\mu_0}}{\sigma_y^*(j+1/2)\Delta y} \\ &\times \left[E_x^n(i,j+1) - E_x^n(i,j) \right] \end{aligned} \tag{8}$$

The eigenmode of this system is given by damped *wave-like* solutions of the form

$$\begin{bmatrix} E_x^n(i,j) \\ E_y^n(i,j) \\ H_{zx}^n(i,j) \\ H_{zy}^n(i,j) \end{bmatrix} = \xi^n e^{-\gamma_x i \Delta x} e^{-\gamma_y j \Delta y} \begin{bmatrix} E_x^0 \\ E_y^0 \\ H_{zx}^0 \\ H_{zy}^0 \end{bmatrix} \tag{9}$$

where $\Re \gamma_p = \alpha_p$ and $\Im \gamma_p = \beta_p$. The attenuation and phase constants in the PML medium are given as

$$\alpha_x = \frac{\sigma_x}{\epsilon_0 c} \cos\phi,\ \ \alpha_y = \frac{\sigma_y}{\epsilon_0 c} \sin\phi \tag{10}$$

$$\beta_x = \frac{\omega}{c} \cos\phi,\ \ \beta_y = \frac{\omega}{c} \sin\phi \tag{11}$$

where ω is the angular frequency, c is the speed of light in free space and ϕ is the angle of incidence. The vector on the right-hand side of eq. (9) is a constant eigenvector, independent of time and space, and $\xi = \xi(\gamma_x, \gamma_y)$ is a complex number known as the amplification factor [6]. **For a stable solution, the magnitude of this factor must be less than unity**. After substituting the eigenvector equation into the difference equations, the characteristic system given by

$$\begin{bmatrix} \xi_y & 0 & \sqrt{\xi}\frac{p_y s_y}{\sigma_y} & \sqrt{\xi}\frac{p_y s_y}{\sigma_y} \\ 0 & \xi_x & -\sqrt{\xi}\frac{p_x s_x}{\sigma_x} & -\sqrt{\xi}\frac{p_x s_x}{\sigma_x} \\ 0 & -\sqrt{\xi}\frac{p_x s_x}{\sigma_x \eta_0^2} & \xi_x & 0 \\ \sqrt{\xi}\frac{p_y s_y}{\sigma_y \eta_0^2} & 0 & 0 & \xi_y \end{bmatrix} \times \begin{bmatrix} E_x^0 \\ E_y^0 \\ H_{zx}^0 \\ H_{zy}^0 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} \tag{12}$$

is obtained, where $\eta_0 = \sqrt{\mu_0/\epsilon_0}$, and

$$s_x = \frac{\sinh(\gamma_x \Delta x/2)}{\Delta x/2},\ \ s_y = \frac{\sinh(\gamma_y \Delta y/2)}{\Delta y/2} \tag{13}$$

$$p_x = 1 - e^{-\sigma_x \Delta t/\epsilon_0} = 1 - e^{-\sigma_x^* \Delta t/\mu_0} \tag{14}$$

$$p_y = 1 - e^{-\sigma_y \Delta t/\epsilon_0} = 1 - e^{-\sigma_y^* \Delta t/\mu_0}. \tag{15}$$

$$\xi_x = \xi - e^{-\sigma_x \Delta t/\epsilon_0},\ \ \xi_y = \xi - e^{-\sigma_y \Delta t/\epsilon_0} \tag{16}$$

The last equality in (14) and (15) follows from the matching condition for the PML, given by [1]

$$\frac{\sigma}{\epsilon_0} = \frac{\sigma^*}{\mu_0}. \tag{17}$$

The characteristic system in (12) will have a solution for the eigenvector only if the determinant of the matrix is zero. Therefore,

$$\xi \left\{ \frac{\xi_y p_x s_x}{\sigma_x \eta_0} \right\}^2 + \xi \left\{ \frac{\xi_x p_y s_y}{\sigma_y \eta_0} \right\}^2 - \{\xi_x \xi_y\}^2 \equiv 0. \tag{18}$$

When the electric and magnetic conductivities vanish, (18) correctly reduces to the characteristic determinant of central differenced equations for the field in free space:

$$
\begin{aligned}
(\xi - 1)^2 \;&+\; 4\xi \left\{ \frac{c\Delta t}{\Delta x} \sin\left(\frac{\beta_x \Delta x}{2}\right) \right\}^2 \\
&+\; 4\xi \left\{ \frac{c\Delta t}{\Delta y} \sin\left(\frac{\beta_y \Delta y}{2}\right) \right\}^2 \equiv 0. \quad (19)
\end{aligned}
$$

2.2. PML Free Space Boundary

A PML adjacent to free space has no conductivity component tangential to the free space interface [1]. Assuming an interface at $x = x_i = i\Delta x$, the characteristic system can be obtained from (12) by replacing $\sigma_y \to 0$, $p_y/\sigma_y \to \Delta t/\epsilon_0$, $s_y \to \jmath\left\{\frac{\sin(\beta_y \Delta y/2)}{\Delta y/2}\right\}$, $\jmath = \sqrt{-1}$, and changing the third and fourth entries in the second row to

$$1 - A\sigma_x(i)\Delta x\sqrt{\xi}e^{-\jmath\beta_x\Delta x/2}\left[e^{-\alpha_x(2i+1/2)\Delta x/2} - 1\right]$$

where

$$A = e^{-\sigma_x(i)\Delta t/\epsilon_0}. \quad (20)$$

The node for E_y falls at the boundary, and the corresponding update equation is obtained from the magnetic field evaluated at two adjacent nodes, one inside free space and the other inside the PML.

A similar procedure is applied to the case when PML is perpendicular to a dielectric interface (*e.g.*, the lateral termination in microstrip problems). The main point of departure in this situation is to ensure that the waves encounter the same exponential decay in PML on either side of the interface. This is accomplished by a self-consistent application of Snell's law and PML matching condition [3].

2.3. Stability Criterion

An upper bound for Δt in terms of the spatial discretization parameters Δx and Δy can be obtained from the quadratic equation (19) by looking for oscillating wave-like soultions in free space which make $|\xi| = 1$. Such solutions lead to the well-known Courant-Levy-Friedrich (CLF) stability criterion for two dimensions, given by

$$c\Delta t \le \left[\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2\right]^{-1/2} \quad (21)$$

However, because of disspation in the PML and the exponential time-differencing employed, the characteristic dispersion equation (18) for a PML is rather complicated, and it does not readily yield a CLF stability criterion akin to (21). Although eq. (18) appears to be quartic upon first glance, it can be simplified to a quadratic equation in ξ, and using a similar procedure as that employed to derive the CLF criterion (21) for free space, one obtains the stability criterion for the PML, given by

$$
\begin{aligned}
c\Delta t \;&\le\; \left[\left(\frac{1}{\Delta x}\right)^2 + \left(\frac{1}{\Delta y}\right)^2\right]^{-1/2} \\
&\times\; \left[1 + \frac{1}{48}\left\{\left(\frac{\sigma_x}{\epsilon_0}\frac{\Delta x}{c}\right)^2 + \left(\frac{\sigma_y}{\epsilon_0}\frac{\Delta y}{c}\right)^2\right\}\right] \quad (22)
\end{aligned}
$$

It is seen that a higher time step can be chosen in the PML when compared to free space. The additional time duration resulting from the conductivity terms may be referred to as diffusion stability limit, in the sense that velocity of propagation inside a PML is damped (or reduced) by the conductive dissipation, similar to a diffusion process. The resulting implication is that one could employ a wider spatial step in the PML medium in comparison to the adjacent free space, without affecting the stability. We are examining this issue further using simulations with a non-uniform grid. Certainly, a larger spatial step could have potential computational savings, as the PML itself comprises of several Yee cells.

3. Results

We have solved (18) for the complex stability factor ξ using Davidenko's method [7], which is an analytical continuation of Newton Raphson's method from a real domain into the complex plane. Fig. 1 shows the magnitude of the stability factor for the case of a plane wave incident on an interface (perpendicular to x-direction) between free space and a four-layer PML medium characterized by $\sigma_y = 0$, $\sigma_x(\rho) = \sigma_m(\rho/\delta)^n$, where ρ is the distance from the interface to a point in the PML, $\delta = 4\Delta x$ is the thickness of the PML, and

$$\sigma_m = -\ln[R(0)]\frac{n+1}{2}\frac{\epsilon_0 c}{\delta}. \quad (23)$$

The lowest desirable reflection coefficient at the boundary, $R(0)$, is chosen as 0.01, n is chosen as 2, and, $\Delta x = \Delta y = 5$ cm, $\Delta t = 0.1$ ns. The stability factor does not change with frequency, but, it does vary slightly with the angle of incidence, perhaps because the reflection varies a little with this angle (see Table 1 in [1]). However, even in the worst case of close to grazing incidence ($\phi = 89^o$), $|\xi|$ is about 0.75, indicating that the solution is stable for all incidence angles and frequencies.

Note that the time step Δt is chosen according to the Courant stability condition (21), and is identical in free space and PML. However, because the diffusion stability limit in (22) for exponentially differenced equations is higher than the conventional Courant limit, it is possible to choose a larger time step in the PML. We have computed the amplification factor for several cases with Δt higher than the conventional Courant limit, but lower than the diffusion stability limit in (22), and found that $|\xi| \le 1$.

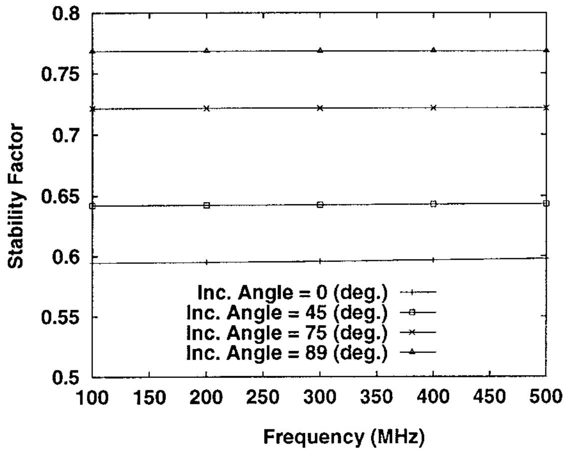

Figure 1: Stability factor at the interface between free space and PML.

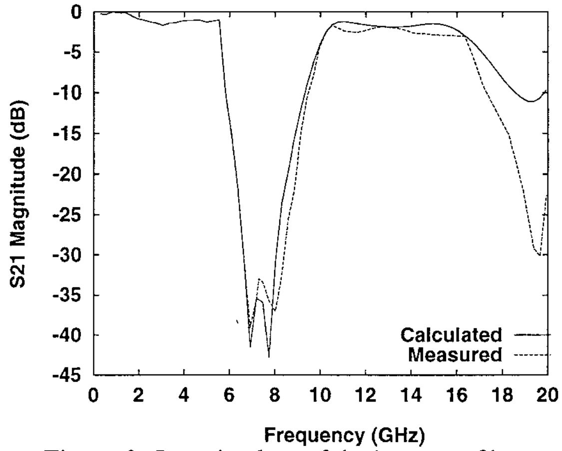

Figure 2: Insertion loss of the low-pass filter.

In order to validate the PML/FDTD implementation and its effectiveness in microwave circuit simulation, we consider a microstrip low-pass filter whose geometry is described in [8]. This is a fairly high-Q filter and requires a long simulation time. Thus, it provides a good check for the stability of the PML algorithm. The computational domain is discretized into $66 \times 42 \times 11$ cells, each of size $\Delta x =$ 0.4064 mm, $\Delta y = 0.4233$ mm and $\Delta z = 0.265$ mm. 3 cells buffer is maintained between the edges of the circuit and the PML boundary, whose thickness is 5 cells. 8000 time steps, each of duration $\Delta t = 0.441$ ps, are employed. The computed insertion loss of the filter, displayed in Fig. 2, corroborates very well with the measurements reported in [8]. No instability was observed in the time-domain field. In comparison with [8], which employs Mur's ABC and the same cell size, we get better accuracy by using PML ABC and 76% fewer cells. Although by no means is the simulation exhaustive, it does provide good insight into the stability, effectiveness (or accuracy in some sense) and computational savings of Berenger's PML absorbing boundary condition for microwave circuit simulation using the FDTD method.

4. Conclusions

The stability of Berenger's PML algorithm for the reflectionless absorption of plane waves at the boundary of a computational domain has been examined rigorously. It is shown that the system of difference equations which govern the EM field in a PML medium, and at the interface between free space and a PML medium, is numerically stable irrespective of the angle of incidence and the frequency. The PML/FDTD implementation has been validated by the efficient simulation of a microstrip filter with a high Q. The transient response does not manifest any instability over long computation times, as demonstrated by good agreement of the frequency-domain S-parameters with measurements. The rigorous stability analysis proves that Berenger's PML boundary condition has significant potential in reducing the computational demands of the FDTD algorithm.

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