Closed-Form Expression of Numerical Reflection Coefficient at PML Interfaces and Optimization of PML Performance

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Abstract— **This letter presents a derivation of the closed-form expression of numerical reflection at interfaces of perfectly matched layer (PML). Reflection coefficients at single interfaces and of finite-thickness absorbers are presented. The derived closed-form expression is found to match identically with the reflection coefficient obtained directly through finite-difference time-domain computation. The closed-form expression of numerical reflection coefficient can significantly facilitate the optimization of PML performance.**

I. Introduction

The PERFECTLY matched layer (PML) has been proven to be very effective for the termination of computation domains in finite-difference time-domain (FDTD) computation [1]. Theoretically, there should be no reflection at interfaces of PML media for incident waves of any angle and frequency so that PML absorbers can be infinitely thin. Reflection does exist in actual numerical computations, however, and the amplitude of the reflection is proportional to the contrast of material parameters on two sides of an interface. Therefore, PML of 8 to 16 cells in thickness and of continuous conductivity profiles are often used to contain the numerical reflection [1], [2].

Many researchers have studied different conductivity profiles in PML in order to minimize the numerical reflection [1]–[3]. These studies were mainly based on numerical experiments by performing many times of numerical computations. It is apparent that the optimization of PML can be done much more efficiently if a closed-form expression of the numerical reflection of PML is available.

The analytical study of numerical reflection at PML interfaces was first done by Chew and Jin with the complex-space stretched coordinate notations [4]. This letter presents an alternative way of deriving the numerical reflection coefficient at an interface of PML media. Reflection coefficients at the interfaces of tangential electric components and of tangential magnetic components are both presented. Numerical reflection coefficients from the analytically derived expression are found to be identical with those obtained directly from numerical computations. The closed-from expression that describes the dependence of the numerical reflection on various parameters of PML media enables efficient determination of optimum values of PML parameters.

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II. Derivation of the Closed-Form Numerical Reflection Coefficients

A. Numerical Dispersion Relation in PML

For the convenience of illustration, the derivation is demonstrated for the two-dimensional (2-D) fields of E_x, E_y, and H_z components. The extension of the conclusion to three-dimensional (3-D) fields is straightforward. Suppose a PML material is of parameters $(\epsilon, \mu, \sigma_x \sigma_x^*)$. Assume Δt and Δh are the FDTD time and space steps and n, i, and j are indices for the time step and for the space in the x and y directions. Substitute a plane wave solution into the finite-difference equations, and settingthe determinant of the resultant homogeneous equations to zero, then the dispersion relation in the PML medium can be optained as

$$\left(\frac{\frac{\sin(k_x \Delta h/2)}{\Delta h}}{1 - j\frac{\sigma_x \Delta t}{2\epsilon \tan(\omega \Delta t/2)}}\right)^2 + \left(\frac{\sin(k_y \Delta h/2)}{\Delta h}\right)^2 = \mu\epsilon\left(\frac{\sin(\omega \Delta t/2)}{\Delta t}\right)^2. \tag{1}$$

B. Numerical Reflection at Single Interface

Consider a uniform PML $(\epsilon, \mu, \sigma_{1x}\sigma_{1x}^*)$, medium 1, in the region $x < 0$ and another uniform PML $(\epsilon, \mu, \sigma_{2x}\sigma_{2x}^*)$, medium 2, in the region $x > 0$. Assume the interface at $x = 0$ coincides with the electric nodes of E_y. An incident plane wave incidents upon the interface from medium 1. The fields in both media can be expressed as follows:

$$E_{1y}^n(i,j) = e^{j(\omega n \Delta t - k_{1x} i \Delta h - k_{1y} j \Delta h)} + R_e e^{j(\omega n \Delta t + k_{1x} i \Delta h - k_{1y} j \Delta h)} \tag{2}$$

$$H_{1z}^n(i,j) = \frac{1}{Z_1}\left[e^{j(\omega n \Delta t - k_{1x} i \Delta h - k_{1y} j \Delta h)} - R_e e^{j(\omega n \Delta t + k_{1x} i \Delta h - k_{1y} j \Delta h)}\right] \tag{3}$$

$$H_{2z}^n(i,j) = \frac{1 + R_e}{Z_2} e^{j(\omega n \Delta t - k_{2x} i \Delta h - k_{2y} j \Delta h)} \tag{4}$$

where R_e is the reflection coefficient to be found at the interface. In (4), it is implied that E_y is continuous at the interface. The impedances Z_1 and Z_2 are defined as E_y/H_z

for a plane wave propagating in $+x$ direction. It can be proved that the impedances on both sides of the interface are the same. Therefore, we denote $Z_1 = Z_2 = Z$. Z can be found as

$$Z = \frac{(\sin(k_{1x}\Delta h/2))/\Delta h}{(\epsilon/\Delta t)\sin(\omega\Delta t/2) - j(\sigma_{1x}/2)\cos(\omega\Delta t/2)} = \frac{(\sin(k_{2x}\Delta h/2))/\Delta h}{(\epsilon/\Delta t)\sin(\omega\Delta t/2) - j(\sigma_{2x}/2)\cos(\omega\Delta t/2)}. \quad (5)$$

The reflection coefficient R_e can be found by substituting (2) to (4) into the finite-difference equation for E_y at the interface as (6), shown at the bottom of the page, where σ_x is the conductivity to be chosen at the interface. If a plane wave incidents upon the interface from medium 2, with the same procedure as above, the reflection coefficient R_e^r can be found as (7), also shown at the bottom of the page.

It can be seen from (6) and (7) that, in general, $R_e \neq -R_e^r$. The reflection coefficients R_e and R_e^r are functions of σ_x at the interface. Typically, σ_x has been chosen to be the average of σ_{1x} and σ_{2x}. Then, the expressions of R_e and R_e^r are reduced to

$$R_e = -R_e^r = -\frac{\cos(k_{2x}\Delta h/2) - \cos(k_{1x}\Delta h/2)}{\cos(k_{2x}\Delta h/2) + \cos(k_{1x}\Delta h/2)}. \quad (8)$$

It can be shown [5] that letting $\sigma_x = (\sigma_{1x} + \sigma_{2x})/2$ is not the best choice. By properly choosing material parameters in the finite-difference equation at the interface, the reflection coefficient at the interface can be substantially smaller than that in (8).

Next, consider the interface coincides with the magnetic nodes of H_z. With the same technique as above and assuming H_z is continuous at the interface, the reflection coefficient R_h of the electric field for the incident wave from medium 1 and R_h^r for the incident wave from medium 2 can be found as (9) and (10), shown at the bottom of the page. Again, it can be seen that, in general, $R_h \neq -R_h^r$, except under the condition $\sigma_x^* = (\sigma_{1x}^* + \sigma_{2x}^*)/2$. In the following derivation, it is assumed that $\sigma_x = (\sigma_{1x} + \sigma_{2x})/2$ and $\sigma_x^* = (\sigma_{1x}^* + \sigma_{2x}^*)/2$.

C. Numerical Reflection of a Finite-Thickness PML Absorber

Suppose a PML absorber is terminated by a perfect electric wall that has reflection coefficient of -1. The total reflection $R_{0.5\Delta h}$ at the H_z node, half Δh away from the electric wall, can be found as

$$R_{0.5\Delta h} = \left(R_h^{0.5\Delta h} - e^{-jk_x\Delta h}\right)/\left(1 - R_h^{0.5\Delta h}e^{-jk_x\Delta h}\right) \quad (11)$$

where $R_h^{0.5\Delta h}$ is the reflection coefficient for the single interface at the H_z node and k_x is the wavenumber in the half-Δh-thick medium next to the electric wall. The total reflection $R_{\Delta h}$ at the E_y node, one Δh away from the electric wall, can be found as

$$R_{\Delta h} = \left(R_e^{\Delta h} + R_{0.5\Delta h}e^{-jk_x\Delta h}\right)/\left(1 + R_e^{\Delta h}R_{0.5\Delta h}e^{-jk_x\Delta h}\right) \quad (12)$$

where $R_e^{\Delta h}$ is the reflection coefficient for the single interface at the E_y node, k_x is the wavenumber in the half-Δh-thick medium between the E_y and the H_z node. The total reflection coefficients at E_y and H_z nodes further away from the electric wall can be found recursively. For a PML absorber of $N\Delta h$ in thickness, the total reflection coefficient at the interface of the PML absorber can be expressed as

$$R_{N\Delta h} = \left(R_e^{N\Delta h} + R_{(N-0.5)\Delta h}e^{-jk_x\Delta h}\right) /\left(1 + R_e^{N\Delta h}R_{(N-0.5)\Delta h}e^{-jk_x\Delta h}\right). \quad (13)$$

III. Numerical Verification and Optimization

In the following numerical tests, $\Delta x = \Delta y = \Delta h = 1$ mm and $\Delta t = 0.5\Delta h\sqrt{\mu\epsilon}$. The reflection coefficient versus frequency is calculated as the ratio of the Fourier-transformed incident and reflected waves. Fig. 1 shows, at the normal incident angle, the reflection coefficient versus frequency at a single interface of the free space and a uniform PML of $\sigma_x = 1$ S/m. Also shown in Fig. 1 is the reflection coefficient for a four-cell PML of parabolic conductivity profile with the theoretical reflection coefficient R_{th} to be 10^{-7}. Here, R_{th} is the reflection coefficient of a PML absorber by ignoring numerical reflection at medium interfaces and numerical dispersion in PML medium [1]. In computing the closed-form numerical reflection coefficient for spatial varying

$$R_e = -\frac{[-\sigma_x + (\sigma_{1x} + \sigma_{2x})/2]\cos(\omega\Delta t/2) - 1/(Z\Delta h)[\cos(k_{2x}\Delta h/2) - \cos(k_{1x}\Delta h/2)]}{[-\sigma_x + (\sigma_{1x} + \sigma_{2x})/2]\cos(\omega\Delta t/2) - 1/(Z\Delta h)[\cos(k_{2x}\Delta h/2) + \cos(k_{1x}\Delta h/2)]} \quad (6)$$

$$R_e^r = -\frac{[-\sigma_x + (\sigma_{1x} + \sigma_{2x})/2]\cos(\omega\Delta t/2) + 1/(Z\Delta h)[\cos(k_{2x}\Delta h/2) - \cos(k_{1x}\Delta h/2)]}{[-\sigma_x + (\sigma_{1x} + \sigma_{2x})/2]\cos(\omega\Delta t/2) - 1/(Z\Delta h)[\cos(k_{2x}\Delta h/2) + \cos(k_{1x}\Delta h/2)]} \quad (7)$$

$$R_h = \frac{[-\sigma_x^* + (\sigma_{1x}^* + \sigma_{2x}^*)/2]\cos(\omega\Delta t/2) - \eta^2/(Z\Delta h)[\cos(k_{2x}\Delta h/2) - \cos(k_{1x}\Delta h/2)]}{[-\sigma_x^* + (\sigma_{1x}^* + \sigma_{2x}^*)/2]\cos(\omega\Delta t/2) - \eta^2/(Z\Delta h)[\cos(k_{2x}\Delta h/2) + \cos(k_{1x}\Delta h/2)]} \quad (9)$$

$$R_h^r = \frac{[-\sigma_x^* + (\sigma_{1x}^* + \sigma_{2x}^*)/2]\cos(\omega\Delta t/2) + \eta^2/(Z\Delta h)[\cos(k_{2x}\Delta h/2) - \cos(k_{1x}\Delta h/2)]}{[-\sigma_x^* + (\sigma_{1x}^* + \sigma_{2x}^*)/2]\cos(\omega\Delta t/2) - \eta^2/(Z\Delta h)[\cos(k_{2x}\Delta h/2) + \cos(k_{1x}\Delta h/2)]} \quad (10)$$

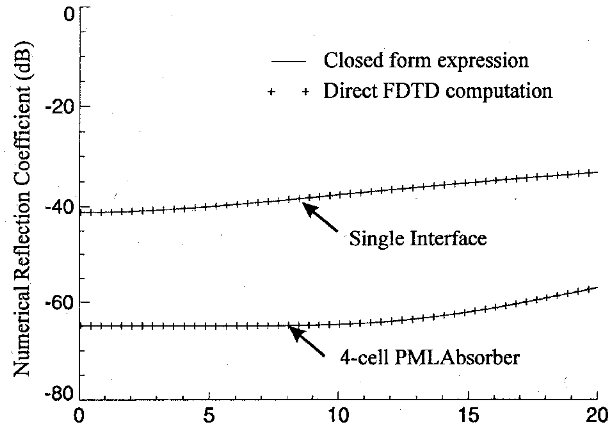

Fig. 1. Comparison of numerical reflection coefficients from the closed-form expression and the direct FDTD computation.

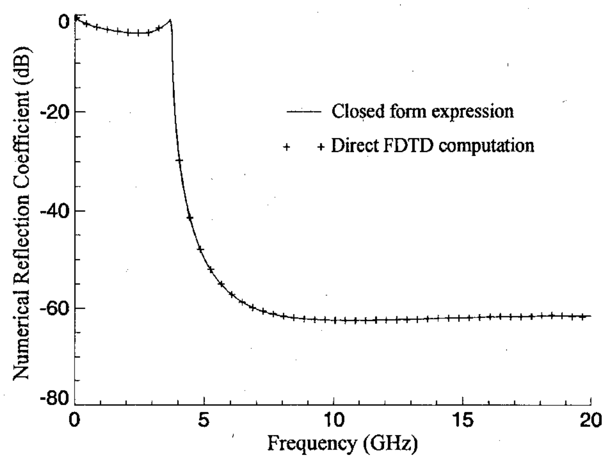

Fig. 2. Comparison of numerical reflection coefficients of a four-cell PML from the closed-form expression and the direct FDTD computation.

conductivity profile, σ_{1x} (or σ_{2x}) is the average conductivity in the half-cell to the left (or right) of the interface. Fig. 2 shows the reflection coefficient of a four-cell PML used to terminate a two-parallel-plate waveguide. The separation between the two metal plates is 40 mm. The theoretical reflection coefficient $R_{\rm th}$ of the PML absorber, which has a parabolic conductivity profile, is 10^{-4}. The incident wave of $\rm TM_1$ mode fields has a cutoff frequency at 3.75 GHz. It can be seen from Figs. 1 and 2 that there is virtually no difference between the reflection coefficients obtained from the closed-form expression and those from the FDTD computation.

The closed-form expression of the numerical reflection coefficient of a PML absorber is a function of space steps Δx and Δy, time step Δt, frequency ω, incident angle θ, thickness of the absorber δ, and the conductivity profile. Assume the conductivity profile is expressed as $\sigma_x = \sigma_m(x/\delta)^n$, where x is the distance to the interface of the PML and the interior

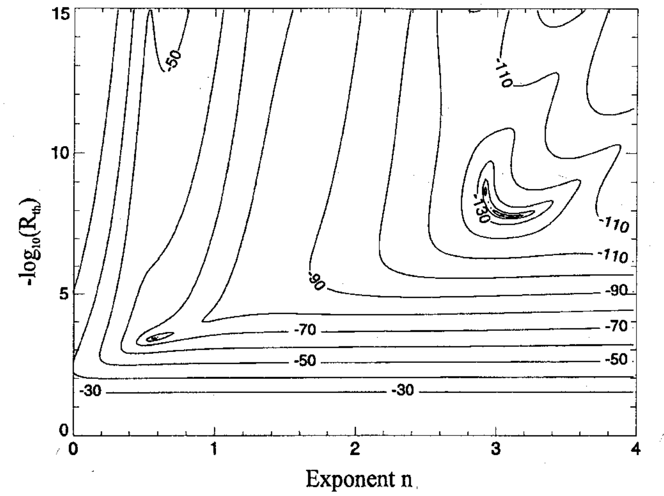

Fig. 3. Contour plot of the numerical reflection coefficient versus the exponent n of the conductivity profile and the theoretical reflection coefficient $R_{\rm th}$ for an eight-cell PML.

medium. If $R_{\rm th}$ at the normal incident angle is specified, the value of σ_m can be found as $-(n+1)/(2\delta\eta)\ln R_{\rm th}$. Depending on different objectives, the PML absorber can be optimized in different ways. Assume we want to find the value of n and $R_{\rm th}$ for minimum reflection at the normal incidence and at the frequency $\lambda = 100\Delta h$, Fig. 3 is the contour plot of the numerical reflection coefficient versus n and $R_{\rm th}$ for an eight-cell PML. Without the closed-form expression, a large number of FDTD computations have to be performed to get the contour plot shown in Fig. 3. From Fig. 3, one can identify that the optimum value of n is about 3.1 and the optimum value of $R_{\rm th}$ is about 10^{-8}.

IV. Conclusion

Closed-form expressions of numerical reflection coefficients at PML interfaces have been derived in this letter. They have also been verified through direct FDTD computations. With the closed-form expression, optimum parameters of PML absorbers can be determined efficiently.

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