Zero Reflection Coefficient in Discretized PML

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***Abstract*—In this paper we present a closed-form reflection coefficient for the perfectly matched layer (PML), when realized using the finite-difference time-domain (FDTD) algorithm. Examining the reflection coefficient, it is found that zero reflection can be obtained for isolated pairs of frequency and angle of incidence.**

***Index Terms*—FDTD, PML.**

I. INTRODUCTION

IN A RECENT study [1] the optimization of the Berenger's perfectly matched layer (PML) absorbing boundary condition (ABC) [2] has been comprehensively discussed. In this letter, we provide closed-form expression for the reflection coefficient from PML as a function of PML parameters, called for in [1].

The optimization has been discussed previously in several papers [3]–[8]. In [3], Wu and Fang make numerical experiments with polynomial profiles and propose optimal polynomial exponent as a function of thickness of the PML. In [4], Berenger analyzes the numerical reflection produced by PML, mainly by numerical experiments and observations, and suggests geometrical progression in the conductivity profile instead of a polynomial one.

In paper [5], Fang and Wu also derive a closed-form expression of the reflection at PML interfaces. Basically, the expression in [5] seems to be derived in similar fashion than ours, but [5] misses the zero-reflection property of the discretized PML. Furthermore, in [1], it is complained that so far published analytical expressions do not accurately predict numerical reflections for all angles and incident waveforms.

In [6], Chew and Jin perform an analysis for the PML in discretized space. The optimization is done via minimization of a cost function, taking into account the angle of incidence as well.

In [7], Lazzi and Gandhi utilize a "pseudoanalytical" formula in optimal design of the PML. However, polynomial profile is again presumed.

Finally, in paper [8], Marengo and Rappaport optimize the profile over polynomials by numerically minimizing a cost function. As in [6], the angle of incidence can be taken into account explicitly.

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In this letter, we demonstrate that PML can be optimized to yield exactly zero reflection for isolated pairs of frequency and angle of incidence. Matlab-codes are given in the Appendix to evaluate the reflection from one-dimensional (1-D) and two-dimensional (2-D) PML layers.

II. 1-D EXPRESSION

In all cases, we assume a PEC condition in the outer boundary of PML. Basically, we proceed recursively from the PEC boundary toward vacuum/PML interface. We assume that incident and reflected waves are plane waves outside the PML region

$$V^n_{inc,\,I} = V_{inc} e^{j(\omega n\Delta t - kI\Delta x)} \tag{1}$$

$$V^n_{ref,\,I} = V_{ref} e^{j(\omega n\Delta t + kI\Delta x)}. \tag{2}$$

Here V stands for both the electric and magnetic fields. Inside PML we do not assume any special form for the fields, but just apply FDTD equations to the unknown fields. Finally, we are able to relate incident and reflected waves outside the PML. Given simulation parameters Δx, Δt and frequency f, we define the dimensionless stability and resolution parameters

$$Q = c_0\Delta t/\Delta x, \qquad R = c_0/(f\Delta x) \tag{3}$$

where c_0 is the speed of light in free space. The electric and magnetic conductivity values of the PML are normalized as follows:

$$\sigma_i^N = \sigma_{i,\,E}\Delta x\eta_0 \qquad \text{for electric conductivity} \tag{4}$$

$$\sigma_i^N = \sigma_{i,\,H}\Delta x/\eta_0 \qquad \text{for magnetic conductivity.} \tag{5}$$

Here $\eta_0 = \sqrt{\mu_0/\varepsilon_0}$. Furthermore, to simplify notations, we define the following parameters:

$$W = 2\sin(\pi Q/R)/Q \tag{6}$$

$$S_i = \sigma_i^N \cos(\pi Q/R) \tag{7}$$

$$T_i = S_i + jW. \tag{8}$$

The index i runs over all conductivity locations, say $i = 1, \ldots, M$. Numerical dispersion relation implies that

$$k\Delta x = 2\sin^{-1}(W/2) \tag{9}$$

where k is the numerical wavenumber. Finally, let

$$U = e^{jk(\Delta x/2)}\left(jW + \left(T_1 + \left(T_2 + \cdots T_M^{-1}\right)^{-1}\right)^{-1}\right). \tag{10}$$

Then the reflection coefficient is

$$\rho = (U - e^{jk\Delta x})/(1+U). \tag{11}$$

TABLE I
SAMPLE OPTIMIZED CONDUCTIVITY PROFILE

σ_1^N	0.0020276	σ_4^N	0.1102515	σ_7^N	0.5736724
σ_2^N	0.0133373	σ_5^N	0.2125432	σ_8^N	0.9464381
σ_3^N	0.0458463	σ_6^N	0.3592777	σ_9^N	1.9711128

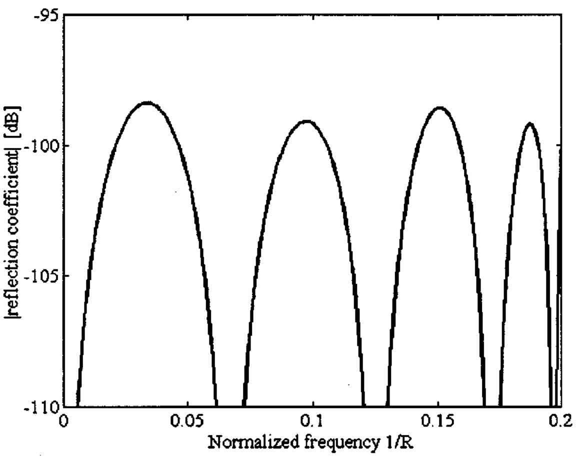

Fig. 1. Reflection characteristics of a sample optimized conductivity profile in one dimension (1-D). Conductivity values given in Table I are used.

Obviously, the zero-reflection condition is

$$U = e^{jk\Delta x}. \tag{12}$$

The following conclusions hold:

- for $2n$ conductivity parameters, it is possible to obtain zero reflection at n distinct frequencies;
- U becomes real at dc. Thus, for $2n+1$ conductivity parameters, it is possible to obtain zero reflection at dc and n distinct frequencies.

As an example, Table I shows normalized conductivity parameters that yield $\rho = 0$ for a set of normalized frequencies $f^N = [0, 0.067, 0.125, 0.172, 0.197]$; here $f^N = R^{-1}$. The conductivity parameters are found by solving (12) using multidimensional Newton iteration. In the following, $Q = 0.99$. Fig. 1 shows corresponding $\rho(f^N)$. For band $f^N = 0 \cdots 0.2 (R > 5)$, the absorption is better than -98 dB.

In the Appendix, the steps (6)–(11) are implemented in a short Matlab-code "rho_1d." For example, the following lines in Matlab produce [1, Fig. 5]:

- $Q = 1$; $a = [0.018, 0.0162, 0.0153]$; $p = 3.675$;
- $b = 376.73^*((1:16)/16).\hat{}p$;
- $s1 = a(1)^*b$; $s2 = a(2)^*b$; $s3 = a(3)^*b$;
- $R = 15 : 100$;
- $r1 = \text{rho\_1d}(Q, R, s1)$; $r2 = \text{rho\_1d}(Q, R, s2)$; $r3 = \text{rho\_1d}(Q, R, s3)$;
- $\text{plot}(R, 20^* \log 10(abs([r1; r2; r3])))$.

Note that the conductivity values are normalized by η_0.

III. TWO-DIMENSIONAL EXPRESSION

The 2-D case can be analyzed in the same way than the 1-D case. The analysis is lengthy, but the result greatly resembles the 1-D case. However, we have found that the approach utilized

TABLE II
OPTIMIZED EIGHT-LAYER CONDUCTIVITY PROFILE FOR WIDE-ANGLE ABSORPTION

σ_1^N	0.0045681	σ_7^N	0.537346	σ_{13}^N	2.568003
σ_2^N	0.0243114	σ_8^N	0.771210	σ_{14}^N	3.784911
σ_3^N	0.0633731	σ_9^N	1.020632	σ_{15}^N	6.009493
σ_4^N	0.120092	σ_{10}^N	1.260711	σ_{16}^N	11.546761
σ_5^N	0.206738	σ_{11}^N	1.508592		
σ_6^N	0.344225	σ_{12}^N	1.881498		

in [1] is more efficient, resulting in faster optimization of the PML parameters. In short, a 2-D wave is considered equivalent to a 1-D wave propagating with a velocity $c/\cos\theta$. Numerical dispersion is discarded here. Given Δx, Δy, Δt and frequency f, we first introduce a cell-shape parameter

$$Z = \Delta x / \Delta y. \tag{13}$$

The stability parameter is

$$Q_2 = \sqrt{1 + Z^2} c_0 \Delta t / \Delta x. \tag{14}$$

We now define the resolution parameter through diagonal dimension of a cell

$$R_2 = \lambda / \sqrt{\Delta x^2 + \Delta y^2} = c_0 Z / (f \Delta x \sqrt{1 + Z^2}). \tag{15}$$

The subscripts highlight the 2-D context. Three-line Matlab-code "rho_2d" in the Appendix evaluates the reflection coefficient, exploiting the 1-D code "rho_1d." For example, the simulated reflection coefficients given in [1, Table I], can be accurately reproduced:

- $Z = 1$; $Q2 = 1$; $th = pi/180^*(0 : 5 : 75)$;
- $Wg = [\text{ones}(1, 13), 10.\hat{}(-0.12^*(5 : 5 : 15))]$;
- $R2 = 1/sqrt(2)^*[15, 20, 30]$; $p = [3.77, 3.74, 3.78]$;
- $Sf = [0.0152, 0.016, 0.0177]$;
- for $i = 1 : 3$, $S = Sf(i)^* 376.73^*((1 : 16)/16).\hat{}p(i)$; for $j = 1 : 16$, $r(i, j) = \text{rho\_2d}(th(j), R2(i), Z, Q2, S)$; end; end;
- $G = \max(20^* \log 10(abs(r.^*[Wg; Wg; Wg])'))$.

The result is $G = \{-90.16, -93.45, -98.79\}$, to be compared with $\{-90.27, -93.71, -98.83\}$ in [1].

IV. WIDE ANGLE ABSORPTION

In a 2-D-problem, it is possible to obtain zero reflection for discrete frequencies and angles. With an n-layer PML having $2n$ parameters, one can obtain zero reflection for n (f, α)-pairs. The corresponding parameters can be found using, e.g., Newton iteration.

We consider two examples. First, we optimize an 8-layer PML in the same angular and frequency range as in [1, Tables I–VII]: θ ranges from 0 to 75° at 5° increments, and R_2 has three values $15/\sqrt{2}$, $20/\sqrt{2}$ and $30/\sqrt{2}$. The optimized and normalized parameters are given in Table II. This single profile yields maximum reflection -113 dB over all R_2, θ combinations involved, even without the weighting function used in [1]. Note that a separate profile is optimized for each resolution in [1].

TABLE III
OPTIMIZED FOUR-LAYER CONDUCTIVITY PROFILE FOR A WAVEGUIDE PROBLEM

σ_1^N	0.001455	σ_4^N	0.3068	σ_7^N	1.7396
σ_2^N	0.02817	σ_5^N	0.5949	σ_8^N	3.4888
σ_3^N	0.1211	σ_6^N	1.0237		

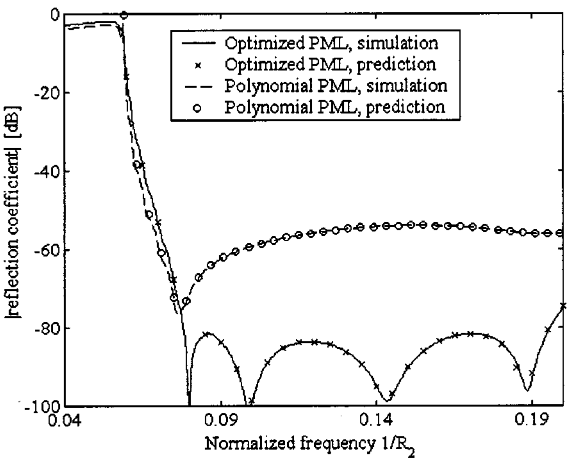

Fig. 2. Predicted and simulated reflection coefficient as functions of frequency in a parallel-plate waveguide problem. Four-layer polynomial and optimized conductivity profiles are used.

As a second example, we consider a parallel-plate waveguide problem ($Z = 1$, $Q_2 = 0.99$, $d = 12\Delta y$). The normalized cut-off frequency of the waveguide is $f_c^N \approx 0.059$. We optimize a 4-layer PML in a band starting from $1.33 \cdot f_c^N = 0.078$. A wave component f^N forms an angle $\alpha(f^N) = \sin^{-1}(f_c^N / f^N)$ with the x-axis. Thus, we choose four frequency-angle pairs $(f^N, \alpha(f^N))$ as design parameters. A good choice is $\mathbf{f}^N =$ [0.08, 0.098, 0.145, 0.187]; the related conductivities are given in Table III.

Fig. 2 presents the predicted and simulated reflection coefficients of the waveguide problem. The reference solution is obtained using a much larger computational volume. Also shown are results due to a polynomial profile of equal thickness with parameters $R_{th} = 10^{-4}$ and $n = 2$, given in [5]. Optimized profile results reflection less than -82 dB over a band $f^N = 0.078 \cdots 80.193$, while the polynomial profile yields reflection less than -54 dB over the same band. Due to numerical dispersion, the zeros in ρ are not perfect. Using a truly 2-D optimization, they can be made exact, but the overall absorption is not improved by doing so. Therefore, 1-D based optimization is recommended.

V. CONCLUSIONS

Closed-form reflection coefficient for discretized PML is given for propagating plane waves. Surprisingly, perfect absorption can be obtained for discrete (f, α)-pairs. Polynomial conductivity profiles are not optimal in general.

The utilization of the 1-D reflection formula in 2-D problem seems to be generalizable to three-dimensional (3-D) case also; this needs still to be confirmed. An analysis for evanescent waves is also a preferred extension of the present work.

APPENDIX

Matlab-code "rho_1d" evaluates the reflection coefficient of a 1-D PML layer. Input parameters are given in (3). The conductivity values are given as a single vector "s."

```
function r = rho_1d(Q, R, s);
%  Jaakko Juntunen 16.11.2000
N = length(s); W = 2/Q*sin(pi*Q./R);
k_delta = 2*asin(W/2);
for i = 1:N,
  T(i, :) = j*W + s(i)*cos(pi*Q./R);
end;
CUM = zeros(size(R));
for i = 1:N,
  CUM = CUM + T(N+1−i, :); CUM = 1./CUM;
end;
U = (j*W + CUM).*exp(j*k_delta/2);
r = (U − exp(j*k_delta))./(1 + U).
```

Matlab-code "rho_2d" evaluates the reflection coefficient of a 2-D PML layer. Input parameters are propagation direction θ and the parameters given in (13)–(15). The conductivity values are given as a single vector "s."

```
function r = rho_2d(th, R2, Z, Q2, s);
%  Jaakko Juntunen 16.11.2000
Q1 = Q2/(cos(th)*sqrt(1+Z^2));
R1 = R2*sqrt(1+Z^2)/(Z*cos(th));
r = rho_1d(Q1, R1, cos(th)*s).
```

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