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A New Absorbing Layer Boundary Condition for the Wave Equation[1]

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A new absorbing boundary condition using an absorbing layer is presented for application to finite-difference time-domain (FDTD) calculation of the wave equation. This algorithm is by construction a hybrid between the Berenger perfectly matched layer (PML) algorithm and the one-way Sommerfeld algorithm. The new prescription contains both of these earlier ones as particular cases, and retains benefits from both. Numerical results indicate that the new algorithm provides absorbing rates superior to those of the PML algorithm. © 2000 Academic Press

Key Words: finite-difference; electromagnetic; wave equation; absorbing boundary condition; ABC; perfectly matched layer; PML; Berenger; Sommerfeld.

1. INTRODUCTION

Absorbing boundary conditions (ABC) are routinely used in electromagnetic simulations to minimize the computer resources required for modeling an open system [5]. Two classes of algorithms are currently in use. The first class uses a discretized approximation of the wave equation at the boundary which is applied only to the waves leaving the computational domain (outgoing waves); such algorithms are called "one-way" ABC. The other class uses an absorbing layer to absorb the outgoing waves at the boundary and is widely used in the form of the Berenger perfectly matched layer (PML) ABC [1]. In contrast with the one-way ABC, the absorbing layer equations treat the waves equally, regardless of their direction of propagation. The advantage of the PML over the one-way ABCs is its flexibility: one may vary the size of the absorbing layer as well as the profile of the absorption coefficient (driven by a numerical conductivity) in the layer in order to optimize the absorption efficiency. However, the PML algorithm is known to give poor performance when a layer of only a few cells is used, because of "numerical reflections" [1, 6]. In contrast, one-way ABCs

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offer no (or very little) flexibility, but are very efficient at absorbing waves on a single-cell boundary.

In this article, we show that it is possible to construct a hybrid algorithm between a one-way and an absorbing layer ABC, retaining the advantages of both. For simplicity, we restricted ourselves to the one-dimensional case in the first part of the article. Using a mathematical condition applying to the FDTD wave equation derived in [4], we derive a recursion relation linking the numerical conductivities in a PML layer. Later in the article, we show from numerical results that the numerical reflections observed with the PML algorithm are due to its violation of this relation. Then, a more general form for a new ABC is given which contains the PML ABC, as well as the Sommerfeld (or first-order Engquist and Majda [3]) ABC as particular cases. Using this form, a new ABC is proposed. This ABC is one-way in the sense that it treats outgoing and ingoing waves differently, and it restricts to the Sommerfeld ABC if the layer is one cell thick. However, as with the PML ABC, it is also possible to absorb the waves in an arbitrary number of layers to obtain higher efficiency. Finally, we show the extension of the algorithm to higher dimension. A numerical comparison is given between this ABC, the Sommerfeld or second-order Engquist and Majda ABC, and the PML algorithm, in one and in two dimensions.

2. A MATHEMATICAL RELATION FOR THE FDTD WAVE EQUATION

2.1. *In Vacuum*

For a FDTD [2] discretization of a wave equation in vacuum, written as

$$E_j^{i+1} = \alpha E_j^i + \beta_1 B_{j+1/2}^{i+1/2} - \beta_2 B_{j-1/2}^{i+1/2} \tag{1}$$

where i is the time index, and j is the space index, we have shown in [4] (see Appendix) that the coefficients α, β_1, and β_2 are linked by

$$\alpha = 1 + \beta_1 - \beta_2 \text{ for waves traveling forward} \tag{2}$$

and

$$\alpha = 1 - \beta_1 + \beta_2 \text{ for waves traveling backward.} \tag{3}$$

We also showed in the same reference, that Eq. (1) is the FDTD discretization of the differential equation

$$\frac{\partial E}{\partial t} = \sigma_E E + \frac{\partial B}{\partial x} + \sigma_B B \tag{4}$$

because it can be written as

$$\frac{E_j^{i+1} - E_j^i}{\delta t} = \sigma_E \frac{E_j^{i+1} + E_j^i}{2} + \frac{B_{j+1/2}^{i+1/2} - B_{j-1/2}^{i+1/2}}{\delta x} + \sigma_B \frac{B_{j+1/2}^{i+1/2} + B_{j-1/2}^{i+1/2}}{2} \tag{5}$$

with

$$\begin{aligned}\sigma_E &= \frac{2}{\delta t}\left(\frac{\alpha - 1}{\alpha + 1}\right)\\ \frac{1}{\delta x} &= \frac{1}{\delta t}\left(\frac{\beta_1 + \beta_2}{\alpha + 1}\right)\\ \sigma_B &= \frac{2}{\delta t}\left(\frac{\beta_1 - \beta_2}{\alpha + 1}\right).\end{aligned} \tag{6}$$

2.2. *In An Absorbing Medium*

In an absorbing medium, the amplitude of the wave changes as it propagates. Assume a wave propagating backward and an attenuation factor t_j, so that the amplitude of the wave is multiplied by t_j each time the wave propagates between grid locations $j + 1/2$ and j. Assuming the transmission of a Heaviside step of amplitude H, we find, after an infinite time, that

$$t_j H = \alpha t_j H + \beta_1 H - \beta_2 H t_j t_{j-1/2} \tag{7}$$

so that

$$\alpha = 1 - \frac{\beta_1}{t_j} + \beta_2 t_{j-1/2}. \tag{8}$$

Symmetrically, for a wave propagating forward, we have

$$\alpha = 1 + \beta_1 t_{j+1/2} - \frac{\beta_2}{t_j}. \tag{9}$$

3. THE PERFECTLY MATCHED LAYER (PML) TECHNIQUE, A RELATION LINKING THE σ

Consider first the existing PML technique [1] to understand the implications of the preceding relations. In one dimension, the basic equation of the PML technique is

$$\frac{\partial E}{\partial t} = \sigma E + \frac{\partial B}{\partial x}, \tag{10}$$

which is Eq. (4) with $\sigma_E = \sigma$ and $\sigma_B = 0$. Once discretized in centered finite-difference form, this becomes

$$E_j^{i+1} = \alpha E_j^i + \beta\left(B_{j+1/2}^{i+1/2} - B_{j-1/2}^{i+1/2}\right), \tag{11}$$

with

$$\alpha = 1 + \sigma a, \quad \beta = \frac{a}{\delta x}. \tag{12}$$

If we directly discretize the differential equation, we have

$$a = \frac{\delta t}{1 - \sigma \delta t/2}, \tag{13}$$

whereas if we integrate the differential equation before discretizing it, as in the original

Berenger paper, we have

$$a = -\frac{1 - \exp(\sigma\delta t)}{\sigma}. \tag{14}$$

Assuming now a wave propagating backward, applying (8) with $\beta = \beta_1 = \beta_2$, we obtain that

$$\alpha = 1 + \beta\left(t_{j-1/2} - \frac{1}{t_j}\right), \tag{15}$$

giving

$$\sigma_j = \frac{t_{j-1/2} - \frac{1}{t_j}}{\delta x}. \tag{16}$$

This gives us a recursion relation on the σ_j which provides an additional constraint on the PML condition and a rule for the progression of the coefficients inside the PML layer. The coefficients t can be chosen independent of each other; this is not the case for the σ_j, which are linked to each other. This relation, which applies at the discretized level and ensures the consistency of the algorithm at this level, is different from the rule $\sigma(\rho) = \sigma_m(\rho/\delta)^n$ (see [1]), which gives *ab initio* the dependency of σ with respect to the distance ρ traveled in the layer at the infinitesimal level.

4. A HYBRID ALGORITHM BETWEEN PML AND ONE-WAY ABCS

4.1. *In One Dimension*

With the previous boundary condition, the limiting case $t_j = 0$ gives $\sigma \to \infty$ and $\beta = 0$, resulting in total reflection of outgoing waves.

We now force the algorithm, at the limit of complete absorption in one cell ($t_j = 0$), to converge to the one-way absorbing boundary condition (Sommerfeld ABC). For example, at the lower bound of the computational domain for waves traveling backward:

$$E_j^{i+1} = \left(1 - \frac{2\delta t}{\delta t + \delta x}\right)E_j^i + \left(\frac{2\delta t}{\delta t + \delta x}\right)B_{j+1/2}^{i+1/2}. \tag{17}$$

We construct a one-way absorbing medium in the form

$$\frac{\partial E}{\partial t} = \sigma_E E + c_E \frac{\partial B}{\partial x} + \sigma_B B, \tag{18}$$

which we discretize in centered finite-difference form with Δ^u, a finite-difference in u, and $\langle\,\rangle_u$, a finite average along u, as

$$\Delta^t E = \sigma_E \langle E\rangle_t + c_E \Delta^x B + \sigma_B \langle B\rangle_x, \tag{19}$$

which we can also write as

$$E_j^{i+1} = \alpha E_j^i + t_j \beta_1 B_{j+1/2}^{i+1/2} - \beta_2 B_{j-1/2}^{i+1/2}. \tag{20}$$

Here t_j has the same meaning as in the preceding section, and α, β_1, and β_2 are three constants to be determined and are linked to σ_E, c_E and σ_B by

$$\sigma_E = -\frac{2}{\delta t}\left(\frac{1-\alpha}{1+\alpha}\right) \tag{21}$$

$$c_E = \frac{\delta x}{\delta t}\left(\frac{t_j\beta_1+\beta_2}{1+\alpha}\right) \tag{22}$$

$$\sigma_B = \frac{2}{\delta t}\left(\frac{t_j\beta_1-\beta_2}{1+\alpha}\right). \tag{23}$$

For this equation, the analysis with the Heaviside step transmission after an infinite time (see Appendix) gives

$$\alpha = 1-\beta_1+t_{j-1/2}\beta_2. \tag{24}$$

For $t_{j-1/2}=0$ and $t_j=1$ (complete absorption in one cell), we force (20) to reduce to (17), giving $\alpha = 1-\beta_1$ and $\beta_1 = \frac{2\delta t}{\delta t+\delta x}$.

On the other hand, for $t_{j-1/2}=t_j=1$ (vacuum), we want the equation to converge to

$$E_j^{i+1} = E_j^i + \frac{\delta t}{\delta x}\left(B_{j+1/2}^{i+1/2}-B_{j-1/2}^{i+1/2}\right); \tag{25}$$

that is, $\beta_1=\beta_2=\frac{\delta t}{\delta x}$.

Noting that $\frac{2\delta t}{\delta t+\delta x} = \frac{\delta t}{\delta x}(1+\frac{\delta x-\delta t}{\delta x+\delta t})$, one solution satisfying these two limits is

$$\begin{aligned}\beta_1 &= \frac{\delta t}{\delta x}\left(1+\left(\frac{\delta x-\delta t}{\delta x+\delta t}\right)\left(1-t_{j-1/2}\right)\right)\\ \beta_2 &= \frac{\delta t}{\delta x}.\end{aligned} \tag{26}$$

In summary, and applying the same analysis for the field B, the new hybrid absorbing layer is now defined as (for waves traveling backward):

$$\begin{aligned}E_j^{i+1} &= \left(1-\beta_{1E}+t_{j-1/2}\beta_{2E}\right)E_j^i + t_j\beta_{1E}B_{j+1/2}^{i+1/2} - \beta_{2E}B_{j-1/2}^{i+1/2}\\ B_{j-1/2}^{i+1/2} &= (1-\beta_{1B}+t_{j-1}\beta_{2B})B_{j-1/2}^{i-1/2} + t_{j-1/2}\beta_{1B}E_j^i - \beta_{2B}E_{j-1}^i\\ \beta_{1E} &= \frac{\delta t}{\delta x}\left(1+\left(\frac{\delta x-\delta t}{\delta x+\delta t}\right)\left(1-t_{j-1/2}\right)\right)\\ \beta_{1B} &= \frac{\delta t}{\delta x}\left(1+\left(\frac{\delta x-\delta t}{\delta x+\delta t}\right)(1-t_{j-1})\right)\\ \beta_{2E} &= \beta_{2B} = \frac{\delta t}{\delta x}\\ 0 &\le t_j \le 1.\end{aligned} \tag{27}$$

This can, equivalently, be written

$$
\begin{aligned}
\Delta^t E &= \sigma_{EE}\langle E\rangle_t + c_E \Delta^x B + \sigma_{EB}\langle B\rangle_x \\
\Delta^t B &= \sigma_{BB}\langle B\rangle_t + c_B \Delta^x E + \sigma_{BE}\langle E\rangle_x \\
\beta_{1E} &= \frac{\delta t}{\delta x}\left(1 + \left(\frac{\delta x - \delta t}{\delta x + \delta t}\right)\left(1 - t_{j-1/2}\right)\right) \\
\beta_{1B} &= \frac{\delta t}{\delta x}\left(1 + \left(\frac{\delta x - \delta t}{\delta x + \delta t}\right)\left(1 - t_{j-1}\right)\right) \\
\beta_{2E} &= \beta_{2B} = \frac{\delta t}{\delta x} \\
0 &\le t_j \le 1,
\end{aligned}
\tag{28}
$$

with

$$
\sigma_{EE} = -\frac{2}{\delta t}\left(\frac{\beta_{1E} - t_{j-1/2}\beta_{2E}}{2 - \beta_{1E} + t_{j-1/2}\beta_{2E}}\right) \tag{29}
$$

$$
c_E = \frac{\delta x}{\delta t}\left(\frac{t_j\beta_{1E} + \beta_{2E}}{2 - \beta_{1E} + t_{j-1/2}\beta_{2E}}\right) \tag{30}
$$

$$
\sigma_{EB} = \frac{2}{\delta t}\left(\frac{t_j\beta_{1E} - \beta_{2E}}{2 - \beta_{1E} + t_{j-1/2}\beta_{2E}}\right) \tag{31}
$$

and

$$
\sigma_{BE} = -\frac{2}{\delta t}\left(\frac{\beta_{1B} - t_{j-1}\beta_{2B}}{2 - \beta_{1B} + t_{j-1}\beta_{2B}}\right) \tag{32}
$$

$$
c_B = \frac{\delta x}{\delta t}\left(\frac{t_{j-1/2}\beta_{1B} + \beta_{2B}}{2 - \beta_{1B} + t_{j-1}\beta_{2B}}\right) \tag{33}
$$

$$
\sigma_{BB} = \frac{2}{\delta t}\left(\frac{t_{j-1/2}\beta_{1B} - \beta_{2B}}{2 - \beta_{1B} + t_{j-1}\beta_{2B}}\right). \tag{34}
$$

The algorithm for waves traveling forward is obtained by symmetry.

4.2. *In Two Dimensions*

The extension of the preceding system to more than one dimension is done, as with the PML ABC, by decomposing the equations along the axes as follows:

$$
\begin{aligned}
\Delta^t E_{zx} &= \sigma_{EE}\langle E_{zx}\rangle_t + c_E \Delta^x B_y + \sigma_{EB}\langle B_y\rangle_x \\
\Delta^t E_{zy} &= -\Delta^y B_x \\
E_z &= E_{zx} + E_{zy} \\
\Delta^t B_y &= \sigma_{BB}\langle B_y\rangle_t + c_B \Delta^x E_z + \sigma_{BE}\langle E_z\rangle_x \\
\Delta^t B_x &= -\Delta^y E_z.
\end{aligned}
\tag{35}
$$

4.3. *Differences with the Berenger PML*

The first equation of (35) has the same form as (4) at the infinitesimal limit. This means that, for the time integration of E, there is an additional term in the form of $\sigma_B B$ in our hybrid ABC compared to the Berenger PML. At the discrete level, our algorithm formally is

$$E_j^{i+1} = \alpha E_j^i + \beta_1 B_{j+1/2}^{i+1/2} - \beta_2 B_{j-1/2}^{i+1/2}, \tag{36}$$

while the Berenger PML formally is

$$E_j^{i+1} = \alpha E_j^i + \beta\left(B_{j+1/2}^{i+1/2} - B_{j-1/2}^{i+1/2}\right). \tag{37}$$

For one iteration, our algorithm is computationally slightly more costly than the Berenger PML; however, it produces significantly less reflection, as shown in the next section.

5. NUMERICAL RESULTS

5.1. *Coefficients of Reflection in 1D*

Measurements of the coefficients of reflection in one dimension have been done, following the same procedure used in [4, Section 3.1.1], using the Harris function as the shape factor of a sinusoidal incident wave. The mesh spacing is defined as δx; the size of the absorbing layer is $8\delta x$.

For the PML case, we used the same progression of conductivity as in [1],

$$\sigma(\rho) = \sigma_m \left(\frac{\rho}{\Delta}\right)^n, \tag{38}$$

with $\sigma_m = 4/\delta x$, $\Delta = 5\delta x$, $n = 1, 2, 3,$ or 4, and ρ the length of penetration in the absorbing layer. In terms of mesh size, $\rho = j\delta x$ with $j = 0$ at the interface, and we define the discrete values of σ to be

$$\sigma_j = \sigma_m \left(\frac{j\delta x}{\Delta}\right)^n, \tag{39}$$

producing, at the location $j\delta x$, a coefficient of transmission t_j given by

$$t_j = e^{-\sigma_j \delta x/2}. \tag{40}$$

These coefficients of transmission were then used to compute a new set of coefficients of conductivity σ(adjusted) with the relation linking the σ defined earlier, that is,

$$\sigma_j = \frac{t_{j+1/2} - \frac{1}{t_j}}{\Delta x}, \tag{41}$$

where the reader is reminded that j has now its origin at the vacuum-absorbing layer interface and increases in the absorbing layer. These σ_j were used to run another case named "PML-σ(adjusted)" and were also used to compute the coefficients for the hybrid algorithm case. A case using the one-way Sommerfeld ABC was also run as a reference.

The results are given in Fig. 1 for all four boundary conditions (one-way, PML, PML-σ(adjusted), hybrid) for $n = 1, 2, 3,$ and 4. For all values of n, the adjustment of the σ gives better results than the PML without adjustment, and the hybrid algorithm considerably reduces the amount of reflection in comparison with the others.

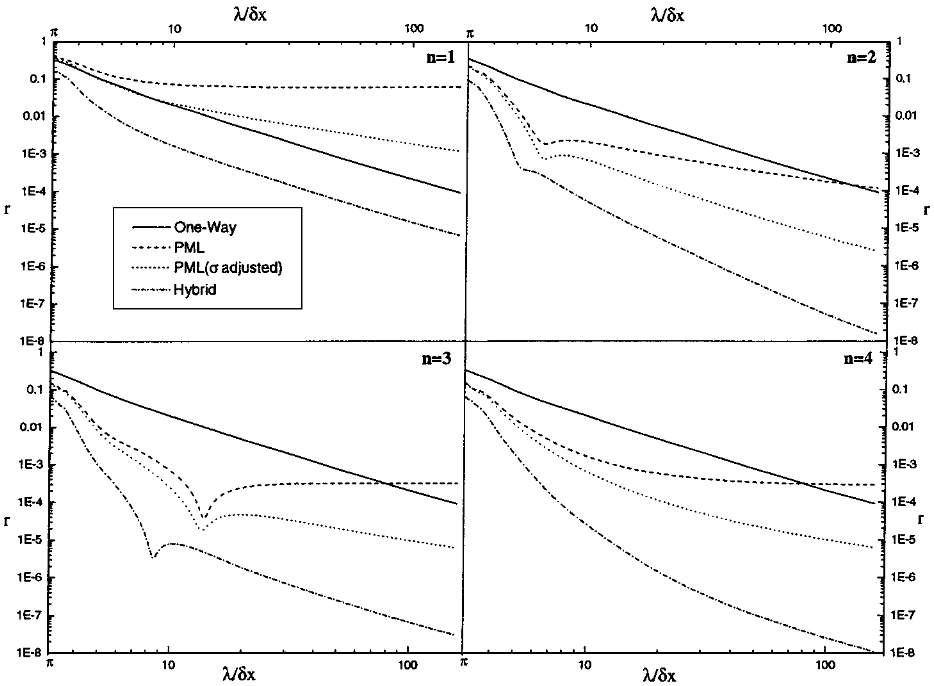

FIG. 1. Coefficient of reflection as a function of wavelength obtained for four ABCs with $n = 1, 2, 3, 4$ (n has no significance for the one-way ABC).

5.2. *Coefficients of Reflection in 2D*

We have measured the coefficient of reflection for a pulse of shape given by the Harris function

$$H(t) = \begin{cases} \frac{10 - 15\cos(2\pi Lt) + 6\cos(4\pi Lt) - \cos(6\pi Lt)}{32} & \text{when } 0 < t < L/c \\ 0 & \text{otherwise,} \end{cases} \tag{42}$$

where c, the wave speed, was normalized to 1, and where L, the support of the function, was given the value $50\delta x$. The size of the test domain was $100\delta x{*}200\delta y$ with an additional surrounding absorbing layer of thickness $8\delta x$. Here, $\delta x = \delta y = 1$. A computation on a reference grid of size $200\delta x{*}200\delta y$ was also performed. Let E_z be the field computed on the test grid and E_{zr} the field computed on the reference grid. The initial signal on both grids was introduced so that $E_z(25,100) = E_{zr}(100,100) = H(t)$. The time step δt was set to $0.5\delta x$, and the simulation was stopped at $t = 200\delta t = 100$. Then the coefficient of reflection was computed on a grid 76*201 by $R(0{:}75, 0{:}200) = E_z(0{:}75, 0{:}200) - E_{zr}(100{:}175, 0{:}200)$. The calculations were made for the PML, the PML-σ(adjusted), and the hybrid ABCs, using, in the direction transverse to the absorbing boundary, the same coefficients as those used for the 1-d numerical tests. The results at the boundary $R(0, 0{:}200)$ are given in Fig. 2 for $n = 1$, 2, 3, and 4. Except for the case $n = 1$ where the PML-σ(adjusted) gives a smaller amount of reflection than the hybrid ABC, the qualitative result found in the 1-d case, which is that the hybrid ABC gives better results than the PML(σ adjusted or not), is obtained again. 3D plots of $R(0{:}75, 0{:}200)$ are given in Fig. 3 (second-order Engquist and Majda, given for reference), Fig. 4 (PML), Fig. 5 (PML-σ(adjusted)), and Fig. 6 (hybrid), all for $n = 2$. The

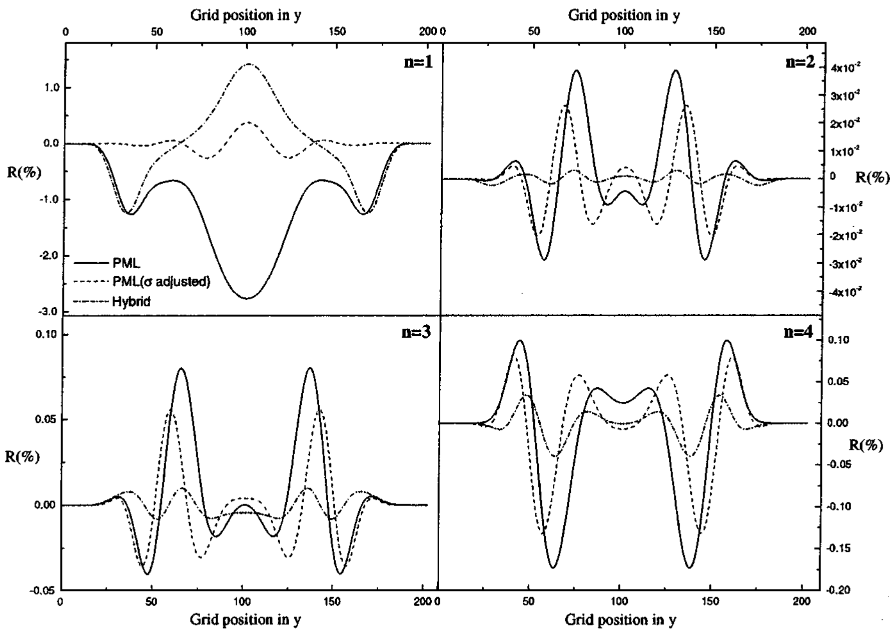

FIG. 2. Coefficients of reflection at the boundary given by the PML, PML-σ(adjusted), and hybrid ABCs.

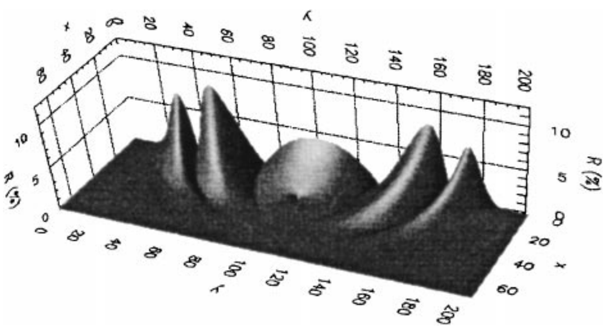

FIG. 3. Reflected signal (in % of the maximum amplitude of the incident pulse measured at the same time) given by the second-order Engquist and Majda ABC.

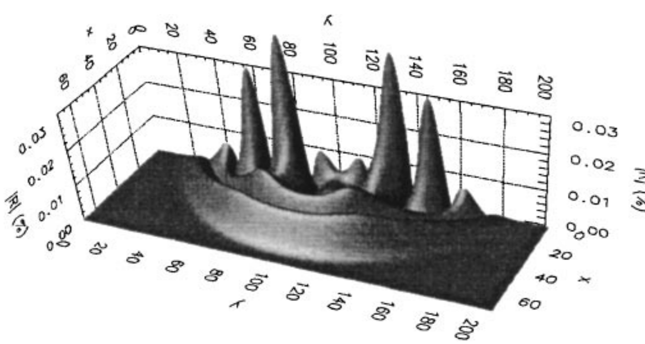

FIG. 4. Reflected signal (in % of the maximum amplitude of the incident pulse measured at the same time) given by PML ABC for an 8-cell absorbing layer with $n = 2$.

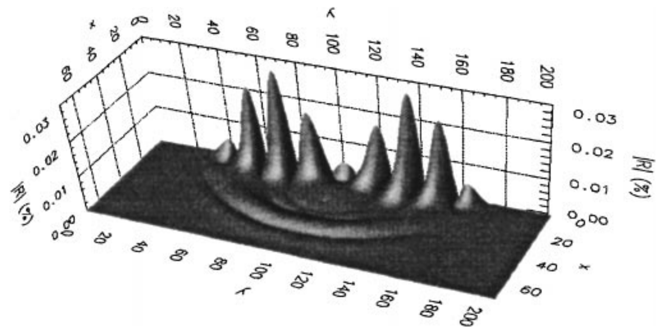

FIG. 5. Reflected signal (in % of the maximum amplitude of the incident pulse measured at the same time) given by the PML-σ(adjusted) ABC for an 8-cell absorbing layer with $n = 2$.

numerical reflection due to the PML ABC, as mentioned by previous authors [1, 6], in the form of a front propagating normally to the boundary, is easy to identify in Fig. 4, while it can be seen in Fig. 5 and Fig. 6 that it is well damped using the PML-σ(adjusted) ABC or the hybrid ABC, which gives the best results of all.

6. CONCLUSION

We have presented a new absorbing boundary condition that has the features of both one-way ABC and PML ABC. Numerical tests show that it yields better results than a PML ABC under the same conditions (same thickness of the absorbing layer and same fall-off of the incident wave amplitude in the layer). This work is still somewhat preliminary, and a full mathematical analysis giving the optimized set of absorbing parameters (t_j) in the layer is needed. Also, a possible improvement may be to take the second-order Engquist and Majda algorithm as the limit of the hybrid algorithm for absorption in one cell, instead of the first-order one, as done in this paper. This implies the addition of a coefficient ξ, in $E_z = E_{zx} + \xi E_{zy}$, to be determined. Whether such a modification will improve the algorithm and is worthwhile are open questions. This hybrid ABC has been implemented in the code EMI2D developed at Ecole Polytechnique (Palaiseau, France) by J. C. Adam, A. Héron, and the author (used for laser-plasma interaction studies).

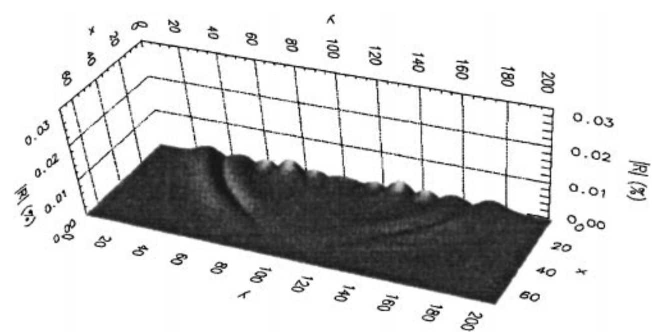

FIG. 6. Reflected signal (in % of the maximum amplitude of the incident pulse measured at the same time) given by the hybrid ABC for an 8-cell absorbing layer with $n = 2$.

APPENDIX: HEAVISIDE STEP ANALYSIS

We consider the discretized wave equation

$$E_j^{i+1} = \alpha E_j^i + \beta_1 B_{j+1/2}^{i+1/2} - \beta_2 B_{j-1/2}^{i+1/2}. \tag{A.1}$$

If we consider the propagation of a Heaviside step of amplitude H traveling forward, we do not know the details of the response of the system for any set $(\alpha, \beta_1, \beta_2)$ but we know from the properties of the wave equation that in vacuum, after an infinite time, all the values must have exactly relaxed to the value H for the magnetic field B and $-H$ for the magnetic field E (we have $E = -B$ for waves traveling forward), giving the relation (true after an infinite time)

$$-H = -\alpha H + \beta_1 H - \beta_2 H, \tag{A.2}$$

and finally

$$\alpha = 1 + \beta_1 - \beta_2. \tag{A.3}$$

The same analysis with waves traveling backward gives

$$\alpha = 1 - \beta_1 + \beta_2. \tag{A.4}$$

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