Exponential discretization of the Perfectly Matched Layer (PML) absorbing boundary condition simulation in FD-TD 3D

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Abstract: We present the discretized equations of the 12 PML (perfectly matched layer) in the three-dimensional case using the Cartesian geometry. These equations can be used in different fields where Maxwell equations need to be solved.

Key words: Absorbing-boundary conditions 3D – perfectly matched layer 3D – finite-differences time-domain 3D

1. Introduction

Solving Maxwell equations for real problems is highly complex and therefore they must be solved by numerical methods. One of these, perhaps the most powerful, is the Yee algorithm [1]. The method called the Finite-Difference Time-Domain (FD-TD) solves time-dependent Maxwell equations, based on the Yee algorithm. This method consists basically of the simulation of time evolution of real and continuous electromagnetic waves in a finite or infinite region of space [2]. In the method FD-TD, with respect to the solution of problems concerning the interaction of electronic waves, the regions are not confined, that is, the space domain has no boundaries in some directions. As it is impossible to store an infinite number of data in any computer, we need to have a finite and limited number of field values. The computational domain must be large enough to include the structure in question, but must also have an appropriate boundary condition on the outside perimeter that simulates an infinite area. These are the conditions of absorbing boundaries. For example, let us use a wave that is propagated within a fiber optics. The resolution of the Maxwell equations invariably provides solutions of movement of these symmetrical waves, or, in other words, a wave travels in the direction of illumination and the other in the opposite direction. Therefore, we need an absorbing condition to eliminate computationally the wave that is propagated in the direction opposite of the illumination.

These conditions cannot be satisfied directly from the numeric algorithm for solving Maxwell equations according to the FD-TD method because this type of system uses a scheme of centered spatial differences that requires knowing the fields at a distance of half a spatial cell on each side of the observation point. That is, the finite differences cannot be implemented at the limits of the lattice.

Berenger [3] published absorbing-boundary conditions for the FD-TD lattice in two dimensions which improved all the ones used up to that time. These were called “Perfectly Matched Layer” (PML), based on the division of the components of the electric and magnetic field in the region of the absorbing boundary with the possibility of assigning losses individually to each division of the field components. The net effect was to create a non-physical absorbing medium adjacent to the outside part of the FD-TD grid, which has a wave impedance independent of the angle of incidence and of the wavelength that spreads outwards. The effective coefficient of reflection is 1/3000 times the coefficients of the previous methods and the noise of the lattice was reduced by $10^{-7}$ times the noise produced by other methods of absorbing-boundary conditions.

Afterwards, the method was extended to three dimensions [4–7] without giving the equations in analytical form. In the present work, we give the discretized expressions of the 12 PML equations for three dimensions in Cartesian geometry. Given in this general form, they can be implemented directly into any type of computational calculus, and thus become greatly useful in all types of research in this field.

2. Method

In the three-dimensional case, the 6 Cartesian components of the field vectors are divided into two, and the resulting PML of the Maxwell equations give us 6 equations dependent on $E_{xy}$, $E_{xz}$, $E_{yx}$, $E_{yz}$, $E_{zx}$, $E_{zy}$ for the electric field and another 6 dependent on...
\( H_{xy}, H_{xz}, H_{zx}, H_{yz}, H_{zx} \) for the magnetic field. By substitution using these components in the Maxwell equations, we get the following expressions [7]:

\[
\begin{align*}
\frac{\partial E_{xy}}{\partial t} + \sigma \frac{E_{xy}}{\partial t} &= \frac{\partial (H_{yz} + H_{zx})}{\partial y}, \\
\frac{\partial E_{yz}}{\partial t} + \sigma \frac{E_{yz}}{\partial t} &= \frac{\partial (H_{xy} + H_{yx})}{\partial z}, \\
\frac{\partial E_{zx}}{\partial t} + \sigma \frac{E_{zx}}{\partial t} &= \frac{\partial (H_{xz} + H_{zy})}{\partial x}, \\
\frac{\partial E_{xy}}{\partial t} + \sigma \frac{E_{xy}}{\partial t} &= \frac{\partial (H_{yz} + H_{zx})}{\partial y}, \\
\frac{\partial E_{yz}}{\partial t} + \sigma \frac{E_{yz}}{\partial t} &= \frac{\partial (H_{xy} + H_{yx})}{\partial z}, \\
\frac{\partial E_{zx}}{\partial t} + \sigma \frac{E_{zx}}{\partial t} &= \frac{\partial (H_{xz} + H_{zy})}{\partial x},
\end{align*}
\]

(1)

(2)

(3)

(4)

(5)

(6)

(7)

(8)

(9)

(10)

(11)

(12)

where the parameters \( \sigma_x, \sigma_y, \sigma_z \) are the electric conductivity, and \( \sigma^*_x, \sigma^*_y, \sigma^*_z \) the magnetic losses; \( \varepsilon \) is the electric permittivity, and \( \mu \) the magnetic permeability.

3. Results

3.1. Exponential discretization in the PML region

The 3D PML technique is now generalized [7] but the equations are not given explicitly. The PMLs surround the zone in question on the 6 sides of the computational domain in such a way, that the wave travelling towards these sides penetrate them without reflection, as well as on the 12 edges and 6 sides. The result of the conductivities, which must be null, is shown in fig. 1 [7].

We shall discretize the 12 subcomponents of the PMLs into 3D.

The discretization of eq. (1) has been already been performed [7], but not eqs. (2–12). These have been approached by generalizing the foregoing result while considering the subcomponents of the electric and magnetic field. eqs. (13–18) were the result.

The discretization of eqs. (7–12) was performed in a similar way while taking into account that, in each equation, \( \mu \) and \( \sigma^* \) appear instead of \( \varepsilon \) and \( \sigma \). The result of the eqs. (19–24) discretized was achieved using the matching-impedance conditions \( \sigma_x = \sigma^*_x, \sigma_y = \sigma^*_y, \sigma_z = \sigma^*_z \) in the medium PML [7].

In this way, with the system of eqs. (13–24), the new value of the field subcomponent to be calculated at any point of the lattice in the PML medium depends on its previous value at this same point and on the previous values of the subcomponents of another field at adjacent points, as shown in fig. 2.

The FD-TD lattice in the PML medium is the same as in the computational domain, the difference being that now, at each point of the network, we calculate two subcomponents (fig. 2). For example, at the points where only \( E_x \) was calculated before, now \( E_{xy}, E_{xz} \) must be calculated. The resulting equations, after all
the calculations, were:

\[ E^{n+1}_{x}(i + \frac{1}{2}, j, k) = \exp\left\{ \frac{-\sigma_z(i + \frac{1}{2}, j, k)}{e(i + \frac{1}{2}, j, k) \Delta t} \right\} E^n_x(i + \frac{1}{2}, j, k) \]

\[ + \frac{1}{\sigma_z(i + \frac{1}{2}, j, k)} \Delta x \left\{ H^{n+1}_{xy}(i + \frac{1}{2}, j, k + \frac{1}{2}) + H^{n+1}_{xz}(i + \frac{1}{2}, j, k) \right\}, \]

\[ - H^{n+1}_{xy}(i + \frac{1}{2}, j, k + \frac{1}{2}) - H^{n+1}_{xz}(i + \frac{1}{2}, j, k) \] \[ E^{n+1}_{z}(i + \frac{1}{2}, j, k) = \exp\left\{ \frac{-\sigma_z(i + \frac{1}{2}, j, k)}{e(i + \frac{1}{2}, j, k) \Delta t} \right\} E^n_z(i + \frac{1}{2}, j, k) \]

\[ + \frac{1}{\sigma_z(i + \frac{1}{2}, j, k)} \Delta y \left\{ H^{n+1}_{zy}(i + \frac{1}{2}, j, k - \frac{1}{2}) + H^{n+1}_{yz}(i + \frac{1}{2}, j, k) \right\}, \]

\[ - H^{n+1}_{zy}(i + \frac{1}{2}, j, k - \frac{1}{2}) - H^{n+1}_{yz}(i + \frac{1}{2}, j, k) \]


\[ H^{n+\frac{1}{2}}_{y}(i + \frac{1}{2}, j, k + \frac{1}{2}) = \exp \left\{ -\frac{\sigma_{z}(i + \frac{1}{2}, j, k + \frac{1}{2})}{\epsilon(i + \frac{1}{2}, j, k + \frac{1}{2})} \Delta t \right\} \left\{ H^{n+\frac{1}{2}}_{y}(i + \frac{1}{2}, j, k + \frac{1}{2}) \right\}

- \exp \left\{ \frac{\sigma_{z}(i + \frac{1}{2}, j, k + \frac{1}{2})}{\epsilon(i + \frac{1}{2}, j, k + \frac{1}{2})} \Delta t \right\}

+ \frac{\mu(i + \frac{1}{2}, j, k + \frac{1}{2})}{\epsilon(i + \frac{1}{2}, j, k + \frac{1}{2})} \sigma_{z}(i + \frac{1}{2}, j, k + \frac{1}{2}) \Delta x \]

\[ E^{n+\frac{1}{2}}_{x}(i + 1, j, k + \frac{1}{2}) + E^{n+\frac{1}{2}}_{y}(i + 1, j, k + \frac{1}{2}) - E^{n+\frac{1}{2}}_{z}(i, j, k + \frac{1}{2}) \]

(22)

\[ H^{n+\frac{1}{2}}_{z}(i + \frac{1}{2}, j, k) = \exp \left\{ -\frac{\sigma_{y}(i + \frac{1}{2}, j + \frac{1}{2}, k)}{\epsilon(i + \frac{1}{2}, j + \frac{1}{2}, k)} \Delta t \right\} \left\{ H^{n+\frac{1}{2}}_{z}(i + \frac{1}{2}, j, k) \right\}

- \exp \left\{ \frac{\sigma_{y}(i + \frac{1}{2}, j + \frac{1}{2}, k)}{\epsilon(i + \frac{1}{2}, j + \frac{1}{2}, k)} \Delta t \right\}

+ \frac{\mu(i + \frac{1}{2}, j + \frac{1}{2}, k)}{\epsilon(i + \frac{1}{2}, j + \frac{1}{2}, k)} \sigma_{y}(i + \frac{1}{2}, j + \frac{1}{2}, k) \Delta y \]

\[ E^{n+\frac{1}{2}}_{x}(i + \frac{1}{2}, j + 1, k) + E^{n+\frac{1}{2}}_{y}(i + \frac{1}{2}, j + 1, k) - E^{n+\frac{1}{2}}_{z}(i + 1, j, k) \]

(23)

where the parameters were defined previously.

When we apply to a real practical situation, these equations can be simplified if certain conditions are met. These restrictions need not be absolutely restrictive, however. Clearly, each case must be evaluated individually, but, in general, the transverse conductivities are equal, and thus we can reduce the 12 foregoing equations to 10 on the sides, as stated above.

The foregoing eqs. (13–24) can be given in terms of two equations, one for the PML subcomponents of the electric field and the other for the magnetic field. The other equations are formulated by cyclic permutations of \(x, y, z\) and \(i, j, k\).

In eq. (13), since the subscript of \(E_{xy}\) are \(x, y, \) the \(H\) component that splits is \(H_{z}\) and does in according to the subscript of \(E_{xy}\); that is, \(H_{z}\) splits in \(H_{zx}\) and \(H_{zy}\). These subcomponents of \(H_{z}\) are spatially evaluated in the direction marked by the second subscript of \(E_{xy}\), this being \(j \pm 1/2\) (fig. 2).

With the second subscript of \(E_{xy}\), \(\sigma\) is noted and evaluated together with \(\epsilon\), in the same position as \(E_{xy}\). Besides, the spatial increase corresponds to the one marked by the second subscript of \(E_{xy}\), that is, \(\Delta y\).

It suffices to take these considerations into account in order to formulate any PML equation of the electric field from eq. (13). For the PML subcomponents of the magnetic field, it would suffice to give the example of eq. (19) and gain the remains in a way analogous to that discussed in \(E_{xy}\).

3.2. FDTD method stability

To test the validity of eqs. (13–24), we calculate the intensity profile at the end of the side of the three planar dielectric waveguides [8] by the FD-TD method using the PML as absorbing conditions. The numeric algorithm of finite differences described above requires the temporal increase \(\Delta t\) to have a specific value with respect to the spatial increase in the Yee lattice \(\Delta x, \Delta y\) and \(\Delta z\). This value is necessary to avoid numerical instability and to ensure that, on resolving the equations, the result does not increase limitlessly with time.

For simplicity, we consider the case of the propagation in one dimension in the direction \(x\). The Maxwell equations in the free space take the form:

\[ \frac{\epsilon_{0} \partial E_{x}}{\partial t} = -\frac{\partial H_{z}}{\partial x} \] (25)

\[ \mu_{0} \frac{\partial H_{z}}{\partial t} = -\frac{\partial E_{x}}{\partial x} \] (26)

derivating eq. (25) respect to \(t\) and taking into account the eq. (26) we can obtain the expression of the one-dimensional wave equation:

\[ \frac{1}{c^{2}} \frac{\partial^{2} E_{x}}{\partial t^{2}} = \frac{\partial^{2} E_{x}}{\partial x^{2}} \]

where \(c = 1/\sqrt{\mu_{0}/\epsilon_{0}}\), is the speed of light in the free space. We develop this expression in finite-differences time-domain:

\[ E^{n+1}(i) = E^{n}(i) - \frac{\epsilon \Delta t^{2}}{2} \frac{E^{n+1}(i) - E^{n-1}(i)}{\Delta x^{2}} \] (27)

This is the centered second-order equation in finite differences. The stability analysis begins by searching for solutions to the differential equation, which we propose to show in this form:

\[ E^{n}(i) = \xi^{n} e^{-ikx_{i+1} \Delta x} \] (29)

where \(j = \sqrt{-1}\) and \(k = 2\pi/\lambda\) is the wavenumber. With this solution, several results are possible, that it increase, diminish or fluctuate in time, depending on the value of \(\xi\). Replacing (29) in differential equation (28),
and eliminating common factors, we get:
\[ \xi^2 - 2A\xi + 1 = 0, \]  
where
\[ A = 1 - 2 \left( \frac{c\Delta t}{\Delta x} \right)^2 \sin^2 \frac{k\Delta x}{2} \]  
we make the replacement in eq. (30) and solve the equation, the result being:
\[ \xi = A \pm (A^2 - 1)^{1/2}. \]  
A growing solution (i.e., unstable) will occur if \(|\xi| > 1\). This happens only if \(|A| > 1\) giving \(c\Delta t > \Delta x\) ⇒ instability. Alternatively, when \(|A| \leq 1\), then \(c\Delta t \leq \Delta x\) and
\[ |\xi| = |A + i(1 - A^2)^{1/2}| = 1. \]  
This implies a solution that fluctuates in time, as was desired. Therefore, the criterion of stability in one dimension takes the form \(c\Delta t \leq \Delta x\).

We extend the above equation to the three-dimensional case, the criterion for the TM mode becoming:
\[ \Delta t \leq \frac{1}{c \sqrt{\frac{1}{(\Delta x)^2} + \frac{1}{(\Delta y)^2} + \frac{1}{(\Delta z)^2}}}. \]  
To develop the program, we chose equality, but placing in \(c\) the speed of light within a vacuum, which is always somewhat greater than its speed inside a fiber optics.

For the case of a cubic lattice in which \(\Delta x = \Delta y = \Delta z\), the stability criterion takes a simpler form:
\[ \Delta t \leq \frac{\Delta x}{c \sqrt{3}}. \]  
However, the stability problem can be more complex than expressed above, leading us to the problem of generalized stability.

Up to now, we have discussed the numerical stability of the basic Yee algorithm in Cartesian coordinates. Nevertheless, the stability of the entire FD-TD method of solving Maxwell equations depends not only on the stability of this algorithm. In fact, the problem of generalized stability is due to the interaction between the Yee algorithm and other algorithms used in resolving the complete problem, e.g., the boundary conditions.

The numerical provision of the boundary conditions for electromagnetic waves can be complex for simulating the structures desired. One major example appears when we implement absorbing-boundary conditions surrounding the Yee lattice, used so that they absorb the electromagnetic wave that travels outwards, without bouncing off the boundary, and to be able to simulate the extension to infinity in a region. These boundary conditions are studied below, examining the problem of stability.

3.3. Illumination

We have simulated a continuous sinusoidal wave. This illumination is achieved simply by varying the electric field in a sinusoidal manner at all the points of one line (in two dimensions) or of a surface (three dimensions), in which we wish to illuminate the fiber optics. In the case of our program, we illuminate in the following way:
\[ E_n^i(i, j_0) = E_n^0(i, j_0) + E_0 \sin \left(2\pi fn_0 \Delta t \right). \]  
As shown in fig. 3, we must solve the problem of the wave transmitting towards \(i\) positive (towards the inside of the guide) as well as negative (towards the back). This is solved by placing behind the illumination an absorbing PML zone (which we shall explain below) which absorbs light as though it travels towards infinity in which there is no reflection.
3.4. Perfectly matched layer boundary conditions

Many geometries of interest are defined in “open regions” where the spatial field domain has no boundary in one direction or more, but no computer can store an unlimited number of data, and therefore the field domain must be limited in size.

This is primarily because the systems use a scheme of centered spatial differences that require the knowledge of the fields at a distance of half a spatial cell to each side of the observation point. The centered differences cannot be implemented at the edges of the network.

We have used the absorbing-PML boundary with a local reflection coefficient on the order of $10^{-4}$. With this, we achieve FD-TD simulations with a dynamic width in the range of some 70dB.

The net effect is to create a non-physical absorbing medium adjacent to the exterior part of the FD-TD lattice that has wave impedance independent of the incidence angle and frequency of the wave that spreads outwards. The effective reflection coefficient is $1/3000$ times the coefficients of other methods and the noise of the network is reduced $10^{-7}$ times.

Figure 4 presents 4 graphs showing the advance of a monochromatic electromagnetic wave of 1550 nm. At the end of the network, between nodes 592 and 600, there is a modeled PML region. The graphs are based on intervals of $10^{-16}$ s. In the last three, the wave has already reached the boundary and, as is clearly shown, there is no reflection in the boundary of the PML zone.

Figure 5 reveals how the affected PML zone affects the propagation of an electromagnetic wave. At node 592 of the Yee lattice the PML begins, from the principle wave it strongly attenuates and there is no reflection backwards in the boundary. Practical application indicates that, in our case, with a thickness of 8 cells of the PML region, the wave completely disappears.

4. Conclusions

In this work, we present the PML of the FD-TD method in 3D, explicitly in Cartesian geometry. These discretized equations are highly useful and can be implemented in all 3-dimensional problems where Maxwell equations need to be solved. Here, we have applied the PML equations given at the beginning of the paper, and the results have been successful, corroborat-
ing that these equations work well. The fields of application are extremely disparate, as in the case of studying the propagation of electromagnetic waves in fiber optics (propagation, curvatures and microcurvatures), propagation of solitons, optical amplifiers, antennae, target detection, bioengineering (hyperthermia, vision).

References