An effective CFS-PML implementation for 2-D WLP-FDTD method

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Abstract: A stretched-coordinate (SC) based complex-frequency-shifted perfectly matched layer (CFS-PML) is presented for the two-dimensional Weighted-Laguerre-polynomials (WLP) finite-difference time-domain (FDTD) method. The proposed CFS-PML is background medium independent, and can be easily extended to dispersive medium. Numerical examples show the effectiveness of the proposed CFS-PML in truncating both air and dispersive medium.

Keywords: complex-frequency-shifted (CFS), perfectly matched layer (PML), Weighted-Laguerre-polynomials (WLP), finite-difference time-domain (FDTD)

Classification: Electromagnetic theory

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1 Introduction

The conventional finite-difference time-domain (FDTD) method is an explicit time-domain technique, its application is constrained by the Courant-Friedrich-Levy (CFL) stability condition especially for the simulation of structures with fine geometries [1]. To overcome this limitation, unconditionally stable schemes have been proposed, such as the alternating-direction-implicit (ADI) FDTD method [2], the Weighted-Laguerre-polynomials (WLP) FDTD method [3], and so on. Among them, the WLP-FDTD method not only removes the CFL stability condition restriction, but also avoids the increasing numerical dispersion error as the time step increasing [4].

The perfectly matched layer (PML) introduced by Berenger [5] has been widely used and proven to be the most efficient technique for the termination of FDTD lattices [6, 7, 8]. However, the traditional split-field PML has been found to be inefficient in absorbing low frequency and evanescent waves [9, 10]. A complex-frequency-shifted (CFS) factor added to the stretched-coordinate (SC) PML helps to improve this case [10, 11]. In recent years, the CFS-PML was implemented in the WLP-FDTD method by using an auxiliary differential equation (ADE) technique [12]. Later, it was extended to periodic structures [13]. More recently, a novel nearly PML implementation for WLP-FDTD is proposed in [14] for general dispersive material.

In this paper, we implement an unsplit-field and stretched-coordinate-based CFS-PML for the 2D WLP-FDTD method. The proposed CFS-PML avoids field splitting and is more convenient to be extended to dispersive media. Numerical results are presented for both air and dispersive plasma to validate the effectiveness of the proposed PML.

2 Formulation in air

Using the stretched coordinate CFS-PML, the 2D TEz formulation of the time-domain Maxwell’s equations with simple and lossless media can be written as:

\[
\frac{\varepsilon_0}{\mu_0} \frac{\partial E_z}{\partial t} = \frac{1}{s_y} \frac{\partial H_z}{\partial y},
\]

(1)
functions, i.e., can be expanded into the polynomial domain with a series of Weighted-Laguerre basis functions, \( s = \frac{1}{\alpha} \frac{\partial E_x}{\partial x} \), \( \mu_0 \frac{\partial H_z}{\partial t} = \frac{1}{s_y} \frac{\partial E_x}{\partial y} - \frac{1}{s_x} \frac{\partial E_y}{\partial x} \). \( \text{(3)} \)

where \( s = \kappa + \sigma/\alpha \).

We introduce the following auxiliary variables:

\[
\begin{align*}
\tilde{H}_{zy} &= \frac{1}{s_y} \frac{\partial H_z}{\partial y} , \quad \tilde{H}_{zx} = \frac{1}{s_x} \frac{\partial H_z}{\partial x} , \quad \tilde{E}_{xy} = \frac{1}{s_y} \frac{\partial E_x}{\partial y} , \quad \tilde{E}_{yx} = \frac{1}{s_x} \frac{\partial E_y}{\partial x}.
\end{align*}
\]

These variables can be written into time domain by replacing \( j/\omega \) in \( \text{(4)} \) with a differential operator \( \partial / \partial t \)

\[
\left( \kappa \alpha + \sigma \right) \tilde{F}_c^q + \kappa \varepsilon_0 \frac{\partial \tilde{F}_c^q}{\partial t} = \alpha \frac{\partial F_q}{\partial t} + \varepsilon_0 \frac{\partial }{\partial t} \left( \frac{\partial F_q}{\partial t} \right) \left( F_q = E_x, E_y, H_z, \right) \ (\eta = y, x).
\]

Following the approach in \[3\], the field components and their time differentials can be expanded into the polynomial domain with a series of Weighted-Laguerre basis functions, i.e.,

\[
\begin{align*}
U(r, t) &= \sum_{p=0}^{\infty} U^p(r) \varphi_p(r) \\
\frac{\partial U(r, t)}{\partial t} &= s \sum_{p=0}^{\infty} \left( 0.5 U^p(r) + \sum_{k=0, p>0}^{p-1} U^k(r) \right) \varphi_p(r),
\end{align*}
\]

where \( U \) stands for \( E_x, E_y, H_z \). \( \varphi_p(r) = e^{-r/2} L_p(r) \) is an entire domain temporal basis function, \( t = s \), \( t \) is the scaled time with a scaling factor \( s > 0 \), and \( L_p(r) \) is the \( p \)-th Laguerre polynomial. Substituting \( \text{(7)} \) into \( \text{(6)} \), and introducing a temporal Galerkin’s testing procedure \[3\], we have

\[
\tilde{F}_c^q = \left( \alpha + 0.5 \varepsilon_0 \right) C_{1q} \frac{\partial F_q}{\partial t} + \varepsilon_0 s C_{1q} h^{-1} (F_c^q),
\]

where

\[
\begin{align*}
C_{1q} &= \frac{1}{\left( \kappa \alpha + \sigma + 0.5 \varepsilon_0 \right)}.
\end{align*}
\]

\( q \) is the WLP order. \( \text{(8)} \) can be solved numerically by employing Yee’s central differencing scheme. More specifically, the detailed field coefficients in the discretized space are expressed as follows:

\[
\begin{align*}
E_x^q|_{i+,j} &= -2 \sum_{k=0}^{q-1} E_x^k|_{i+,j} + 2 C_{1q} \left( h^{-1} (H_c)|_{i+,j} + 2 \right) \\
&= \frac{C_{2q} C_{1q}}{\Delta y} \left( H_c^q|_{i+,j} - H_c^q|_{i+,j-\frac{1}{2}} \right) + 2 C_{1q} \left( h^{-1} (H_c)|_{i+,j} + 2 \right)
\end{align*}
\]

\( \text{(11)} \)
\[ E_{y}^{q} |_{i,j+\frac{1}{2}} = -2 \sum_{k=0,q>0}^{q-1} E_{y}^{k} |_{i,j+\frac{1}{2}} - 2C_{1x} |_{j+\frac{1}{2}} - 2C_{1x} |_{i+\frac{1}{2}} \]

\[
\frac{C_{2x} C_{1x}}{\Delta x} \left( H_{x}^{q} |_{i+1/2,j+1} - H_{x}^{q} |_{i-1/2,j+1} \right),
\]

\[
\frac{C_{3} C_{2x} C_{1y}}{\Delta y} \left( E_{y}^{q} |_{i+\frac{1}{2},j+1} - E_{y}^{q} |_{i+\frac{1}{2},j} \right),
\]

\[
- 2C_{3} C_{1x} |_{j+\frac{1}{2}} + \frac{C_{3} C_{2x} C_{1x}}{\Delta x} \left( H_{x}^{q} |_{i+\frac{1}{2},j+1} - H_{x}^{q} |_{i+\frac{1}{2},j} \right)
\]

where

\[
C_{2q} = \left( \frac{2a_{q}}{\varepsilon_{0} \sigma} + 1 \right), \quad C_{3} = \varepsilon_{0}/\mu_{0}.
\]

Inserting (11) and (12) into (13), we get

\[
\left( 1 + C_{3} \frac{C_{2x} C_{1y}}{\Delta y} \left( j+\frac{1}{2} \right) + C_{3} \frac{C_{2x} C_{1y}}{\Delta y} \left| j+\frac{1}{2} \right| \right) \left( \frac{C_{3} C_{2x} C_{1x}}{\Delta x} \left| j+\frac{1}{2} \right| \right) H_{x}^{q} |_{i+\frac{1}{2},j+\frac{1}{2}}
\]

\[
+ C_{3} \frac{C_{2x} C_{1x}}{\Delta x} \left( i+\frac{1}{2} \right) \left( C_{3} \frac{C_{2x} C_{1y}}{\Delta y} \left| j+\frac{1}{2} \right| \right) - C_{3} \frac{C_{2x} C_{1y}}{\Delta y} \left| j+\frac{1}{2} \right| \right) H_{x}^{q} |_{i+\frac{1}{2},j+\frac{1}{2}}
\]

\[
- C_{3} \frac{C_{2x} C_{1x}}{\Delta x} \left( i+\frac{1}{2} \right) \left( C_{3} \frac{C_{2x} C_{1x}}{\Delta x} \left| i+\frac{1}{2} \right| \right) - C_{3} \frac{C_{2x} C_{1x}}{\Delta x} \left| i+\frac{1}{2} \right| \right) H_{x}^{q} |_{i+\frac{1}{2},j+\frac{1}{2}}
\]

\[
= -2 \sum_{k=0,q>0}^{q-1} H_{x}^{q} |_{i+\frac{1}{2},j+\frac{1}{2}} + 2C_{3} C_{1x} |_{j+\frac{1}{2}} H_{x}^{q-1} (E_{y} |_{i+\frac{1}{2},j+\frac{1}{2}})
\]

\[
- 2C_{3} C_{1x} |_{j+\frac{1}{2}} H_{x}^{q-1} (E_{y} |_{i+\frac{1}{2},j+\frac{1}{2}})
\]

\[
- 2C_{3} \frac{C_{2x} C_{1y}}{\Delta y} \left| j+\frac{1}{2} \right| \left( \sum_{k=0,q>0}^{q-1} E_{x}^{q} |_{i+\frac{1}{2},j+1} - \sum_{k=0,q>0}^{q-1} E_{x}^{q} |_{i+1/2,j} \right)
\]

\[
+ 2C_{3} \frac{C_{2x} C_{1x}}{\Delta x} \left| i+\frac{1}{2} \right| \left( \sum_{k=0,q>0}^{q-1} E_{x}^{q} |_{i+1/2,j+2} - \sum_{k=0,q>0}^{q-1} E_{x}^{q} |_{i,j+1/2} \right)
\]

\[
+ 2C_{3} \frac{C_{2x} C_{1y}}{\Delta y} \left| j+\frac{1}{2} \right| \left( C_{1y} |_{j+1} H_{x}^{q-1} (H_{x} |_{j+1/2,j+1}) - C_{1y} |_{j+1} H_{x}^{q-1} (H_{x} |_{j+1/2,j+1}) \right)
\]

\[
+ 2C_{3} \frac{C_{2x} C_{1x}}{\Delta x} \left| i+\frac{1}{2} \right| \left( C_{1x} |_{i+1} H_{x}^{q-1} (H_{x} |_{i+1/2,j+1}) - C_{1x} |_{i+1} H_{x}^{q-1} (H_{x} |_{i+1/2,j+1}) \right)
\]

The right side of (15) consists of lower order fields and auxiliary variables in Laguerre polynomial domain. Therefore all the field coefficients can be solved by using a back-substitution routine. Afterwards, the time-domain fields can be reconstructed using (7). The proposed PML is theoretically equivalent to the split-field PML in [12, 13], the number of additional variables are the same. The
advantage of the unsplit formulation lies in its ease extension to a general dispersive material, which is discussed in detail in the next section.

3 Formulation in plasma

In this section, we extend the CFS-PML into frequency-dependent dispersive medium. For the sake of simplicity, we take plasma as an example. It is worth mentioning that the extension to general dispersive material could be done by introducing some auxiliary variables following [15].

The constitutive relation of plasma is given by

\[
D(\omega) = \varepsilon_0 \left( 1 - \frac{\omega_p^2}{\omega^2 - j\omega \sigma} \right) E(\omega),
\]

where \(\omega_p\) is the plasma frequency, \(\nu\) is the collision frequency. Assuming

\[
\psi(\omega) = \frac{\omega_p^2}{\omega^2 - j\omega \sigma} E(\omega),
\]

and replacing \(j\omega\) with a differential operator \(\partial / \partial t\) [15], (16) and (17) can be written as:

\[
D(r, t) = \varepsilon_0 (E(r, t) - \psi(r, t))
\]

\[
-\frac{\partial^2}{\partial t^2} \psi(r, t) - \nu \frac{\partial}{\partial t} \psi(r, t) = \omega_p^2 E(r, t).
\]

Now following the coordinate stretching scheme, and repeating the same process as in section 2, inside plasma, (11) and (12) become

\[
E_x^q|_{i+1/2,j} = -2 \sum_{k=0,q>0}^{q-1} E_x^{k+1/2,j} + 2 C_1 x_jH^{q-1}(H_x|i+1/2,j)
\]

\[
+ \left( \psi_x^{k+1/2,j} + 2 \sum_{k=0,q>0}^{q-1} \psi_x^{k,j+1/2,j} \right) + \frac{C_2 x_j}{\Delta y} \left| H_z^p |_{i+1/2,j+1/2} - H_z^p |_{i+1/2,j-1/2} \right|
\]

\[
E_y^q|_{i,j+1/2} = -2 \sum_{k=0,q>0}^{q-1} E_y^{k+1/2,j+1/2} - 2 C_1 x_jH^{q-1}(H_z|i,j+1/2)
\]

\[
+ \left( \psi_y^{k+1/2,j+1/2} + 2 \sum_{k=0,q>0}^{q-1} \psi_y^{k,j+1/2,j} \right) - \frac{C_2 x_j}{\Delta x} \left| H_z^p |_{i+1/2,j+1/2} - H_z^p |_{i-1/2,j+1/2} \right|
\]

Noting the second derivative relation ship

\[
\frac{\partial^2 U(r, t)}{\partial t^2} = s^2 \sum_{p=0}^{\infty} \left( 0.25U^p(r) + \sum_{k=0, p>0}^{p-1} (p-k)U^k(r) \right) \varphi_p(t),
\]

the update equation of \(\psi\) in Laguerre polynomial domain can be derived from (19) as:

\[
\psi^q(r) = -\omega_p^2 E^q(r) - s^2 \sum_{k=0,q>0}^{q-1} (q-k)\psi^k(r) - \nu s \sum_{k=0,q>0}^{q-1} \psi^k(r)
\]

\[
\frac{0.25s^2 + 0.5\nu s}{0.25s^2 + 0.5\nu s}.
\]
Substituting (20) and (21) into (13), we can get the update equation of the polynomial coefficients.

4 Numerical study

In this section, numerical examples are shown to validate the accuracy and efficiency of the proposed CFS-PML for the WLP-FDTD method. First, we consider air as the background material. The computational domain is divided into 32 × 32 lattices along the $x$ and $y$ direction, respectively. The grid size is defined as $dx = dy = 0.15$ mm, $\Delta t = 0.25$ ps. A magnetic current source in shape of differential Gaussian pulse given by

$$I_{me}(t) = (t - t_0)/\tau \times \exp(-(t - t_0)^2/\tau^2)$$

(24)

is excited at $Hz$ in the center of the simulation domain with $t_0 = 10$ ps, $\tau = 3$ ps. Five PML layers are patched to each of the four boundaries, as shown in Fig. 1. The PML parameters are scaled following [10]:

$$\sigma_\zeta = \sigma_{\zeta_{\text{max}}} |\zeta - \zeta_0|^m/d^m,$$

(25)

$$\sigma_{\text{opt}} = (m + 1)/150\pi \Delta \zeta,$$

(26)

$$\kappa_\zeta = 1 + (\kappa_{\zeta_{\text{max}}} - 1)|\zeta - \zeta_0|^m/d^m,$$

(27)

where $\zeta = x, y, \zeta_0$ represents the interface between FDTD and PML grids. $d$ is the thickness of the PML. $m = 4$ is a constant number. In the first example, the parameter for SC-PML without CFS are $\kappa_{\text{max}} = 1, \sigma_{\text{max}} = 1 \times \sigma_{\text{opt}}, \alpha = 0$, denoted by $(1,1,0)$. With the same denotation, parameters $(1,1,0.27)$ are used for SC-PML with CFS. The observation point is located at the corner grid (25,25). The order of Laguerre polynomial is 300, and $s = 4 \times 10^{11}$.

Fig. 2 shows the magnetic field at the observation point as compared to the conventional FDTD method. As we can see, the two results agree with each other very well.

The relative reflection error was computed as:
where $H^\text{Ref}_z(t)$ is the reference solution based on an extended model where no reflection can be captured within the observation period of time. Fig. 3 shows the relative reflection error at the observation point for the proposed CFS-PML compared to that of the SC-PML without CFS. It is seen that the CFS-PML achieves a better absorption performance at late time.

Next, we take plasma ($\omega_p = 1.803 \times 10^{11} \text{rad/s}$, $v = 2 \times 10^{10} \text{rad/s}$) as background material and repeat the same simulation model. The PML parameters $(1, 1.15, 0.3)$ and $(1, 1, 0)$ are used for SC-PML with CFS, SC-PML without CFS respectively. Fig. 4 shows the relative reflection error at $(25, 25)$. Again, the CFS-PML is compared to the SC-PML without CFS. Similar result is found for plasma.

As the third example, we validate the correctness of the WLP-FDTD method in dispersive media via computing the reflection coefficient of a plasma slab. The

![Fig. 2. Transient magnetic field at the observation point.](image1)

![Fig. 3. Relative reflection error at (25, 25) for air.](image2)
The simulation model is shown in Fig. 5. The computational domain is discretized into $100 \times 50$ cells, with a cell size of $\Delta x = \Delta y = 150 \mu m$. The plasma occupies grids $(69-99)$ in $x$ direction, with $\omega_p = 1.803 \times 10^{11} \text{rad/s}$, $v = 2 \times 10^{10} \text{rad/s}$.

The excitation source located at grid $(x = 50)$ is a differential Gaussian pulse given by (24) with $t_0 = 0.05 \text{ns}$, $\tau = 0.01 \text{ns}$. The order of WLP is 500, and $s = 2 \times 10^{11}$. The WLP-FDTD takes a time step of $\Delta t = 1 \text{ps}$. The simulation runs
for 1 ns, and the time domain signal is transferred to frequency domain afterwards to calculate the reflection coefficient of the plasma slab. The WLP-FDTD result is compared to the analytic solution [16] in Fig. 6 for both magnitude and phase of the reflection coefficient. Very good agreements verify the correctness of the WLP-FDTD algorithm.

5 Conclusion

In this paper, we presented a stretched coordinate CFS-PML absorbing boundary condition for the WLP-FDTD method. The formulation was given for both air and plasma as background media. Numerical results indicate that the proposed CFS-PML performs better than the traditional PML.

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