Numerical Method for Wave Propagation Problem by FDTD Method with PML

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1 Introduction

It is necessary to set a computational domain appropriately for the numerical simulation of wave propagation phenomena in unbounded region. There are several approaches for this problem. In 1994, J.-P. Bérenger introduced the technique of Perfectly Matched Layer (PML). It is said that PML technique gives the best performance for Finite Difference Time Domain (FDTD) method in unbounded region. Some researchers expanded this idea into the linearized Euler equation and acoustic wave equation. In this paper, we consider some mathematical and numerical problem of PML technique, and propose a new discretization scheme that is better than the original scheme.

2 PML Method

2.1 Formulation of PML

The Maxwell equation is written as:

$$\frac{\partial \mathbf{E}}{\partial t} = -\frac{\sigma}{\epsilon} \mathbf{E} + \frac{1}{\epsilon} \nabla \times \mathbf{H}, \qquad \frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \mathbf{E}. \tag{1}$$

where, **E** is electric field, **H** is magnetic field, and ϵ , μ and σ are permittivity, magnetic permeability and electrical conductivity, respectively.

To treat the problem in unbounded region, we introduce PML technique which surrounds interior region by an absorption medium introduced in [1]. In the PML region, the electromagnetic wave propagates without reflection and decreases amplitude exponentially, and there is no reflection on the boundary between the interior and PML regions. The solution in interior region is not polluted. This behavior is realized by introducing dissipation term into the Maxwell equation (1), and imposing the impedance matching condition $\sigma/\epsilon_0 = \sigma^*/\mu_0$:

$$\frac{\partial \mathbf{E}}{\partial t} = -\frac{\sigma}{\epsilon_0} \mathbf{E} + \frac{1}{\epsilon_0} \nabla \times \mathbf{H}, \qquad \frac{\partial \mathbf{H}}{\partial t} = -\frac{\sigma^*}{\mu_0} \mathbf{H} - \frac{1}{\mu_0} \nabla \times \mathbf{E}, \tag{2}$$

where, σ^* is magnetic conductivity.

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2.2 Exact Solution in PML Region

In this section, we investigate some properties of PML technique. First, we consider one dimensional continuous problem. In case that the solutions of (2) depend only on t and x, the equation is rewritten as:

$$\epsilon_0 \frac{\partial E_y}{\partial t} + \sigma E_y = -\frac{\partial H_z}{\partial x}, \qquad \mu_0 \frac{\partial H_z}{\partial t} + \sigma^* H_z = -\frac{\partial E_y}{\partial x}.$$
(3)

We take a unit such that $\epsilon_0 = \mu_0 = 1$, then the impedance matching condition becomes $\sigma = \sigma^*$. Also, we put $E_y = u$ and $H_z = v$, then (3) becomes the wave equation for u and v:

$$\frac{\partial u}{\partial t} + \sigma u = -\frac{\partial v}{\partial x}, \qquad \frac{\partial v}{\partial t} + \sigma v = -\frac{\partial u}{\partial x}.$$
(4)

The exact solutions of (4) with initial values u(0, x) and v(0, x) at t = 0 are given as:

$$u(t,x) = \frac{1}{2} \left(e^{-\int_0^x \sigma(s)ds} f(x-t) + e^{\int_0^x \sigma(s)ds} g(x+t) \right),$$

$$v(t,x) = \frac{1}{2} \left(e^{-\int_0^x \sigma(s)ds} f(x-t) - e^{\int_0^x \sigma(s)ds} g(x+t) \right),$$

where,

$$f(x) = e^{\int_0^x \sigma(s)ds} (u(0,x) + v(0,x)),$$

$$g(x) = e^{-\int_0^x \sigma(s)ds} (u(0,x) - v(0,x)).$$

3 FDTD Method and PML

3.1 Discretization of Dissipation Term in FDTD Method

In 1966, K.S. Yee [2] introduced FDTD method to treat electromagnetic wave problem. In this section, we consider a discretization scheme for (4). We set $\Delta t = \Delta x \equiv \tau$ and $\sigma_s \equiv \sigma(s\Delta x)$, s = m or m + 1/2, and make use of the approximation:

$$\sigma(s\Delta x)u(s\Delta x) \approx \sigma_s \frac{1}{2}(u_{s+\frac{1}{2}}^n + u_{s-\frac{1}{2}}^n).$$

Then, the difference approximation of (4) becomes

$$u_m^{n+1} = a_m u_m^n - b_m (v_{m+\frac{1}{2}}^{n+\frac{1}{2}} - v_{m-\frac{1}{2}}^{n+\frac{1}{2}}),$$
(5)

$$v_{m+\frac{1}{2}}^{n+\frac{1}{2}} = a_{m+\frac{1}{2}}u_{m+\frac{1}{2}}^{n-\frac{1}{2}} - b_{m+\frac{1}{2}}(v_{m+1}^n - v_m^n),$$
(6)

with

$$a_s = \frac{1 - \frac{\tau}{2}\sigma_s}{1 + \frac{\tau}{2}\sigma_s}, \ b_s = \frac{1}{1 + \frac{\tau}{2}\sigma_s}, \ s = m \text{ or } m + \frac{1}{2}.$$
 (7)

We call (5) - (7) a plain scheme.

3.2 Artificial Reflection Caused by Discretization

In this section, we consider the artificial reflection caused by discretization. We set $\sigma = 0$ in $x \le 0$ and $\sigma > 0$ in x > 0. Then the solution given as:

$$\{u_m^n, v_{m-\frac{1}{2}}^{n-\frac{1}{2}}\}, \ u_m^n = \delta_{0,n-m}, \ v_{m-\frac{1}{2}}^{n-\frac{1}{2}} = \delta_{0,n-m}$$

which propagates towards the positive direction of x. When t = 0 (n = 0), the solution is one at x = 0 which is boundary between interior and PML regions and zero elsewhere. When n=1/2, we have from (6):

$$v_{m+\frac{1}{2}}^{\frac{1}{2}} = \begin{cases} b_{1/2} : m = 0, \\ 0 : \text{otherwise}. \end{cases}$$

When n = 1, we have from (5):

$$u_m^1 = \begin{cases} a_0 - b_0 b_{1/2} : m = 0, \\ b_1 b_{1/2} : m = 1, \\ 0 : \text{otherwise.} \end{cases}$$

Hence, u_0^1 propagates towards the negative direction of x. We can express u_0^1 concretely

$$\begin{split} u_0^1 &= a_0 - b_0 b_{1/2} \\ &= \frac{1 - \frac{\tau \sigma_0}{2}}{1 + \frac{\tau \sigma_0}{2}} - \frac{1}{1 + \frac{\tau \sigma_0}{2}} \frac{1}{1 + \frac{\tau \sigma_{1/2}}{2}} = \frac{\frac{\tau \sigma_{1/2}}{2}}{1 + \frac{\tau \sigma_{1/2}}{2}}. \end{split}$$

Then, if $\sigma > 0$, an artificial reflection occurs. Therefore, when we set non-trivial PML, an artificial reflection occurs inevitably. We assume that $\sigma(x)$ can be expanded in the Tayler series in $[0, +\infty)$ as:

$$\sigma(x) = \sigma_0 + \sum_{k=1}^{N} \frac{1}{k!} \frac{d^k}{dx^k} \sigma(0) x^k + O(x^{N+1}).$$

Then, the artificial reflection coefficient R is given as:

$$R = \sigma_o \tau + \frac{\sigma'(0)}{2}\tau^2 + O(\tau^3).$$

In particular, the artificial reflection is almost proportional to the product of jump of σ and τ . In case the jump of σ is zero, it is proportional to the product of derivative of σ and τ^2 by neglecting $O(\tau^3)$ term. Furthermore, if σ is differentiable at the boundary, the artificial reflection is at most order τ^3 .

3.3 A New Scheme with Lower Reflection

From the analysis in the previous section, even if the dissipation is constant, an artificial reflection occurs in PML region. To eliminate this spurious reflection at PML region where σ is constant, we propose the new scheme. The new scheme is defined as:

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$$u_m^{n+1} = a_m^{new} u_m^n - b_m^{new} (v_{m+\frac{1}{2}}^{n+\frac{1}{2}} - v_{m-\frac{1}{2}}^{n+\frac{1}{2}}),$$
(8)

$$v_{m+\frac{1}{2}}^{n+\frac{1}{2}} = a_{m+\frac{1}{2}}^{new} u_{m+\frac{1}{2}}^{n-\frac{1}{2}} - b_{m+\frac{1}{2}}^{new} (v_{m+1}^n - v_m^n),$$
(9)

with

$$a_s^{new} = e^{-\tau\sigma_s}, \ b_s^{new} = e^{-\tau\sigma_s/2}, \ s = m \text{ or } m + \frac{1}{2}.$$
 (10)

 σ_s is constant with respect s, we can show easily that $a_s - b_s b_{s+1/2} = 0$. This concludes that there is no spurious reflection in PML region where σ is constant.

4 Some Numerical Examples

4.1 Comparison among Various Schemes in 1D Case

In this section, we give some numerical examples to confirm our analysis. In the first example, we compare the spurious reflections among various schemes in 1D case. The whole region [0, 2] is set to be PML with constant dissipation: $\sigma(x) \equiv \log 10 = 2.302585 \cdots$, $x \in [0, 2]$. We set the initial values u and v to be

$$u(0,x) = \begin{cases} \cos^2\left(20\pi(x-1.0)\right), & 0.95 < x < 1.05, \\ 0, & \text{otherwise,} \end{cases} \quad v(0,x) \equiv 0.$$

We assume the homogeneous Dirichlet condition on both ends of [0, 2]. In this case, the analytical reflection coefficient for this PML is $e^{-2\int_0^2 \sigma(x)dx} = 10^{-4}$. Namely the incident wave from the left end has a primal reflection with the magnitude 10^{-4} .

Figure 1 - 3 show the comparison of reflection waves computed by Bérenger's original scheme, plain scheme and our new scheme. We take a common mesh size $\tau = 1/160$ for space and time. The horizontal coordinate represents the time t and the vertical coordinate shows the value of u(t, x) at time t = 0.0, 0.2, 0.4, 0.6 respectively. Plain scheme and Bérenger's scheme give spurious reflective trail behind the wave front whereas our new scheme is pollution free. The magnitude of the spurious waves is proportional to $\sigma^2 \tau^2$, it could be controlled to be small enough in practical applications.



Fig. 1. The initial shape of u(0, x).

In the second example, we compare the reflection waves from PML for three different shapes of function $\sigma(x)$ in our new scheme. Figure 4 shows the shapes of function $\sigma(x)$. The vacuum region is [0.0, 1.0] and PML one is [1.0, 1.2]. In the first case, $\sigma(x)$ increases discontinuously at the boundary between interior and PML



Fig. 2. Comparison of reflection waves at t = 0.4 for Bérenger (left), plain (middle) and new scheme (right).



Fig. 3. Comparison of reflection waves at t = 0.8 for Bérenger (left), plain (middle) and new scheme (right).

regions with magnitude $\sigma_0 = 10 \log 10 = 23.025 \cdots$. In the second case, $\sigma(x)$ increases linearly on [1.0, 1.1]. In the last case, $\sigma(x)$ increases as the 3rd order spline on [1.0, 1.1]. In all cases, the integrals of $\sigma(x)$ on [1.0, 1.2] are the same. Next, we measure the reflection at x = 0.5. In figure 5 - 6, the horizontal coordinate is time and the vertical one is the value of u(t, 0.5) at the observation point. The wave form during the time between 1.9-2.0 propagate from the interior vacuum region to the PML region, and reflects back at an edge of a PML region, and comes back to the interior region again. We call this wave the real reflection wave. The wave in the neighborhood of t = 1.6 is spurious one. In the first, the second and the last cases, the spurious waves are proportional to τ, τ^2, τ^4 respectively.



Fig. 4. Shapes of function $\sigma(x)$ for three different cases: discontinuous (left), linear (middle) and 3rd order spline (right).



Fig. 5. Comparison of reflection wave to depend on three different shapes of $\sigma(x)$: $\tau = 1/160$.



Fig. 6. Comparison of reflection wave to depend on three different shapes of $\sigma(x)$: $\tau = 1/320$.

4.2 Application to Two-Dimensional Electromagnetic Problem

We extend our scheme to the two-dimensional Maxwell equation for TE mode, and give some numerical examples. The concrete algorithm satisfies the CFL stability condition and $\Delta x = \Delta y = \Delta l = 1/160$ and $\Delta t = \Delta l/\sqrt{2}$. Bérenger's scheme is

$$H_{zx}(i,j) = e^{-\sigma_x(i)\Delta t} H_{zx}(i,j) - \frac{1 - e^{-\sigma(i)\Delta t}}{\sigma_x(i)\Delta l} \{ E_y(i+1,j) - E_y^n(i,j) \},\$$

and our new scheme is

$$H_{zx}(i,j) = e^{-\sigma_x(i)\Delta t} H_{zx}(i,j) - \frac{\Delta t}{\Delta l} e^{-\sigma_x(i)\frac{\Delta t}{2}} \{ E_y(i+1,j) - E_y^n(i,j) \}.$$

We set the computational domain to be a square $[-0.7, 0.7] \times [-0.7, 0.7]$ and the vacuum region is a square $[-0.5, 0.5] \times [-0.5, 0.5]$. The shapes of the dissipation functions $\sigma(x)$ and $\sigma(y)$ are the 3rd order spline like in the 1D case. The initial value is set to be

$$H_z(0, x, y) = e^{-(x-2+y^2)/16}, \quad E_x(0, x, y) = 0, \quad E_y(0, x, y)) = 0.$$

Figure 7 - 9 show the time history of the wave. The horizontal coordinate is x and the vertical one is y, and the value of u(t, x, y) is represented by gradation of brightness. The results show good numerical performance with little reflection from the PML region.



Fig. 7. Two-dimensional results, t = 0.0 (left), t = 0.2 (right).



Fig. 8. Two-dimensional results, t = 0.4 (left), t = 0.6 (right).



Fig. 9. Two-dimensional results, t = 0.8 (left), t = 1.0 (right).

5 Conclusion and Future Works

We explained the origin of the artificial reflection based on the mathematical analysis for 1D problem, and proposed a new scheme for which the artificial reflection does

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not occur in the region where $\sigma(x)$ is constant. By some numerical examples, we confirmed our mathematical analysis and effectiveness of our new scheme. Moreover, we extended the new scheme to 2D problem and got good results. As the result of these numerical performance, we conclude that the new PML is efficient in 1D and 2D computation of wave propagation problems.

The theoretical analysis for 2D problem and the proposal of stable 3D numerical method are future works. We will then proceed to the application in the real world problem such as the transient phenomena in various wave propagation problems including the voice generation simulation and the electromagnetic wave simulation in MRI problem.

References

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