A Finite Difference Time Domain Method for Two Dimensional Electromagnetic Wave Propagation In Lossy Dielectric Media With Cyclic and Perfectly Matched Layer Boundary Conditions

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Abstract

In this work, the foundations behind the one- and two-dimensional finite-difference time-domain (FDTD) method in the context of electromagnetic wave propagation are presented. Two different boundary conditions, cyclic and perfectly matched layer (PML), are presented and discussed. This work includes implementations of the method using both boundary conditions, written in standard Python 3.

Keywords: Electromagnetic wave simulation, finite-difference time-domain, perfectly matched layer

1   Introduction

The goal of the finite-difference time-domain (FDTD) method is to simulate the propagation of electromagnetic waves in complex geometry. For instance, propagation through several different materials with different dielectric constants, or electrical conductivities. Problems such as these are often impossible to solve analytically, and so numerical approaches, such as this one, are required.

This work is an overview of the derivation of the necessary expressions used in the FDTD method as well as two types of boundary conditions. Implementations of the method for both boundary conditions with results are presented and discussed.

2   Governing Equations for Electromagnetic Waves

The differiential form of Maxwell's equations for the electric field, $\mathbf{E}$, and magnetic field, $\mathbf{B}$, in vacuum, are [1]

$$\boldsymbol{\nabla} \cdot \mathbf{E} = \frac{\rho}{\epsilon_0}, \tag{1}$$

$$\boldsymbol{\nabla} \cdot \mathbf{B} = 0, \tag{2}$$

$$\boldsymbol{\nabla} \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}, \tag{3}$$

$$\boldsymbol{\nabla} \times \mathbf{B} = \mu_0 \mathbf{J} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}. \tag{4}$$

Where

- ρ is the free electric charge density

- $\mathbf{J}$ is the free current density

- ϵ_0 is the permittivity of free space

- μ_0 is the permeability of free space

- c is the speed of light, $c \equiv \frac{1}{\sqrt{\epsilon_0 \mu_0}}$

In the context of electromagnetic wave propagation, only Eqs. 3 and 4 are of interest. Assuming there is no free current, rewriting these two equations in terms of the magnetic field strength, $\mathbf{H} = \mathbf{B}/\mu_0$, and subsituting $c \equiv \frac{1}{\sqrt{\epsilon_0 \mu_0}}$ yields

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0}\boldsymbol{\nabla} \times \mathbf{E}, \tag{5}$$

$$\epsilon_0 \frac{\partial \mathbf{E}}{\partial t} = \boldsymbol{\nabla} \times \mathbf{H}. \tag{6}$$

In a dielectric medium, we introduce the relative permittivity, ϵ_r, which is material-specific. This allows us to write the permittivity as $\epsilon = \epsilon_r \epsilon_0$. We could also introduce the relative permeability, but in this work we will assume all materials are nonmagnetic, meaning $\mu_r = 1$ and so $\mu = \mu_0$. Eqs. 5 and 6 become

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0}\boldsymbol{\nabla} \times \mathbf{E}, \tag{7}$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\epsilon}\boldsymbol{\nabla} \times \mathbf{H}. \tag{8}$$

A more general form of these equations uses the electric displacement, $\mathbf{D}$, which can be written as $\mathbf{D}(\omega) = \epsilon_0 \epsilon_r^*(\omega)\mathbf{E}(\omega)$, where ω is the frequency of the wave and ϵ_r^* is the frequency dependent dielectric constant of the medium [2]. If we assume, for a lossy dielectric medium with relative permittivity ϵ_r and conductivity σ, that ϵ_r^* is of the form

$$\epsilon_r^*(\omega) = \epsilon_r + \frac{\sigma}{i\omega\epsilon_0}, \tag{9}$$

then we see that the electric displacement is

$$\mathbf{D}(\omega) = \epsilon_0 \epsilon_r \mathbf{E}(\omega) + \frac{\sigma}{i\omega} \mathbf{E}(\omega). \qquad (10)$$

Transforming this from the frequency domain to the time domain requires an identity which is derived in Appendix A. In the time domain, the above equation is

$$\mathbf{D}(t) = \epsilon_0 \epsilon_r \mathbf{E}(t) + \sigma \int_0^t \mathbf{E}(\tau) d\tau. \qquad (11)$$

So that the relevant equations for electromagnetic waves are then

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu_0} \boldsymbol{\nabla} \times \mathbf{E}, \qquad (12)$$

$$\mathbf{D}(t) = \epsilon_0 \epsilon_r \mathbf{E}(t) + \sigma \int_0^t \mathbf{E}(\tau) d\tau, \qquad (13)$$

$$\frac{\partial \mathbf{D}}{\partial t} = \boldsymbol{\nabla} \times \mathbf{H}. \qquad (14)$$

Finally, we express everything in Gaussian units instead of SI. The purpose for this is so that E, D, and H are around the same order of magnitude [2]. In Gaussian units,

$$\tilde{\mathbf{E}} = \sqrt{\frac{\epsilon_0}{\mu_0}} \mathbf{E}, \qquad (15)$$

$$\tilde{\mathbf{D}} = \sqrt{\frac{1}{\epsilon_0 \mu_0}} \mathbf{D}. \qquad (16)$$

This normalization yields the final set of equations that will be used to govern the propagation of electromagnetic waves in a lossy dielectric medium,

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\sqrt{\epsilon_0 \mu_0}} \boldsymbol{\nabla} \times \tilde{\mathbf{E}}, \qquad (17)$$

$$\tilde{\mathbf{D}}(t) = \epsilon_r \tilde{\mathbf{E}}(t) + \frac{\sigma}{\epsilon_0} \int_0^t \tilde{\mathbf{E}}(\tau) d\tau, \qquad (18)$$

$$\frac{\partial \tilde{\mathbf{D}}}{\partial t} = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \boldsymbol{\nabla} \times \mathbf{H}. \qquad (19)$$

In these equations, the two parameters that are material-specific appear only in Eq. 18. Larger relative permittivities, ϵ_r, decrease the strength of the electric field per unit charge, which has the effect of slowing electromagnetic waves. The dielectric conductivity, σ, represents the total dissipative effect of the material, accounting for any energy loss of the waves in the material.

3 Finite Difference Approximation of the Derivative

Let $f(x)$ be any continuous and thrice differentiable function with bounded derivatives. If we want to obtain an approximation of $f'(x)$, we start by considering $f(x + h)$ and $f(x - h)$, where h is a small displacement. Theorem 1 in Appendix B allows us to write $f(x + h)$ and $f(x - h)$ as shown in Eq. 20.

$$f(x + h) = f(x) + hf'(x) + \frac{h^2}{2} f''(x) + \frac{h^3}{3!} f'''(\eta_1)$$

$$f(x - h) = f(x) - hf'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f'''(\eta_2)$$

$$(20)$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2}{6} \frac{f'''(\eta_1) + f'''(\eta_2)}{2} \tag{21}$$

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{h^2}{6} f'''(\eta) \tag{22}$$

Subtracting both expressions in Eq. 20 and rearranging yields Eq. 21. Here, η_1 and η_2 are two unknown points in the domain of f. By applying the intermediate value theorem to the last term in Eq. 21, the two unknown points can be reduced to a single unknown point, η. This leads to Eq. 22. This equation suggests an approximation for the first derivative,

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}. \tag{23}$$

With an error of

$$E = \frac{h^2}{6} f'''(\eta). \tag{24}$$

Since f and all derivatives of f are bounded, we may introduce M, the absolute maxmimum value of $f'''(x)$, meaning $|f'''(x)| \leq M \; \forall \; x$. Thus, the error term is a constant multiplied by h^2. We say then that this error is an order of h^2, or

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2). \tag{25}$$

This is known as the central difference approximation of the derivative. Due to the error being in h^2, this is a second order approximation. There are many other approximations of the first derivative as well as higher order derivatives. However, this is the only derivative approximation necessary in FDTD.

4 Formulation of FDTD in 1D

For example purposes, a formulation of the FDTD method in 1D is presented here. First, we must choose an axis of propagation. Arbitrarily, suppose the wave travels only in the $\hat{z}$ direction. Eqs. 17 and 19 become

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\sqrt{\epsilon_0 \mu_0}} \frac{\partial \tilde{E}_x}{\partial z} \tag{26}$$

$$\frac{\partial \tilde{D}_x}{\partial t} = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \frac{\partial H_y}{\partial z} \tag{27}$$

Using the central difference approximation of the derivative, in Eq. 23, on each of the derivatives—using $h/2$ for the spatial stepsize and $k/2$ for the temporal stepsize—leads us to Eqs. 28 and 29.

$$\frac{H_y(z, t+k/2) - H_y(z, t-k/2)}{k} = -\frac{1}{\sqrt{\epsilon_0 \mu_0}} \frac{\tilde{E}_x(z+h/2, t) - \tilde{E}_x(z-h/2, t)}{h} \tag{28}$$

$$\frac{\tilde{D}_x(z, t+k/2) - \tilde{D}_x(z, t-k/2)}{k} = \frac{1}{\sqrt{\epsilon_0 \mu_0}} \frac{H_y(z+h/2, t) - H_y(z-h/2, t)}{h} \tag{29}$$

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References

[1] J. D. Jackson, *Classical Electrodynamics.* Wiley, 1999.

[2] D. M. Sullivan, *Electromagnetic Simulation Using The FDTD Method.* IEEE Press, 2000.

A   Inverse Fourier Transform of $E(\omega)/i\omega$

First, we must develop some Fourier transforms of useful functions. Starting with the constant function, $x(t) = a$. Instead of directly evaluating the transform, we instead look at the inverse transform of $X(\omega)$,

$$F^{-1}(X(\omega)) = x(t) = a = \frac{1}{2\pi} \int_{-\infty}^{\infty} X(\omega)e^{i\omega t}d\omega.$$

Clearly, then $X(\omega)$ must be $2\pi a\delta(\omega)$. So,

$$a \rightleftharpoons 2\pi a\delta(\omega). \tag{30}$$

Now, we examine the signum function,

$$sgn(t) = \begin{cases} +1 & \text{if } t > 0 \\ 0 & \text{if } t = 0 \\ -1 & \text{if } t < 0 \end{cases}. \tag{31}$$

Which has the property

$$\frac{d}{dt}sgn(t) = 2\delta(t). \tag{32}$$

Taking the Fourier transform of this function follows, using integration by parts

$$F(sgn(t)) = \int_{-\infty}^{\infty} sgn(t)e^{-i\omega t}dt$$

$$= \left[\frac{-1}{i\omega}sgn(t)e^{-i\omega t} \right]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{-2}{i\omega}\delta(t)e^{-i\omega t}dt$$

$$= \frac{2}{i\omega}.$$

So,

$$sgn(t) \rightleftharpoons \frac{2}{i\omega}. \tag{33}$$

The last function we need is the Heaviside step function,

$$H(t) = \begin{cases} 1 & \text{if } t \geq 0 \\ 0 & \text{if } t < 0 \end{cases}. \tag{34}$$

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Noticing that $H(x) = \frac{sgn(t)+1}{2}$ we take the Fourier transform of H,

$$F(H(t)) = F\left(\frac{sgn(t)+1}{2}\right)$$

$$= F\left(\frac{sgn(t)}{2}\right) + F\left(\frac{1}{2}\right)$$

$$= \frac{1}{i\omega} + \pi\delta(\omega).$$

So,

$$H(t) \rightleftharpoons \frac{1}{i\omega} + \pi\delta(\omega). \tag{35}$$

Now, consider a general function, $f(t)$ which can be written as the integral from $-\infty$ to t of some other function, $g(t)$,

$$f(t) = \int_{-\infty}^{t} g(\tau)d\tau. \tag{36}$$

This can be expressed as a convolution integral with the Heaviside function,

$$f(t) = \int_{-\infty}^{t} g(\tau)d\tau = \int_{-\infty}^{\infty} g(\tau)H(t-\tau)d\tau = (g * H)(t). \tag{37}$$

Fourier's convolution theorem states that for any two functions, $\theta(t)$ and $\phi(t)$, whose Fourier transforms exist,

$$F((\theta * \phi)(t)) = \Theta(\omega)\Phi(\omega). \tag{38}$$

Applying this to our function, $f(t)$, yields,

$$F(f(t)) = G(\omega)\left[\frac{1}{i\omega} + \pi\delta(\omega)\right]. \tag{39}$$

So,

$$\int_{-\infty}^{t} g(\tau)d\tau \rightleftharpoons G(\omega)\left[\frac{1}{i\omega} + \pi\delta(\omega)\right]. \tag{40}$$

Finally, we can use this identity to find $\mathbf{E}(t)$, given $\mathbf{E}(\omega)$. We apply the above identity to each of the components of $\mathbf{E}(\omega)\left[\frac{1}{i\omega} + \pi\delta(\omega)\right]$. Then,

$$\int_{-\infty}^{t} \mathbf{E}(\tau)d\tau \rightleftharpoons \mathbf{E}(\omega)\left[\frac{1}{i\omega} + \pi\delta(\omega)\right]. \tag{41}$$

We may assume that $\mathbf{E}(t)$ is zero for $t < 0$ and $\mathbf{E}(\omega = 0) = 0$, in which case the above equation reduces to the desired identity,

$$\int_{0}^{t} \mathbf{E}(\tau)d\tau \rightleftharpoons \frac{\mathbf{E}(\omega)}{i\omega}. \tag{42}$$

B   The Lagrange Remainder Theorem

Theorem 1. *Let $f(x)$ be a function which is continuous on $[a, b]$ and $(n + 1)$ differientiable on (a, b). Then, for each $x \in [a, b]$ there exists $\eta \in [a, b]$ such that*[1]

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \frac{f^{(n+1)}(\eta)}{(n+1)!}(x-a)^{n+1}. \quad (43)$$

Proof. Let T_n be the nth Taylor polynomial of f, centered at a. That is,

$$T_n(x) = f(a) + f'(a)(x - a) + \frac{f''(a)}{2}(x - a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x - a)^n. \quad (44)$$

Now choose $K \in \mathbb{R}$ such that

$$f(b) = T_n(b) + K(b - a)^{n+1}. \quad (45)$$

We will show that this K is coefficient of the final term in Eq. 43. First we consider the function F, defined as

$$F(x) = f(x) - T_n(x) - K(x - a)^{n+1}. \quad (46)$$

Notice that $F^{(k)}(a) = 0$ for $k \leq n$ since

$$T_n^{(k)}(x) = f^{(k)}(a) + f^{(k+1)}(a)(x - a) + \cdots + \frac{f^{(n)}(a)}{(n - k)!}(x - a)^{n-k} \text{ for } k \leq n. \quad (47)$$

So $T_n^{(k)}(a) = f^{(k)}(a)$ for $k \leq n$. And,

$$\frac{d^k}{dx^k} K(x - a)^{n+1} = \frac{K(n+1)!}{(n+1-k)!}(x - a)^{n+1-k}. \quad (48)$$

This demonstrates that $F^{(k)}(a) = 0$ for $k \leq n$. Our choice of K garuntees $F(b) = 0$, so we see that $F(a) = F(b) = 0$. This allows us to apply Rolle's theorem to F. The theorem is an extension to the mean value theorem, and it states that for any function, g, that is continuous on $[a, b]$ and differientiable on (a, b), if $g(a) = g(b)$ then there exists at least one $c \in [a, b]$ such that $g'(c) = 0$. Applying this theorem to F tells us that there exists a $c_1 \in [a, b]$ such that $F'(c_1) = 0$. Now we examine F'. We have shown above that $F'(a) = 0$,

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[1]The final term in this equation is called the remainder term of the nth Taylor polynomial of f. This is because it is the error between f and the nth Taylor polynomial of f, T_n. That is to say, $f(x) - T_n(x) = \frac{f^{(n+1)}(\eta)}{(n+1)!}$ for some $\eta \in [a, b]$

and we have just demonstrated that $F'(c_1) = 0$, thus $F'(a) = F'(c_1) = 0$. Applying Rolle's theorem now to F' tells us that there exists $c_2 \in [a, c_1]$ such that $F''(c_2) = 0$. We continue this process on the higher derivatives of F up to $F^{(n+1)}$. Here, Rolle's theorem garuntees the existence of a $c_{n+1} \in [a, c_n]$ such that $F^{(n+1)}(c_{n+1}) = 0$. However, since $T_n^{(n+1)} \equiv 0$, we know that $F^{(n+1)}$ is

$$F^{(n+1)}(x) = f^{(n+1)}(x) - K(n+1)!. \tag{49}$$

So, using the fact that $F^{(n+1)}(c_{n+1}) = 0$,

$$K = \frac{f^{(n+1)}(c_{n+1})}{(n+1)!}. \tag{50}$$

Let $\eta = c_{n+1}$. Since $[a, c_{n+1}] \subseteq [a, c_n] \subseteq [a, c_{n-1}] \subseteq \cdots \subseteq [a, b]$, we know $\eta \in [a, b]$. Moreover, since our choice of K in Eq. 45 could be repeated with b replaced by any $x \in [a, b]$, the entire process could be done with any point in $[a, b]$, yielding a not-necessarily different η for each point. However, each η would still be in $[a, b]$ since $[a, x] \subseteq [a, b] \; \forall \; x \in [a, b]$. Plugging this expression for K back into Eq. 45 shows that for each $x \in [a, b]$, there exists $\eta \in [a, b]$ such that

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \cdots + \frac{f^{(n)}(a)}{n!}(x-a)^n + \frac{f^{(n+1)}(\eta)}{(n+1)!}(x-a)^{n+1}. \tag{51}$$

$\square$