Finite Difference Time Domain method applied to a specific problem

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0.1 Overview of the problem

The field of electromagnetics has a wide range of applications in both physics and engineering. However, what is so interesting is that these applications can all be explained by Maxwell's equations, a set of four partial differential equations that describe the properties of electric and magnetic fields and relate them to their sources, current density and charge density. Maxwell's differential equations are listed below:

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (1)$$

$$\nabla \times \vec{B} = \mu_0 \epsilon_0 \frac{\partial \vec{E}}{\partial t} + \mu_0 \vec{J} \quad (2)$$

$$\nabla \cdot \vec{E} = \frac{\rho}{\epsilon_0} \quad (3)$$

$$\nabla \cdot \vec{B} = 0 \quad (4)$$

where $\nabla \times$ denotes curl, $\nabla \cdot$ denotes divergence, $\vec{E}$ is the electric field, $\vec{B}$ is the magnetic field, $\vec{J}$ is the total current density, ρ is the total charge density, ϵ_0 is the permittivity of free space and μ_0 is the permeability of free space. (cite Nanophotonics or EM textbook)

Combined, these four equations can be used to explain the electromagnetic phenomena in the universe. When these equations can be solved with proper initial and boundary conditions, the electric and magnetic fields for a system can be determined over both space and time. However, it is often difficult to determine the electric and magnetic fields of a system through analytic methods.

One of the most popular ways to solve Maxwell's equations numerically is the finite difference time domain method (FDTD for short). Since its introduction in 1966, FDTD has become popular because of several important reasons. The basic FDTD method does not use any linear algebra and it is accurate and robust. The sources of error with the method are well understood and can be bounded. FDTD also treats impulsive behavior and nonlinear behavior naturally. It is a systematic approach which does not require a problem to be remodeled each time it needs to be solved. Also as computer capabilities increase, FDTD is easily implemented to provide visualizations of electric and magnetic fields since the method generates arrays of fields over time.

The FDTD method works by discretizing the computational space into a grid. Then, using discrete steps in time, the fields are evolved over time at these grid points. By making the space and time steps finer, solutions will become closer to the continuous solution.

0.2 The Yee Algorithm

The Finite Difference Time Domain method was first introduced in 1966 by Kane S. Yee in his paper, *Numerical Solution of Initial Boundary Value Problems Involving Maxwell's Equations in Isotropic Media*. Although the method did not gain popularity until the 1980s, it is fundamentally robust and provides the basis behind many variations used today. The basic algorithm is discussed below.

FTDT works by discretizing the computational space where one desires to know the electric and magnetic fields into a mesh. Then, using discrete steps in time, the fields are evolved over time at the points in the mesh. The fields are calculated using basic finite difference methods in a leapfrogging manner where electric fields are calculated in one time step and then at the next time step, the magnetic fields are calculated using the electric field time steps that were calculated in the previous time step. Although base of Yee's algorithm has remained the same over time, there have been many improvements to the original FTDT method to improve its accuracy and handling of geometries and boundary conditions.

The basic algorithm is as discussed above. The first thing that is done is converting Maxwell's equations into a set of six coupled scalar equations as seen below. Although Gauss's Laws (equations 3 and 4) are not explicitly mentioned within these six equations, these relations are maintained in the FDTD algorithm.

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu}\left[\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - (M_{source_x} + \sigma^* H_x)\right] \tag{5}$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu}\left[\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - (M_{source_y} + \sigma^* H_y)\right] \tag{6}$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu}\left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - (M_{source_z} + \sigma^* H_z)\right] \tag{7}$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon}\left[\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - (J_{source_x} + \sigma E_x)\right] \tag{8}$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\epsilon}\left[\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - (J_{source_y} + \sigma E_y)\right] \tag{9}$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\epsilon}\left[\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - (J_{source_z} + \sigma E_z)\right] \tag{10}$$

The other important thing needed is creating the mesh of points where the fields will be calculated. Yee's algorithm uses a 3-D grid of points so that in any plane, any point where the $\vec{E}$ field is calculated is surrounded by four $\vec{B}$ components, perpendicular to the $\vec{E}$ field vector and vice versa. A diagram of a cubic unit cell is inserted below. This design is known as Yee's lattice. See Appendix A for a copy of image (need to figure out how to include images in document). FDTD can make use of other grid structures. Grids can be in Cartesian coordinates, or they can also be expressed as hexagonal grids and other polygonal/polyhedron shapes as well. Hexagonal grids reduce certain types of error to a much greater percentage than Yee lattices can. However the Yee lattice is one of the simplest grids.dcc

The Yee algorithm uses leapfrogging time stepping which is fully explicit. A diagram of leapfrog time stepping in one dimension is included below (see Appendix B, need to figure how to include images once again). In Yee's notation, the partial differential equations for a given point are determined by using values that are half a time step away. The use of centered finite-difference expressions produces derivatives that are second-order accurate.

The derivation of the formulas for computation of the fields are displayed below.

$$\frac{\partial E_x}{\partial t} = \frac{1}{\epsilon}\left[\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - (J_{source_x} + \sigma E_x)\right]$$

$$\begin{aligned}&\frac{E_x|^{n+1/2}_{i,j+1/2,k+1/2} - E_x|^{n-1/2}_{i,j+1/2,k+1/2}}{\Delta t} = \\ &\quad \frac{1}{\epsilon_{i,j+1/2,k+1/2}} \cdot \Bigg(\frac{H_z|^n_{i,j+1,k+1/2} - H_z|^n_{i,j,k+1/2}}{\Delta y} - \frac{H_y|^n_{i,j+1/2,k+1} - H_y|^n_{i,j+1/2,k}}{\Delta z} \\ &\quad -J_{source_x}|^n_{i,j+1/2,k+1/2} - \sigma_{i,j+1/2,k+1/2} E_x|^n_{i,j+1/2,k+1/2}\Bigg)\end{aligned} \tag{11}$$

As can be seen, the calculation for $E_x|^{n+1/2}$ requires $E_x|^n$ however only $E_x|^{n-1/2}$ is stored. The following semi-approximation is used to calculate $E_x|^n$.

$$E_x|^n = \frac{E_x|^{n+1/2} - E_x|^{n-1/2}}{2} \tag{12}$$

When this formula is plugged into equation 11, the following formula for $E_x|^{n+1/2}_{i,j+1/2,k+1/2}$ is obtained. This same method can be used to determine the other components of the electric field and the magnetic field.

$$\begin{aligned}E_x|^{n+1/2}_{i,j+1/2,k+1/2} &= \left(\frac{1 - \frac{\sigma_{i,j+1/2,k+1/2}\Delta t}{2\epsilon_{i,j+1/2}}}{1 + \frac{\sigma_{i,j+1/2,k+1/2}\Delta t}{2\epsilon_{i,j+1/2}}}\right) E_x|^{n+1/2}_{i,j+1/2,k+1/2} \\ &+ \left(\frac{\frac{\Delta t}{\epsilon_{i,j+1/2,k+1/2}}}{1 + \frac{\sigma_{i,j+1/2,k+1/2}\Delta t}{2\epsilon_{i,j+1/2}}}\right)\Bigg(\frac{H_z|^n_{i,j+1,k+1/2} - H_z|^n_{i,j,k+1/2}}{\Delta y} - \frac{H_y|^n_{i,j+1/2,k+1} - H_y|^n_{i,j+1/2,k}}{\Delta z} \\ &-J_{source_x}|^x_{i,j+1/2,k+1/2}\Bigg)\end{aligned} \tag{13}$$

0.3 FDTD in Two Dimensions

In many cases, Yee's algorithm will require calculations in all three dimensions. However, in some cases however, the solution can be condensed into two dimensions. (p 138) For example, let us assume that the wave that is being modeled can be extended out to infinity in the z direction. That is to say that the beam is propagating solely in the x-y plane. Then, all the partial derivatives with respect to z equal zero. When this occurs, the six equations can be reduced into two groups of three.

$$\begin{aligned}
\frac{\partial H_x}{\partial t} &= \frac{1}{\mu}\left[-\frac{\partial E_z}{\partial y} - (M_{source_x} + \sigma^* H_x)\right] && (14)\\
\frac{\partial H_y}{\partial t} &= \frac{1}{\mu}\left[\frac{\partial E_z}{\partial x} - (M_{source_y} + \sigma^* H_y)\right] && (15)\\
\frac{\partial E_z}{\partial t} &= \frac{1}{\epsilon}\left[\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - (J_{source_z} + \sigma E_z)\right] && (16)\\
\frac{\partial H_z}{\partial t} &= \frac{1}{\mu}\left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - (M_{source_z} + \sigma^* H_z)\right] && (17)\\
\frac{\partial E_x}{\partial t} &= \frac{1}{\epsilon}\left[\frac{\partial H_z}{\partial y} - (J_{source_x} + \sigma E_x)\right] && (18)\\
\frac{\partial E_y}{\partial t} &= \frac{1}{\epsilon}\left[-\frac{\partial H_z}{\partial x} - (J_{source_y} + \sigma E_y)\right] && (19)\\
& && (20)
\end{aligned}$$

The first group of equations contain only E_z, H_x, and H_y. These field components make up the transverse-magnetic mode or TM_z mode where the electric field does not have any component in the direction of propagation but the magnetic field does. Likewise, the second group of equations comprise the transverse-electric mode or TE_z mode where the electric field has a component in the direction of propagation but the magnetic field does not. These two modes have no common field vector components and as a result, they can exist simultaneously without any mutual interactions.

Knowledge that the wave that is being modeled is uniform in one plane can reduce the problem significantly. If this is the case, the vector field components in the space lattice can be reduced to a plane. This in turn reduces the memory requirements and number of computations that the algorithm needs to implement. As a result, reducing the problem to either a TM or TE case is highly desireable. The number of points is reduced by a factor of the number of points in the removed dimension. Most commercial programs provide the option for solving in either two or three dimensions based on the incident wave enabling the algorithm that will be most efficient.

0.4 Examining the FDTD Method

Although the equations used to calculate the electric fields look large, the derivation of the FDTD method is intuitive and straightforward. However, in order to fully understand the FDTD method, its benefits and its weaknesses, it needs to be analyzed for stability and accuracy.

FDTD is not unconditionally stable. However the requirements for the FDTD method to be stable are well-known. The time step and the spatial step are related by the Courant factor, S. This factor is further bounded based on the smallest refractive index of the system (usually 1) and the number of dimensions in which the fields are being calculated. (cite MEEP).

$$\Delta t = S \Delta x \tag{21}$$

$$S < \frac{n_{min}}{\sqrt{\#numbers}} \tag{22}$$

However, while this sets the requirement for the size of the time step, it is important to consider the spatial step as well. FTDT is dependent on continuity between adjacent grid points. If the grid points are spaced too far apart, the fields will be incorrectly calculated. A standard grid spacing that is commonly used is $\frac{\lambda_{min}}{20}$. This in turn brings up the point that if the electric field needs to be calculated a large distance from the source, FDTD will take a large amount of time to run as it functions at a rather high precision.

One of the problems with the original FDTD algorithm is that it did not handle the boundaries of the computational space very well. In the real world, electromagnetic waves propagate infinitesimally as they continue to attenuate. However when solving for the electric and magnetic fields numerically with a computer, the solution is restricted to a finite space and time. In problems where unbounded regions are being simulated, an absorbing boundary condition must be implemented to simulate the extension of the lattice to infinity. In 1994, J.P. Berenger developed the *perfectly matched layer*. The purpose of this layer is to absorb all waves. When FDTD is used, the PML is almost always used. Otherwise, oblique waves bounce back from the boundaries and corrupt the solution. Although its derivation is not discussed in this paper, the PML layer was a break through in improving the accuracy of modeled results and is almost always used in current modeling software using DFDT.

0.5 1-D FDTD Modeling

A 1-dimensional FDTD method was developed in MATLAB for the project. A 1-D simulation was chosen because of the complexities associated with 2-D and 3-D simulations along with the time it takes and problems that can emerge from boundary conditions. A single frequency sinusoidal electric field source was added at the left hand side. As can be seen in the code (attached in the Appendices), at each time step, the script calculates the E field and the B field based on one another. The incident source is introduced gradually in the script. To ensure smoothness, an exponential component is added to the source.

0.6 Applications of FDTD

Although Yee's paper did not gain significant recognition for nearly 20 years after it was published, FDTD methods are referenced in thousands of paper and several commercial and open-source software versions of FDTD are available. One of the new fields where FDTD is gaining popularity is nanophotonics. Since nanophotonics is at the scale of wavelengths or even less, it becomes feasible to use FDTD to model components and and the transmission of electromagnetic waves. Furthermore, there is a desire to model structures before and after the fabrication of these structures especially with respect to electric and magnetic fields. One such example is the photonic crystal waveguide. Photonic crystals are materials that possess a periodicity in their refractive index. For these structures, there are certain frequency regions where electromagnetic propagation is forbidden or severely attenuated resulting in a material with a photonic bandgap. By introducing a line defect into such a material (a wire-like shape where the refractive index is constant), a waveguide can be created by taking advantage of the fact that electromagnetic radiation of certain frequencies cannot propagate through the main photonic crystal. It is highly important to model the behavior of electromagnetic radiation within these photonic crystal waveguides. FDTD which provides snapshots of the fields over time provides the perfect method to derive the fields but also to convert into images of the electric and magnetic fields.

0.7 Sources

Taflove, Allen and Susan Hagness. *Computational Electrodynamics: The finite-difference time-domain method*. Boston: Artech House, 2000.

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