

Chapter 1

Methods

1.1 Introduction

Electromagnetic simulations in this dissertation were performed using the Finite-Difference Time-Domain (FDTD) method.

1.2 FDTD Overview

The Finite-Difference Time-Domain (FDTD) method is a technique for iteratively solving Maxwell's curl equations. Using the finite difference approximation, the equations are discretized for computational use and thus is second order accurate. The modern method for FDTD simulation, initially proposed by Yee in 1966 REF, constructs a grid where the electric field components are offset in space by half a grid dimension as can be seen in <FIGURE>. We call a single cell of this arrangement the *Yee Cell*. To calculate the electric field value at a grid point the simulation needs to know the value at that point one time step earlier and the magnetic field value in the surrounding grid points half a time step earlier. Thus, the simulation alternately calculates the entire magnetic field and in the simulation field before calculating the electric field one “half” time step later.

$$\begin{aligned}
\nabla \times \mathbf{E} &= -\mu \frac{\partial \mathbf{H}}{\partial t} & \nabla \times \mathbf{H} &= -\varepsilon \frac{\partial \mathbf{E}}{\partial t} \\
\frac{\partial \mathbf{H}}{\partial t} &= -\frac{1}{\mu} \nabla \times \mathbf{E} & \frac{\partial \mathbf{E}}{\partial t} &= -\frac{1}{\varepsilon} \nabla \times \mathbf{H} \\
\frac{\mathbf{H}(t + \frac{\Delta t}{2}) - \mathbf{H}(t - \frac{\Delta t}{2})}{\Delta t} &= -\frac{1}{\mu} \nabla \times \mathbf{E}(t) & \frac{\mathbf{E}(t + \Delta t) - \mathbf{E}(t)}{\Delta t} &= \frac{1}{\varepsilon} \nabla \times \mathbf{H}(t + \frac{\Delta t}{2}) \\
\mathbf{H}(t + \frac{\Delta t}{2}) &= \mathbf{H}(t - \frac{\Delta t}{2}) - \frac{\Delta t}{\mu} \nabla \times \mathbf{E}(t) & \mathbf{E}(t + \Delta t) &= \mathbf{E}(t) + \frac{\Delta t}{\varepsilon} \nabla \times \mathbf{H}(t + \frac{\Delta t}{2})
\end{aligned} \tag{1.1}$$

These equations are then solved for each vector component

$$H_x(x, y, z)^{t+\frac{\Delta t}{2}} = H_x(x, y, z)^{t-\frac{\Delta t}{2}} - \frac{\Delta t}{\mu} \left(\frac{E_y^t(x, y+1, z) - E_y^t(x, y, z)}{\Delta y} - \frac{E_z^t(x, y, z+1) - E_z^t(x, y, z)}{\Delta z} \right) \tag{1.2}$$

where x, y, z represent coordinates in simulation space, $\Delta x, \Delta y, \Delta z$ are the lengths of the Yee cell in that dimension and Δt is the simulation time step. As can be seen in (1.1) and (1.2) these formulations of Maxwell's curl equations are second order accurate. It has been shown that to maintain numerical stability the ratio of the time step to spatial step must satisfy the condition $c\Delta t \leq \frac{1}{\Delta x^2 + \Delta y^2 + \Delta z^2}$. The maximum value, $S_c = \frac{c\Delta t}{\Delta x^2 + \Delta y^2 + \Delta z^2}$, is known as the *Courrant number* <REF>.

1.2.1 Generic explanation

The time domain nature of FDTD means that multiple frequencies of interest can be studied from a single simulation by using a broad band source. In this dissertation frequency domain analysis is performed with the FDTD code to produce electric field colormaps for a range of frequencies, reflectance and transmittance spectra and photonic band diagrams.

1.2.2 Types of Analysis done with FDTD

1.2.3 Utility of FDTD

The purpose of a FDTD simulation is to determine the electromagnetic response of some material structure. While simple methods for determining the response of layered structures, such as the transfer matrix method (TMM) <REF>, are effective, FDTD has the added flexibility to simulate more complexly patterned structures. The time domain nature of FDTD, unlike its frequency domain counterparts, allows for broad band simulation while also allowing for the portrayal of specific frequency responses in post processing analysis. The method is accurate, robust and scalable. FDTD has been used to simulate macro scale objects, such as low visibility aircraft, scattering radar waves, cell phone signals interacting with human brain tissue and nano scale structures interacting with infrared scale wavelengths, which is the subject matter of this dissertation. Furthermore FDTD naturally handles nonlinear behavior, can handle anisotropic media and is easily parallelizable.

1.2.3.1 Limits of FDTD

1.3 Sources

In order to perform useful stimulations an electromagnetic excitation needs to be introduced. Two common methods for this are discussed here: a pointwise hard source and a total field/scattered field (TFSF) source. For either source a time domain function is used to evolve the field value(s) at a specified location within the simulation space. While a harmonic source could be used this would fail to utilize the broadband frequency functionality of FDTD. For this reason much of the work in this dissertation was done using simulations excited by a Ricker wavelet <REF>.

1.3.0.1 The Ricker Wavelet

$$\nu_r(t) = (1 - 2(\pi\nu_p(t - d_r)^2))e^{-(\pi\nu_p(t-d_r)^2)} \quad (1.3)$$

Where ν_p is the peak frequency and d_r is the temporal delay. The Ricker wavelet, (1.3), is a pulsed source equivalent to the second derivative of a Gaussian. The pulsing of the source enabled broad band simulations to be performed. Unlike a Gaussian pulse there is no dc component. The delay was able to be set such that the source "turned on" gradually. This gradual nature combined with a lack of a dc component reduced the occurrence of non-physical numerical artifacts in simulations. The spectral content was centered around a peak frequency in the spectral range of interest for each study.

1.3.1 Point Sources

A point source in FDTD is simulated by varying a single (or array of single) grid points using a source function of the form discussed in the previous section. These sources are useful for simulating dipoles or artificial point sources, such as an afm tip.

1.3.2 TFSF Source

A Total Field Scatter Field (TFSF) source allows the simulation of a "one-way" plane wave. By subtracting the backwards propagating portion of the source from the grid point half a cell dimension "behind" the source a space in the simulation is created where only non-negligible electric or magnetic field strength is due to signal which has been reflected, or scattered, from an object in the simulation. This is particularly useful when it comes to calculating reflection spectra.

1.4 Boundary Conditions

In order to simulate realistic structures it was necessary to incorporate boundaries into our simulation. For periodic structures their properties were ascertained by utilizing *periodic* boundaries. Where a photonic band structure was the desired output these boundaries were varied to become Bloch periodic boundaries. In the case of a terminal boundary, such as an "infinite" substrate or incident medium, an absorbing boundary was used called a Perfectly Matched Layer (PML).

1.4.1 PEC Boundary

1.4.2 Periodic Boundary

To simulate an infinite sheet of meta materials the most basic unit cell was repeated 'infinitely'. This was accomplished by bounding the simulation in the x - and y -direction with a periodic boundary. this is accomplished by updating the discretized curl equation along the upper boundary (lower boundary for the magnetic field curl equation) explicitly. An example can be seen in (1.4)

$$E_y^t(x, 0, z) - E_y^t(x, N_y, z) \quad (1.4)$$

Where N_y is the size of the simulation space in the y -direction. When the cells at $y = N_y$ are updated the term $E_y^t(x, y + 1, z)$ is replaced with $E_y^t(x, 0, z)$. Thus any signal exiting through a cell along the $y = N_y$ boundary reenters the simulation at $y = 0$. To create an infinite two dimensional simulation space this procedure is repeated along the x axis as well.

1.4.2.1 Bloch Periodic Boundary

1.4.3 Perfectly Matched Layers

1.4.4 UPML

1.4.5 CPML

1.5 Materials Models

1.5.1 Isotropy

1.5.1.1 Isotropic

1.5.1.2 Anisotropic

1.5.1.3 Diagonally Anisotropic

1.5.2 Dielectric Materials

1.5.3 Dispersive materials

1.5.3.1 Z Transform

1.5.3.2 Drude Model

1.5.3.3 Debye Drude Model

1.5.3.4 Lorentz

1.5.3.5 Diagonally Anisotropic

1.6 Sensors

1.6.1 Time domain sensors

1.6.2 Frequency Domain Sensors

1.6.2.1 Heat Maps

1.6.2.2 BTA Spectra