The Finite-Difference Time-Domain Method for Photonic Crystal Simulations
Parallel Computing Final Project Report
Nicole Saulnier

The finite-difference time-domain method is used to simulate the propagation of electric and magnetic fields through space with time. The method can be applied to one, two, or three dimensional problems. This document provides a brief summary of the method and the computer program that is being developed for 3D finite-difference time-domain simulations.

Introduction:
Propagation of the electric and magnetic fields are described fully by Maxwell's equations shown in equation 1.

$$\left.\begin{array}{l} \nabla \times H = \dfrac{\partial D}{\partial t} + J \\[2mm] \nabla \times E = -\dfrac{\partial B}{\partial t} \\[2mm] \nabla \cdot B = 0 \\[2mm] \nabla \cdot D = \rho \end{array}\right\} \qquad (1)$$

In the 3D finite-difference time-domain method, the Maxwell equations are solved numerically using finite-difference equations derived from the Maxwell differential equations. The central-difference approximation can be used to write the spatial and time derivatives of the magnetic, H_y, and electric field, E_x, components of the first two Maxwell equations as:

$$\left.\begin{array}{l} H_y^{n+1}(i+\tfrac{1}{2},j,k+\tfrac{1}{2}) = H_y^n(i+\tfrac{1}{2},j,k+\tfrac{1}{2}) - \dfrac{\Delta t}{\Delta x\sqrt{\varepsilon_o\mu_o}}\left(E_x^{n+1/2}(i+\tfrac{1}{2},j,k+1) - E_x^{n+1/2}(i+\tfrac{1}{2},j,k) - E_z^{n+1/2}(i+1,j,k+\tfrac{1}{2}) + E_z^{n+1/2}(i,j,k+\tfrac{1}{2})\right) \\[4mm] E_x^{n+1/2}(i,j,k+\tfrac{1}{2}) = E_x^{n-1/2}(i,j,k+\tfrac{1}{2}) + \dfrac{\Delta t}{\Delta x\sqrt{\varepsilon_o\mu_o}}\left(H_z^n(i+\tfrac{1}{2},j+\tfrac{1}{2},k) - H_z^n(i+\tfrac{1}{2},j-\tfrac{1}{2},k) - H_y^n(i+\tfrac{1}{2},j,k+\tfrac{1}{2}) + H_y^n(i+\tfrac{1}{2},j,k-\tfrac{1}{2})\right) \end{array}\right\} (2)$$

Here, Δt is the time step, Δx is the spatial step, ε_o is the vacuum permittivity and μ_o is the vacuum permeability. These equations closely follow the approach first used by Yee, where the electric and magnetic field grid points are interlaced in space and time and a leapfrog scheme is used to solve the system of equations [1]. The electric and magnetic field strengths in the equations are normalized so that they are of the same order of magnitude. The rest of the field components can be written down in an analogous manner.

Computer Code Implementation:
For simplicity and numerical stability the time step is chosen as $\Delta t = \Delta x/(2c)$, where c is the velocity of light in free space. The spacial step is chosen to be at most one twentieth of the wavelength of light used for the simulation. The equations above can be written in the following form for creating computer code:

$$hy[i][j][k] = hy[i][j][k] + .5\big(ez[i+1][j][k] - ez[i][j][k] - ex[i][j][k+1] + ex[i][j][k]\big)$$
$$ex[i][j][k] = ex[i][j][k] + .5\big(hz[i][j][k] - hz[i][j-1][k] - hy[i][j][k] + hy[i][j][k-1]\big)$$

$$(3)$$

The factor of .5 is obtained by substituting the relationship between the spacial and time steps into equation 2 and noting that c is inversely proportional to the square root of the permittivity times the permeability.

The equations discussed thus far assume light propagation in vacuum. A more interesting situation involves light propagation in dielectric media. For this, the equations are simply modified through the constitutive relation $D=\varepsilon E$. The electric and magnetic fields evolve in time by solving the equations at each time step in the following order. First, the electric flux components are calculated from the initial magnetic field components and an input is applied to the system as an electric flux. Next, the electric field components are found from the electric flux using the constitutive relation. Finally, new magnetic field components are found from the electric field. This is illustrated in the flowchart at the end of the document.

Because a problem space can not be infinite, it is necessary to model infinite conditions at the boundary of the problem space. This can be done using the perfectly matched layer techniques developed by Berniger [2,3]. Typically for the case of optical waveguides and lasers, materials are chosen with permeabilities close to that of free space. The perfectly matched layer takes advantage of the properties of lossy and magnetic material to attenuate and eliminate reflections as the electromagnetic waves reach the boundary of the problem space. The specifics of the numerical development will not be discussed here.

Results:

The equations above have been coded into a C program and Fig. 1 shows the simulation results of a photonic crystal slab waveguide suspended in air. For this structure, $r = 219$ nm, $a = 547$ nm, slab thickness $d = 301$ nm and guide length $l = 30$ μm. A Gaussian wave packet with wavelength $\lambda=1.5$ μm is taken as the input. The x component of the electric field is shown at the center of the slab (x slice) and the wave packet propagates down the length of the guide with relatively low loss.
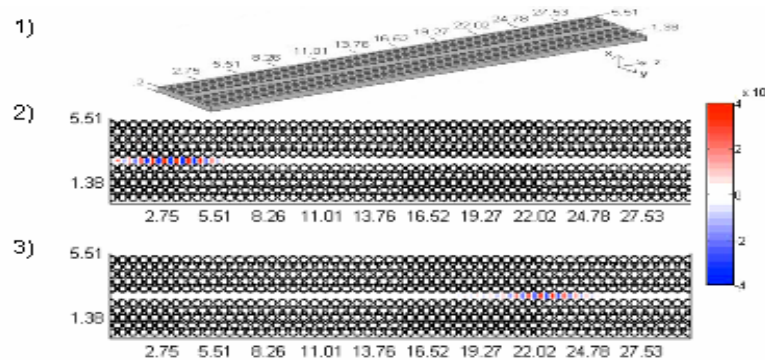

Fig. 1. 3D FDTD simulation results for a Gaussian pulse of wavelength $\lambda = 1.5$ μm traveling along a PC waveguide. Length in microns 1) 3D view of guide 2) zoomed view, time $= 9.17$ x 10^{-14} sec 3) zoomed view, time $= 4.13$ x 10^{-13} sec.

The simulation results are shown more clearly in the included movie. This shows the propagation of the wave packet with time. The top portion of the movie is the propagation of the x component of the electric field and the bottom portion is the y

component of the magnetic field. The guide length is still $l = 30$ μm and the x slice is shown.

Future Work:
   The program has been used primarily for waveguide simulations however it is possible to examine the modes of a cavity using this FDTD program. Several cases will be tested in the near future. Also it is possible to use the FDTD data to create the photonic band diagram for a particular crystal structure. This is done by taking the Fourier transform of the data at several spacial steps along the reciprocal space unit cell. The program will be modified slightly to allow for the creation of these diagrams, and a function may be added to perform the Fourier transform.
   Computation can take several days and it may be reasonable to examine the possibility of using MPI to create a parallelized program. As of yet it is unclear whether the performance will be enhanced significantly, but I hope that use of MPI will allow for the computation of field propagation over larger problem spaces.

[1] K.S. Yee, "Numerical solution to initial boundary value problems involving Maxwell's equations in isotropic media", *IEEE Trans. Antennas Propagat.*, Vol. AP-14, pp. 302-307, 1966.
[2] J.P. Berenger, "Perfectly Matched Layer for the FDTD solution of Wave-Structure Interaction Problems", *IEEE Trans. Antennas Propagat.*, Vol. 44, pp. 110-117, 1996.
[3 J.P. Berenger, "Three-Dimensional Perfectly Matched Layer for the Absorption of Electromagnetic Waves", *Journal Compt. Phys.*, Vol. 127, pp. 363-379, 1996.