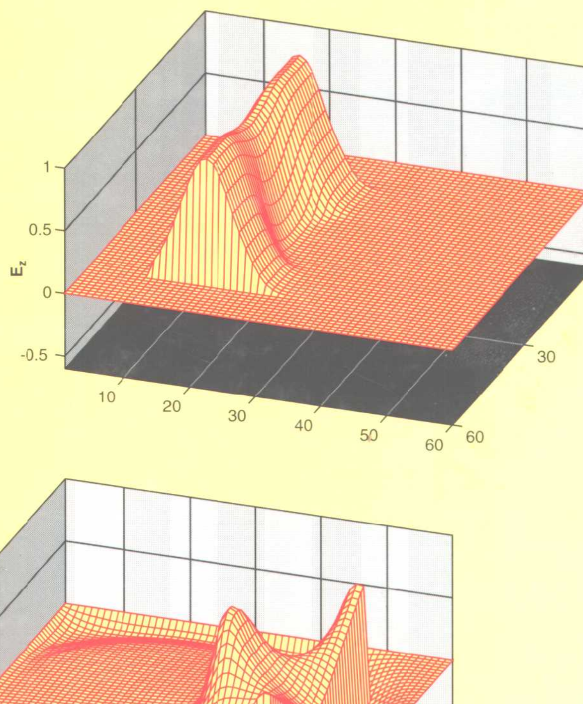
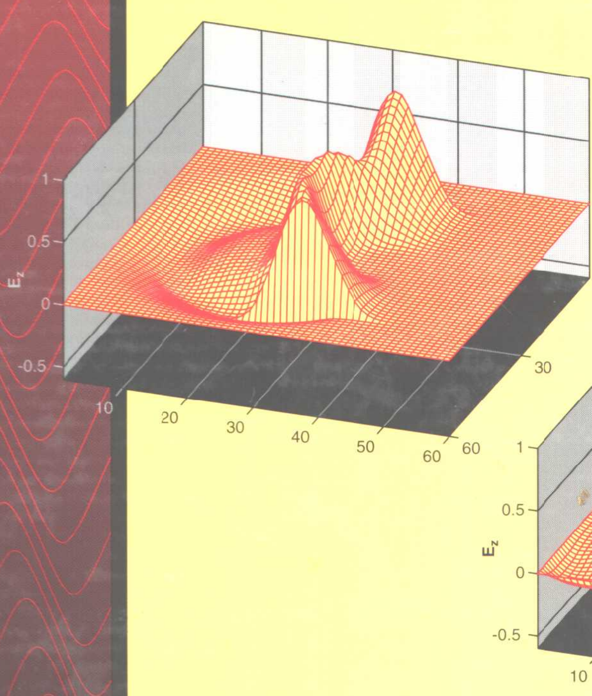
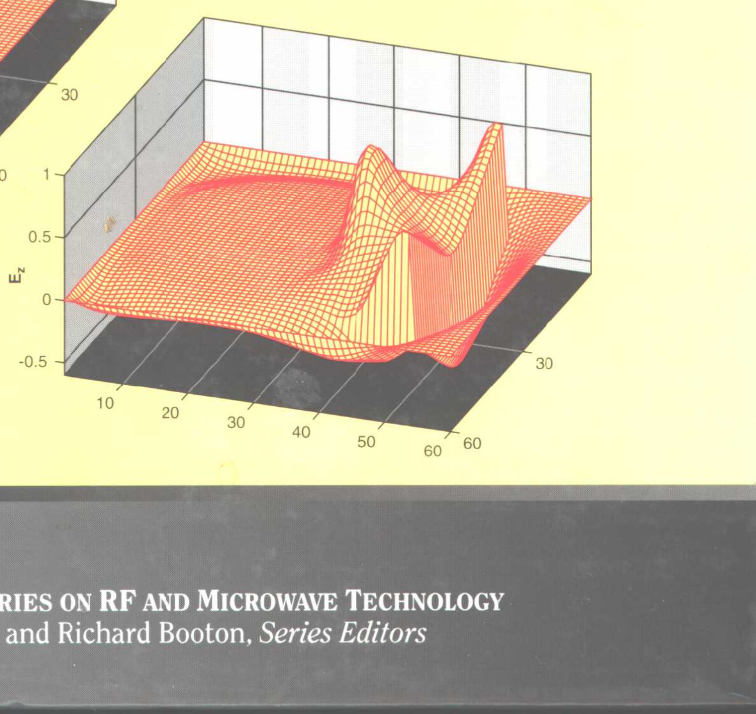
ELECTROMAGNETIC SIMULATION USING THE FDTD METHOD

DENNIS M. SULLIVAN







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To
Sully and Jane

Guide to the Book

PURPOSE

This book has one purpose only: to enable the reader or student to learn how to do three-dimensional electromagnetic simulation using the finite-difference time-domain (FDTD) method. It does not attempt to explain the theory of FDTD simulation in great detail. It is not a survey of all possible approaches to the FDTD method nor is it a "cookbook" of applications. It is aimed at those who would like to learn to do FDTD simulation in a reasonable amount of time.

FORMAT

This book is tutorial in nature. Every chapter attempts to address an additional level of complexity. The text increases in complexity in two major ways:

Dimension of Simulation	Type of Material
One-dimensional	Free space
Two-dimensional	Dielectric material
Three-dimensional	Lossy dielectric material
	Frequency-dependent material

The first section of Chapter 1 is one-dimensional simulation in free space. From there it progresses to more complicated media. In Chapter 2, the simulation of frequency-dependent media is addressed. Chapter 3 introduces two-dimensional simulation, including the simulation of plane waves and how to implement the perfectly matched layer. Chapter 4 introduces three-dimensional simulation. This is the approach taken throughout the book.

SPECIFIC CHOICES DEALING WITH SOME TOPICS

There are many ways to handle individual topics having to do with FDTD simulation. This book does not attempt to address all of them. In most cases, one single approach is taken and used throughout the book for the sake of clarity. My philosophy is that when first learning the FDTD method, it is better to learn one specific approach and learn it well rather than to be confused by switching among different approaches. In most cases, the approach being taught is this author's preference. That does not make it the only approach or even the best; it is just the approach that this author has found to be effective. In particular, the following are some of the choices that have been made.

1. **The use of normalized (Gaussian) units.** Maxwell's equations have been normalized by substituting

$$\tilde{\boldsymbol{E}} = \sqrt{\frac{\varepsilon_0}{\mu_0}}\boldsymbol{E}.$$

   This is a system called *Gaussian units,* which is frequently used by physicists. The reason for using it here is simplicity in the formulations. The E field and the H fields have the same order of magnitude. This has an advantage in formulating the perfectly matched layer (PML), which is a crucial part of FDTD simulation.
2. **The PML for boundary conditions.** The absorbing boundary conditions (ABCs) are an important topic in FDTD simulation. The ABCs prevent spurious reflections from the edge of the problem space. There are numerous approaches to this, but this book will use the perfectly matched layer (PML) for two- and three-dimensional simulation exclusively. (A simpler boundary condition will be used in one dimension just for convenience.) The reason is its effectiveness and versatility in working with different media.
3. **Maxwell's equations with flux density.** There is some leeway in forming the time-domain Maxwell's equations from which the FDTD formulation is developed. The following is used in Chapter 1:

$$\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{\varepsilon_0}\nabla\times\boldsymbol{H} - \frac{\sigma}{\varepsilon_0}\boldsymbol{E} \tag{1}$$

$$\frac{\partial \boldsymbol{H}}{\partial t} = \frac{1}{\mu_0}\nabla\times\boldsymbol{E}. \tag{2}$$

   This is a straightforward formulation and among the most commonly used. However, by Chapter 2, the following formulation using the flux density is adopted:

$$\frac{\partial \boldsymbol{D}}{\partial t} = \nabla\times\boldsymbol{H} \tag{3}$$

$$\boldsymbol{D} = \varepsilon\boldsymbol{E} \tag{4}$$

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

   In this formulation, it is assumed that the materials being simulated are nonmagnetic; that is, $\boldsymbol{H} = \frac{1}{\mu_0}\boldsymbol{B}$. However, we will be dealing with a broad range of dielectric properties, so Eq. (4) could be a complicated convolution. There is a reason for using this formulation: Eqs. (3) and (5) remain the same regardless of the material; any complicated mathematics stemming from the material is in Eq. (4). We will see that the solution of Eq. (4) can be looked upon as a digital filtering problem. In fact, the use of signal processing techniques in FDTD simulation will be a recurring theme in this book.

Z TRANSFORMS

As mentioned above, the solution of Eq. (4) for most complicated material can be viewed as a digital filtering problem. That being the case, the most direct approach to solving the problem is to take Eq. (4) into the Z domain. Z transforms are a regular part of electrical engineering education, but not that of physicists, mathematicians, and others. In teaching a graduate class on FDTD simulation, I begin the semester by teaching two topics in parallel: FDTD simulation and Z transforms. When we have progressed to the simulation of complicated dispersive materials, the students are ready to apply the Z transform theory. This had two distinct advantages over and above the simulation applications: (1) Electrical engineering students have had another application of Z transforms to strengthen their understanding of signal processing and filter theory; and (2) physics students and others now know and can use Z transforms, something that had not previously been part of their formal education. Based on my positive experience, I would encourage anyone using this book when teaching an FDTD course to consider this approach. However, I have left the option open to simulate dispersive methods with other techniques. The sections on Z transforms are optional and may be skipped. An appendix of Z transform theory is provided.

PROGRAMMING EXERCISES

The philosophy behind this book is that the student will learn by doing. Therefore, the majority of exercises involve programming. Each chapter has one or more FDTD programs written in C. If there is more than one program per chapter, typically only the first will be a complete program listing. The subsequent programs will not be complete, but will only show changes as compared to the first program. For instance, section 1 of Chapter 1 describes one-dimensional FDTD simulation in free space. The program fd1d_1.1.c at the end of the chapter is a simulation of a pulse in free space. Section 3 describes how a simple absorbing boundary condition is implemented. The program fd1d_1.2.c is not a complete program, but shows the changes necessary to fd1d_1.1.c to implement the boundary condition. Furthermore, important lines of code are highlighted in boldface.

PROGRAMMING LANGUAGE

The programs at the end of each chapter are written in the C programming language. The reasons for this are the almost universal availability of C compilers on UNIX workstations, and the fact that so many engineers and scientists know C. However, the reader should keep one fact in mind: most researchers who do large scientific programming use FORTRAN because FORTRAN was written for scientific programming. The structured style of C may have aesthetic appeal, but it typically runs slower than FORTRAN. This is particularly true of supercomputers.

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Contents

1

One-Dimensional Simulation with the FDTD Method

This chapter is a step-by-step introduction to the FDTD method. It begins with the simplest possible problem, the simulation of a pulse propagating in free space in one dimension. This example is used to illustrate the FDTD formulation. Subsequent sections lead to the formulation for more complicated media

1.1 ONE-DIMENSIONAL FREE SPACE FORMULATION

The time-dependent Maxwell's curl equations in free space are

$$\frac{\partial \boldsymbol{E}}{\partial t} = \frac{1}{\varepsilon_0} \nabla \times \boldsymbol{H} \tag{1.1a}$$

$$\frac{\partial \boldsymbol{H}}{\partial t} = -\frac{1}{\mu_0} \nabla \times \boldsymbol{E}. \tag{1.1b}$$

$\boldsymbol{E}$ and $\boldsymbol{H}$ are vectors in three dimensions, so in general, Eq. (1.1a) and (1.1b) represent three equations each. We will start with a simple one-dimensional case using only E_x and H_y, so Eq. (1.1a) and (1.1b) become

$$\frac{\partial E_x}{\partial t} = -\frac{1}{\varepsilon_0} \frac{\partial H_y}{\partial z} \tag{1.2a}$$

$$\frac{\partial H_y}{\partial t} = -\frac{1}{\mu_0} \frac{\partial E_x}{\partial z}. \tag{1.2b}$$

These are the equations of a plane wave with the electric field oriented in the x direction, the magnetic field oriented in the y direction, and traveling in the z direction.

Taking the central difference approximations for both the temporal and spatial derivatives gives

$$\frac{E_x^{n+1/2}(k) - E_x^{n-1/2}(k)}{\Delta t} = -\frac{1}{\varepsilon_0} \frac{H_y^n(k+1/2) - H_y^n(k-1/2)}{\Delta x} \tag{1.3a}$$

$$\frac{H_y^{n+1}(k+1/2) - H_y^n(k+1/2)}{\Delta t} = -\frac{1}{\mu_0} \frac{E_x^{n+1/2}(k+1) - E_x^{n+1/2}(k)}{\Delta x}. \tag{1.3b}$$

In these two equations, time is specified by the superscripts, i.e., "n" actually means a time $t = \Delta t \cdot n$. Remember, we have to discretize everything for formulation into the computer. The term "$n + 1$" means one time step later. The terms in parentheses represent distance, i.e., "k" actually means the distance $z = \Delta x \cdot k$. (It might seem more sensible to use Δz as the incremental step, since in this case we are going in the z direction. However, Δx is so commonly used for a spatial increment that I will use Δx.) The formulation of Eq. (1.3a) and (1.3b) assumes that the $\boldsymbol{E}$ and $\boldsymbol{H}$ fields are interleaved in both space and time. $\boldsymbol{H}$ uses the arguments $k + 1/2$ and $k - 1/2$ to indicate that the $\boldsymbol{H}$ field values are assumed to be located between the $\boldsymbol{E}$ field values. This is illustrated in Fig. 1.1. Similarly, the $n + 1/2$ or $n - 1/2$ superscript indicates that it occurs slightly after or before n, respectively.

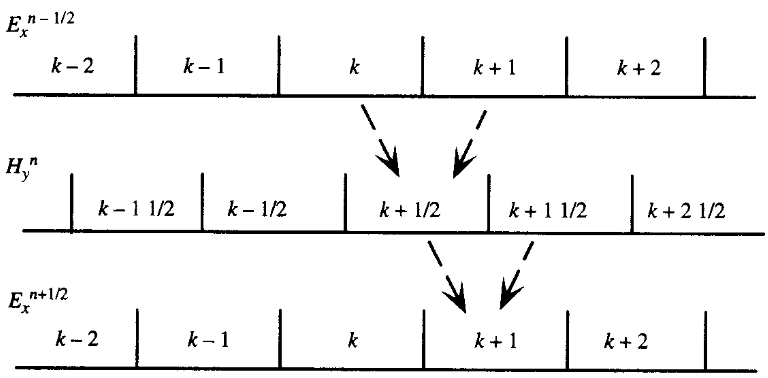

Figure 1.1 Interleaving of the E and H fields in space and time in the FDTD formulation. To calculate $H_y(k + 1/2)$, for instance, the neighboring values of E_x at k and $k + 1$ are needed. Similarly, to calculate $E_x(k + 1)$, the value of H_y at $k + 1/2$ and $k + 1\ 1/2$ are needed.

Eq. (1.3a) and (1.3b) can be rearranged in an iterative algorithm:

$$E_x^{n+1/2}(k) = E_x^{n-1/2}(k) - \frac{\Delta t}{\varepsilon_0 \cdot \Delta x}[H_y^n(k + 1/2) - H_y^n(k - 1/2)] \tag{1.4a}$$

$$H_y^{n+1}(k + 1/2) = H_y^n(k + 1/2) - \frac{\Delta t}{\mu_0 \cdot \Delta x}[E_x^{n+1/2}(k + 1) - E_x^{n+1/2}(k)]. \tag{1.4b}$$

Notice that the calculations are interleaved in both space and time. In Eq. (1.4a), for example, the new value of E_x is calculated from the previous value of E_x and the most recent values of H_y. This is the fundamental paradigm of the finite-difference time-domain (FDTD) method [1].

Eqs. (1.4a) and (1.4b) are very similar, but because ε_0 and μ_0 differ by several orders of magnitude, E_x and H_y will differ by several orders of magnitude. This is circumvented by making the following change of variables [2]:

$$\tilde{E} = \sqrt{\frac{\varepsilon_0}{\mu_0}}E. \tag{1.5}$$

Substituting this into Eqs. (1.4a) and (1.4b) gives

$$\tilde{E}_x^{n+1/2}(k) = \tilde{E}_x^{n-1/2}(k) - \frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{\Delta t}{\Delta x}[H_y^n(k + 1/2) - H_y^n(k - 1/2)] \tag{1.6a}$$

$$H_y^{n+1}(k + 1/2) = H_y^n(k + 1/2) - \frac{1}{\sqrt{\varepsilon_0\mu_0}}\frac{\Delta t}{\Delta x}[\tilde{E}_x^{n+1/2}(k + 1) - \tilde{E}_x^{n+1/2}(k)] \tag{1.6b}$$

Once the cell size Δx is chosen, then the time step Δt is determined by

$$\Delta t = \frac{\Delta x}{2 \cdot c_0} \tag{1.7}$$

where c_0 is the speed of light in free space. (The reason for this will be explained later.) Therefore,

$$\frac{1}{\sqrt{\varepsilon_0 \mu_0}} \frac{\Delta t}{\Delta x} = c_0 \cdot \frac{\Delta x / 2 \cdot c_0}{\Delta x} = \frac{1}{2} \tag{1.8}$$

Rewriting Eqs. (1.6a) and (1.6b) in C computer code gives the following:

```
ex[k] = ex[k] + 0.5*( hy[k-1] - hy[k] )          (1.9a)
hy[k] = hy[k] + 0.5*( ex[k] - ex[k+1] ).          (1.9b)
```

Note that the n or $n + 1/2$ or $n - 1/2$ in the superscripts is gone. Time is implicit in the FDTD method. In Eq. (1.9a), the ex on the right side of the equal sign is the previous value at $n - 1/2$, and the ex on the left side is the new value, $n + 1/2$, which is being calculated. Position, however, is explicit. The only difference is that $k + 1/2$ and $k - 1/2$ are rounded off to k and $k - 1$ in order to specify a position in an array in the program.

The program fd1d_1.1.c at the end of the chapter is a simple one-dimensional FDTD program. It generates a Gaussian pulse in the center of the problem space, and the pulse propagates away in both directions as seen in Fig. 1.2. The E_x field is positive in both directions, but the H_y field is negative in the negative direction. The following things are worth noting about the program:

1. The E_x and H_y values are calculated by separate loops, and they employ the interleaving described above.
2. After the E_x values are calculated, the source is calculated. This is done by simply specifying a value of E_x at the point k = kc, and overriding what was previously calculated. This is referred to as a "hard source," because a specific value is imposed on the FDTD grid.

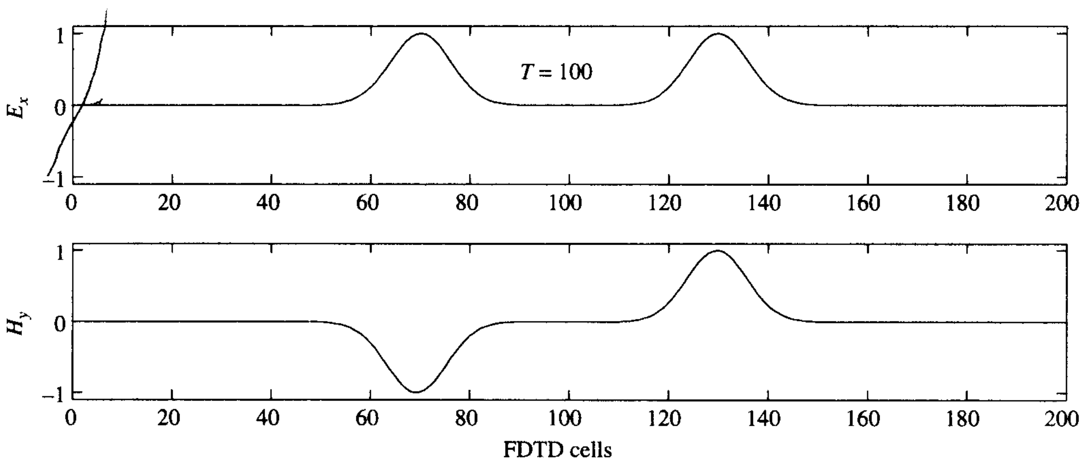

Figure 1.2 FDTD simulation of a pulse in free space after 100 time steps. The pulse originated in the center and travels outward.

PROBLEM SET 1.1

1. Get the program fd1d_1.1.c running. What happens when the pulse hits the end of the array? Why?
2. Modify the program so it has two sources, one at `kc - 20` and one at `kc + 20` (Notice that kc is the center of the problem space). What happens when the pulses meet? Explain this from basic EM theory.
3. Instead of E_x as the source, use H_y at `k = kc` as the source. What difference does it make? Try a two-point magnetic source at `kc - 1` and kc such that `hy[kc-1] = -hy[kc]`. What does this look like? What does it correspond to physically?

1.2 STABILITY AND THE FDTD METHOD

Let us return to the discussion of how we determine the time step. An electromagnetic wave propagating in free space cannot go faster than the speed of light. To propagate a distance of one cell requires a minimum time of $\Delta t = \Delta x / c_0$. When we get to two-dimensional simulation, we have to allow for the propagation in the diagonal direction, which brings the time requirement to $\Delta t = \Delta x / (\sqrt{2} c_0)$. Obviously, three-dimensional simulation requires $\Delta t = \Delta x / (\sqrt{3} c_0)$. This is summarized by the well-known "Courant Condition" [3, 4]:

$$\Delta t \leq \frac{\Delta x}{\sqrt{n} \cdot c_0}, \tag{1.10}$$

where n is the dimension of the simulation. Unless otherwise specified, throughout this book we will determine Δt by

$$\Delta t = \frac{\Delta x}{2 \cdot c_0}. \tag{1.11}$$

This is not necessarily the best formula; however, we will use it for simplicity.

PROBLEM SET 1.2

1. In fd1d_1.1.c, go to the two governing equations, Eq. (1.9a) and (1.9b), and change the factor 0.5 to 1.0. What happens? Change it to 1.1. Now what happens? Change it to .25 and see what happens.

1.3 THE ABSORBING BOUNDARY CONDITION IN ONE DIMENSION

Absorbing boundary conditions are necessary to keep outgoing $\boldsymbol{E}$ and $\boldsymbol{H}$ fields from being reflected back into the problem space. Normally, in calculating the $\boldsymbol{E}$ field, we need to know the surrounding $\boldsymbol{H}$ values; this is a fundamental assumption of the FDTD method. At the edge of the problem space we will not have the value to one side. However, we have an advantage because we know there are no sources outside the problem space. Therefore, the fields at the edge must be propagating outward. We will use these two facts to estimate the value at the end by using the value next to it [5].

Suppose we are looking for a boundary condition at the end where $k = 0$. If a wave is going toward a boundary in free space, it is traveling at c_0, the speed of light. So in one time step of the FDTD algorithm, it travels

$$\text{distance} = c_0 \cdot \Delta t = c_0 \cdot \frac{\Delta x}{c_0} = \frac{\Delta x}{2}.$$