Computing the Flow of Light

NONSTANDARD FDTD METHODOLOGIES FOR PHOTONICS DESIGN

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Contents

Preface

People often speak of *the* finite difference time domain (FDTD) method, as if there were only one such method, formulated long ago by wise sages and fixed for all time. This is not so. FDTD is a topic of active research, and its methodology is constantly evolving. FDTD and FDTD-like methods can be used to solve a wide variety of problems, including—but not limited to—the wave equation, Maxwell's equations, and the Schrödinger equation.

FDTD is particularly useful for investigating time-dependent phenomena. As the name suggests, the time evolution of a system is computed at discrete time steps, and periodic visualizations can show its time evolution—information that is not available in a frequency domain technique. This yields useful physical insights into transient processes as well as an intuitive feel for what is happening; often, one can see at a glance if something is wrong with a calculation—saving not only computer time, but more importantly, human time.

In essence, *an* FDTD algorithm is derived from *a* difference equation model of the differential equation to be solved by replacing the derivatives with finite difference (FD) expressions. (We use indefinite articles to indicate that there can be more than one FD model and more than one FDTD algorithm.) As we shall demonstrate in this book, the accuracy and stability of FDTD algorithms can be greatly improved by using what are called *nonstandard* FD models on which nonstandard FDTD is based.

High-precision FDTD is the primary—but not the only—subject of this book. Although the basic FDTD algorithm is simple, you will encounter many 'devils in the details' when you actually try to use it to solve a problem. Throughout this book we address these devilish details.

Green's functions, although an elegant analytical construct, are of limited practical use to solve differential equations because they can be difficult to find, but the discrete Green's function (DGF) of a difference equation model of a differential equation can be found using FDTD. The DGF methodology is a useful alternative to conventional FDTD for certain problems.

Besides introducing useful new methodologies, we have written this book to give our readers new insights, along with the analytical background necessary to develop their own methodologies to solve new problems on the leading edges of photonics and electromagnetics research. We explain not only how FDTD works, but why it works. We delve into the details of a few analytical solutions against which the numerical solutions can be compared to validate FDTD algorithms and to elucidate their limitations.

We make no attempt to be encyclopedic; rather, we delve deeply (devils in the details) into a few of the most important and basic methodologies. We hope that our readers can use this book to write their own working programs and improve on our methods, and that they will share what they have learned with the community.

Our experience in solving real-life applications with FDTD has taught us that there are two distinct communities: those who see FDTD from the algorithmic–computational point of view and those who see themselves primarily as users of black-box software. We believe that FDTD simulations must be guided by an understanding of Maxwell's equations and how these equations incorporate material properties. This premise is an important focus of this book. Through the simulation examples presented, we have attempted to show that FDTD and related techniques can be very useful in solving practical problems.

Summary of the Contents

- **Chapter 1** introduces FD expressions and develops the notation that is used throughout this book. The appendices give some supplementary advanced topics.
- **Chapter 2** introduces algorithms in general. We analyze a few example algorithms in detail and discuss their accuracy and numerical stability. In the appendices we introduce additional advanced topics. Working programs illustrate some of the main ideas.
- **Chapter 3** develops the basic concepts of the FDTD methodology using the simple harmonic oscillator as a vehicle. We then introduce the nonstandard FDTD methodology. We go on to develop analytic solutions for both the differential equations and their corresponding difference equations using Green's functions. In the appendices we review some basic mathematical concepts and derive Green's functions for differential and difference equations. We also analyze the accuracy and stability of a few simple FDTD algorithms.
- **Chapters 4–7** present FDTD for the wave equation. Following a strategy of stepwise increasing complexity, we start with the one-dimensional wave equation and develop the machinery needed to solve useful problems using FDTD. The appendices contain advanced

material (Green's function solutions, including the development of a Green's function for the finite difference form of the wave equation) and deal with various devilish details. We then extend these developments to two and three dimensions, and give some working example programs.
- **Chapter 8** provides a brief review of electromagnetic theory.
- **Chapters 9 and 10** present FDTD for Maxwell's equations. We first develop standard and nonstandard FDTD (the Yee algorithm) in one dimension, and then extend the methodology to two and three dimensions. This completes the development of conventional and *nonstandard* FDTD. Working programs illustrate some the main ideas.
- **Chapter 11** provides example problems.
- **Chapters 12–14** present FDTD for the dispersive case and provide example problems in photonics design. We introduce some of our latest research results on how to improve accuracy in the dispersive case. We solve some interesting photonics problems and discuss photonics design for engineering a subwavelength structure to have desired optical properties.

Audience

Our intended audience includes intelligent beginners such as students, experimental scientists who want to model their experiments, practical engineers, and theoretical researchers grappling with problems that cannot be solved analytically.

We introduce our nonstandard FDTD methodology as a useful tool for computational professionals as well as for beginners.

Very few members of the physics community are aware of the wide utility of FDTD methods, and we hope that our book will inform this group.

We include working FDTD programs that bring wave and electromagnetic phenomena to life. Our analytic solutions motivate the study of mathematical physics as a practical tool. Indeed, this book could be useful for teaching a mathematical physics, applied mathematics, or engineering class.

We also hope that advanced practitioners of FDTD can use this book to extend the nonstandard approach to other FDTD methodologies not covered here.

Finally, this book is written for researchers who want to develop new methodologies that go beyond those we have presented.

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