Advances in FDTD Computational Electrodynamics: Photonics and Nanotechnology

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Advances in FDTD Computational Electrodynamics

Photonics and Nanotechnology

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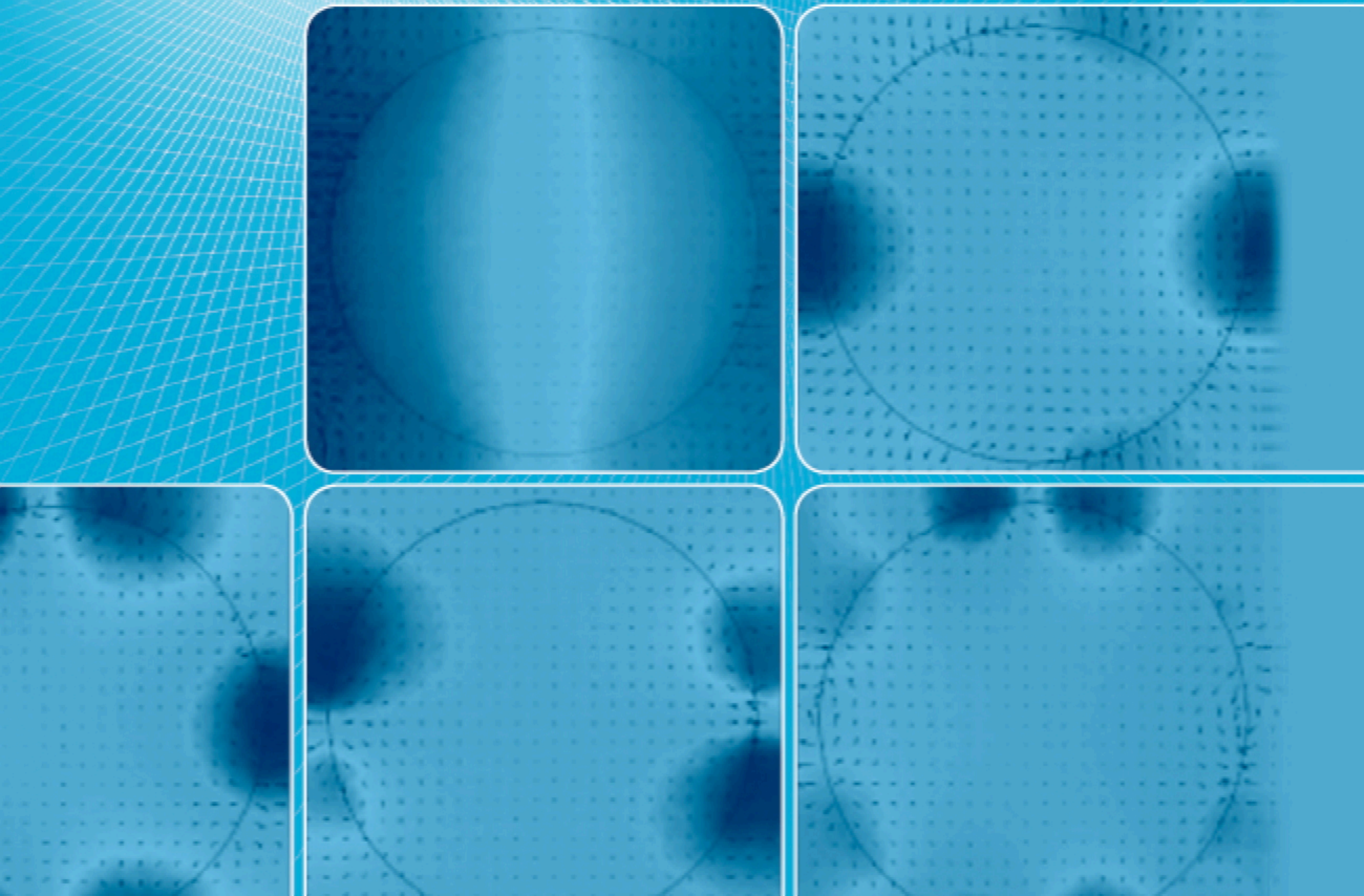

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Preface

Advances in photonics and nanotechnology have the potential to revolutionize humanity's ability to communicate and compute, to understand fundamental life processes, and to diagnose and treat dread diseases such as cancer. To pursue these advances, it is crucial to understand and properly model the interaction of light with nanometer-scale, three-dimensional (3-D) material structures. Important geometric features and material inhomogeneities of such structures can be as small as a few tens of atoms laid side by side. Currently, it is recognized that the most efficient computational modeling of optical interactions with such nanoscale structures is based on the numerical solution of the fundamental Maxwell's equations of classical electrodynamics, supplemented as needed by spatially localized hybrids with (the even more fundamental, but computationally much more intense) quantum electrodynamics.

Aimed at academic and industrial researchers working in all areas of photonics and nanotechnology, this book reviews the current state-of-the-art in formulating and implementing computational models of optical interactions with nanoscale material structures. Maxwell's equations are solved using the finite-difference time-domain (FDTD) technique, investigated over the past 40 years primarily in the context of electrical engineering by one of us (Taflove),[1] and over the past 12 years primarily in the context of physics by two of us (Oskooi and Johnson).[2]

On one level, this book provides an update (for general applications) of the FDTD techniques discussed in the 2005 Taflove-Hagness Artech book, *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, 3rd ed.[3] (It is assumed that the readers of this book are familiar with the fundamentals of FDTD solutions of Maxwell's equations, as documented therein.) On another level, this book provides a wide-ranging review of recent FDTD techniques aimed at solving specific current problems of high interest in photonics and nanotechnology.

Chapters 1 through 7 of this book present important recent advances in FDTD and pseudospectral time-domain (PSTD) algorithms for modeling general electromagnetic wave interactions. Capsule summaries of these chapters follow.

Chapter 1: "Parallel-Processing Three-Dimensional Staggered-Grid Local-Fourier-Basis PSTD Technique," by M. Ding and K. Chen. This chapter discusses a new staggered-grid, local-Fourier-basis PSTD technique for efficient computational solution of the full-vector Maxwell's equations over electrically large, open-region, 3-D domains. The new PSTD formulation scales more efficiently with the size of the computational domain than previous collocated-grid PSTD approaches, and very importantly, *avoids the Gibbs phenomenon artifact*. This allows accurate

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[1] See the online article, http://www.nature.com/milestones/milephotons/full/milephotons02.html, in which *Nature Milestones | Photons* cites Prof. Taflove as one of the two principal pioneers of numerical methods for solving Maxwell's equations.

[2] Dr. Oskooi and Prof. Johnson have led the development of a powerful, free, open-source implementation of a suite of FDTD Maxwell's equations solvers at the Massachusetts Institute of Technology (MIT): *Meep* (acronym for MIT Electromagnetic Equation Propagation), available online at http://ab-initio.mit.edu/meep. Meep has been cited in over 600 journal publications, and has been downloaded more than 54,000 times.

[3] As of September 2012, the combined citations of the three editions (1995, 2000, and 2005) of *Computational Electrodynamics: The Finite-Difference Time-Domain Method*, rank this book 7th on the *Google Scholar®* list of the most-cited books in physics, according to the Institute of Optics of the University of Rochester. See: http://www.optics.rochester.edu/news-events/news/google_scholar.html.

PSTD modeling of dielectric structures having high-contrast material interfaces. The complete algorithm is presented, including its implementation for a uniaxial perfectly matched layer (UPML) absorbing boundary condition (ABC).

Chapter 2: "Unconditionally Stable Laguerre Polynomial-Based FDTD Method," by B. Chen, Y. Duan, and H. Chen. This chapter discusses an efficient algorithm for implementing the unconditionally stable 3-D Laguerre polynomial-based FDTD technique with an effective PML ABC. In contrast to the conventional Laguerre-based FDTD method, which requires solving a very large sparse matrix, the new technique requires solving only six tri-diagonal matrices and three explicit equations for a full update cycle. This provides excellent computational accuracy — much better than alternating-direction-implicit FDTD approaches — and can be efficiently parallel-processed on a computing cluster.

Chapter 3: "Exact Total-Field/Scattered-Field Plane-Wave Source Condition," by T. Tan and M. Potter. This chapter discusses an efficient exact FDTD total-field/scattered-field plane-wave source suitable for arbitrary propagation and polarization angles, stability factors, and non-unity aspect ratios. This technique provides *zero leakage* of the incident plane wave into the scattered-field region to machine-precision levels. The incremental computer memory and execution time are essentially negligible compared to the requirements of the primary 3-D grid.

Chapter 4: "Electromagnetic Wave Source Conditions," by A. Oskooi and S. G. Johnson. This chapter provides a tutorial discussion of relationships between current sources and the resulting electromagnetic waves in FDTD simulations. The techniques presented are suitable for a wide range of modeling applications, from deterministic radiation, scattering, and waveguiding problems to nanoscale material structures interacting with thermal and quantum fluctuations. The chapter begins with a discussion of incident fields and equivalent currents, examining the principle of equivalence and the discretization and dispersion of equivalent currents in FDTD models. This is followed by a review of means to separate incident and scattered fields, whether in the context of scatterers, waveguides, or periodic structures. The next major topic is the relationship between current sources and the resulting local density of states. Here, key sub-topics includes the Maxwell eigenproblem and the density of states, radiated power and the harmonic modes, radiated power and the local density of states, computation of the local density of states in FDTD, Van Hove singularities in the local density of states, and resonant cavities and Purcell enhancement. Subsequent major topics include source techniques that enable covering a wide range of frequencies and incident angles in a small number of simulations for waves incident on a periodic surface; sources to efficiently excite eigenmodes in rectangular supercells of periodic systems; moving sources to enable modeling of Cherenkov radiation and Doppler-shifted radiation; and finally thermal sources via a Monte-Carlo/Langevin approach to enable modeling radiative heat transfer between complex-shaped material objects in the near field.

Chapter 5: "Rigorous PML Validation and a Corrected Unsplit PML for Anisotropic Dispersive Media," by A. Oskooi and S. G. Johnson. This chapter discusses a straightforward technique to verify the correctness of any proposed PML formulation, irrespective of its implementation. Several published claims of working PMLs for anisotropic media, periodic media, and oblique waveguides are found to be just instances of adiabatic pseudo-PML absorbers. This chapter also discusses an efficient, corrected, unsplit PML formulation for anisotropic dispersive media, involving a simple refactorization of typical UPML proposals. Appendixes to this chapter provide a tutorial discussion of the complex-coordinate-stretching basis of PML, and the application of coupled-mode theory to analyze and design effective adiabatic pseudo-PML absorbers for FDTD modeling of photonic crystals.

Chapter 6: "Accurate FDTD Simulation of Discontinuous Materials by Subpixel Smoothing," by A. Oskooi and S. G. Johnson. This chapter discusses an efficient local ("subpixel") dielectric smoothing technique for achieving second-order accuracy when modeling non-grid-aligned isotropic and anisotropic dielectric interfaces in a Cartesian FDTD grid. This technique is based on a rigorous perturbation theory (summarized in an Appendix), rather than on an *ad hoc* heuristic. It provides greatly improved accuracy relative to previous approaches without increasing the required computational storage or running time. Subpixel smoothing has an additional benefit: it allows the simulation to respond continuously to changes in the geometry, such as during optimization or parameter studies, rather than changing in discontinuous jumps as dielectric interfaces cross pixel boundaries. Additionally, it yields much smoother convergence of the error with grid resolution, which makes it easier to evaluate the accuracy of a simulation, and enables the possibility of extrapolation to gain another order of accuracy. Unlike methods that require modified field-update equations or larger stencils and complicated position-dependent difference equations for higher-order accuracy, subpixel smoothing uses the standard center-difference expressions, and is easy to implement in FDTD by simply preprocessing the materials.

Chapter 7: "Stochastic FDTD for Analysis of Statistical Variation in Electromagnetic Fields," by S. M. Smith and C. M. Furse. This chapter discusses a new stochastic FDTD (S-FDTD) technique that provides an efficient means to evaluate statistical variations in numerical simulations of electromagnetic wave interactions caused by random variations of the electrical properties of the model. The statistics of these variations are incorporated *directly* into FDTD, which computes an estimate of the resulting mean and variance of the fields at every point in space and time with a *single run*. The field variances computed using only two S-FDTD runs can effectively "bracket" the results using the brute-force Monte Carlo technique, the latter obtained after hundreds or thousands of runs. Hence, the S-FDTD technique offers a potentially huge savings in computation time, and opens up the possibility of assessing statistical parameters for applications in bioelectromagnetics, biophotonics, and geophysics where the material electrical properties have uncertainty or variability.

Chapters 8 through 20 provide a wide-ranging review of recent FDTD techniques aimed at solving specific current problems of high interest in photonics and nanotechnology. In order of presentation, the topics include:

- Plasmonics (emphasizing hybrid models with quantum mechanics), including active plasmonics, nonlocal electrodynamics, and modification of the optical properties of dye molecules closely bound to adjacent metal nanostructures
- Transformation electromagnetics, including non-diagonal anisotropic metamaterial cloaks
- Metamaterials, including periodic sub-wavelength optical structures comprised of non-rectangular-shaped plasmonic components
- Extensive tutorials on computational optical imaging for microscopy and nanoscale lithography
- Biophotonics applications, including imaging/characterization of intracellular structure and sensing of nanoscale intracellular anomalies indicative of early-stage cancer

- Non-paraxial spatial soliton propagation and interactions with nanoscale material structures
- Vacuum quantum phenomena, including blackbody radiation and electromagnetic fluctuations in dissipative open systems, and Casimir forces in arbitrary material geometries
- MIT's flexible, free FDTD software package, *Meep*.

Capsule summaries of these chapters follow.

Chapter 8: "FDTD Modeling of Active Plasmonics," by I. Ahmed, E. H. Khoo, and E. P. Li. This chapter discusses a recent hybrid FDTD/quantum mechanics technique for modeling plasmonic devices having integral semiconductor elements capable of providing gain upon pumping. The new technique integrates a Lorentz-Drude model to simulate the metal components of the device with a multi-level, multi-electron quantum model of the semiconductor component. Two examples of applications are summarized: amplification of a 175-fs optical pulse propagating in a thin, electrically pumped GaAs medium between two gold plates; and the resonance shift and radiation from a GaAs microcavity resonator with embedded gold nanocylinders. An appendix reviews the recent critical-points model for metal optical properties. This model is capable of providing a more accurate treatment of the bulk dielectric dispersion properties of various metals over a wider range of optical wavelengths than previously possible.

Chapter 9: "FDTD Computation of the Nonlocal Optical Properties of Arbitrarily Shaped Nanostructures," by J. M. McMahon, S. K. Gray, and G. C. Schatz. At length scales of less than ~10 nm, quantum-mechanical effects can lead to unusual optical properties for metals relative to predictions based on assuming bulk dielectric values. A full quantum-mechanical treatment of such nanostructures would be best, but is not practical for these structure sizes. However, it is possible to incorporate some quantum effects within classical electrodynamics via the use of a different dielectric model than that for the bulk metal. In this chapter, the quantum effect of primary interest requires a dielectric model wherein the material polarization at a point in space depends not only on the local electric field, but also on the electric field in its neighborhood. This chapter discusses a technique to calculate the optical response of an arbitrarily shaped nanostructure described by such a spatially nonlocal dielectric function. This technique is based on converting the hydrodynamic Drude model into an equation of motion for the conduction electrons, which then serves as a current field in the Maxwell-Ampere law. The latter is incorporated in a self-consistent manner in the FDTD solution of Maxwell's curl equations. Using this hybrid technique, modeling results for one-dimensional (1-D), two-dimensional (2-D), and 3-D gold nanostructures of variable size are presented. These results demonstrate the increasing importance of including nonlocal dielectric phenomena when modeling optical interactions with gold nanostructures as characteristic length scales of interest fall below ~10 nm.

Chapter 10: "Classical Electrodynamics Coupled to Quantum Mechanics for Calculation of Molecular Optical Properties: An RT-TDDFT/FDTD Approach," by H. Chen, J. M. McMahon, M. A. Ratner, and G. C. Schatz. This chapter discusses a new multiscale computational methodology to incorporate the scattered electric field of a plasmonic nanoparticle into a quantum-mechanical optical property calculation for a nearby dye molecule. For a given location of the dye molecule with respect to the nanoparticle, a frequency-dependent scattering response function is first computed using FDTD. Subsequently, the time-dependent scattered electric field at the dye molecule is calculated using this response function through a multidimensional Fourier transform to reflect the effect of polarization of the nanoparticle on the local field at the dye molecule. Finally, a real-time time-dependent density function theory (RT-TDDFT) approach is employed to obtain the desired optical property of the dye molecule in the presence of the nanoparticle's local electric field. Using this technique, enhanced absorption spectra of the N3 dye molecule and enhanced Raman spectra of the pyridine molecule are modeled, assuming proximity to a 20-nm-diameter silver nanosphere. The computed signal amplifications reflect the strong coupling between the wavelike response of the dye molecule's individual electrons and the collective action of the silver nanosphere's dielectric medium. Overall, this hybrid method provides a bridge spanning the gap between quantum mechanics and classical electrodynamics (i.e., FDTD) with respect to both length and time scales.

Chapter 11: "Transformation Electromagnetics Inspired Advances in FDTD Methods," by R. B. Armenta and C. D. Sarris. Transformation electromagnetics exploits the coordinate-invariance property of Maxwell's equations to synthesize the permeability and permittivity tensors of artificial materials to guide electromagnetic waves in specified manners. This chapter shows how employing a coordinate system-independent representation of Maxwell's equations based on the invariance principle provides powerful additional FDTD capabilities, including conformal modeling of curved material boundaries, incorporation of artificial materials providing novel wave-propagation characteristics, and time-dependent discretizations for high-resolution tracking of moving electromagnetic pulses. Examples of these enhanced FDTD capabilities are derived from coordinate transformations of Maxwell's equations involving projections onto the covariant-contravariant vector bases associated with a general curvilinear coordinate system.

Chapter 12: "FDTD Modeling of Non-Diagonal Anisotropic Metamaterial Cloaks," by N. Okada and J. B. Cole. Without proper care, the direct application of FDTD to simulate transformation-based metamaterials having non-diagonal anisotropic constitutive parameters is prone to numerical instabilities. This chapter discusses the basis, formulation, and validation of a technique to solve this instability problem by ensuring that the numerically derived FDTD equations are exactly symmetric. The crucial step in this technique involves finding the eigenvalues and diagonalizing the constitutive tensors. After this diagonalization, any of the previously reported FDTD algorithms for purely diagonal metamaterial cases can be applied. The technique is illustrated with a 2-D FDTD model of a transformation-based elliptical cylindrical cloak comprised of a non-diagonal anisotropic metamaterial. The cloak is found to greatly reduce both the bistatic radar cross-section and the total scattering cross-section of the enclosed elliptical perfect electric conductor (PEC) cylinder at the design wavelength. In fact, as the grid of the FDTD model is progressively refined, scattering by the cloaked PEC cylinder trends rapidly toward zero. However, the bandwidth of the effective scattering reduction is only ~4%; so narrow that it may be described as just a scattering null. This narrow bandwidth appears to limit practical applications of such cloaks.

Chapter 13: "FDTD Modeling of Metamaterial Structures," by Costas D. Sarris. This chapter provides an overview of the application of FDTD to several key classes of problems in metamaterial analysis and design, from two complementary perspectives. First, FDTD analyses of the transient response of several metamaterial structures of interest are presented. These include negative-refractive-index media and the "perfect lens," an artificial transmission line exhibiting a negative group velocity, and a planar anisotropic grid supporting resonance cone phenomena. Second, periodic geometries realizing metamaterial structures are studied. The primary tool used here is the sine-cosine method, coupled with the array-scanning technique. This tool is applied to obtain the dispersion characteristics (and, as needed, the electromagnetic field) associated with planar periodic positive-refractive-index and negative-refractive-index transmission lines, as well as the planar microwave "perfect lens" comprised of sections of 2-D transmission lines exhibiting both positive and negative equivalent refractive indices. The chapter continues with a review of the triangular-mesh FDTD technique for modeling optical metamaterials with plasmonic components, and how this technique could be coupled with the sine-cosine method to analyze periodic plasmonic microstructures requiring much better modeling of slanted and curved metal surfaces than is possible using a Cartesian FDTD grid and simple staircasing. Finally, the periodic triangular-mesh FDTD technique is applied to accurately obtain the dispersion characteristics and electromagnetic modes of a sub-wavelength plasmonic photonic crystal comprised of an array of silver microcylinders.

Chapter 14: "Computational Optical Imaging Using the Finite-Difference Time-Domain Method," by I. R. Capoglu, J. D. Rogers, A. Taflove, and V. Backman. This chapter presents a comprehensive and rigorous tutorial discussion of the theoretical principles that comprise the foundation for emerging electromagnetic-field models of optical imaging systems based on 3-D FDTD solutions of Maxwell's curl equations. These models provide the capability to computationally synthesize images formed by *every* current form of optical microscopy (bright-field, dark-field, phase-contrast, etc.), as well as optical metrology and photolithography. Focusing, variation of the numerical aperture, and so forth can be adjusted simply by varying a few input parameters – literally a *microscope in a computer*. This permits simulations of both existing and proposed novel optical imaging techniques over a 10^7:1 dynamic range of distance scales, i.e., from a few nanometers (the FDTD voxel size within the microstructure of interest) to a few centimeters (the location of the image plane where the amplitude and phase spectra of individual pixels are calculated). This tutorial shows how a general optical imaging system can be segmented into four self-contained sub-components (illumination, scattering, collection and refocusing), and how each of these sub-components is mathematically analyzed. Approximate numerical methods used in the modeling of each sub-component are explained in appropriate detail. Relevant practical applications are cited whenever applicable. Finally, the theoretical and numerical results are illustrated via several implementation examples involving the computational synthesis of microscope images of micro-scale structures. Overall, this chapter constitutes a useful starting point for those interested in modeling optical imaging systems from a rigorous electromagnetic-field point of view. A distinct feature of this approach is the extra attention paid to the issues of discretization and signal processing — a key issue in finite methods such as FDTD, where the electromagnetic field is only computed at a finite set of spatial and temporal points.

Chapter 15: "Computational Lithography Using the Finite-Difference Time-Domain Method," by G. W. Burr and J. T. Azpiroz. This chapter presents a comprehensive and rigorous tutorial discussion of the fundamental physical concepts and FDTD numerical considerations whose understanding is essential to perform electromagnetic-field computations for very large-scale integration (VLSI) optical lithography in the context of semiconductor microchip manufacturing. As the characteristic dimensions of VLSI technology shrink and complexity increases, the usual geometrical approximations of the electromagnetic field interactions underlying optical lithographic technology can become increasingly inaccurate. However, the accurate simulation of both immersion and extreme ultraviolet (EUV) lithographic systems is expected to be an increasingly critical component of semiconductor manufacturing for the foreseeable future. While rigorous computations of the required 3-D electromagnetic fields can be much slower than approximate methods, rapid turnaround is still crucial. The FDTD method offers advantages such as flexibility, speed, accuracy, parallelized computation, and the ability to simulate a wide variety of materials. In fact, FDTD computation of the electromagnetic fields underlying VLSI optical lithography currently offers the best combination of accuracy and turn-around time to understand and model field effects involved with relatively small patterns.

Chapter 16: "FDTD and PSTD Applications in Biophotonics," by I. R. Capoglu, J. D. Rogers, C. M. Ruiz, J. J. Simpson, S. H. Tseng, K. Chen, M. Ding, A. Taflove, and V. Backman. This chapter discusses qualitatively the technical basis and representative applications of FDTD and PSTD computational solutions of Maxwell's curl equations in the area of biophotonics. The FDTD applications highlighted in this chapter reveal its ability to provide ultrahigh-resolution models of optical interactions within individual biological cells, and furthermore to provide the physics kernel of advanced computational microscopy techniques. The PSTD applications highlighted in this chapter indicate its ability to model optical interactions with clusters of many biological cells and even macroscopic sections of biological tissues, especially in regard to developing an improved understanding of the physics of enhanced optical backscattering and turbidity suppression. In all of this, a key goal is to inform readers how FDTD and PSTD can put Maxwell's equations to work in the analysis and design of a wide range of biophotonics technologies. These technologies exhibit promise to advance the basic scientific understanding of cellular-scale processes, and to provide important medical applications (especially in early-stage cancer detection).

Chapter 17: "GVADE FDTD Modeling of Spatial Solitons," by Z. Lubin, J. H. Greene, and A. Taflove. The general vector auxiliary differential equation (GVADE) FDTD method, discussed in this chapter, is a powerful tool for first-principles, full-vector solutions of electromagnetic wave interactions in materials having combined linear and nonlinear dispersions. This technique provides a direct time-domain solution of Maxwell's curl equations without any simplifying paraxial, slowly varying envelope, or scalar approximations. Furthermore, it can be applied to arbitrary inhomogeneous material geometries, and both linear and nonlinear polarizations can be incorporated through the Maxwell-Ampere law. This chapter derives the GVADE FDTD time-stepping algorithm for the electromagnetic field in a realistic 2-D model of fused silica characterized by a three-pole Sellmeier linear dispersion, an instantaneous Kerr nonlinearity, and a dispersive Raman nonlinearity. (Here, the electric field is assumed to have both a longitudinal and a transverse component in the plane of incidence.) Next, the technique is extended to model a plasmonic metal characterized by a linear Drude dispersion. The GVADE FDTD method is then applied to model the propagation of single nonparaxial and overpowered spatial solitons; the interaction of a pair of closely spaced, co-propagating, nonparaxial spatial solitons; spatial soliton scattering by subwavelength air holes; and interactions between nonparaxial spatial solitons and thin gold films. It is concluded that the GVADE FDTD technique will find emerging applications in optical communications and computing involving micro- and nano-scale photonic circuits that require controlling complex electromagnetic wave phenomena in linear and nonlinear materials with important subwavelength features.

Chapter 18: "FDTD Modeling of Blackbody Radiation and Electromagnetic Fluctuations in Dissipative Open Systems," by J. Andreasen. This chapter discusses how the FDTD method can simulate fluctuations of electromagnetic fields in open cavities due to output coupling. The foundation of this discussion is the fluctuation-dissipation theorem, which dictates that cavity field dissipation by leakage is accompanied by thermal noise, simulated here by classical electrodynamics. The absorbing boundary of the FDTD grid is treated as a blackbody that radiates into the grid. Noise sources are synthesized with spectra equivalent to that of blackbody radiation at various temperatures. When an open dielectric cavity is placed in the FDTD grid, the thermal radiation is coupled into the cavity and contributes to the thermal noise for the cavity field. In the Markovian regime, where the cavity photon lifetime is much longer than the coherence time of thermal radiation, the FDTD-calculated amount of thermal noise in a cavity mode agrees with that given by the quantum Langevin equation. This validates the numerical model of thermal noise that originates from cavity openness or output coupling. FDTD simulations also demonstrate that, in the non-Markovian regime, the steady-state number of thermal photons in a cavity mode exceeds that in a vacuum mode. This is attributed to the constructive interference of the thermal field inside the cavity. The advantage of the FDTD numerical model is that the thermal noise is added in the time domain without any prior knowledge of cavity modes. Hence, this technique can be applied to simulate complex open systems whose modes are not known prior to the FDTD calculations. This approach is especially useful for very leaky cavities whose modes overlap strongly in frequency, as the thermal noise related to the cavity leakage is introduced naturally without distinguishing the modes. Therefore, the method discussed here can be applied to a wide range of quantum optics problems.

Chapter 19: "Casimir Forces in Arbitrary Material Geometries," by A. Oskooi and S. G. Johnson. This chapter discusses how FDTD modeling provides a flexible means to compute Casimir forces for essentially arbitrary configurations and compositions of micro- and nanostructures. Unlike other numerical techniques proposed for this application, FDTD is not structure specific, and hence, very general codes such as MIT's freely available *Meep* software (Chapter 20) can be used with no modifications. The chapter begins by establishing the theoretical foundation for the FDTD-Casimir technique. This is followed by a discussion of an efficient implementation employing a rapidly convergent harmonic expansion in the source currents. Then, means to extend the FDTD-Casimir technique to account for nonzero temperatures are presented. The chapter provides five FDTD-Casimir modeling examples, concluding with a fully 3-D simulation where the Casimir force transitions from attractive to repulsive depending on a key separation parameter. Overall, in addition to providing simulations of fundamental physical phenomena, these developments in FDTD-Casimir modeling may permit the design of novel micro- and nano-mechanical systems comprised of complex materials.

Chapter 20: "Meep: A Flexible Free FDTD Software Package," by A. Oskooi and S. G. Johnson. This chapter discusses aspects of the free, open-source implementation of the FDTD algorithm developed at the Massachusetts Institute of Technology (MIT): *Meep* (acronym for MIT Electromagnetic Equation Propagation), available online at http://ab-initio.mit.edu/meep. Meep is a full-featured software package, including, for example, arbitrary anisotropic, nonlinear, and dispersive electric and magnetic media modeling capabilities; a variety of boundary conditions including symmetries and PMLs; distributed-memory parallelism; spatial grids in Cartesian coordinates in one, two, and three dimensions as well as in cylindrical coordinates; and flexible output and field computations. Meep also provides some unusual features: advanced signal processing to analyze resonant modes; subpixel smoothing to accurately model slanted and curved dielectric interfaces in a Cartesian grid; a frequency-domain solver that exploits the time-domain code; complete scriptability; and integrated optimization facilities. This chapter begins with a discussion of the fundamental structural unit of "chunks" that constitute the FDTD grid and enable parallelization. Next, an overview is provided of Meep's core design philosophy of approaching the goal of continuous space-time modeling for inputs and outputs. The discussion continues with an explanation and motivation of Meep's somewhat-unusual design intricacies for nonlinear materials and PMLs; important aspects of Meep's computational methods for flux spectra and resonant modes; a demonstration of the formulation of Meep's frequency-domain solver that requires only minimal modifications to the underlying FDTD algorithm; and how Meep's features are accessible to users via a scripting interface. Overall, a free/open-source, full-featured FDTD package like Meep can play a vital role in enabling new research in electromagnetic phenomena. Not only does it provide a low barrier to entry for standard FDTD simulations, but the simplicity of the FDTD algorithm combined with access to the Meep source code offers an easy route to investigate new physical phenomena coupled with classical electrodynamics.

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