1

Introduction

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1.1 Photonics: The Countless Possibilities of Light Propagation

Following the advances in semiconductor physics that have allowed us to fully exploit the conducting properties of certain materials, thereby initiating the transistor revolution in electronics, in the last few decades a new frontier has opened up. The goal in this case is to control the optical properties of materials. An enormous range of technological developments would become possible if we could engineer materials that respond to light waves over a desired range of frequencies by perfectly reflecting them, or allowing them to propagate only in certain directions, or confining them within a specified volume.

Optical solutions to engineering problems are being increasingly found in many fields of application, including medicine, communication, entertainment, sensing and homeland security. Already, fibre optic cables, which simply guide light, have revolutionised the telecommunications industry. Laser engineering, high-speed computing and spectroscopy are just a few of the fields next in line to reap the benefits of the advances in optical materials. Photonics as a field covers today a huge range, from communications to science and technology applications, including laser manufacturing, biological and chemical sensing, display technology and optical computing.

For a number of reasons, ranging from a higher bandwidth to the inexpensiveness of optical fibre materials, components based on electric currents are more and more complemented or replaced by technology based on light. Relatively cheap, compact and highly sensitive photonic devices have already been commercialised for a variety of areas, and are expected to be basic blocks for all-optical integrated circuits, truly revolutionising the way we live.

All-optical systems are believed to be the best solution for the realisation of devices capable of meeting the high-performance characteristics required today and by next-generation telecommunications. In recent decades, with the advent of photonic crystals (PhCs) technology, the goal of a system capable of all-optical signal processing

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has made a giant step towards becoming a reality. PhC technology has brought the possibility of manipulating the light in a way that is basically not possible with conventional optical technology. Moreover, this capability of manipulating light is also obtained with an efficiency that is far greater than that obtained with conventional optical devices. However, the complex geometry of devices realised with PhC technology is still a challenge for fabrication technology, although significant progress has been made in this field, making it possible to fabricate new devices exploiting such technology. On the other hand, the mass production of these devices is still far from becoming a reality, and this can pose a serious threat to the development of PhC technology and, most of all, to the development of all-optical systems for ultra-fast telecommunication applications. In this aspect, numerical methods can be of vital help. Generally speaking, the possibility to predict the performance of a device before its practical fabrication can be a key factor towards the development of new and innovative technologies. With the exponential growth of the computational capabilities of modern personal computers (PCs), numerical methods have experienced a sudden expansion in all fields of engineering. This has made possible the development of new applications at a rate that was unthinkable just few decades ago.

Up to now, there have been many books on the market that treat numerical modelling techniques. However, the majority only concentrate on one or two numerical methods. The main goal of this book is to present a comprehensive state-of-the art of the latest modelling possibilities for the analysis and design of innovative devices for next-generation optical communications. Through a thorough analysis of the latest advances in numerical methods, weaknesses and drawbacks will be addressed in order to develop new techniques capable of dealing with simulations of optical devices in an innovative fashion, so as to increase either the accuracy or the efficiency. This aim will be reached through a deep theoretical analysis which will involve the physics behind the functionality of the optical device more directly in the core of the numerical techniques. In this way, the obtained numerical tools will be considered to be more state-of-the-art computational techniques than mere 'number-crunching' algorithms for the solution of Maxwell's equations. The gain in terms of efficiency can be usefully employed for the extension of the methods to dealing with three-dimensional (3D) problems without requiring a prohibitive amount of computational resources, making it possible to obtain simulation results closer to reality.

The information in the book will be essential for the reader to perform and excel in the following:

- Understanding the physics of light propagation in various photonic devices.
- Understanding Maxwell's equations, governing the propagation phenomena.
- Grasping basic concepts of general numerical modelling techniques.
- Deriving the equations underlying the numerical modelling techniques.
- Applying the gained knowledge of computational modelling to modelling photonic devices.

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These functions range from introductory (understanding the basic concepts) to advanced levels (application of the concepts to the numerical modelling of photonic devices).

1.2 Modelling Photonics

The last decade has witnessed dramatic progress and interest in micro- and nano-fabrication techniques of complex photonic devices. In almost all cases, an accurate quantitative theoretical modelling of these devices has to be based on advanced computational techniques that solve the corresponding, numerically very large linear, nonlinear or coupled partial differential equations.

Photonics is especially suitable for computation because Maxwell's equations are practically exact, the relevant material properties are well known and the length scales are not too small. Therefore, an exciting aspect of this field is that quantitative theoretical predictions can be made from first principles, without any questionable assumptions or simplifications. The results of such computations have consistently agreed with experiments. This makes it possible and preferable to optimise the design of photonic devices on a computer at an early stage, prior the actual fabrication. The computer becomes the pre-laboratory.

1.2.1 History of Computational Modelling

Many standard numerical techniques for the solution of partial differential equations have been applied to electromagnetics (EM), and each has its own particular strengths and weaknesses. High-quality 'black-box' software is widely available, including free, open-source programs. Indeed, computational photonics has matured so much that many are familiar only with the general principles and capabilities of the different tools.

In the last decades, a wide variety of numerical techniques have been developed and utilised for the design and optimisation of optical devices. Most of them have been successfully employed for the simulation of novel devices, mostly in two-dimensional (2D) space domains. Despite their powerful numerical capabilities, all these techniques possess drawbacks which pose limitations in the range of applicability of the methods to specific classes of problems. These drawbacks become more severe once the extension of these techniques to full-vectorial 3D space domains is considered. These limitations are mainly due to the huge growth in the computational burden required for 3D problems. Furthermore, if nonlinear phenomena are also taken into account, the limitations appear to be even more stringent.

Typically, the existing different numerical schemes can be divided into two main categories: time-domain and frequency-domain methods.

1.2.2 Frequency Domain

Before 1960, the principal approaches in the area of frequency-domain (FD) based numerical techniques involved closed-form and infinite-series analytical solutions, with numerical results from these analyses obtained using mechanical calculators. After 1960, the increasing availability of programmable electronic digital computers permitted such FD approaches to increase significantly in sophistication. Researchers were provided with a whole new range of capabilities offered by powerful high-level programming languages, such as Fortran, rapid random-access storage of large arrays of numbers, and computational speeds orders of magnitude faster than possible with mechanical calculators. In this period, the principal computational techniques for Maxwell's equations included high-frequency asymptotic methods and integral equations. However, these FD methods have some difficulties and drawbacks. For instance, while asymptotic analyses are well suited for modelling the scattering properties of large electrical shapes, such approaches are find it difficult to deal with nonmetallic material compositions and the volumetric complexity of a structure. On the other hand, integral equation methods can deal with material and structural complexity, however their need to construct and solve systems of linear equations limits the electrical size of possible models, especially those requiring detailed treatment of geometric details within a volume.

Although significant progress has been made in solving the ultra-large systems of equations generated by these FD integral equations, the capabilities of even the latest of such technologies cannot keep up with many volumetrically complex structures of recent engineering interest. This also holds for FD finite-element techniques, which generate sparse rather than dense matrices. Moreover, properties of material such as nonlinearities cannot be easily incorporated into the FD solutions of Maxwell's equations, which is a severe constraint, as research today is very active in the fields of active electromagnetic/electronic and electromagnetic/quantum-optical systems, such as high-speed digital circuits, and microwave and millimetre-wave amplifiers and lasers.

1.2.3 Time Domain

Since the arrival of the digital computer, which has profoundly changed the possibilities, time-domain (TD) modelling has offered efficient and flexible techniques to study computational electromagnetic propagation in linear and nonlinear optics.

There are two basic reasons for the success of TD over FD modelling: computational efficiency and problem requirements. Generally, when broadband information is analysed, a TD approach is intrinsically a more immediate choice because it provides a transient response whose bandwidth is limited only by the frequency content of the source, and the time and space sampling adopted in the numerical approach. Moreover, the computational efficiency of TD is also derived from its natural ability

P1: OTA/XYZ P2: ABC
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to adapt to parallel computer architectures. In addition, the TD approach can usually model problems involving time-varying media and components in a more straightforward way.

A representative example of the rapid growth in TD research is the popularity of the finite-difference time-domain (FDTD) method developed by Taflove.

There are general steps that need to be carried out in order to perform numerical modelling in the time domain:

- Develop time-dependent integral or Maxwell's curl equations.
- Discretise the equations in space and in time by means of an appropriate grid in space, and suitable basis and testing functions.
- Derive a set of equations that relate unknown with known quantities (starting from an initial value that usually is given by the source field).
- Generate a numerical solution of this initial-value problem in space and time.

1.2.4 Chapter Overview

Following this Introduction, from Chapter 2 to Chapter 4, beam propagation method (BPM) based numerical techniques in the frequency domain are considered. Amongst them, Chapter 2 presents the governing equations for the full-vectorial BPM, including the finite-element analysis, the perfectly matched layer (PML) scheme for the treatment of boundary conditions and the imaginary-distance BPM that provides the mode solver. Full-vectorial BPM is then assessed in Chapter 3, where modal analysis of rectangular waveguides is given together with analysis of photonic crystal fibres and liquid-crystal-based photonic crystal fibres.

The bidirectional BPM is presented in Chapter 4. The chapter focuses on the optical waveguide discontinuity problem, giving the formulation of a numerical method able to perform its simulation. After deriving the governing equations, the bidirectional BPM is assessed in several optical examples.

From Chapter 5, numerical techniques belonging to the area of time-domain schemes are presented. Chapter 5 starts with a recent innovative modification of the conventional finite-difference time-domain (FDTD) method: complex-envelope alternating-direction-implicit FDTD. After derivation of the fundamental equations to solve Maxwell's equations, assessment of the technique is driven by the specific problem of photonic crystal cavities.

In Chapter 6, the finite-volume time-domain (FVTD) method is proposed as a novel alternative technique to FDTD for the study of electromagnetic problems. The scheme is presented in detail, providing mathematical formulations, analysis of numerical stability and dispersion, and an efficient scheme for the treatment of the boundary conditions. The FVTD is then assessed in Chapter 7, where both linear and nonlinear devices are investigated.

Further modelling possibilities are given in Chapter 8, with the multiresolution time domain (MRTD) method. Basic concepts of the multiresolution analysis are given and its application to the solution of Maxwell's equations is explained. An accurate and innovative extension of the method to the analysis of second-order nonlinear effects is given. Assessment of the MRTD scheme is presented in Chapter 9, providing code validation in linear photonic devices. Assessment of the technique for the study of second-order nonlinear photonic devices follows in Chapter 10. Chapter 11 shows improvement of the nonlinear-MRTD scheme, with the inclusion of auxiliary differential equations (ADE) that enable the accurate analysis of linear dispersion of the media. Chapter 11 also presents validation of the code with generation of second harmonics in a planar waveguide and in a one-dimensional (1D) photonic crystal.

1.2.5 Overview of Commercial Software for Photonics

The continuous advancement of microwave circuits and electromagnetic devices towards increased functionality and performance requires simultaneous development of modelling tools that are able to keep up with the growing level of sophistication. In order to get a deeper insight into the field of computational electromagnetics (CEM) and grasp what is available in the market, the most widely used commercial packages are listed as follows:

– *COMSOL Multiphysics* (formerly *FEMLAB*) is a finite element analysis, solver and simulation software package for various physics and engineering applications, especially coupled phenomena, or multiphysics. COMSOL Multiphysics also offers an extensive interface to MATLAB and its toolboxes for a large variety of programming, pre-processing and post-processing possibilities.
– *FIMMWAVE* is a generic full-vectorial mode-finder for waveguide structures. FIMMWAVE combines both methods based on semi-analytical techniques with other more numerical methods such as finite difference or finite element.
– *CST MICROWAVE STUDIO®* (CST MWS) offers five solver modules; the Transient, Eigenmode, Frequency Domain, 'Resonant: Fast S-Parameter', 'Resonant: S-Parameter, Fields' (formerly known as Modal Analysis), and the Integral Equation Solver, each offering distinct advantages in their own domains. There are numerical advantages offered by the method used in most of the solvers, the finite integration technique (FIT).
– *CrystalWave* is a design environment for the layout and design of integrated optics components optimised for the design of photonic crystal structures. It is based on both FDTD and finite-element frequency-domain (FEFD) simulators and includes a masque file generator carefully optimised for planar photonic crystal structures.
– *Optiwave* is a suite of engineering design tools. Amongst these, there are *OptiFDTD,* which is based on the FDTD algorithm with second-order numerical accuracy

and the most advanced boundary condition – the uniaxial perfectly matched layer (UPML) boundary condition, and *OptiBPM*, which is based on the BPM.

– *RSoft's Photonic Component Design Suite* allows the design and the simulation of both passive and active photonic devices for optical communications, optoelectronics and semiconductor manufacturing. *FullWAVE* is a simulation tool for studying the propagation of light in a wide variety of photonic structures, including integrated and fibre-optic waveguide devices, as well as circuits and nanophotonic devices, such as photonic crystals. The software employs the FDTD method for the full-vector simulation of photonic structures. *BandSOLVE* is a design tool for the calculation of photonic band structures for all photonic crystal (PC) devices which employs the plane wave expansion (PWE) algorithm.

Indeed, commercial EM simulation programs available today provide powerful design tools, however no single numerical method provides a universal solution, and commercial codes often fail to accurately simulate high-end problems found in cutting-edge research. Therefore, research in computational EM is still essential to keep up with the increasing complexity of devices throughout the EM spectrum and has to develop parallel to fabrication technologies to allow the full establishment of the new photonic solutions in the market.

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