Computational Methods for Electromagnetic Phenomena

A unique and comprehensive graduate text and reference on numerical methods for electromagnetic phenomena, from atomistic to continuum scales, in biology, optical-to-micro waves, photonics, nano-electronics, and plasmas.

The state-of-the-art numerical methods described include:

- Statistical fluctuation formulae for dielectric constants
- Particle mesh Ewald, fast multipole method, and image-based reaction field methods for long-range interactions
- High-order singular/hyper-singular (Nyström collocation/Galerkin) boundary and volume integral methods in layered media for Poisson–Boltzmann electrostatics, electromagnetic wave scattering, and electron density waves in quantum dots
- Absorbing and UPML boundary conditions
- High-order hierarchical Nédélec edge elements
- High-order discontinuous Galerkin (DG) and Yee scheme time-domain methods
- Finite element and plane wave frequency-domain methods for periodic structures
- Generalized DG beam propagation methods for optical waveguides
- NEGF (non-equilibrium Green's function) and Wigner kinetic methods for quantum transport
- High-order WENO, Godunov and central schemes for hydrodynamic transport
- Vlasov–Fokker–Planck, PIC, and constrained MHD transport in plasmas

Wei Cai has been a full Professor at the University of North Carolina since 1999. He has also taught and conducted research at Peking University, Fudan University, Shanghai Jiaotong University, and the University of California, Santa Barbara. He has published over 90 refereed journal articles, and was awarded the prestigious Feng Kang prize in scientific computing in 2005.

"A well-written book which will be of use to a broad range of students and researchers in applied mathematics, applied physics and engineering. It provides a clear presentation of many topics in computational electromagnetics and illustrates their importance in a distinctive and diverse set of applications."

— Leslie Greengard, Professor of Mathematics and Computer Science,
Courant Institute, New York University

"... This is a truly unique book that covers a variety of computational methods for several important physical (electromagnetics) problems in a rigorous manner with a great depth. It will benefit not only computational mathematicians, but also physicists and electrical engineers interested in numerical analysis of electrostatic, electrodynamic, and electron transport problems. The breadth (both in terms of physics and numerical analysis) and depth are very impressive. I like, in particular, the way the book is organized: A physical problem is described clearly first and then followed by the presentation of relevant state-of-the-art computational methods..."

— Jian-Ming Jin, Y. T. Lo Chair Professor in Electrical and Computer Engineering,
University of Illinois at Urbana-Champaign

"This book is a great and unique contribution to computational modeling of electromagnetic problems across many fields, covering in depth all interesting multi-scale phenomena, from electrostatics in biomolecules, to EM scattering, to electron transport in plasmas, and quantum electron transport in semiconductors. It includes both atomistic descriptions and continuum based formulations with emphasis on long-range interactions and high-order algorithms, respectively. The book is divided into three main parts and includes both established but also new algorithms on every topic addressed, e.g. fast multipole expansions, boundary integral equations, high-order finite elements, discontinuous Galerkin and WENO methods. Both the organization of the material and the exposition of physical and algorithmic concepts is superb and make the book accessible to researchers and students in every discipline."

— George Karniadakis, Professor of Applied Mathematics, Brown University

"This is an impressive ... excellent book for those who want to study and understand the relationship between mathematical methods and the many different physical problems they can model and solve."

— Weng Cho Chew, First Y. T. Lo Endowed Chair Professor in Electrical and
Computer Engineering, University of Illinois at Urbana-Champaign

Computational Methods for Electromagnetic Phenomena

Electrostatics in Solvation, Scattering, and Electron Transport

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To my wife, Xiaoyan,

and

my children, Angela and Richard

Contents

Foreword

This is an impressive book by Wei Cai. It attempts to cover a wide range of topics in electromagnetics and electronic transport. In electromagnetics, it starts with low-frequency solutions of Poisson–Boltzmann equations that find wide applications in electrochemistry, in the interaction between electromagnetic fields and biological cells, as well as in the drift-diffusion model for electronic transport. In addition to low-frequency problems, the book also addresses wave physics problems of electromagnetic scattering, and the Schrödinger equation. It deals with dyadic Green's function of layered media and relevant numerical methods such as surface integral equations, and finite element, finite difference, and discontinuous Galerkin methods. It also addresses interesting problems involving surface plasmons and periodic structures, as well as wave physics in the quantum regime.

In terms of quantum transport, the book discusses the non-equilibrium Green's function method, which is a method currently in vogue. The book also touches upon hydrodynamic electron transport and the germane numerical methods.

This is an excellent book for those who want to study and understand the relationship between mathematical methods and the many different physical problems they can model and solve.

Weng Cho Chew, First Y. T. Lo Endowed Chair Professor, UIUC

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Preface

工若善其事，必先利其器

-Analects

Electromagnetic (EM) processes play an important role in many scientific and engineering applications such as the electrostatic forces in biomolecular solvation, radar wave scattering, the interaction of light with electrons in metallic materials, and current flows in nano-electronics, among many others. These are the kinds of electromagnetic phenomena, from atomistic to continuum scales, discussed in this book.

While the focus of the book is on a wide selection of various numerical methods for modeling electromagnetic phenomena, as listed under the entry "numerical methods" in the book index, attention is also given to the underlying physics of the problems under study. As computational research has become strongly influenced by the interaction from many different areas such as biology, physics, chemistry, and engineering, etc., a multi-faceted and balanced approach addressing the interconnection among mathematical algorithms and physical principles and applications is needed to prepare graduate students in applied mathematics, sciences, and engineering, to whom this book is aimed, for innovative advanced computational research.

This book arises from courses and lectures the author gave in various universities: the UNC Charlotte and the UC Santa Barbara in the USA, and Peking University, Fudan University, and Shanghai Jiao Tong University in China, to graduate students in applied mathematics and engineering. While attempts are made to include the most important numerical methods, the materials presented are undoubtedly affected by the author's own research experience and knowledge. The principle of selecting the materials is guided by Confucius's teaching above – "For a man to succeed in his endeavors, he must first sharpen his tools." So, emphasis is on the practical and algorithmic aspects of methods ready for applications, instead of detailed and rigorous mathematical elucidation.

The book is divided into three major parts according to three broadly defined though interconnected areas: electrostatics in biomolecules, EM scattering and guiding in microwave and optical systems, and electron transport in semiconductor and plasma media. The first two areas are based on atomistic and continuum

EM theory, while the last one is based on Schrödinger quantum and also Maxwell EM theories. Part I starts with a chapter on the statistical molecular theory of dielectric constants for material polarization in response to an electric field, an important quantity for molecular dynamics simulation of biomolecules and understanding optical properties of materials addressed in the book. Then, the Poisson–Boltzmann (PB) theory for solvation is given in Chapter 2, together with analytical approximation methods such as the generalized Born method for solvation energy and image methods for reaction fields in simple geometries. Chapter 3 contains various numerical methods for solving the linearized PB equations including the boundary integral equation methods, the finite element methods, and the immersed interface methods. Chapter 4 presents three methods to handle the long-range electrostatic interactions – a key computational task in molecular dynamics algorithms: the particle-mesh Ewald, the fast multipole method, and a reaction field based hybrid method.

Part II contains a large collection of numerical techniques for solving the continuum Maxwell equations for scattering and propagation in time- and frequency-domains. This part starts with Chapter 5 on Maxwell equations with physical and artificial boundary conditions; the former includes dielectric interface conditions and Leontovich impedance boundary conditions for conductors with a perfect electric conductor (PEC) as a limiting case, and the latter includes local absorbing boundary conditions and uniaxial perfectly matched layer (PML) boundary conditions. Chapter 6 discusses the dyadic Green's functions in layered media for the Maxwell equations in the frequency-domain and an algorithm for fast computation. High-order surface integral methods for electromagnetic scattering form the subject of Chapter 7, which includes the Galerkin method using mixed vector–scalar potentials and the Nyström collocation method for both the hyper-singular integral equations and the mixed vector–scalar potential integral equations, and combined integral equations for the removal of resonance in cavities. Finally, the high-order surface current basis for the Galerkin integral equation methods is discussed. Chapter 8 on edge elements begins with Nédélec's original construction of the $H(\text{curl})$ conforming basis, and then presents hierarchical high-order elements in 2-D rectangles and 3-D cubes and simplexes in both 2-D and 3-D spaces. Next, time-domain methods, including the discontinuous Galerkin (DG) methods with a high-order hierarchical basis and the finite difference Yee scheme, are given in Chapter 9. Numerical methods for periodic structures and surface plasmons in metallic systems are covered in Chapter 10, including plane-wave-based methods and transmission spectra calculations for photonics band structures, finite element methods, and volume integral equation (VIE) methods for the Maxwell equations. For the surface plasmons, the DG methods for dispersive media using auxiliary differential equations (ADEs) are given for Debye and Drude media. The final chapter (Chapter 11) of Part II contains numerical methods for Schrödinger equations for dielectric optical waveguides and quantum dots: a generalized DG method for the paraxial approximation in optical waveguides, and a VIE method for Schrödinger equations in quantum dots embedded in layered semiconductor materials.

Part III starts with Chapter 12 on the electron quantum transport models in semiconductors, which also includes the Fermi–Dirac distribution for electron gas within the Gibbs ensemble theory, density operators, and kinetic descriptions for quantum systems. The quantum transport topics discussed in this chapter include the Wigner transport model in phase space for electrons, the Landauer transmission formula for quantum transport, and the non-equilibrium Green's function (NEGF) method. Then, the non-equilibrium Green's function method in Chapter 13 contains the treatment of quantum boundary conditions and finite difference and finite element methods for the NEGF; the latter allows the calculation of the transmission coefficients in the Landauer current formula for general nano-devices. Chapter 14 includes numerical methods for the quantum kinetic Wigner equations with the upwinding finite difference and an adaptive cell average spectral element method. Chapter 15 first presents the semi-classical Boltzmann and continuum hydrodynamic models for multi-species transport, including electron transport, and then follows with the numerical methods for solving the hydrodynamic equations by Godunov methods and WENO and central differencing methods. In the final chapter of the book, Chapter 16, we first present the kinetic Vlasov–Fokker–Planck (VFP) model and the continuum magneto-hydrodynamic (MHD) transport model for electrons in plasma media. Then, several numerical methods are discussed including the VFP scheme in phase space, and the particle-in-cell and constrained transport methods for the MHD model, where the divergence-free condition for the magnetic field is specifically enforced.

In making this book a reality, I credit my education and ways of doing research to my teachers Prof. Zhongci Shi at the University of Science and Technology of China (USTC), who exposed me to the power of non-conforming finite element methods and reminded me that computational research must not be devoid of real science and engineering relevance, and Prof. David Gottlieb (my doctoral thesis advisor) at Brown University, who taught me that simplicity is the beauty in sciences. Also, my scientific research has benefited greatly from encouragements and interactions from the late Prof. Steven Orszag over many years. I have learnt much from interactions with my colleague physicist Prof. Raphael Tsu (a co-inventor of the resonant tunneling diode and a pioneer in quantum superlattices), whose sharp physics insight has always been an inspiration and pleasure during many of our discussions. My former colleague Prof. Boris Rozovsky has provided much encouragement, spurring me to undertake the challenge of writing this book, which started in 2004 during one of my many research collaboration visits with Prof. Pingwen Zhang at Peking University through the Beijing International Center for Mathematical Research. This book would not be possible without the joint research work undertaken in the past few decades with my colleagues Pingwen Zhang and Shaozhong Deng, and my former students and postdoctoral researchers Tiejun Yu, Yijun Yu, Yuchun Lin, Tiao Lu, Xia Ji, Haiyan Jiang, Min hyung Cho, Kai Fan, Sihong Shao, Zhenli Xu, and Jianguo Xin. Special thanks are given for the many useful discussions with my friends and other colleagues, which have contributed to my understanding of various topics in the book, including Achi Brandt, Alexandre Chorin, Weinan E, George Karniadakis, Chiwang Shu, Leslie Greengard, Jan Hesthaven, Tom Hagstrom, Eitan Tadmor, Shiyi Chen, Roger Temam, Weng Cho Chew, Jian-ming Jin, Dian Zhou, Xuan Zeng, Jinchao Xu, Jianguo Liu, Shi Jin, Houde Han, Jing Shi, Ann Gelb, Gang Bao, Jingfang Huang, Bob Eisenberg, Chun Liu, Xianjun Xing, Benzhuo Lu, Tao Tang, Jie Shen, Huazhong Tang, Tsinghua Her, Andrij Baumketner, Donald Jacobs, Guowei Wei, Vasily Astratov, and Greg Gbur. I would like to thank Dr. Shaozhong Deng for his careful reading of the manuscript; many improvements in the presentation of the book have resulted from his suggestions. The author is also grateful for the professional help and great effort of Ms. Irene Pizzie during the copy-editing of the book.

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