Wei Cai

Deterministic, Stochastic, and Deep Learning Methods for Computational Electromagnetics

Second Edition

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To my wife, Xiaoyan Duan (段晓艳) and my children, Angela Cai (蔡安琪) and Richard Cai (蔡敏琪)

Preface to the Second Edition

Since the publication of the first edition of this book over 11 years ago under the title "*Computational Methods for Electromagnetic Phenomena: Electrostatics in Solvation, Scattering, and Electron Transport*" [1], many new developments in numerical methods have occurred, especially in stochastic and deep learning approaches. To update it with the new results in these and other areas, this book is expanded with work from the research community as well as the author. The current edition, with a new title, includes numerical methods using stochastic and deep neural network learning as well as deterministic approaches.

The intended application area of the computational methods is still electromagnetics, and as in the first edition, the term "electromagnetics" is interpreted in a broader scope than the conventional one, which usually only covers classic electromagnetic (EM) processes described by Maxwell's equations such as EM wave scattering and propagation. Thus, in this book, electromagnetic processes in quantum systems governed by the Schrödinger equation such as electron transport in nanoelectronics and electronic structures of molecules and nanosystems, and their computations are also considered. As in the first edition, the book is divided into three parts: Part I, *Electrostatics*; Part II, *Electromagnetic Scattering*; and Part III, *Electron Transport and Electronic Structure*. Five new chapters have been included in the second edition, giving the book a total of 21 chapters. Corrections and minor changes and literature updates have also been made to other chapters.

The following summarizes the material in the new five chapters, while the synopsis of other 16 chapters can be found in the Preface to the First Edition. Chapter 4 discusses stochastic and probabilistic methods for solving electrostatic problems based on the Feynman–Kac formula, and hybrid boundary integral and random walk-on-spheres methods for solving mixed boundary value problems of the Laplace equation. A concise review of basic stochastic calculus, including Itô's formula and Dynkin's formula as well as stochastic differential equations (SDEs), is included for completeness, and their applications in SDE-based deep neural networks for PDEs are presented in Chap. 6. Chapter 5 discusses stochastic spectral methods for uncertainty quantification and their application in assessing the effect of geometric randomness on the capacitance of rough microchip interconnects. In Chap. 6, several deep neural network learning methods for solving PDEs are discussed, including Deep-Ritz, PINN, and WAN learning methods, as well as SDE-based learning algorithms by leveraging the connection between classic elliptic and parabolic PDEs and forward and backward SDEs. Then, methods to mitigate spectral biases of DNN learning toward lower frequencies are discussed, including phase-shift DNN (PhaseDNN) and multiscale DNN (MscaleDNN). Chapter 10 presents a newly developed fast multipole method for wave source interactions in layered media in three-dimensional space governed by Green's function of the Helmholtz equation. Finally, Chap. 17 discusses density functional theory for electronic structures of quantum systems and its computational methods, including plane wave and finite element methods as well as a linear scaling $O(N)$ density matrix minimization method using the discontinuous Galerkin discretization for computing ground state of quantum systems.

Acknowledgements

The second edition is based on author's lectures given at Southern Methodist University, and includes research work since the first edition by the author and his collaborators, particularly, Bo Wang, Wenzhong Zhang, Pei Elton Hsu, Chanhao Yan, Cuiyan Ding, Yijing Zhou, Ziqi Liu, Zhiqin Xu, Xiaoguang Li, Lizuo Liu, Qing He, Tiao Lu, Haiyan Jiang, and Hengliang Zhu. The author has benefited greatly from many discussions with Weinan E and George Karniadakis on deep learning and uncertainty quantification for scientific computing. The author thanks the following researchers for their help and input during the research, which led to some of the results covered in the book, including Minhyung Cho, Jack Douglas, Qiang Du, Tom Hagstrom, Jiequn Han, Jan Hesthaven, Shi Jin, Lin Lin, Chun Liu, Jianguo Liu, Qing Huo Liu, Jianfeng Lu, Michael Mascagni, Vassilis Papanicoloau, Karl K. Sabelfeld, Chiwang Shu, Tao Tang, Johannes Tausch, Lilian Wang, Dongbin Xiu, Jinchao Xu, Zhenli Xu, Haizhao Yang, George Yin, Lexing Ying, Haomin Zhou, and Tao Zhou. Moreover, the Preface to the First Edition credited many other collaborators of the author for contributing to the results covered in this book.

The author is also thankful for the support of the Betty Clements Chair in Applied Mathematics at Southern Methodist University for providing resources and time, which made the writing of this book possible. Appreciation is given to the US NSF for partially supporting some of the research presented in this book. The author thanks Science Press editor Liping Wang and Springer editors Daniel Wang and Prasanth Anandan for their support and efforts in publishing this book.

Notations

- The symbol Ω denotes random sample space in the probability space triplet $(\Omega, \mathcal{F}, P)$ when discussing stochastic methods in Chaps. 4–6 or a physical domain $\Omega \in \mathbb{R}^d$, $d = 2, 3$ in other chapters.
- The symbol E denotes the mathematical expectation in Chaps. 4–6 or an energy level of a physical system in Part III.

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July 2024

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Reference

1. W. Cai. Computational Methods for Electromagnetic Phenomena: electrostatics in solvation, scattering, and electron transport. Cambridge University Press; 2013.

Preface to the First Edition[1]

工欲善其事，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 multifaceted 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

[1] Published by Cambridge University Press, 2013 [1]. Chapter numbers in parentheses refer to the second edition.

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's 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(7) 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's equations for scattering and propagation in time and frequency domains. This part starts with Chapter 5(8) on Maxwell's 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(9) discusses the dyadic Green's functions in layered media for Maxwell's 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(11), 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(12) 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(13). Numerical methods for periodic structures and surface plasmons in metallic systems are covered in Chapter 10(14), including plane-wave-based methods and transmission spectra calculations for photonics band structures, finite element methods, and volume integral equation (VIE) methods for Maxwell's 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(15) 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(16) 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(18) 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(19) includes numerical methods for the quantum kinetic Wigner equations with the upwinding finite difference and an adaptive cell average spectral element method. Chapter 15(20) 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(21), 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.

Finally, special acknowledgements are given to the continual support of the Advanced Scientific Computing Research, Office of Science at the Department of Energy (under program managers Sandy Landsberg and Karen Pao) and the Army Research Office (under program manager Joseph Myers) over the years, and to NSF and NIH for allowing me to undertake the research that is behind many results contained in this book.

Charlotte, North Carolina, USA Wei Cai
September 2012

Reference

1. W. Cai. *Computational Methods for Electromagnetic Phenomena: electrostatics in solvation, scattering, and electron transport*. Cambridge University Press; 2013.

Contents

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Deterministic, Stochastic, and Deep Learning Methods for Computational Electromagnetics

Second Edition

This book provides a well-balanced and comprehensive treatment of computational electromagnetics based on clear physics, solid mathematical formulation, and state-of-the-art useful numerical methods in deterministic, stochastic, and deep neural network machine learning approaches for computer simulations of electromagnetic and transport processes in biology, microwave and optical wave devices, and nano-electronics. Computational research has become strongly influenced by interactions from many different areas including biology, physics, chemistry, and engineering. A multifaceted approach that addresses the interconnections among mathematical algorithms, physical foundations, and applications is much needed.

The second edition includes five new chapters and covers the following numerical methods: • Multi-scale DeepRitz and PINN, SDE-based, and spectral bias-free deep neural networks for solving PDEs. • Random walk-on-spheres methods for electrostatics. • Stochastic spectral methods for uncertainty quantifications in microchip designs. • Plane wave, finite element, and density matrix minimization DFT methods for electronic structure. • Fast multipole methods for Helmholtz equations in 3D layered media, particle-mesh Ewald, and image-based reaction field method for long-range interactions.• Discontinuous Galerkin, Bloch plane waves, hierarchical Nedelec edge elements, and high-order surface/volume integral equation methods for Maxwell's equations, periodic structures, and quantum dots. • Vlasov-Fokker-Planck and PIC methods for plasma MHD. • Quantum non-equilibrium Green's function and Wigner equation, and hydrodynamic WENO methods for electron transport. • Absorbing and PML boundary conditions for EM scattering, etc.

"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."

on the first edition, **Weng Cho Chew**, Distinguished Professor of Electrical and Computer Engineering, Purdue University.

"The second edition of this book is an even great and unique contribution to modern computational methods in modeling electromagnetic problems across classical and quantum fields. Both the organization of the material and the exposition of physical and algorithmic concepts are superb and make the book accessible to researchers and students in every discipline. Highly recommended!"

George Em Karniadakis, The Charles Pitts Robinson and John Palmer Barstow Professor of Applied Mathematics and Engineering, Brown University.

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