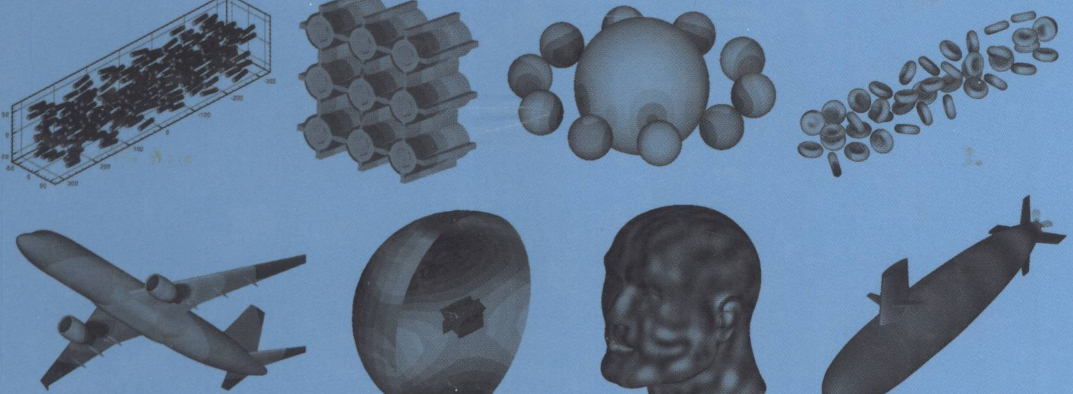
Fast Multipole Boundary Element Method

Theory and Applications in Engineering



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FAST MULTIPOLE BOUNDARY ELEMENT METHOD

The fast multipole method is one of the most important algorithms in computing developed in the 20th century. Along with the fast multipole method, the boundary element method (BEM) has also emerged as a powerful method for modeling large-scale problems. BEM models with millions of unknowns on the boundary can now be solved on desktop computers using the fast multipole BEM. This is the first book on the fast multipole BEM, which brings together the classical theories in BEM formulations and the recent development of the fast multipole method. Two- and three-dimensional potential, elastostatic, Stokes flow, and acoustic wave problems are covered, supplemented with exercise problems and computer source codes. Applications in modeling nanocomposite materials, biomaterials, fuel cells, acoustic waves, and image-based simulations are demonstrated to show the potential of the fast multipole BEM. This book will help students, researchers, and engineers to learn the BEM and fast multipole method from a single source.

Dr. Yijun Liu has more than 25 years of research experience on the BEM for subjects including potential; elasticity; Stokes flow; and electromagnetic, elastic, and acoustic wave problems, and he has published extensively in research journals. He received his Ph.D. in theoretical and applied mechanics from the University of Illinois and, after a postdoctoral research appointment at Iowa State University, he joined the Ford Motor Company as a CAE (computer-aided engineering) analyst. He has been a faculty member in the Department of Mechanical Engineering at the University of Cincinnati since 1996. Dr. Liu is currently on the editorial board of the international journals *Engineering Analysis with Boundary Elements* and the *Electronic Journal of Boundary Elements.*

Preface

This book is an introduction to the fast multipole boundary element method (BEM), which has emerged in recent years as a powerful and practical numerical tool for solving large-scale engineering problems based on the boundary integral equation (BIE) formulations. The book integrates the classical results in BIE formulations, the conventional BEM approaches applied in solving these BIEs, and the recent fast multipole BEM approaches for solving large-scale BEM models. The topics covered in this book include potential, elasticity, Stokes flow, and acoustic wave problems in both two-dimensional (2D) and three-dimensional (3D) domains.

The book can be used as a textbook for a graduate course in engineering and by researchers in the field of applied mechanics and engineers from industries who would like to further develop or apply the fast multipole BEM to solve large-scale engineering problems in their own field. This book is based on the lecture notes developed by the author over the years for a graduate course on the BEM in the Department of Mechanical Engineering at the University of Cincinnati. Many of the results are also from the research work of the author's group at Cincinnati and from the collaborative research conducted by the author with other researchers during the last 20 years.

The book is divided into six chapters. Chapter 1 is a brief introduction to the BEM and the fast multipole method. Discussions on the advantages of the BEM are highlighted. A simple beam problem is used to illustrate the idea of transforming a problem cast in a differential equation formulation to a boundary equation formulation. The mathematical background needed in this book is also reviewed in this chapter.

Chapter 2 is on the potential problems governed by the Poisson equation or the Laplace equation. This is the most important chapter of this book, which presents the procedures in developing the BIE formulations and the conventional BEM to solve these BIEs. The fundamental solution and its properties are discussed. Both the conventional (singular) and hypersingular BIE formulations are presented, and the weakly singular nature of these BIEs is emphasized. Discretization of the BIEs using constant and higher-order elements is presented, and the related issues in handling multidomain problems, domain integrals, and indirect BIE formulations are also reviewed. Finally, programming for the conventional BEM is discussed, followed by numerical examples solved by using the conventional BEM.

Chapter 3 is on the fast multipole BEM for solving potential problems, which lays the foundations for all the subsequent chapters. Detailed derivations of the formulations, discussions on the algorithms, and computer programming for the fast multipole BEM are presented for 2D potential problems, which will serve as the prototype of the fast multipole BEM for all other problems discussed in the subsequent chapters. Then, the fast multipole formulation for 3D potential problems is presented. Numerical examples of both 2D and 3D problems are presented to demonstrate the efficiency and accuracy of the fast multipole BEM for solving large-scale problems. This chapter should be considered the focus of this book and studied thoroughly if one wishes to develop his or her own fast multipole BEM computer codes for solving other problems.

The approaches and results developed in Chapters 2 and 3 are extended in the following three chapters to solve 2D and 3D elasticity problems (Chapter 4), Stokes flow problems (Chapter 5), and acoustic wave problems (Chapter 6). In each case, the related BIE formulations are presented first, and the same systematic fast multipole BEM approaches developed for 2D and 3D potential problems are extended to the related fast multipole formulations for the subject of the chapter. In all of these chapters, the use of the dual BIE formulations (a linear combination of the conventional and hypersingular BIEs) is emphasized because of the faster convergence rate they have for the fast multipole BEM solutions.

One important objective of this book is to demonstrate the applications of the fast multipole BEM in solving large-scale practical engineering problems. To this end, many numerical examples are presented in Chapters 3–6 to demonstrate the relevance and usefulness of the fast multipole BEM, not only in academic research but also in real engineering applications. Many of the large-scale models solved by using the fast multipole BEM are still beyond the reach of the domain-based numerical methods, which clearly demonstrates the huge potentials of the fast multipole BEM in many emerging areas such as modeling of advanced composites, biomaterials, microelectromechanical systems, structural acoustics, and image-based modeling and analysis.

Exercise problems are provided at the end of each chapter for readers to review the materials covered in the chapter. More exercise problems or course projects on computer-code development and software applications can be utilized to help further understand the methods and enhance the skills. All of the computer programs of the fast multipole BEM for potential, elasticity, Stokes flow and acoustic wave problems that are discussed in this book are available from the author's website (http://urbana.mie.uc.edu/yliu).

Analytical integration of the kernel functions for 2D potential, elasticity, and Stokes flow cases and the sample computer source codes for both the 2D potential conventional BEM and the fast multipole BEM are provided in the two appendices. Electronic copies of these source codes can be downloaded from this book's webpage at the Cambridge University Press website. References for all the chapters are provided at the end of the book.

The author hopes that this book will help to advance the fast multipole BEM – an elegant numerical method that has huge potential in solving many large-scale problems in engineering. The author welcomes any comments and suggestions on further improving this book in its future editions and also takes full responsibility for any mistakes and typographical errors in this current edition.

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The author would like to dedicate this book to Professor Frank J. Rizzo, a pioneer in the development of the BIE and BEM and now retired after teaching for more than 30 years at four universities in the United States. The author was fortunate enough to have the opportunity of conducting research under the guidance of Professor Rizzo from 1988 to 1994, first as a Ph.D. student and later as a postdoctoral research associate, at three of the four universities. His insightful views on the BIE and BEM, his serious attitude toward research, and his thoughtfulness to his students have had an immense and long-lasting impact on the author's academic career.

The author is also indebted to Professor Tianqi Ye, now retired from the Northwestern Polytechnical University in Xi'an, China, who introduced the author to the interesting subject of the BIE and BEM and taught the author that "everything important is simple" in order to pursue the best solutions for seemingly complicated problems.

The author would also like to thank Professor Naoshi Nishimura at Kyoto University for his tremendous help in the research on the fast multipole BEM in the past few years. During 2003–2004, the author spent eight months in Professor Nishimura's group and gained in-depth knowledge of the fast multipole BEM through almost daily discussions with Professor Nishimura. Much of the content presented in this book is based on the collaborative work of the author with Professor Nishimura's group at Kyoto University.

During the course of his research in the last 20 years, the author received a great deal of advice and help from many other researchers in the field of BIE and BEM. He would like to thank Professor David J. Shippy at the University of Kentucky and Professor Thomas J. Rudolphi at Iowa State University for their advice in different stages of his graduate studies, and Professor Subrata Mukherjee at Cornell University for the continued exchange of ideas and collaborations on several research endeavors that have benefited the author greatly.

The author would also like to sincerely thank his former and current students at the University of Cincinnati for their contributions to the research on the fast multipole BEM, especially to Drs. Liang Shen (3D potential and acoustics), Xiaolin Chen (image-based modeling with the fast multipole BEM), and Milind Bapat (2D and 3D acoustics). Without the students' research contributions, this book would not have been possible.

The author sincerely acknowledges the U.S. National Science Foundation for supporting his research and the Japan Society for the Promotion of Science Fellowship for Senior Researchers. Permission from Advanced CAE Research, LLC (ACR) in using the software package *FastBEM Acoustics*® for solving the 3D examples in Chapter 6 is also acknowledged.

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Finally, the author would like to express his gratitude to his wife Rue Yuan, son Fred, and family back in China for their understanding, encouragement, patience, and sacrifice during the last 20 years.

Acronyms Used in This Book

1D:	one-dimensional
2D:	two-dimensional
3D:	three-dimensional
BC:	boundary condition
BEM:	boundary element method
BIE:	boundary integral equation
BNM:	boundary node method
CBIE:	conventional boundary integral equation
CHBIE:	dual BIE formulation
CNT:	carbon nanotube
CPU:	central processing unit
CPV:	Cauchy principal value
DOF:	degree of freedom
EFM:	element-free method
FDM:	finite difference method
FEM:	finite element method
FFT:	fast Fourier transform
FMM:	fast multipole method
GMRES:	generalized minimal residual
HBIE:	hypersingular boundary integral equation
HFP:	Hadamard finite part
L2L:	local-to-local
M2L:	moment-to-local
M2M:	moment-to-moment
M2X:	multipole-to-exponential

MD: molecular dynamics
MEMS: microelectromechanical system

NURBS: nonuniform rational B spline

ODE: ordinary differential equation

PC: personal computer
PDE: partial differential equation

Q8: eight-node
Q4: four-node

RAM: random-access memory
RBC: red blood cell
RVE: representative volume element

SOFC: solid oxide fuel cell
STL: stereolithography

X2L: exponential-to-local
X2X: exponential-to-exponential

Contents

1 Introduction

1.1 What Is the Boundary Element Method?

The *boundary element method* (BEM) is a numerical method for solving boundary-value or initial-value problems formulated by use of *boundary integral equations* (BIEs). In some literature, it is also called the boundary integral equation method. Figure 1.1 shows the relation of the BEM to other numerical methods commonly applied in engineering, namely the *finite difference method* (FDM), *finite element method* (FEM), *element-free* (or *meshfree*) *method* (EFM), and *boundary node method* (BNM). The FDM, FEM, and EFM can be regarded as domain-based methods that use ordinary differential equation (ODE) or partial differential equation (PDE) formulations, whereas the BEM and BNM are regarded as boundary-based methods that use the BIE formulations. It should be noted that the ODE/PDE formulation and the BIE formulation for a given problem are equivalent mathematically and represent the local and global statements of the same problem, respectively. In the BEM, only the boundaries – that is, surfaces for three-dimensional (3D) problems or curves for two-dimensional (2D) problems – of a problem domain need to be discretized. However, the BEM does have similarities to the FEM in that it does use elements, nodes, and shape functions, but on the boundaries only. This reduction in dimensions brings about many advantages for the BEM that are discussed in the following sections and throughout this book.

1.2 Why the Boundary Element Method?

The BEM offers some unique advantages for solving many engineering problems. The following are the main advantages of the BEM:

- *Accuracy:* The BEM is a semianalytical method and thus is more accurate, especially for stress concentration problems such as fracture analysis of structures.