MULTIPHYSICS MODELING VOLUME 1

Numerical Modeling of Coupled Phenomena in Science and Engineering

Practical Use and Examples

M.C. Suárez Arriaga, J. Bundschuh and F.J. Dominguez-Mota
EDITORS

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NUMERICAL MODELING OF COUPLED PHENOMENA
IN SCIENCE AND ENGINEERING

Multiphysics Modeling

Series Editors

Jochen Bundschuh
International Technical Cooperation Program, CIM (GTZ/BA), Frankfurt, Germany
Instituto Costarricense de Electricidad (ICE), San José, Costa Rica
Royal Institute of Technology (KTH), Stockholm, Sweden

Mario-César Suárez Arriaga
Faculty of Sciences, Michoacan University UMSNH, Morelia, Mexico

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Volume 1

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M.C. Suárez Arriaga

Faculty of Sciences, Michoacan University UMSNH, Morelia, Mexico

J. Bundschuh

International Technical Co-operation Program, CIM (GTZ/BA), Frankfurt, Germany
Instituto Costarriense de Electricidad (ICE), San José, Costa Rica
Royal Institute of Technology (KTH), Stockholm, Sweden

F.J. Domínguez-Mota

Faculty of Sciences, Michoacan University UMSNH, Morelia, Mexico

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Numerical modeling is the process of obtaining approximate solutions to problems of scientific and/or engineering interest. The book series addresses novel mathematical and numerical techniques with an interdisciplinary emphasis that cuts across all fields of science, engineering and technology. It focuses on breakthrough research in a richly varied range of applications in physical, chemical, biological, geoscientific, medical and other fields in response to the explosively growing interest in numerical modeling in general and its expansion to ever more sophisticated physics. The goal of this series is to bridge the knowledge gap among engineers, scientists, and software developers trained in a variety of disciplines and to improve knowledge transfer among these groups involved in research, development and/or education.

This book series offers a unique collection of worked problems in different fields of engineering and applied mathematics and science, with a welcome emphasis on coupling techniques. The book series fills a need for up-to-date information on numerical modeling.

Faster computers and newly developed or improved numerical methods such as boundary element and meshless methods or genetic codes have made numerical modeling the most efficient state-of-art tool for integrating scientific and technological knowledge in the description of phenomena and processes in engineered and natural systems. In general, these challenging problems are fundamentally coupled processes that involve dynamically evolving fluid flow, mass transport, heat transfer, deformation of solids, and chemical and biological reactions.

This series provides an understanding of complicated coupled phenomena and processes, its forecasting, and approaches in problem solving for a diverse group of applications, including natural resources exploration and exploitation (e.g. water resources and geothermal and petroleum reservoirs), natural disaster risk reduction (earthquakes, volcanic eruptions, tsunamis), evaluation and mitigation of human-induced phenomena as climate change), and optimization of engineering systems (e.g. construction design, manufacturing processes).

Jochen Bundschuh
Mario-César Suárez Arriaga
(Series Editors)

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Preface

The behavior of solids and fluids in response to external forcings is of fundamental importance in many engineering fields as well as in the geosciences. Examples include recovery of oil and gas from subsurface reservoirs, hydrology of groundwater and surface water systems, stability of mechanical structures such as bridges, dams and mines, propagation of seismic waves and electrical current through geologic media, and assessment and mitigation of seismic and volcanic hazards. Much of the fundamental physics of the mechanics of continua—solids as well as fluids—was developed in the nineteenth and early twentieth century, and has been expressed as mathematical models that usually take the form of partial differential equations. Analytical solutions to these equations are possible only for idealized circumstances; hence the need for numerical approaches.

Numerical modeling is the process of obtaining approximate solutions to problems of scientific and/or engineering interest. It is as much an art as it is a science. Indeed, although the fundamental physics involved as well as the mathematical algorithms certainly are “science”, posing and solving numerical problems in a manner that will provide useful insights is an “art”, in the sense that it requires much creativity and intuition on behalf of the numerical analyst. Continuum mechanics problems when posed "rigorously" often defy solution, while approximations or simplifications may change the problem in such a way that it is no longer a good model of the real world process of interest. In addition, parameters and data defining a numerical problem are often incomplete, of limited accuracy, or unavailable. It is the art of the numerical analyst to find a middle ground between rigor and simplification, and to identify and implement conceptualizations and approximations that will be practically feasible while being responsive to the desired objectives.

Numerical methods have a long history and were broadly practiced in fields such as civil engineering long before the advent of the digital computer. The interest in and practice of these methods has grown explosively with the wide availability of ever faster computers at ever lower cost. At the same time the demands placed on numerical models have also greatly increased. Extraction of subsurface resources, such as oil, gas, minerals, and geothermal energy, demands ever more detailed models with more accurate representation of coupled processes that involve fluid flow, mass transport, deformation of solids, heat transfer, chemical reactions, and even microbial activity. Such processes may operate on a broad range of spatial scales. Similar trends are present in environmental protection, such as groundwater resources, subsurface disposal of chemical and radioactive wastes, and understanding human impacts on global climate, where insight is required for unprecedented time scales of hundreds to thousands of years or more. Problems involving multiple spatial and temporal scales are very difficult to solve, and are among the most active areas of current research.

The chapters in this monograph grew out of presentations made at the 4th International Congress and 2nd National Congress of Numerical Methods in Engineering and Applied Sciences, held in the beautiful city of Morelia, Michoacan, Mexico, in January 2007. The Congress brought together an international group of applied mathematicians, engineers, and geoscientists active in applications and further developments of numerical methods. Emphasizing the great diversity in numerical modeling problems and approaches in different fields of science and engineering, the articles assembled in this monograph also testify to the fact that there is much commonality and cross-fertilization. It is my hope that the studies presented in this volume will benefit researchers and practitioners alike by encouraging awareness and promoting new developments beyond narrow fields of specialization.

Karsten Pruess
Senior Scientist
Lawrence Berkeley National Laboratory
Earth Science Division
Berkeley, California, August 2007

Authors' CVs by Chapter

CHAPTER 1

Ismael Herrera-Revilla is one of the most distinguished personalities in science in Mexico. His undergraduate training was in engineering, chemistry, physics and mathematics, at the *Universidad Nacional Autónoma de México* (UNAM) in Mexico City. He obtained his PhD from the Division of Applied Mathematics at Brown University (Providence, Rhode Island, USA). He was awarded the three most prestigious scientific prizes in Mexico: the National Science Prize, the prize for Outstanding Research from the Mexican Academy of Sciences, and the "Luis Elizondo Prize", offered by the *Instituto Tecnológico de Monterrey*. He was the founder of the National Council for Science and Technology (CONACYT).
E-mail: iherrera@geofisica.unam.mx

CHAPTER 2

Igor Brilla graduated from the Faculty of Mathematics and Physics of Comenius University in Bratislava, Slovakia. He received his RNDr (*Rerum Naturalis* Doctor) degree and PhD degree in Applied Mathematics. He was a scientific researcher at the Institute of Applied Mathematics and Computing Technique of Comenius University and is currently a member of the Department of Mathematics, Faculty of Electrical Engineering and Information Technology, Slovak Technical University, Bratislava. His research activity is oriented to numerical solution of problems in engineering and applied sciences.
E-mail: igor.brilla@stuba.sk

CHAPTER 3

Lucas Jódar Sánchez received his *Licenciatura* of Mathematics and a PhD in Mathematics from the *Universidad de Valencia* (Spain). He is currently Professor of Mathematics at the *Universidad Politécnica de Valencia* (UPV), and he is the Director of the *Instituto de Matemática Multidisciplinar*. He is the author of more than 200 papers published in a variety of international journals of mathematics. His current research involves analytical and numerical solutions to deterministic and random differential equations.
E-mail: ljodar@imm.upv.es

Juan Carlos Cortés López received his *Licenciatura* of Mathematics degree from *Universidad de Valencia* (Spain). He was awarded a PhD in Mathematics from *Universidad Politécnica de Valencia* and is currently a Professor of Mathematics at the *Instituto de Matemática Multidisciplinar* at this university. His research interests include random differential equations and its applications to engineering, economy and life sciences.
E-mail: jccortes@imm.upv.es

Laura Villafuerte Altúzar received a Bachelor of Mathematics degree from the *Universidad Veracruzana* (Mexico), MSc in Applied Mathematics at the *Centro de Investigación en Matematicas* CIMAT (Mexico), and PhD in Mathematics at the *Universidad Politécnica de Valencia* (Spain). She is now a Professor of Mathematics at the *Universidad Autónoma de Chiapas* (Mexico). Her research interests include random differential equations and their applications.
E-mail: lva5@hotmail.com

CHAPTER 4

Pablo Barrera-Sánchez completed his BSc, MSc and PhD in Mathematics at the *Facultad de Ciencias* of the *Universidad Nacional Autónoma de México*. He has been a Lecturer at the *Universidad Nacional* since 1971. He is the main author or co-author of more than 50 research papers and proceedings, and thesis advisor for 34 undergraduates and 15 graduate students. He has been the main speaker at many scientific meetings and is the leader of the UNAMALLA workgroup. His research interests include numerical grid generation, nonlinear programming, numerical linear algebra, and computer programming.
E-mail: pablo@athena.fciencias.unam.mx

Guilmer González Flores is a student of the professor Pablo Barrera Sánchez, *Facultad de Ciencias* of the *Universidad Nacional Autónoma de México* (UNAM). His is interested in several areas of scientific computing.
E-mail: guilmerg@yahoo.com, gfgf@athena.fciencias.unam.mx

Francisco Javier Domínguez Mota completed undergraduate work in Physics and Mathematics at the *Facultad de Ciencias*, *Universidad Michoacana de San Nicolás de Hidalgo* in Morelia, Mexico. He obtained a Master in Mathematics from the Center of Research in Mathematics in Guanajuato, Mexico, and a PhD in Mathematics from the Faculty of Sciences of the *Universidad Nacional Autónoma de México*. He is a member of the National System of Researchers (SNI), and is a Professor and Researcher in Applied Mathematics at the *Facultad de Ciencias* of the *Universidad Michoacana de San Nicolás de Hidalgo*. Areas of research include numerical generation of structured grids from a direct variational setting and theory and applications of optimization in large scale problems.
E-mail: dmota@umich.mx

Justina Longina Castellanos Noda graduated in Mathematics-Cybernetics at the *Universidad de La Habana* (Cuba) and received a PhD in Mathematics from the Cuban Academy of Sciences (La Habana, Cuba). She has been an Invited Professor and Researcher at many institutions in Mexico including UNAM, UMSNH, IIMAS, IMTA and at the Department of Mathematics of the *Universidad Nacional del Sur* (Argentina). She developed several software codes for nonlinear optimization; optimal grid generation and linear and nonlinear parameter estimation. Her areas of research include large scale optimization methods, numerical methods for linear algebra, differential equations and applications, curvilinear grid generation, global optimization methods, aquifer parameter estimation, and theory and methods for inverse problems in dynamic systems.
E-mail: longinac@gmail.com

Angel Albeo Pérez Domínguez graduated in Mathematics from the Moscow State University "Lomonosov" (Russia), and obtained his PhD in Mathematics from the Computing Center of the Russian Academy of Sciences (Moscow, Russia). He is a researcher at the Institute of Cybernetics, Mathematics and Physics in Cuba. He is a permanent member of the Cuban National Committee for Scientific Degrees in Physics and Mathematics. He is also Head of the Numerical Methods group at the Institute of Cybernetics, Mathematics and Physics. Areas of research include numerical methods for linear algebra, differential equations, curvilinear grid generation, global optimization methods, aquifer parameter estimation, and theory and methods for inverse problems in dynamic systems.
E-mail: aperezdom@gmail.com

CHAPTER 5

Sergio Ivvan Valdez Peña received a BSc in Mechanical Engineering from the *Instituto Tecnológico de Celaya* (Mexico) and an MSc in Computer Sciences from the Center for Research in Mathematics. He is a graduate student pursuing a PhD in Computer Science in the Department of

Computer Science at *Centro de Investigación en Matemáticas* (CIMAT) in Guanajuato, Mexico. He has authored several papers about optimization and evolutionary computation. His research interests are evolutionary computation, multi-objective optimization, the finite element method, and estimation of distribution algorithms.
E-mail: ivvan@cimat.mx

Salvador Botello Rionda received a BSc degree in civil engineering from the *Universidad de Guanajuato* (Mexico), MSc in structures engineering from the *Instituto Tecnológico de Monterrey* (Mexico) and his PhD in *Ingeniero de Caminos Canales y Puertos* from the *Universitat Politècnica de Catalunya* (Barcelona, Spain). He is a Research Professor in the Department of Computer Sciences at the *Centro de Investigación en Matemáticas* (CIMAT) in Guanajuato, Mexico. His research interests are image processing and computational vision, optimization, the finite element method, evolutionary computation, multi-objective optimization and the development of finite element software for solid mechanics applications.
E-mail: botello@cimat.mx

Arturo Hernández Aguirre received a BSc in Electronics from the *Universidad Autónoma Metropolitana* (Mexico) and MSc and PhD in Computer Science from Tulane University (New Orleans, LA, USA). Dr. Hernández joined the Center for Research in Mathematics, where he works as a researcher at the Computer Science Department of the *Centro de Investigación en Matemáticas* (CIMAT) in Guanajuato, Mexico. He has authored over 14 journal papers, 100 conference papers and 6 book chapters. His areas of interest are evolutionary computation and bio-inspired algorithms for global and constrained optimization.
E-mail: artha@cimat.mx

CHAPTER 6

Arturo Ortiz-Tapia received a BSc, Biotechnological Agricultural Engineer from the *Universidad de Celaya* (Mexico), Part III Mathematical Tripos, University of Cambridge (UK), M.Phil. in Theoretical Chemistry, Cambridge University (UK), and PhD in Plasma Physics, Czech Technical University. He is currently a Scientific Researcher at the *Instituto Mexicano del Petroleo* in the Department of Molecular Engineering. His areas of interests are mathematical, numerical and computational modeling of fluids in porous media, and plasmas, numerical and computational analysis of differential equations, Analytical number theory and its applications in the solution of physical and engineering problems.
E-mail: aortizt@imp.mx

CHAPTER 7

Joel A. Rodriguez-Ceballos graduated from the School of Physics and Mathematics at the *Universidad Michoacana de San Nicolás de Hidalgo* (UMSNH) in Morelia, Mexico, and obtained his PhD degree from the Institute of Physics and Mathematics at the same university. He taught mathematics and physics at the *Instituto Tecnológico de Morelia* and UMSNH. Currently he is a postdoctoral fellow at the Institute of Mathematics of the *Universidad Nacional Autónoma de México* (UNAM). His specific research interests are applications of asymptotic methods to problems of wave propagation.
E-mail: joel@ifm.umich.mx

Petr Zhevandrov graduated from the Moscow State University (Russia) and obtained his PhD degree at the same university. He taught mathematics and worked as a researcher at the Moscow State University, Russian Academy of Sciences at the Institute for Problems in Mechanics, and the Center of Research and Advanced Studies of the *Instituto Politécnico Nacional* (Mexico). Currently he holds a professorship at the *Universidad Michoacana de San Nicolás de Hidalgo* in Morelia, Mexico and teaches mathematics at the *Universidad de La Sabana* (Chía, Cundinamarca,

Colombia). He is the author of various papers on applications of asymptotic methods to problems of wave propagation.
E-mail: pzhevand@zeus.umich.mx

CHAPTER 8

Ismael Herrera-Revilla (*see Chapter 1*)

CHAPTER 9

Rainald Löhner is the Director of the Center for Computational Fluid Dynamics at George Mason University (USA). He has received numerous awards in recognition of his work, serves on the editorial board of five international journals, has authored more than 500 scientific papers and has written a book on Applied CFD Techniques. His areas of interest include grid generation, field solvers (compressible and incompressible flow, acoustics, electromagnetics, heat and mass transfer), grid generation, visualization, optimal shape and process design and parallel computing, with particular emphasis on unstructured grids.
E-mail: rlohner@gmu.edu

Chi Yang is an Associate Professor at George Mason University (USA). She has been working in Computational Fluid Dynamics (CFD) to develop computational methods and tools for marine hydrodynamics applications for more than 20 years. She has over 120 scientific publications on a wide range of topics, including efficient Euler/RANS solvers based on unstructured grids and finite element method for compressible and incompressible flows; potential flow solvers based on a new boundary integral representation and Fourier-Kochin approach for free surface flows; fluid-structure interaction; shape optimization using CFD tools. She has given numerous invited lectures at conferences, universities, research institutes and private companies worldwide.
E-mail: cyang@gmu.edu

Eugenio Oñate directs the International Center for Numerical Methods (CIMNE) at the *Universitat Politècnica de Catalunya* in Barcelona, Spain. An internationally recognized figure, he is the author, co-author and editor of many books and scientific papers. He has been the president of the International Association of Computational Mechanics. His works covers many areas and aspects of computational mechanics: solids (beams, shells and solids, discrete elements, plasticity and damage models), fluids (solidification, hydro- and aerodynamics), electromagnetics, control and numerical methods (shell elements, fractional step procedures, particle finite element methods, finite point methods, finite calculus methods).
E-mail: onate@cimne.upc.edu

CHAPTER 10

Mustapha Benaouicha has a PhD in Mechanics from the University of La Rochelle, France. At present, he is Assistant Professor and Researcher at the Research Institute of French Naval Academy. Research interests include mathematical modeling and numerical simulation of fluid/structure interaction (FSI), reduction of models and Proper Orthogonal Decomposition (POD) method in FSI, and the Arbitrary Lagrangian-Eulerian (ALE) method.
E-mail: mustapha.benaouicha@ecole-navale.fr

Erwan Liberge holds a PhD in Mechanics in the University of La Rochelle (France). Research interest includes modeling and numerical simulation in Fluid Structure Interaction, Reduced Order Modeling (ROM) in mechanics. His main research concerns the use of the Proper Orthogonal Decomposition (POD) as a ROM tool in Fluid Structure Interaction. He works actually on the modeling of infiltration in buildings in the LEPTIAB, a research laboratory at the University of La Rochelle.
E-mail: erwan.liberge@univ-lr.fr

Aziz Hamdouni is a Professor of Theoretical Mechanics and it's responsible for the *Numerical Methods and Turbulence Modeling* group of the LEPTIAB laboratory at University of La Rochelle (France). Research interests include mathematical modeling and numerical simulation of fluid structure interaction (FSI), *reduced models*, modeling of turbulence, geometrical methods in mechanics (Lie groups and algebra, symmetry groups) and modeling of thin structures.
E-mail: aziz.hamdouni@univ-lr.fr

CHAPTER 11

Humberto Varum holds a Master's degree in Structures and a degree in Civil Engineering, both from the University of Porto, Portugal and a PhD in Civil Engineering from the University of Aveiro. He is an Assistant Professor in the Civil Engineering Department of the University of Aveiro, Portugal. His research combines experimental testing and nonlinear analytical modeling of structures. In his teaching he has specialized in the dynamic of structures, strength of materials and rehabilitation of structures. His main research interests include assessment, strengthening and repair of existing structures, structural testing and modeling, earthquake engineering and structural dynamics, and earth construction.
E-mail: hvarum@ua.pt

Aníbal Costa holds a PhD and a degree in Civil Engineering from the University of Porto. He is a Full Professor in the Civil Engineering Department of the University of Aveiro, Portugal. He is Vice-President of the Portuguese Society of Seismic Engineering. His research combines experimental testing and nonlinear analytical modelling of structural systems. In his teaching he has specialised in the reinforced concrete, dynamic of structures, and rehabilitation of structures. His main research interests include assessment, strengthening and repair of existing structures, structural testing and modeling, earthquake engineering and structural dynamics, and earth construction.
E-mail: agc@ua.pt

Hugo Rodrigues is a PhD student in the Civil Engineering Department of the University of Aveiro, Portugal. His MSc research focused on new numerical models for the representation of the seismic behavior of reinforced concrete structures. He is currently carrying out his PhD research in the field of seismic study of irregular reinforced concrete structures. His research interests include nonlinear modeling and analysis of reinforced concrete structures, seismic assessment and design of existing structures, and earthquake engineering.
E-mail: hrodrigues@ua.pt

CHAPTER 12

Israel Enrique Herrera Díaz obtained his Civil Engineer degree from the *Instituto Politécnico Nacional* (IPN) of Mexico and a Master of Science degree from the same institution. He is a PhD student in the Postgrade Division of the *Universidad Nacional Autónoma de México* (Mexico). He published a mathematical model of total sediment transport in estuarine and coastal zones at the 11th World Multiconference on Systemics, Cybernetics and Informatics in 2007.
E-mail: enrique_herrera@att.net.mx

Hermilo Ramírez-Leon obtained a Civil Engineer degree from the Faculty of Engineering of the *Universidad Nacional Autónoma de México* (Mexico), his Hydraulic Master Degree at the same institution and his PhD at the ECN-France. He was a Postdoctoral fellow at the same institution. He has held research positions at the Hydraulic Group of the Engineering Institute and the Environmental Pollution Group of the Research Electrical Institute. Presently, he works at the Mathematics and Computation Group of the *Instituto Mexicano del Petroleo*. He has published several papers and articles and three book chapters.
E-mail: hrleon@imp.mx

Carlos Couder Castañeda obtained his Bachelor of Applied Mathematics degree from the *Universidad Nacional Autónoma de México*. He received a Master of Science in Computer Science from the Research Center in Computation of the *Instituto Politécnico Nacional* in Mexico City. Presently, he works at the *Instituto Mexicano del Petroleo* and is in a doctoral program in Industrial Mathematics. He published a paper on the baroclinic mathematical modeling of fresh water plumes in the interaction river-sea in the International Journal of Numerical Analysis in 2005.
E-mail: ccouder@imp.mx, ccouder@hotmail.com

Ivan Campos obtained his degree of Civil Engineer from *Escuela Superior de Ingenieria y Arquitectura* (ESIA) of *Instituto Politécnico Nacional* in Mexico City. He has a MSc of Hydraulics from the same institution. At present, he works at the *Comisión Federal de Electricidad* (CFE) in the Department of Mathematical Models on modeling lakes, rivers, estuaries and coastal waters.
E-mail: bao_campos@hotmail.com

CHAPTER 13

Oleksandr Tkachenko received his PhD from the Kharkov National Aerospace University (Ukraine). Currently, he is an Associate Professor in the Department of Mechanical Engineering, *Instituto Tecnológico de Monterrey*, Campus Mexico in Monterrey. He has about 25 years of research experience in the field of aircraft mechanical engineering, CAD/CAE and computational mechanics. He has published papers in the area of foam properties and simulation. His research interests include computational mechanics, finite element methods, micromechanics, mechanics of composites, and numerical analysis.
E-mail: oleksandr.tkachenko@itesm.mx

Sergey Kanaoun received his Doctor of Science in Physics and Mathematics from the Russian Academy of Science (Moscow, Russia), and his PhD in Physics and Mathematics from the Saint Petersburg State University (Saint Petersburg, Russia). He is a Professor of the Mechanical Engineering Department of the *Instituto Tecnológico de Monterrey* (ITESM), State Mexico Campus. He is a member of the System of National Researchers (Level II), leader of the cathedra of composite materials. He is the author of three books and more than 100 papers in peer-reviewed international journals. His areas of interest include applied mathematics, numerical methods, continuum mechanics, the mechanics of composite materials, elasticity, plasticity, and wave propagation. His latest book "Self-Consistent Methods for Composites" vol. 1 and 2 was published by Springer in 2008.
E-mail: kanaoun@itesm.mx

CHAPTER 14

Dulce Yolotzin Medina received a BSc in Metallurgical and Materials Engineering from the *Instituto Politécnico Nacional* (Mexico), BSc in Industrial Engineering from the *Universidad Autónoma Metropolitana Azcapotzalco* (Mexico), and MSc in Materials Engineering from the same institution. He is currently an Assistant Professor at the *Universidad Autónoma Metropolitana Azcapotzalco*. Research interests include process modeling and simulation and luminescent films.
E-mail: dyolotzin@hotmail.com

Miguel Angel Barrón received a BSc in Metallurgical Engineering from *Universidad Nacional Autónoma de México*, MSc in Chemical Engineering from *Universidad Autónoma Metropolitana Iztapalapa* (Mexico); and PhD in Materials Science from *Instituto Politécnico Nacional* (Mexico). He is currently a Full Professor at the *Universidad Autónoma Metropolitana Azcapotzalco*. He has pursued research at the *Universidad Politécnica de Catalunia* (Barcelona, Spain) and the University of Notre Dame (Notre Dame, IN). His research interests include mathematical modeling of manufacturing processes, and nonlinear dynamics.
E-mail: bmma@correo.azc.uam.mx

CHAPTER 15

Carlos I. Rivera-Solorio received a BSc with honors from *Instituto Tecnológico de Monterrey*, (Mexico), MSc from the *Universidad Nacional Autónoma de México* and PhD in Mechanical Engineering from the University of Houston (USA). He is an Assistant Professor of the Mechanical Engineering Department at the *Instituto Tecnológico de Monterrey* (Mexico). He is also a current member of the National Research System of México. He specializes in fluid dynamics and thermal science. He has collaborated in projects on air pollution, solar energy, refrigeration, bioengineering and thermal design of power oil transformers.
E-mail: rivera.carlos@itesm.mx

Alejandro J. García-Cuéllar received his BSc degree in Chemical Engineering from *Instituto Tecnológico de Monterrey* (Mexico) and his PhD degree in Chemical Engineering from Rice University (Houston, Texas, USA). He is an Assistant Professor in the Department of Mechanical Engineering and Head of the Research Chair in Solar Energy and Thermal-Fluid Sciences of *Instituto Tecnológico de Monterrey*, Campus Monterrey. He is a member of the American Society of Heating, Refrigerating and Air Conditioning Engineers. His research interests and consulting experience include thermodynamics, process heat transfer and solar energy applications.
E-mail: ajgarcia@itesm.mx

Jesús J. González Villafaña received his M.S. degree in Energy Technology from *Instituto Tecnológico de Monterrey*, Mexico. He has held engineering positions within the oil services industry.
E-mail: A00789976@itesm.mx

Ramón Ramírez-Tijerina He received a BS degree in Mechanical Engineering and his MS degree in Energy Technology (both with honors) from *Instituto Tecnológico de Monterrey* (Mexico). He has worked as an engineer in the automotive industry and has collaborated on projects with industry in the thermal sciences. His research areas of interest are computational fluid dynamics and heat transfer.
E-mail: ramon.ramirez@claut.com.mx

CHAPTER 16

Alfonso Campos-Amezcua holds a PhD in Mechanical Engineering from *Universidad de Guanajuato* (Mexico). Since 1994 he is working at the *Instituto de Investigaciones Eléctricas* from Mexico (IIE) as a researcher, involved in developing technologies for maintenance, diagnostics and remaining life prediction of turbine components using thermodynamic, fluid flow and heat transfer analysis. He has 33 publications at internationals conferences and journals and also he has worked as a professor at two Mexican universities.
E-mail: acampos@iie.org.mx

Zdzislaw Mazur holds a PhD in Mechanical Engineering. He worked as turbine manufacturer in "Zamech Elblag" Poland for 20 years. Since 1988 he is working at the *Instituto de Investigaciones Eléctricas* from Mexico as a researcher, involved in developing technologies for repair, maintenance, remaining life prediction and life extension of turbine components. He has 154 publications at internationals conferences and journals, also 17 patents awarded and he is reviewer of 6 International journals.
E-mail: mazur@iie.org.mx"mazur@iie.org.mx

Gloria Ma. García-Gómez graduated as Bachelor of Computer Science at the School of Statistics and Informatics of the *Universidad de Veracruz* (Mexico). She works at the *Instituto de Investigaciones Eléctricas* since 1997, where she has participated in the development of several diagnostic systems based on personal computers that allow to monitor the behavior of turbomachinery. She has 11 registered copyrights and 3 publications at international conferences.
E-mail: gmgarcia@iie.org.mx

Armando Gallegos-Muñoz is a professor at the *Universidad de Guanajuato* (Mexico) and his activity inside of the research is oriented to the analysis of heat transfer and dynamics of fluids applying CFD. He has participated in the direction of 3 PhD theses, 20 MSc and 20 bachelor's degrees. He has 12 papers published in journals and 40 papers at international conferences.
E-mail: gallegos@salamanca.ugto.mx

José M. Riesco-Ávila obtained his degree in Mechanical Engineering in 1984, and his MSc degree in 1986, in Mexico. He holds a PhD from *Universidad Politécnica de Valencia* (Spain). Over the last five years, his research activities have included a project funded by national administrations and two R&D projects funded by the industry. Scientific publications include 11 articles published in international journals and 38 papers at scientific conferences.
E-mail: riesco@salamanca.ugto.mx

Jorge A. Alfaro-Ayala is a Mechanical Engineer from the *Universidad de Guanajuato* (Mexicio); he is a MSc Student and he works in the analysis of heat transfer and dynamics of fluids applying CFD.
E-mail: elronaldodi@hotmail.com

Vicente Pérez-García is a Mechanical Engineer from the *Universidad de Guanajuato* (Mexico); he is a MSc. Student and he works in finite element analyses.
E-mail: eniac04@hotmail.com

J. J. Pacheco-Ibarra holds a PhD in Mechanical Engineering from the *Universidad de Guanajuato* (Mexico). He is a professor at the *Universidad Michoacana de San Nicolás de Hidalgo* and he works on thermoeconomic evaluation of power plants.
E-mail: jjpi15@hotmail.com

CHAPTER 17

Soheil Porkhial is a Professor associated of the Mechanical Engineering Department of the Azad University, Karaj Branch. He obtained a PhD degree in Mechanical Engineering from the University of Amirkabir (former Tehran Polytechnic). He has been working as a renewable energy expert since 1996. Presently he is the Head of the Iranian Geothermal Energy Agency (IGEA) and the Head of geothermal department in the renewable energy organization (SUNA). He teaches courses in dynamics, heat transfer, thermodynamics and refrigerators. He has published twelve conference papers, three ISI papers and three books. His research field is heat transfer, cooling and renewable energy.
E-mail: porkhial@yahoo.com

CHAPTER 18

Sadegh Babaii Kochekseraii holds a BS ME from Imperial College London (UK), MSc in Engineering Solid Mechanics, and PhD in Applied Mechanics from UMIST Manchester (UK). He was invited to *Instituto Tecnológico de Monterrey*, Campus Estado de Mexico as an International Visiting Professor of Mechanical Engineering and is currently a full time Professor and researcher there. His previous industrial experience included international consultancy in the oil and power generation industry. He is currently supervisor of all advanced engineering and computational mechanics areas of *Chrysler de Mexico*. He is a member of Mexico's National System of Investigators.
E-mail: sb878@chrysler.com

Sergey Kanaoun (*see Chapter 13*)

CHAPTER 19

José Manuel Arnau Pilar received his *Licenciatura* of Mathematics degree from the *Universidad de Valencia* (Spain) and a PhD in Mathematics from the *Universidad Politécnica de Valencia* (UPV),

Spain. He develops his research at the *Instituto de Matemática Multidisciplinar* at the UPV. His research interests include numerical methods for conservation laws and fluid dynamics.
E-mail: jmarnau@uv.es

José Vicente Romero Bauset received his *Licenciatura* of Physics degree from the *Universidad de Valencia* (Spain) and a PhD in Physics from the *Universidad de Valencia*. He is currently Professor of Mathematics at the *Instituto de Matemática Multidisciplinar* in the *Universidad Politécnica de Valencia*. His research interests include numerical methods for conservation laws and fluid dynamics.
E-mail: jvromero@imm.upv.es

María Dolores Roselló Ferragud received her *Licenciatura* of Mathematics degree from the *Universidad de Valencia* (Spain) and a PhD in Mathematics from the *Universidad Politécnica de Valencia*. She is currently Professor of Mathematics in the *Instituto de Matemática Multidisciplinar* at this university. Her research interests include numerical methods for conservation laws and fluid dynamics.
E-mail: drosello@imm.upv.es

Antonio J. Torregrosa Huguet received his *Licenciatura* of Physics degree from the *Universidad de Valencia* (Spain) and a PhD in Physics from *Universidad Politécnica de Valencia*. He is currently Professor of Thermal Engines at this university. He develops his research at the *Instituto CMT—Motores Térmicos* at the UPV. His research interests include gas dynamics and acoustics of internal combustion engines, and heat transfer and thermal management of diesel engines.
E-mail: atorreg@mot.upv.es

CHAPTER 20

Raymundo Antonio Cordero Cuevas is a Civil Engineer from *Instituto Tecnológico de Monterrey*, Mexico, and a postgraduate in Computer Science and Structures. He was granted a PhD degree in Civil Engineering by University of Wales Swansea (Swansea University, UK) for his research work on computational mechanics, particularly on limit state analysis. His work has focused on the development and application of computer methods for the analysis of structures and mechanical components, including elastic and plastic models. Other recent research interests include the development of deployable structures and the use of modern optimization techniques for the solution of a variety of finite element models.
E-mail: rcordero@itesm.mx

Javier Bonet graduated in Civil Engineering in Barcelona and completed a PhD at Swansea University (UK). He has carried out research in finite element methods and computational mechanics for over 20 years, specializing in areas such as large strain solid mechanics, superplastic forming, membrane analysis, meshless methods, limit analysis and fluid structure interaction. He has co-authored two books in the field: "Finite Elements—A Gentle Introduction" and "Nonlinear continuum Mechanics for Finite Element Analysis" and published over 150 academic papers in international journals and conference proceedings. He is currently a Professor of Civil Engineering at Swansea University and the Head of the School of Engineering.
E-mail: j.bonet@swansea.ac.uk

CHAPTER 21

Arturo Ortiz-Tapia (*see Chapter 6*)

CHAPTER 22

Sergio Gallegos-Cázares obtained a BSc in Civil Engineering from *Universidad Anahuac* (Mexico), and MSc and PhD from the University of Illinois at Urbana-Champaign (USA), with a specialty

in Structural Engineering. He has consulted for the Mexican Institute of Cement and Concrete, 1980–1981 and performed research at the *Instituto de Investigaciones Eléctricas*. He is a Professor of Civil Engineering at the *Instituto Tecnológico de Monterrey,* Campus Monterrey and has served as Head of the program and Graduate Program Coordinator. His teaching experience includes basic and advanced solid mechanics, finite elements, plates, shells, structural dynamics and reinforced concrete. His research interests are computational mechanics, modeling of concrete structures and blood flow simulation.
E-mail: sergio.gallegos@itesm.mx

Jorge Cortés is a Professor of Mechanical Engineering, *Instituto Tecnológico de Monterrey*, Mexico. He conducts research in bioengineering with the School of Medicine focusing in the design of medical devices and medical simulation.
E-mail: jcortes@itesm.mx
Lucio Florez is a Professor of Bioengineering, *Instituto Tecnológico de Monterrey*. He conducts research on endothelial cells and on vascular flow and behavior.
E-mail: lflorez@itesm.mx

Alfredo Robles is a graduate student in the Civil Engineering department of *Instituto Tecnológico de Monterrey*, Mexico.

CHAPTER 23

Roger González Herrera obtained his BEng in Civil Engineering at the *Universidad Autónoma de Yucatán* (Mexico), Master's degree at the University of Waterloo (Canada), and PhD studies in the Geophysics Institute at the *Universidad Nacional Autónoma de México*. He is a Research Associate and a member of the Hydraulics and Hydrology Academic Group, at the Engineering School of the *Universidad Autónoma de Yucatán*. His research interests are coastal zones hydrodynamics, saline intrusion and its controlling factors, groundwater resources evaluation, groundwater flow and contaminant transport modeling in karstic aquifers and the application of science to practical problems of contamination.
E-mail: gherrera@uady.mx

CHAPTER 24

Dennys Armando López-Falcón holds BS and PhD degrees from the Physic-Mathematical Science Faculty and the Institute of Physics, respectively, both in the *Benemérita Universidad Autónoma de Puebla* (BUAP), in Puebla, Mexico, and MS degree from the Center of Research and Advanced Studies of the *Instituto Politécnico Nacional* (CINVESTAV-IPN), all in physics. He is a member of the Society of Petroleum Engineers. Currently, he is a scientist in the Hydrocarbon Recovery Program of the *Instituto Mexicano del Petroleo*. His research interests include mathematical modeling and numerical simulation of multiphase flow and transport through porous media and physics of enhanced oil recovery methods.
E-mail: dalopez@imp.mx

Martín Díaz-Viera is an Engineer in Applied Mathematics from the Moscow Power Engineering Institute (Russia). He obtained both his MSc and PhD degrees in Mathematical Modeling of Earth Systems from *Universidad Nacional Autónoma de México*. He is currently working at the *Instituto Mexicano del Petroleo*. His research areas are mathematical modeling, numerical methods for PDEs, geostatistics and stochastic modeling for reservoir characterization.
E-mail: mdiazv@imp.mx

Ismael Herrera-Revilla (*see Chapter 1*)

Ezequiel Rodríguez-Jáuregui obtained his PhD in Theoretical Physics from the *Instituto de Fisica*, *Universidad Nacional Autónoma de México*. He was a Posdoctoral research fellow at DESY Theory Group in Hamburg, Germany as well as a Research Associate at the *Instituto Mexicano del*

Petroleo. He is currently a Research Professor at the *Departamento de Fisica Universidad de Sonora* (Mexico).
E-mail: ezequiel.rodriguez@correo.fisica.uson.mx

CHAPTER 25

Martín Díaz-Viera (*see Chapter 24*)

Dennys Armando López-Falcón (*see Chapter 24*)

Ismael Herrera-Revilla (*see Chapter 1*)

CHAPTER 26

Jesús Alberto Rodríguez Castro has a PhD in Civil Engineering from the University of Kansas (USA). His dissertation was on a groundwater management model using conditional simulation and chance-constrained optimization. Presently he is Professor and Researcher at the *Universidad Michoacana de San Nicolás de Hidalgo* (Mexico). His main areas of research are design, analysis, and operation of water resources systems, groundwater resources management modeling, hydrologic and hydraulic modeling, storm water engineering, flood control systems design and operation, and hydrodynamic and water quality modeling.
E-mail: jealroca@yahoo.com.mx

CHAPTER 27

Mario César Suárez Arriaga studied Physics at the *Facultad de Ciencias* of the *Universidad Nacional Autónoma de México* (UNAM), Mathematics and Mechanics in the University of Toulouse-III and at the Institute of Theoretical and Applied Mechanics, University of Paris VI, France. He was granted a PhD degree on mathematical modeling of geothermal systems from the Faculty of Engineering of UNAM. He co-founded *Geotérmia*, a Mexican journal specialized on geothermal energy. He worked 19 years in geothermal reservoir engineering at the federal utility producing electricity in Mexico. Presently he is Professor-Researcher at the *Facultad de Ciencias* of the *Universidad Michoacana de San Nicolás de Hidalgo* (Morelia, Mexico). His areas of research include mathematical modeling of complex natural systems, continuum mechanics and geothermal energy. He is member of the National Researchers System (SNI) since 1991, has published numerous papers in technical journals and in international conference proceedings, books, chapters and he is editor of the new book series "Multiphysics Modeling".
E-mail: mcsa50@gmail.com

Fernando Samaniego V. earned his BS and MS degrees from the *Universidad Nacional Autónoma de México* and a PhD degree from Stanford University (USA), all in Petroleum Engineering. He has worked in the *Instituto Mexicano del Petroleo*, the *Instituto de Investigaciones Eléctricas* and PEMEX (all in Mexico). He has published 175 studies, 92 of them in the English literature. He was President of the Mexican Section of the Society of Petroleum Engineers (SPE) and received an SPE Distinguished Service Award, as well as the 2004 SPE Lester C. Uren Award and the SPE Honorary Member Award. He was elected as a Foreign Associate of the National Academy of Engineering (USA).
E-mail: fsamaniegov@pep.pemex.com

Jochen Bundschuh completed his PhD on numerical modeling of heat transport in aquifers in Tübingen, Germany. He has been working worldwide in international academic and technical co-operation programs in different fields of subsurface hydrology and integrated water resources management as well as in geothermics. He served as an expert for the German Agency for Technical Cooperation (GTZ) and as long-term Professor for the DAAD (German Academic Exchange Service) in Argentina. He was appointed to the Integrated Expert Program of CIM (GTZ/BA),

Frankfurt, Germany, and still works within the framework of German governmental cooperation as adviser in geothermics in a mission to Costa Rica at the *Instituto Costarricense de Electricidad*. He is an Affiliate Professor of the Royal Institute of Technology, Stockholm, Sweden and Vice-President of the International Society of Groundwater for Sustainable Development (ISGSD). He is chief editor of the book series "Arsenic in the Environment", and principal organizer of the homonymous International Congress series, and editor of the book series "Multiphysics Modeling".
E-mail: jochenbundschuh@yahoo.com

CHAPTER 28

M.H. Ferri Aliabadi is a Professor of Aerospace Structures and Head of Aerostructures, Department of Aeronautics. Imperial College, London (UK) and has served as a Professor of Computational Mechanics and Director of Research, Department of Engineering, Queen Mary, University of London (UK); Reader and Head of Damage Tolerance Division, Wessex Institute of Technology, Southampton; Director of the Aerospace Engineering Programme, Queen Mary, London; and is currently Editor of the International Journal for Structural Integrity and Durability, Editor in Chief of Computational and Experimental Methods in Structures, and Editor of Electronic Journal for Boundary Elements. He has published numerous books, chapters and papers in technical journals and conference proceedings and obtained several grants from different institutions.
E-mail: m.h.aliabadi@imperial.ac.uk

CHAPTER 29

Luis Rodríguez-Tembleque received a BSc degree in Mechanical Engineering from the *Universidad de Málaga* (Spain), MSc in Mechanical Engineering from the *Universidad de Sevilla* (Spain), and is finishing his PhD Thesis under the supervision of Prof. Abascal, at the *Universidad de Sevilla*. He is a Teaching Assistant in the Continuum Mechanics Department of the *Escuela Técnica Superior de Ingenieros*, *Universidad de Sevilla*. His research interests are numerical methods in engineering, particularly the application of boundary element and finite element methods (BEM-FEM) in contact, rolling and wear problems, and BEM-FEM coupling.
E-mail: luisroteso@us.es

José A. González received his BSc and PhD degrees in Mechanical Engineering from the *Universidad de Sevilla* (Spain). He is currently an Assistant Professor of Construction Engineering at the *Universidad de Sevilla*. His research involves the application of finite element and boundary element methods in structural problems, the numerical solution of contact problems, BEM-FEM coupling techniques and partitioned formulations using localized Lagrange multipliers.
E-mail: japerez@us.es

Ramón Abascal received his BSc and PhD degrees in Mechanical Engineering from the *Universidad de Sevilla* (Spain). Currently he is a Professor in the Department of Continuum Mechanics at *Universidad de Sevilla*. His research is focused on the Boundary Element Method and its application to elastodynamics (seismic wave propagation and scattering in non-homogenous viscoelastic soils, seismic response of foundations including dynamic soil-structure interaction and nonlinear contact effects due to uplift, guided wave scattering, and ultrasonic waves), fracture mechanics, contact problems (including friction and rolling) and substructure coupling techniques using Lagrange Multipliers.
E-mail: abascal@us.es

CHAPTER 30

Carlos A. Gómez de La Garza is currently working on his PhD Thesis under the supervision of Dr. Gilberto López at the *Centro de Investigación Científica y de Educación Superior de Ensenada*

(Mexico). His research involves the numerical solution of differential equations using pseudo-spectral methods. He obtained his Master's degree from the Computer Science department in CICESE and his Bachelor's degree from *Instituto Tecnológico de Monterrey*, Campus Monterrey.
E-mail: gcarlos100@yahoo.com

Gilberto López-Mariscal received his PhD in Applied Mathematics from Northwestern University (Evanston/Chicago, IL, USA). He was a postdoctoral associate at the Institute of Mathematics and its Applications (Minnesota, USA). He is currently a Professor in the Computer Science Department at the *Centro de Investigación Científica y de Educación Superior de Ensenada* (Mexico), where he does research in mathematical and numerical models for fluid flow.
E-mail: glopez@cicese.mx

CHAPTER 31

Juan José Pérez Gavilán E. graduated from the Engineering Faculty of the *Universidad Nacional Autónoma de México.* He became a consultant and later obtained a PhD in Computational Mechanics at University of London (UK). He is a researcher of the Institute of Engineering, *Universidad Nacional Autónoma de México*. He taught the postgraduate finite element course and lectures on the analysis and design of masonry structures. He is a board member of the Mexican Society of Numerical Methods, Vice-President of the Mexican Society of Structural Engineers and President of its Masonry Committee. His research interests include wave propagation in the neighborhood of oil wells, hybrid simulation of masonry structures, and design and analysis of hyperbolic cooling towers.
E-mail: jjpge@pumas.iingen.unam.mx

CHAPTER 32

Miguel X. Rodríguez Paz has a Civil Engineering degree from the *Tecnológico de Oaxaca* (Mexico) and a Master's degree in Structural Engineering from *Instituto Tecnológico de Monterrey* (ITESM), Mexico. He received his PhD from the University of Wales, Swansea, where he worked as a Senior Research Assistant. He is currently the Head the Engineering and Architecture School at the *Instituto Tecnológico de Monterrey* (Puebla, Mexico). His research work has been published in several scientific journals and presented in several international conferences. He is member of the National Researchers System (SNI-Conacyt). His research areas include numerical methods, computational engineering and particle methods.
E-mail: rodriguez.miguel@itesm.mx

David Ricardo Sol Martínez earned a degree in Computer Engineering, *Universidad de las Américas* (UA) in Puebla, Mexico. He developed software for several companies in Mexico and prepared his doctoral thesis at Université de Savoie, France. His dissertation was on the representation and interpretation of dynamics scenes. He was Professor at UA and directed several undergraduate projects and theses. He is the former Chair of the Computer Science department, UA and is currently Professor and director of Computing Engineering and Information Technologies Management at *Instituto Tecnológico de Monterrey*, Campus Puebla, Mexico. He has projects with researchers of the FIRST Fraunhofer in Berlin, Germany and France (LIRIS Lab) at INSA-Lyon. He has published several international papers in journals and congresses.
E-mail: dsol@itesm.mx

CHAPTER 33

David Ricardo Sol Martínez (*see Chapter 32*)

Miguel X. Rodríguez Paz (*see Chapter 32*)

Claudia Zepeda received a joint PhD in Computer Science at the *Institut National des Sciences Appliqueés de Lyon*, France and the *Universidad de las Américas in Puebla*, Mexico. Currently she

is a full-time professor at the *Benemérita Universidad Autónoma de Puebla*. Her current research focuses on the definition of evacuation plans based on logical approaches.
E-mail: czepeda@gmail.com

CHAPTER 34

Carlos Couder Castañeda (*see Chapter 12*)

Hermilo Ramirez-Leon obtained his degree as Civil Engineer from the Faculty of Engineering of *Universidad Nacional Autónoma de México*, his MSc in Hydraulics from the Faculty of Physics from the same university and earned his PhD in Ingineering Sciences, Option Computational Fluid Dynamics in 1991 (ECN-France). At present, he is a Researcher at the *Instituto Mexicano del Petroleo*, Applied and Computational Research Group and also Professor at the *Universidad Nacional Autónoma de México* and the *Instituto Politécnico Nacional* (Mexico).
E-mail: hrleon@imp.mx

ISRAEL E. Herrera D. (*see Chapter 12*)

CHAPTER 35

Cuauhtémoc Castañeda-Roldán earned his Bachelor's degree at *Benemérita Universidad Autónoma de Puebla* (BUAP), Mexico. He also earned his PhD in Mathematics for his work in approximation theory at BUAP. He has been co-author in studies of approximation theory (Elsevier) and optical surfaces polishing (OSA). He is currently a Research Professor at *Universidad Tecnológica de la Mixteca* (UTM) in Oaxaca, Mexico. His research interests include the application of mathematical programming to problems in physics and engineering as well as approximation of functions.
E-mail: ccroldan@yahoo.com.mx

Liliana Jeanett Manzano-Sumano earned her Bachelor's degree at *Universidad Tecnológica de la Mixteca*, Oaxaca, Mexico, in Applied Mathematics.
E-mail: limasu@hotmail.com

Jorge González Garcia earned his Bachelor's degree at *Benemérita Universidad Autónoma de Puebla* (BUAP), Mexico, in electronics, his Master's degree at BUAP in optical instrumentation and his PhD with a focus on optical surfaces polishing. He performed scientific research at the Instituto de Astronomia, *Universidad Nacional Autónoma de México* (UNAM) in Ensenada, Baja California, Mexico. He has been co-author in studies about optical design (Elsevier), adaptive optics (Proc. SPIE.), mechanical design (SOMI) and optical surfaces polishing (OSA). He has been working for the last 4 years as a research professor at *Universidad Tecnológica de la Mixteca* (UTM) in Oaxaca, Mexico.
E-mail: jgonzal@mixteco.utm.mx

Alberto Cordero Dávila earned his Bachelor's degree at *Benemérita Universidad Autónoma de Puebla* (BUAP), Mexico, in physics, he earned his Master's and his PhD at *Instituto Nacional de Astrofísica Óptica y Electrónica* INAOE, Mexico. He is a member of the *Sistema Nacional de investigadores* since 1989. He is coauthor of more than 70 papers, most of them are about design, construction and testing of optical systems. He won the "*Cabrillo de oro*" prize for his design work of the fluorescence detector telescope of the Pierre Auger Observatory. He has directed more than 40 Bachelor, Masters and Doctoral level thesis. He is currently a Research Professor at *Benemérita Universidad Autónoma de Puebla*, Mexico.

Part 1
Computational mathematics, modeling and numerical methods

CHAPTER 1

Mathematical and computational modeling in Mexico

Ismael Herrera-Revilla

1.1 INTRODUCTION

I want to thank the editors, for having invited me to write this introductory chapter, whose initial intention was to give a historical background of mathematical and computational modeling (MMC: Modelación Matemática y Computacional in Spanish) in Mexico. However, I must confess that in order to give a fair and balanced account of the past and present state of MMC a very thorough study and research would be required. This, however, is beyond the available time and resources. Thus, the scope of this chapter was severely limited. It only contains a rather schematic and general historical perspective, together with a few examples, drawn from my own personal experience, of the MMC activities that have been carried out in Mexico up to now. We hope these examples will be useful as illustrations of what has been done so far, but the resulting picture is far from representing an integrated and fair image of the MMC activity in Mexico. In particular, there are many people working in MMC whose work deserves attention and are not here included; my apologies to them all.

1.2 WHAT IS MMC?

Predicting nature's behavior is an ancestral human aspiration. For this purpose, our forefathers used supra-natural means, including magical and religious thinking. However, throughout history, this ambition of mankind has been a basic motivation for scientific development. This actually covered a considerable time-span, but eventually it was recognized that scientific means were the most effective for performing nature-behavior prediction, and that in turn "scientific prediction" required deep knowledge of nature and its phenomena. Furthermore, it must be pointed out that scientific and technological knowledge by itself is not enough for predicting the behavior of nature and of other systems that are important to humans, since behavior prediction requires integrating such knowledge into models to mimic those systems. In addition, it was also eventually recognized that the most effective models are mathematical models. Newton, in the seventeenth century, was the pioneer and founder of this school of thought when he developed the required mathematical methods and illustrated their power by successfully modeling the planetary system's motion. This awoke the consciousness of his contemporaries to the potential of mathematical modeling and stimulated further expansion of his basic concepts.

Newton was followed by many generations of physicists and mathematicians who developed his ideas and applied them to an amazing diversity of systems in science and engineering. As far as continuous macroscopic systems are concerned, among which most systems from engineering and science are included, the theoretical framework was crowned by the axiomatic formulation developed during the twentieth century under the leadership of Truesdell, Noll and others [1, 2]. Such a theoretical framework was very impressive, albeit insufficient because although its range of applicability included practically all systems of interest, the analytical tools available were very limited and only capable of dealing with simple systems. Linearity of the models was an ever-present assumption, but even so, simple geometry and simple properties were always required. This was not suitable for supplying the detailed information that is needed in many scientific and engineering applications. When that was the state of the art, the usefulness of mathematical modeling as an engineering tool was severely hampered. However, that situation changed sharply during the second half of the twentieth century with the advent of electronic computing. Nowadays mathematical and computational modeling is the most efficient method for integrating scientific and technological knowledge, with the purpose of performing effectively scientific prediction.

1.3 THE ANTECEDENTS

1.3.1 *Science and engineering in ancient Mexico*

Indigenous scientific development in Mexico was quite significant. Autochthonous advances in astronomy and mathematics are proverbial, as were the outstanding advances in hydraulics and engineering, although these are not as well known [3, 4]. In the eighth century, in the time when the Teotihuacán culture flourished, irrigation was based on the use of springs. Later, the water of the lake in which Tenochtilán, the ancient Aztec capital on the site of present-day Mexico City, was located was salty and unsuited for human consumption. However, in the Valley of Mexico springs were abundant and the fresh water they produced was a valuable source of water for the people who lived there. Thus, large aqueducts were constructed; among them, one carried the water from Chapultepec springs, and another from Coyoacán springs. It is also known that the works used for supplying water to Texcoco were built by Nezahualcóyotl, the legendary king, poet and engineer.

On the other hand, through history the cities located in the Valley of Mexico have been susceptible to flooding during the annual rainy season. To diminish such risks and reduce the damages, the Aztecs built boulevards, ditches and other hydraulic works, dividing with them the water into sectors and controlling the water flow in this manner. The Nezahualcóyotl ditch is especially famous, and it was used to traverse the Valley of Mexico from north to south.

1.3.2 *Mexico's scientific renaissance*

That not withstanding, contemporary scientific and engineering activity of Mexico actually started after the 1910 Mexican Revolution. Political stability was reestablished in the 1930s, and at the end of that decade and beginning of the next one the foundations of contemporary scientific development were laid down. Nationalism, one of the revolutionary ideology's components, included the idea that a new nation had to be built and that in this endeavor every Mexican citizen should participate. Social demands, as well as a thorough revision of material needs, required modernization of the country, which also had an important bearing in the post-revolutionary governmental programs.

The *Comisión Nacional de Caminos* (National Roads Commission) was created in the 1920s as a governmental agency in charge of an ambitious road construction program that had just begun. Similarly, the *Comisión Nacional de Irrigación* (National Irrigation Commission) was also created. This commission eventually became the *Secretaría de Recursos Hidráulicos*, with visible responsibility in dam construction and dam operation, while the *Comisión Nacional de Caminos* became the *Secretaría de Obras Públicas*, with responsibility for roads and also dam construction. Furthermore, the oil industry was nationalized in 1938, and the enterprise *Petróleos Mexicanos* that has been in charge of its administration ever since, was established. Safe water supply for the population and emerging activities, together the need to generate electricity required for the modernization of the country soon led to a boom in road building and construction of other public works such as dams. A nationalistic private sector also played an important role in these developments. In the 1940s, a group of young, distinguished Mexican engineers created what eventually became a very important construction enterprise; namely, *Ingenieros Civiles Asociados* (ICA), that was instrumental in carrying out many of the governmental projects.

The "Golden Age" of Mexican engineering (especially civil engineering) that thrived during the 1940s and extended over many decades thereafter must of course be attributed to the needs created by the above-mentioned boom in public works, but ICA was the main catalyst. In the chemical industrial sector, *Bufete Industrial* played a similar role. In summary, the Mexican Revolution of 1910 created a new consciousness of social needs and aspirations, which in turn gestated many new activities that in turn generated a boom of engineering activities. But the chain-reaction did not end there, because the demand for engineering professionals soon stimulated engineering education, which pushed science education, and science education pushed science research. It was then when the precursors of present-day research institutions were established.

The ancestral *Real y Pontificia Universidad de la Nueva España*, which was founded in 1551 and was reopened in the twentieth century as the *Universidad Nacional de México*, became today's *Universidad Nacional Autónoma de México* (UNAM) in 1929 when it achieved autonomy. UNAM played a central role in the initiation of research activities in contemporary Mexico. Most of the civil engineers needed in post-revolutionary Mexico, including ICA's engineers, were trained at the *Escuela Nacional de Ingenieros*, UNAM's *Facultad de Ingeniería* today, while petroleum engineers and geologists were educated at the recently created *Instituto Politécnico Nacional* (IPN). Furthermore, the *Escuela Nacional de Ingenieros* was the womb in which the present day research institutions in engineering and hard sciences (physics and mathematics) were gestated.

As for chemistry, a corresponding role was played by the *Escuela Nacional de Ciencias Químicas*. Teaching of pure sciences began at the *Facultad de Ciencias*, created in 1939 within the *Escuela Nacional de Ingenieros*, and during the period of 1939–1950 the institutes of basic research in mathematics, physics, geophysics, chemistry and astronomy were established. The "Mexican School of Thought" in physics and mathematics owes much to Ivy League universities, particularly Princeton, and the influence of Solomon Lefchetz should be mentioned.

On the other hand, some of the most distinguished applied mathematicians in Mexico were trained at Brown University.

Those developments not withstanding, most of the activities in mathematical and computational modeling (MMC) were associated with specific endeavors related to engineering work, and a certain number of applied research institutions were created. With ICA as its main promoter, the *Instituto de Ingeniería* was created in 1956 within the *Facultad de Ingeniería*. The first computer devoted to research, a 650 IBM, was installed at the *Facultad de Ciencias* in 1958. Other institutes of applied research and development were the *Instituto de Investigaciones Eléctricas*, the *Instituto Mexicano del Petróleo* and the *Instituto Mexicano de Tecnología del Agua* (IMTA), established in 1962, 1966 and 1981, respectively.

1.4 SAMPLING MMC IN MEXICO

The Pacific volcanic rim frames a large part of the Mexican territory on the west coast; furthermore, the Transmexican Volcanic Belt runs across the country, from the Pacific Ocean to the Gulf of Mexico. Seismicity is high in Mexico, so that the observation and study of earthquakes and their effects have had high priority since the beginning of the twentieth century. The National Seismological Service was established in 1910 and has been in charge of the Institute of Geophysics since it was established in 1949.

Mexico, together with USA, Japan and a few other countries, was pioneer in the study, research and application of 'seismic engineering' also called 'earthquake engineering'. In Mexico, a very strong and still highly respected seismic engineering research group was created under Emilio Rosenblueth's leadership. Rosenblueth, whose friendship I enjoyed until his death in 1994, was a worldwide leader, pioneer and founder, together with Newmark, of earthquake engineering as an engineering discipline [5]. One of the main objectives of seismic engineering is to predict, combining both deterministic and statistical models, the occurrence and the effects of earthquakes, especially on civil engineering structures. Thus, MMC is a fundamental tool in this area of engineering. Models built in Mexico include: statistical models for predicting the probability of earthquake occurrence, along with time and location, magnitude and other features such as the predominant period [6, 7]; models of the focal behavior of earthquakes; the effect of the structure of the crust and upper mantle in the transmission of the elastic waves from the seism focus to the structure location; the effect of the local geology on the characteristics of the motion that excite the engineering structure under study; soil-structure interaction models that take into account the effect of the structure in the motion of the soil; deterministic models for predicting the response of different engineering structures, such as buildings and dams, when the motion that excites them is known; and models of the stochastic processes in structures that are governed by differential equations of the Fokker-Plank type [8].

The results of all this research has been very useful not only in Mexico but in many other parts of the world. Mexican experts in earthquake engineering, such as Luis Esteva, have traveled to many other seismic active countries to advise local experts due the high prestige of the Mexican earthquake-engineering institutions. The research results obtained in this area have been incorporated in building regulations not only in Mexico City, but in many other cities of the world. This has been a great contribution to the safety of the people and their material possessions.

For a time, long ago, the author of this chapter was an active participant of the earthquake engineering research group and at that time he also did some research on seismology, which deals less directly with practical problems, but the new knowledge generated by it is rapidly incorporated by disciplines with a more practical orientation, such as seismic engineering. Many such studies are carried out with the purpose of establishing the physics and structure of the Earth's interior. One of the main tools used for this purpose are models of the elastic motion in the crust, mantle and deep interior. Therefore, such research frequently investigates basic properties of elastic motion. For a time there was worldwide interest in establishing the distribution of the upper mantle of the Earth, and including features such as its thickness. Besides some deep drilling projects, which were very costly, MMC models of elastic surface-waves, mainly Love and Rayleigh waves, were used for this purpose. Mexico participated in the Gulf of California Project that was carried out in collaboration with the University of California at Los Angeles (UCLA). Among the results of that project that were obtained in Mexico and should be cited is the derivation of orthogonality relations for Rayleigh waves. Orthogonality relations for Love waves had been known for a long time, but for Rayleigh waves they were not known until 1964 [9].

One of our most important problems is securing the daily water supply throughout our large country, and the best way of coping with this is with scientific management of our resources [10], which requires a great variety of mathematical and computational models of surface and groundwater. In the case of the former, water flow, including flood prediction, and contaminant transport in rivers and channels, deterministic and statistical modeling of basin response, and dam design, are a few of the necessary models. Flood prediction, for example, is essential for the design of bridges, and requires the modeling of the basin response. The administration of groundwater also poses important challenges in the modeling of subsurface water flow and contaminant transport. On the other hand, urbanization is a reality of our changing world that is causing the birth and growth of many megalopolises. A central question is, "*How can our cities be sustained under these circumstances?*". The Mexico City Metropolitan Area (MCMA) exemplifies these problems to an extreme degree [3, 4]. There, a very important problem is land subsidence, which is induced by the severe pumping of the aquifer, due to the leaky character of the subsurface hydrologic system.

In Mexico, modeling of surface water systems has being going on for a long time, at least since the 1950s. The leader who organized a very prestigious group in this area was José Luis Sánchez Bribiesca. Many of the most distinguished Mexican hydrologists of today were his students; to cite just one: Álvaro Aldama, who was not only a former general director of IMTA but also consolidated that national institute.

As for groundwater, it would be difficult to overstate its importance for a country in which more than 60% of the territory is arid or semiarid. A pioneer and worldwide leader of the application of MMC to groundwater is George F. Pinder; first at the US Geological Survey (USGS) and later at Princeton University. In Mexico, scientific research of groundwater using mathematical and computational models was initiated in the late 1960s at the Institute of Geophysics under Herrera's leadership [11, 12]. Later, he was invited to join the Advisory Council at Princeton, and since then Herrera and Pinder have had a very fruitful collaboration. The main scientific contribution to the mathematical modeling of groundwater made by Herrera and his collaborators at UNAM was the invention and development of the "Integro-differential equations approach to leaky aquifers" [13–15], sometimes called "Herrera's integrodifferential equations approach to leaky aquifers".

Thereby, it should be mentioned that the subsurface hydrologic system of Mexico City is precisely a multilayered leaky aquifer system. The software developed by the USGS in 1994 [16] is based on Herrera's approach. Because of his pioneering results, Herrera has been considered to be founder, together with Neumann and Witherspoon, of the "multilayered aquifer systems theory" [17]. Mathematical and computational models were developed for the construction of the artificial lakes at the Texcoco Basin [18], the subsurface hydrologic system of Mexico City (the MCMA system) [19, 20] and the geothermal systems of Cerro Prieto, B.C. and Los Azufres, Michoacán. Today, MCM models are used routinely in Mexico to deal with many groundwater problems, albeit there is a shortage of professionals and engineers adequately trained in subsurface hydrology.

As for basic contributions to the methodology of MMC, probably the most conspicuous group doing research in that area is the *Grupo de Modelación Matemática y Computacional* of the *Instituto de Geofísica*, UNAM [21–43], whose leader is also editor and founder of the international journal "Numerical Methods for Partial Differential Equations", published by Wiley (New York) since 1985. Many of its research themes stem from an "algebraic theory of boundary value problems" for partial differential equations and the "theory of partial differential equations on discontinuous piecewise-defined functions" that derived from it. The algebraic theory has been developed over a long time-span [21–43]. It identifies and makes extensive use of some algebraic properties of boundary value problems. In the first part of its development, the research that originated it was oriented to construct a general framework for variational principles of boundary value problems that at the time were being extensively studied all over the world. This was the period of the initial stages of the application of computers to solving partial differential equations, and variational principles were the means used for discretizing such equations. The theory that was so obtained accommodates practically all variational principles for boundary value problems known at that a time. Furthermore, it also encompasses Trefftz methods, bi-orthogonal systems of functions and a criterion for completeness of systems of functions (originally introduced as 'C-completeness', but later known as 'T-completeness', or 'TH-completeness'). This theory also yields a suitable framework for the development of complete systems of solution of partial differential equations (see [44], Ch. II, where the exposition is based on Herrera's 'T-completeness' or 'TH-completeness' concept). Furthermore, according to Begehr and Gilbert the algebraic theory supplies the basis for effectively applying to boundary value problems the function theoretic method of partial differential equations. Indeed, in [44], p. 115, these authors assert:

> *The function theoretic approach which was pioneered by Bergman and Vekua and then further developed by Colton, Gilbert, Kracht-Kreyszig and Lanckau and others, may now be effectively applied because of this result of the formulation by Herrera [21] as an effective means to solving boundary value problems.*

On the other hand, the algebraic theory has also been useful for establishing the theoretical foundations of 'Trefftz methods'. This time the citation comes from J. Jirousek, one of the most conspicuous representatives of Trefftz methods [45, p. 324]: "...the mathematical foundations of which (referring to Trefftz methods) have been laid mainly by Herrera and co-workers." In 1984, the Pitman's Advanced Publishing Program collected many of the results of the theory in a book [21]. An important element of the theory of differential equations in discontinuous functions that was introduced by Herrera immediately afterwards, in 1985, is a kind of Green's formula applicable to them and referred to as Green-Herrera formulas. They have played a central role in later developments. Their relevance is two-fold: firstly, they supply more explicit expressions for the distributional derivatives and, secondly, they extend the notion of distributional derivative in a way that permits applying 'fully discontinuous trial and test functions' simultaneously, something that is not possible when the standard theory of distributions is used. Apparently, it had been this latter fact which had prevented, until recently, the development of more direct approaches to partial differential equations formulated in discontinuous piecewise-defined functions.

This more recent work-phase of the theory includes a number of applications. Among them: the introduction of the 'localized adjoint method' (LAM) that in turn supplied the theoretical basis of the

'Eulerian-Lagrangean LAM' (ELLAM), a numerical method that has had considerable success in treating advection-dominated transport; more advanced applications to Trefftz method and studies of several aspects of domain decomposition methods; and a general class of methods that are collectively denominated 'finite elements methods with optimal functions (FEM-OF)'. This latter kind of methods is more general than LAM and has yielded some very effective procedures for applying orthogonal collocation; and also for developing some classes of enhanced finite elements (see [43], chapter 8 in this volume).

A truly general and systematic theory of finite element methods (FEM) should be formulated using, as 'trial and test functions, piecewise-defined functions' that can be fully discontinuous across the internal boundary which separates the elements from each other. Some of the most relevant work addressing such formulations is contained in the literature on 'discontinuous Galerkin (dG) methods' and on 'Trefftz methods'. However, the formulations of partial differential equations in discontinuous functions used in both of those fields are indirect approaches which are based on the use of 'Lagrange multipliers' and mixed methods in the case of dG methods, and the frame in the case of Trefftz method. The "theory of partial differential equations on discontinuous piecewise-defined functions" [41] addresses this problem from a different point of view and formulates the partial differential equations in discontinuous piecewise-defined functions. Such an approach is more direct and systematic, and furthermore it avoids the use of Lagrange multipliers or a frame, while mixed methods are incorporated as particular cases of more general results implied by the theory. When boundary value problems are formulated in discontinuous functions, well-posed problems are boundary value problems with prescribed jumps (BVPJ) in which the boundary conditions are complemented by suitable jump conditions to be satisfied across the internal boundary of the domain-partition. One result of the theory shows that for elliptic equations of order $2m$, with $m \geq 1$, the problem of establishing conditions for existence of solution for the BVPJ reduces to that of the 'standard boundary value problem', without jumps, which has been extensively studied. Background material of the "theory of partial differential equations on discontinuous piecewise-defined functions" appeared in scattered publications; however, the question of developing a 'theory of partial differential equations in discontinuous piecewise-defined functions' in a systematic manner was only recently addressed and published [41].

It should also be mentioned that a very important achievement of the theory just described has been recently obtained and published in two papers [42, 46]. Its relevance is in connection with the application of parallel computing to partial differential equations. The paper introduces a new approach to iterative substructuring methods that, without recourse to Lagrange multipliers, yields positive definite preconditioned formulations of the Neumann-Neumann and FETI types. Standard formulations are done using Lagrange multipliers to deal with discontinuous functions, and this is the first time that such formulations have been made without resource to Lagrange multipliers.

A numerical advantage that is concomitant to such multipliers-free formulations is the reduction of the degrees of freedom associated with the Lagrange multipliers. The general framework of the new approach is rather simple and stems directly from the discretization procedures that are applied; in it, the differential operators act on discontinuous piecewise-defined functions. Thus, the Lagrange multipliers are not required, because in such an environment the function-discontinuities are not anomalies that need to be corrected.

To finish, I hope that soon a new document, covering in a more complete manner MMC activities in Mexico, will be written. Then, I am sure, many other scholars whose work deserves attention will be included.

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CHAPTER 2

Numerical solution of boundary inverse problems for orthotropic solids

Igor Brilla

2.1 INTRODUCTION

Inverse problems are very important from a practical point of view and interesting from a theoretical point of view as they are improperly posed problems. An important class of inverse problems is a class of identification problems. These problems are important, for example, in the non-destructive testing of materials, the identification of material parameters, the study of aquifer problems as well as for electrical impedance tomography, etc.

Numerical analysis of these problems encounters difficulties connected with the improperness of inverse problems.

However, the majority of papers on inverse problems deal with isotropic problems modeled by second order differential equations. Additional difficulties arise in the case of orthotropic and anisotropic inverse problems and problems modeled by differential equations of higher order or by systems of differential equations.

We deal with analysis of inverse problems for orthotropic solids when measured data is given only on the boundary of the domain. The inverse problems for orthotropic solids have special features in comparison with those for isotropic solids. In order to solve orthotropic problems, more unknown material parameters of governing differential equations than the total number of equations must be determined and therefore, in order to determine them, we need input data measured from more than one field state. These input states as we show cannot be chosen arbitrarily. This fact leads to new theoretical problems in the analysis of inverse problems for orthotropic solids and also complicates numerical analysis.

For numerical analysis of such problems we apply discrete methods. These are very convenient because in the case of practical problems we have to measure input states in discrete points. In this chapter, we have elaborated an iterative procedure to the numerical solution of plane orthotropic boundary inverse problem when the input data measured from suitable states is sufficient to determine the unknown material parameters. We derive the number of measured input states and conditions for these measured input states which secure determinability of the numerical solution. We also deal with numerical experiments. Since input data is measured in the case of practical problems, we also study its influence on the stability of the numerical solutions. This approach is based on the methods derived by Brilla [1, 2]. Another approach is derived in Grebennikov [3, 4].

2.2 FORMULATION OF THE PROBLEM

Governing equations of plane anisotropic solids have the following form:

$$(c_{ijkl}u_{k,l})_{,j} + f_i = 0 \quad \text{in } \Omega, \quad i,j,k,l = 1,2 \tag{2.1}$$

where c_{ijkl} are elastic coefficients, u_i are displacements and f_i are volume forces. We assume that Ω is a two dimensional Lipschitz domain. We apply the summation and differentiation rule with respect to indices. Elastic coefficients are symmetric. It holds $c_{ijkl} = c_{klij} = c_{jikl} = c_{ijlk}$.

In the 2D orthotropic case c has 4 components and the equation (2.1) can be written in the following forms:

$$\begin{aligned}(Au_{x,x})_{,x} + (Cu_{y,y})_{,x} + (Du_{y,x})_{,y} + (Du_{x,y})_{,y} + f_x = 0 \quad \text{in } \Omega\\(Bu_{y,y})_{,y} + (Cu_{x,x})_{,y} + (Du_{y,x})_{,x} + (Du_{x,y})_{,x} + f_y = 0 \quad \text{in } \Omega\end{aligned} \tag{2.2}$$

where we use following notations $c_{1111} = A$, $c_{2222} = B$, $c_{1122} = C$, $c_{1212} = D$.

In the case of the inverse problems, u_x and u_y are given and A, B, C and D are unknown, in the case of non-constant elastic coefficients we obtain two differential equations of first order for determination of the unknown functions A, B, C and D.

In the case of the inverse problems we have to determine the elastic coefficients we need for their determination boundary conditions:

$$A(s) = a(s), \quad B(s) = b(s), \quad C(s) = c(s), \quad D(s) = d(s), \quad s \in \partial\Omega \tag{2.3}$$

In the case of boundary inverse problems we also have to determine the displacements u_x and u_y using measured values of the displacements u_x and u_y on the boundary $\partial\Omega$. We consider the Dirichlet boundary conditions for the u_x and u_y displacements:

$$u_x(s) = g_1(s), \quad u_y(s) = g_2(s), \quad s \in \partial\Omega \tag{2.4}$$

and over specified Neumann boundary conditions:

$$u_{x,n}(s) = g_3(s), \quad u_{y,n}(s) = g_4(s), \quad s \in \partial\Omega \tag{2.5}$$

where $(.)_{,n}$ denotes the differentiation in the direction of the outer normal.

In our approach, we consider Neumann's boundary problem (2.2), (2.3), (2.5) in the following way. Considering Hooke's law:

$$\tau_{ij} = c_{ijkl}\,\varepsilon_{kl}$$

where τ is the stress tensor and ε is the strain tensor. Hooke's law can be written for our 2D orthotropic problem in the following forms:

$${}^u\tau_{xx} = Au_{x,x} + Cu_{y,y}, \quad {}^u\tau_{yy} = Cu_{x,x} + Bu_{y,y}, \quad {}^u\tau_{xy} = D(u_{x,y} + u_{y,x}) \tag{2.6}$$

Using equations (2.6) equations (2.2) and (2.5) can be written in the forms:

$$\begin{aligned}&{}^u\tau_{xx,x} + {}^u\tau_{xy,y} + f_x = 0, \quad {}^u\tau_{xy,x} + {}^u\tau_{yy,y} + f_y = 0 \quad \text{in } \Omega\\&{}^u\tau_{xx}(s) = {}^u j_1(s), \quad {}^u\tau_{yy}(s) = {}^u j_2(s), \quad {}^u\tau_{xy}(s) = {}^u j_3(s), \quad s \in \partial\Omega\end{aligned} \tag{2.7}$$

However, in the case of a 2D orthotropic problem, the system of equations (2.2)–(2.4), (2.7) does not form a complete system of equations and is not sufficient for the determination of the unknown elastic coefficients. We show that for the determination of the unknown elastic coefficients, it is necessary to add input data measured from the next state of the displacements v_x and v_y. For this next state of input data, we consider the equations analogical to equations (2.2):

$$\begin{aligned}(Av_{x,x})_{,x} + (Cv_{y,y})_{,x} + (Dv_{y,x})_{,y} + (Dv_{x,y})_{,y} + q_x = 0 \quad \text{in } \Omega \\ (Bv_{y,y})_{,y} + (Cv_{x,x})_{,y} + (Dv_{y,x})_{,x} + (Dv_{x,y})_{,x} + q_y = 0 \quad \text{in } \Omega\end{aligned} \tag{2.8}$$

and boundary conditions analogical to Dirichlet boundary conditions (2.4):

$$v_x(s) = g_5(s), \quad v_y(s) = g_6(s), \quad s \in \partial\Omega \tag{2.9}$$

corresponding equations of Hooke's law:

$$^{v}\tau_{xx} = Av_{x,x} + Cv_{y,y}, \quad ^{v}\tau_{yy} = Cv_{x,x} + Bv_{y,y} \quad ^{v}\tau_{xy} = D(v_{x,y} + v_{y,x}) \tag{2.10}$$

and corresponding equations and boundary conditions for stresses:

$$\begin{aligned}&^{v}\tau_{xx,x} + {}^{v}\tau_{xy,y} + q_x = 0, \quad ^{v}\tau_{xy,x} + {}^{v}\tau_{yy,y} + q_y = 0 \quad \text{in } \Omega \\ &^{v}\tau_{xx}(s) = {}^{v}j_1(s), \quad ^{v}\tau_{yy}(s) = {}^{v}j_2(s), \quad ^{v}\tau_{xy}(s) = {}^{v}j_3(s), \quad s \in \partial\Omega\end{aligned} \tag{2.11}$$

Now the question of whether the states u_x, u_y and v_x, v_y can be chosen arbitrarily arises. We show that these states cannot be chosen arbitrarily.

2.3 NUMERICAL ANALYSIS OF THE PROBLEM

For numerical analysis we can apply discrete methods. They are very convenient because in practical problems we have to measure input states in discrete points. We assume that the domain Ω is rectangular $(m+1)h \times (n+1)h, h > 0$. Using central differences, equations (2.2) assume following discrete forms:

$$\begin{aligned}&(A_{i+1;k} - A_{i-1;k} + 4A_{i;k})(u_x)_{i+1;k} + (A_{i-1;k} - A_{i+1;k} + 4A_{i;k})(u_x)_{i-1;k} \\ &\quad + (D_{i;k+1} - D_{i;k-1} + 4D_{i;k})(u_x)_{i;k+1} + (D_{i;k-1} - D_{i;k+1} + 4D_{i;k})(u_x)_{i;k-1} \\ &\quad - 8(A_{i;k} + D_{i;k})(u_x)_{i;k} + (C_{i+1;k} - C_{i-1;k})[(u_y)_{i;k+1} - (u_y)_{i;k-1}] \\ &\quad + (C_{i;k} + D_{i;k})[(u_y)_{i+1;k+1} + (u_y)_{i-1;k-1} - (u_y)_{i-1;k+1} - (u_y)_{i+1;k-1}] \\ &\quad + (D_{i;k+1} - D_{i;k-1})[(u_y)_{i+1;k} - (u_y)_{i-1;k}] + 4h^2(f_x)_{i;k} = 0, \\ &(D_{i+1;k} - D_{i-1;k} + 4D_{i;k})(u_y)_{i+1;k} + (D_{i-1;k} - D_{i+1;k} + 4D_{i;k})(u_y)_{i-1;k} \\ &\quad + (B_{i;k+1} - B_{i;k-1} + 4B_{i;k})(u_y)_{i;k+1} + (B_{i;k-1} - B_{i;k+1} + 4B_{i;k})(u_y)_{i;k-1} \\ &\quad - 8(B_{i;k} + D_{i;k})(u_y)_{i;k} + (D_{i+1;k} - D_{i-1;k})[(u_x)_{i;k+1} - (u_x)_{i;k-1}] \\ &\quad + (C_{i;k} + D_{i;k})[(u_x)_{i+1;k+1} + (u_x)_{i-1;k-1} - (u_x)_{i-1;k+1} - (u_x)_{i+1;k-1}] \\ &\quad + (C_{i;k+1} - C_{i;k-1})[(u_x)_{i+1;k} - (u_x)_{i-1;k}] + 4h^2(f_y)_{i;k} = 0, \\ &\quad i = 1, 2, \ldots, m, \quad k = 1, 2, \ldots, n\end{aligned} \tag{2.12}$$

where:

$$A_{0;k},\ A_{m+1;k},\ C_{0;k},\ C_{m+1;k},\ D_{0;k},\ D_{m+1;k},\quad k=1,2,\ldots,n$$
$$B_{i;0},\ B_{i;n+1},\ C_{i;0},\ C_{i;n+1},\ D_{i;0},\ D_{i;n+1},\quad i=1,2,\ldots,m$$

are given from the boundary conditions (2.3) and:

$$(u_x)_{0;k},\ (u_x)_{m+1;k},\ (u_y)_{0;k},\ (u_y)_{m+1;k},\quad k=0,1,\ldots,n+1$$
$$(u_x)_{i;0},\ (u_x)_{i;n+1},\ (u_y)_{i;0},\ (u_y)_{i;n+1},\quad i=0,1,\ldots,m+1$$

are given from Dirichlet boundary conditions (2.4). Similar equations are obtained for other ν_x, ν_y states.

In order to solve the boundary inverse problems (2.2)–(2.4), (2.7)–(2.9), (2.11) we can use the following iterative procedure which is a generalization of the method for the solution of 2D orthotropic and 2D anisotropic boundary inverse conductivity problems derived in [1, 2]:

- determination of an initial approximation of the elastic coefficients $A^0_{i;k}$, $B^0_{i;k}$, $C^0_{i;k}$, $D^0_{i;k}$, $i=1,2,\ldots,m,\ k=1,2,\ldots,n$ as the linear interpolation of the boundary conditions (2.3);
- determination of the displacements $(u^0_x)_{i;k}$ and $(u^0_y)_{i;k}, i=1,2,\ldots,m,\ k=1,2,\ldots,n$ from equations (2.12) and $(\nu^0_x)_{i;k}$ and $(\nu^0_y)_{i;k}$ from the discrete form of equations (2.8);
- determination of the stresses $({}^u\tau^0_{xx})_{i;k}$, $({}^u\tau^0_{yy})_{i;k}$, $({}^u\tau^0_{xy})_{i;k}$, $i=1,2,\ldots,m,\ k=1,2,\ldots,n$ from equations (2.7) and (2.6) rewritten in the following forms:

$$
\begin{aligned}
&{}^u\tau^0_{xx,x}=-f_x-\{D^0(u^0_{x,y}+u^0_{y,x})\}_{,y},\ {}^u\tau^0_{yy,y}=-f_y-{}^u\tau^0_{xy,x},\\
&{}^u\tau^0_{xy,y}=-f_x-(A^0u^0_{x,x}+C^0u^0_{y,y})_{,x}
\end{aligned}
$$

  and $({}^\nu\tau^0_{xx})_{i;k}, ({}^\nu\tau^0_{yy})_{i;k}, ({}^\nu\tau^0_{xy})_{i;k},\ i=1,2,\ldots,m,\ k=1,2,\ldots,n$ using similar equations which we obtain from equations (2.11) and (2.10), which are ordinary first order differential equations. Solutions for these equations can be found using a modified Euler method, for example;
- determination of new state of the elastic coefficients $A^1_{i;k}$, $B^1_{i;k}$, $C^1_{i;k}$, $D^1_{i;k}$, $i=1,2,\ldots,m,\ k=1,2,\ldots,n$ from equations (2.6) and (2.10) using following formulas:

$$
\begin{aligned}
A^1_{i;k}=2h\{&[({}^\nu\tau^0_{yy})_{i;k}[(\nu^0_y)_{i;k+1}-(\nu^0_y)_{i;k-1}]\\
&-({}^\nu\tau^0_{xx})_{i;k}[(\nu^0_x)_{i+1;k}-(\nu^0_x)_{i-1;k}]][(u^0_y)_{i;k+1}-(u^0_y)_{i;k-1}]^2\\
&-[({}^u\tau^0_{yy})_{i;k}[(u^0_y)_{i;k+1}-(u^0_y)_{i;k-1}]\\
&-({}^u\tau^0_{xx})_{i;k}[(u^0_x)_{i+1;k}-(u^0_x)_{i-1;k}]][(\nu^0_y)_{i;k+1}-(\nu^0_y)_{i;k-1}]^2\}/\Delta,
\end{aligned}
$$

$$
\begin{aligned}
B^1_{i;k} &= 2h\{[({}^{v}\tau^0_{yy})_{i;k}[(v^0_y)_{i;k+1} - (v^0_y)_{i;k-1}] \\
&\quad - ({}^{v}\tau^0_{xx})_{i;k}[(v^0_x)_{i+1;k} - (v^0_x)_{i-1;k}]][(u^0_x)_{i+1;k} - (u^0_x)_{i-1;k}]^2 \\
&\quad - [({}^{u}\tau^0_{y/y})_{i;k}[(u^0_y)_{i;k+1} - (u^0_y)_{i;k-1}] \\
&\quad - ({}^{u}\tau^0_{xx})_{i;k}[(u^0_x)_{i+1;k} - (u^0_x)_{i-1;k}]][(v^0_x)_{i+1;k} - (v^0_x)_{i-1;k}]^2\}\big/\Delta, \qquad (2.13)\\
C^1_{i;k} &= \frac{2h({}^{u}\tau^0_{xx})_{i;k} - A^1_{i;k}[(u^0_x)_{i+1;k} - (u^0_x)_{i-1;k}]}{(u^0_y)_{i;k+1} - (u^0_y)_{i;k-1}}, \\
D^1_{i;k} &= 2h({}^{u}\tau^0_{xy})_{i;k}\big/\Delta_1, \\
&\quad i = 1,2,\ldots,m, \quad k = 1,2,\ldots,n
\end{aligned}
$$

where:

$$
\begin{aligned}
\Delta &= [(u^0_x)_{i+1;k} - (u^0_x)_{i-1;k}]^2[(v^0_y)_{i;k+1} - (v^0_y)_{i;k-1}]^2 \\
&\quad - [(u^0_y)_{i;k+1} - (u^0_y)_{i;k-1}]^2[(v^0_x)_{i+1;k} - (v^0_x)_{i-1;k}]^2, \\
\Delta_1 &= [(u^0_x)_{i;k+1} - (u^0_x)_{i;k-1}] + [(u^0_y)_{i+1;k} - (u^0_y)_{i-1;k}], \\
&\quad i = 1,2,\ldots,m, \quad k = 1,2,\ldots,n
\end{aligned}
$$

- in order to arrive at the final solution, we have to reiterate this procedure and thus minimize the error.

  From equations (2.13) we can see that the iterative procedure can be used only if:

$$
\begin{aligned}
&[(u^j_x)_{i+1;k} - (u^j_x)_{i-1;k}]^2[(v^j_y)_{i;k+1} - (v^j_y)_{i;k-1}]^2 \\
&\quad - [(u^j_y)_{i;k+1} - (u^j_y)_{i;k-1}]^2[(v^j_x)_{i+1;k} - (v^j_x)_{i-1;k}]^2 \neq 0, \\
&[(u^j_x)_{i;k+1} - (u^j_x)_{i;k-1}] + [(u^j_y)_{i+1;k} - (u^j_y)_{i-1;k}] \neq 0 \qquad (2.14)\\
&(u^j_y)_{1;k+1} - (u^j_y)_{i;k-1} \neq 0 \\
&\quad i = 1,2,\ldots, m, \quad k = 1,2,\ldots, n, \quad j = 0,1,\ldots
\end{aligned}
$$

The conditions (2.14) are discrete forms of the conditions:

$$(u_{x,x}v_{y,y})^2 - (u_{y,y}v_{x,x})^2 \neq 0, \quad u_{x,y} + u_{y,x} \neq 0, \quad u_{y,y} \neq 0 \quad \text{in } \Omega.$$

This means that the input states cannot be chosen arbitrarily.

2.4 NUMERICAL EXPERIMENTS

We deal with numerical experiments from a mathematical point of view. This means that we construct the exact solution of the problem under consideration, afterwards we compute the numerical solution of this problem using the iterative procedure and in the end compare it with the exact one.

We use the iterative procedure with the stopping condition such that the difference of two computed consecutive states of the elastic coefficients is less than 10^{-10}. We consider the following domain $\Omega = \langle 0, 2\rangle \times \langle 0, 1\rangle$. For example, for the following elastic coefficients:

$$\begin{aligned} &A = (x+1)(y+1)^2, \quad B = (x+1)^2(y+1), \\ &C = (x+1) + (y+1), \quad D = (x+1)(y+1) \end{aligned} \tag{2.15}$$

displacements:

$$\begin{aligned} &u_x = (x+1)^2 + (y+1)^2, \quad u_y = (x+1)(y+1), \\ &v_x = (x+1), \quad v_y = (y+1) \end{aligned} \tag{2.16}$$

corresponding stresses:

$$\begin{aligned} &{}^u\tau_{xx} = 2(x+1)^2(y+1)^2 + [(x+1) + (y+1)](x+1) \\ &{}^u\tau_{yy} = (x+1)^3(y+1) + 2[(x+1) + (y+1)](x+1) \\ &{}^u\tau_{xy} = 3(x+1)(y+1)^2, \quad {}^v\tau_{xy} = 0 \\ &{}^v\tau_{xx} = (x+1)(y+1)^2 + (x+1) + (y+1) \\ &{}^v\tau_{yy} = (x+1)^2(y+1) + (x+1) + (y+1) \end{aligned} \tag{2.17}$$

and corresponding volume forces:

$$\begin{aligned} &f_x = 4(x+1)(y+1)^2 + 2(x+1) + (y+1) + 6(x+1)(y+1) \\ &f_y = (x+1)^3 + 3(y+1)^2 + 2(x+1) \\ &q_x = (y+1)^2 + 1, \quad q_y = (x+1)^2 + 1 \end{aligned} \tag{2.18}$$

using equations (2.18) the boundary conditions constructed from equations (2.15)–(2.17) and the iterative procedure in the Table 2.1 we are able to see the percentage of errors in the computed solutions in the second column with respect to the exact solutions of the meshes given in the first column. In the third column we report the number of iterations after which we obtained the numerical solution with the specific stopping condition on the given mesh. We can see from the results that we obtain very small errors for a course mesh and when the number of grid points increases, errors also increase slightly but are still small.

If we change the displacements:

$$\begin{aligned} &u_x = (x+1) + (y+1), \quad u_y = (x+1) + 2(y+1) \\ &v_x = 2(x+1), \quad v_y = (y+1) \end{aligned} \tag{2.19}$$

Table 2.1. Results for the problem (2.15)–(2.18).

Mesh	Error (%)	Number of iterations
8×4	$6.2\ 10^{-8}$	182
12×6	$2.1\ 10^{-7}$	470
16×8	$6.7\ 10^{-7}$	1006

Table 2.2. Results for the problem (2.15), (2.19)–(2.21).

Mesh	Error	Number of iterations
8×4	$4.0\ 10^{-8}$	160
16×8	$1.6\ 10^{-7}$	522
12×6	$4.9\ 10^{-7}$	1319

for corresponding stresses:

$$\begin{aligned}
{}^u\tau_{xx} &= (x+1)(y+1)^2 + 2[(x+1)+(y+1)] \\
{}^u\tau_{yy} &= 2(x+1)^2(y+1) + (x+1) + (y+1) \\
{}^u\tau_{xy} &= 2(x+1)(y+1), \quad {}^v\tau_{xy} = 0 \\
{}^v\tau_{xx} &= 2(x+1)(y+1)^2 + (x+1) + (y+1) \\
{}^v\tau_{yy} &= (x+1)^2(y+1) + 2[(x+1)+(y+1)]
\end{aligned} \tag{2.20}$$

and corresponding volume forces:

$$\begin{aligned}
f_x &= (y+1)^2 + 2(x+1) + 2, \quad q_x = 2(y+1)^2 + 1 \\
f_y &= 2(x+1)^2 + 2(y+1) + 1, \quad q_y = (x+1)^2 + 2
\end{aligned} \tag{2.21}$$

we obtain similar results for the same elastic coefficients as it is shown in the Table 2.2.
For other elastic coefficients:

$$\begin{aligned}
A &= (x+1)^2(y+1), \quad B = (x+1)(y+1)^2, \\
C &= (x+1) + (y+1), \quad D = (x+1)(y+1)
\end{aligned} \tag{2.22}$$

the displacements given by equations (2.16) and for their corresponding stresses:

$$\begin{aligned}
{}^u\tau_{xx} &= 2(x+1)^3(y+1) + [(x+1)+(y+1)](x+1) \\
{}^u\tau_{yy} &= (x+1)^2(y+1)^2 + 2[(x+1)+(y+1)](x+1)
\end{aligned}$$