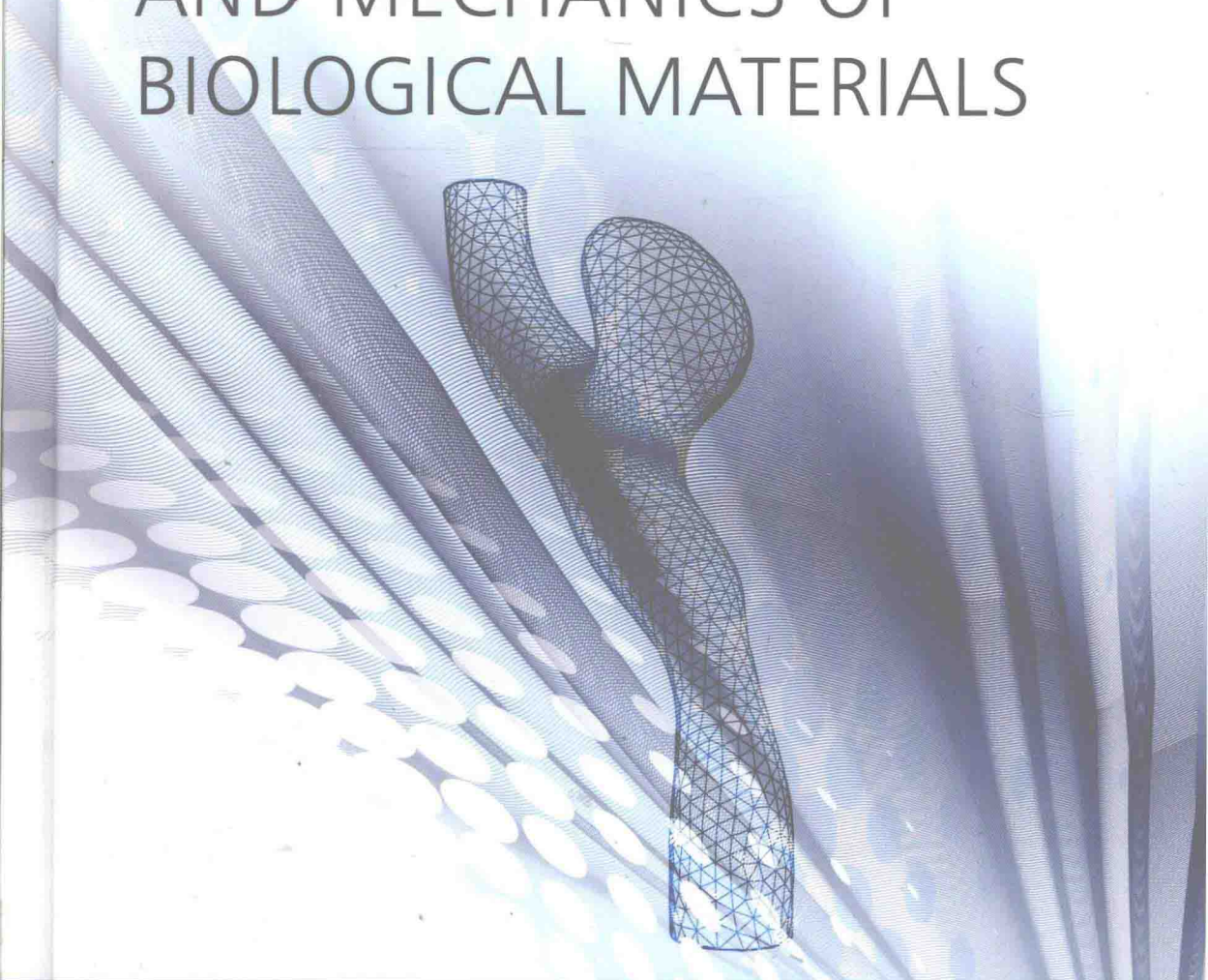


EDITORS | SHAOFAN LI | DONG QIAN

MULTISCALE SIMULATIONS AND MECHANICS OF BIOLOGICAL MATERIALS



 WILEY

MULTISCALE SIMULATIONS AND MECHANICS OF BIOLOGICAL MATERIALS

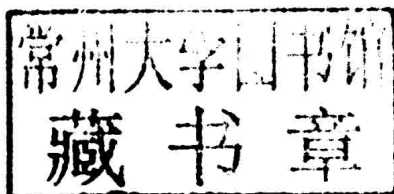
Edited by

Shaofan Li

University of California at Berkeley, USA

Dong Qian

University of Texas at Dallas, USA



 **WILEY**

A John Wiley & Sons, Ltd., Publication

This edition first published 2013
© 2013 John Wiley & Sons, Ltd

Registered office

John Wiley & Sons Ltd, The Atrium, Southern Gate, Chichester, West Sussex, PO19 8SQ, United Kingdom

For details of our global editorial offices, for customer services and for information about how to apply for permission to reuse the copyright material in this book please see our website at www.wiley.com.

The right of the author to be identified as the author of this work has been asserted in accordance with the Copyright, Designs and Patents Act 1988.

All rights reserved. No part of this publication may be reproduced, stored in a retrieval system, or transmitted, in any form or by any means, electronic, mechanical, photocopying, recording or otherwise, except as permitted by the UK Copyright, Designs and Patents Act 1988, without the prior permission of the publisher.

Wiley also publishes its books in a variety of electronic formats. Some content that appears in print may not be available in electronic books.

Designations used by companies to distinguish their products are often claimed as trademarks. All brand names and product names used in this book are trade names, service marks, trademarks or registered trademarks of their respective owners. The publisher is not associated with any product or vendor mentioned in this book. This publication is designed to provide accurate and authoritative information in regard to the subject matter covered. It is sold on the understanding that the publisher is not engaged in rendering professional services. If professional advice or other expert assistance is required, the services of a competent professional should be sought.

Library of Congress Cataloging-in-Publication Data

Multiscale simulations and mechanics of biological materials / edited by Professor Shaofan Li, Dr Dong Qian.
pages cm

Includes bibliographical references and index.

ISBN 978-1-118-35079-9 (cloth)

1. Biomechanics. 2. Biomedical materials—Mechanical properties. 3. Multiscale modeling. I. Li, Shaofan, editor of compilation. II. Qian, Dong, editor of compilation.

QH513.M85 2013

612.7'6—dc23

2012040166

A catalogue record for this book is available from the British Library.

ISBN: 9781118350799

Typeset in 9/11pt Times by Aptara Inc., New Delhi, India
Printed and bound in Singapore by Markono Print Media Pte Ltd



WILEY

**MULTISCALE
SIMULATIONS AND
MECHANICS OF
BIOLOGICAL
MATERIALS**

About the Editors

Dr. Shaofan Li is currently a Professor of Applied and Computational Mechanics at the University of California–Berkeley. Dr. Li graduated from the Department of Mechanical Engineering at the East China University of Science and Technology (Shanghai, China) with a Bachelor Degree of Science in 1982; he also holds Master Degrees of Science from both the Huazhong University of Science and Technology (Wuhan, China) and the University of Florida (Gainesville, FL, USA) in Applied Mechanics and Aerospace Engineering in 1989 and 1993, respectively. In 1997 Dr. Li received a PhD degree in Mechanical Engineering from the Northwestern University (Evanston, IL, USA), and he was also a post-doctoral researcher at the Northwestern University during 1997–2000. In 2000 Dr. Li joined the faculty of the Department of Civil and Environmental Engineering at the University of California–Berkeley. Dr. Shaofan Li has also been a visiting Changjiang professor in the Huazhong University of Science and Technology, Wuhan, China (2007–2010). Dr. Shaofan Li is the recipient of the A. Richard Newton Research Breakthrough Award (2008) and an NSF Career Award (2003). Dr. Li has published more than 100 articles in peer-reviewed scientific journals, and he is the author and co-author of two research monographs/graduate textbooks. (li@ce.berkeley.edu)

Dr. Dong Qian is an associate professor in the Department of Mechanical Engineering at the University of Texas at Dallas. He obtained his BS degree in Bridge Engineering in 1994 from Tongji University in China. He came to the USA in 1996 and obtained an MS degree in Civil Engineering at the University of Missouri–Columbia in 1998. He continued his study at Northwestern University from 1998 and received his PhD in Mechanical Engineering in 2002. Shortly after his graduation, he was hired as an assistant professor at the University of Cincinnati. In 2008 he was promoted to the rank of associate professor with tenure and served as the Director of Graduate Studies from 2010. In the Fall of 2012 he joined the mechanical engineering department at the University of Texas at Dallas as an associate professor (tenured). His research interests include nonlinear finite-element and meshfree methods, fatigue and failure analysis and life prediction, surface engineering, residual stress analysis, and modeling and simulation of manufacturing processes (peening, forming, etc.) and nanostructured materials with a focus on mechanical properties and multiphysics coupling mechanisms. (dong.qian@utdallas.edu)

List of Contributors

Ashfaq Adnan, Mechanical and Aerospace Engineering, University of Texas at Arlington, USA (aadnan@uta.edu)

Facundo J. Bellomo, INIQUI (CONICET), Faculty of Engineering, National University of Salta, Argentina (facundobellomo@yahoo.com.ar)

Eduard Benet, Department of Civil, Environmental and Architectural Engineering, University of Colorado, USA (ebenetcerda@gmail.com)

Sagar Bhamare, School of Dynamic Systems College of Engineering and Applied Science, University of Cincinnati, USA (bhamare.sagar@gmail.com)

Jiun-Shyan Chen, Department of Civil and Environmental Engineering, University of California, Los Angeles, USA (jschen@seas.ucla.edu)

Sheng-Wei Chi, Department of Civil and Environmental Engineering, University of Illinois at Chicago, USA (swchi@uic.edu)

Jae-Hyun Chung, University of Washington, USA (jae71@uw.edu)

Suvranu De, Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, New York, USA (des@rpi.edu)

Michel Devel, FEMTO-ST Institute, Université de Franche-Comté, France (michel.devel@ens2m.fr)

Khalil I. Elkhodary, Department of Mechanical Engineering, Northwestern University, USA (k-elkhodary@northwestern.edu)

Xavier Espinet, Department of Civil, Environmental and Architectural Engineering, University of Colorado, USA (xavier.espinetalegre@colorado.edu)

Leonora Felon, X-spine Systems, Inc., USA (lfelon@x-spine.com)

Sheikh F. Ferdous, Mechanical and Aerospace Engineering, University of Texas at Arlington, USA (sheikh.ferdous@mavs.uta.edu)

Jacob Fish, Columbia University, USA (fishj@columbia.edu)

Louis Foucard, Department of Civil, Environmental and Architectural Engineering, University of Colorado, USA (louis.foucard@colorado.edu)

Yao Fu, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, USA (yaf11@pitt.edu)

Michael Steven Greene, Theoretical & Applied Mechanics, Northwestern University, USA (greenes@u.northwestern.edu)

Shaolie S. Hossain, Institute for Computational Engineering and Sciences, The University of Texas at Austin, USA (sshossain@tmhs.org)

Jia Hu, Department of Mechanical Engineering and Mechanics, Lehigh University, USA; School of Mechanical Mechanics and Engineering, Southwest Jiaotong University, People's Republic of China (jih511@lehigh.edu)

Daeyong Kim, Korea Institute of Materials Science, South Korea (daeyong@kims.re.kr)

Ji Hoon Kim, Korea Institute of Materials Science, South Korea (kimjh@kims.re.kr)

- Jong-Hoon Kim**, University of Washington, USA (jhkim78@uw.edu)
David Kirschman, X-spine Systems, Inc., USA (dk@x-spine.com)
Nikolay Kostov, Mechanical Engineering, Rice University, USA (nmk1@tafsm.org)
Hyun-Boo Lee, University of Washington, USA (hyunboo@uw.edu)
Myoung-Gyu Lee, Pohang University of Science and Technology, South Korea (mglee@postech.ac.kr)
Lisheng Liu, Department of Civil and Environmental Engineering, The University of California at Berkeley, USA; Department of Engineering Structure and Mechanics, Wuhan University of Technology, People's Republic of China (liulish@mail.whut.edu.cn)
Yaling Liu, Department of Mechanical Engineering and Mechanics, Lehigh University, USA; Bio-engineering Program, Lehigh University, USA (yal310@lehigh.edu)
Seetha Ramaiah Mannava, School of Dynamic Systems College of Engineering and Applied Science, University of Cincinnati, USA (mannavr@ucmail.uc.edu)
Virginia Monteiro, International Center for Numerical Method in Engineering (CIMNE), Technical University of Catalonia, Spain (virginiamonteiro@yahoo.com)
Liz G. Nallim, INIQI (CONICET), Faculty of Engineering, National University of Salta, Argentina (lgnallim@yahoo.com.ar)
Devin O'Connor, Department of Mechanical Engineering, Northwestern University, USA (devinoconnor2014@u.northwestern.edu)
Sergio Oller, International Center for Numerical Method in Engineering (CIMNE), Technical University of Catalonia, Spain (oller@cimne.upc.edu)
Eugenio Oñate, International Center for Numerical Method in Engineering (CIMNE), Technical University of Catalonia, Spain (onate@cimne.upc.edu)
Harold S. Park, Department of Mechanical Engineering, Boston University, USA (parkhs@bu.edu)
Anthony Puntel, Mechanical Engineering, Rice University, USA (anthony.puntel@tafsm.org)
Farzad Sarker, Mechanical and Aerospace Engineering, University of Texas at Arlington, USA (md.sarker@mavs.uta.edu)
Kathleen Schjodt, Mechanical Engineering, Rice University, USA (kms@tafsm.org)
Daniel C. Simkins, Jr., University of South Florida, USA (dsimkins@eng.usf.edu)
Kenji Takizawa, Department of Modern Mechanical Engineering and Waseda Institute for Advanced Study, Waseda University, Japan (kenji.takizawa@tafsm.org) or (ktakiz@gmail.com)
Shaoqiang Tang, HEDPS, CAPT & Department of Mechanics, Peking University, People's Republic of China (maotang@pku.edu.cn)
Tayfun E. Tezduyar, Mechanical Engineering, Rice University, USA (tezduyar@gmail.com)
Albert C. To, Department of Mechanical Engineering and Materials Science, University of Pittsburgh, USA (albertto@pitt.edu)
Vijay Vasudevan, School of Dynamic Systems College of Engineering and Applied Science, University of Cincinnati, USA (vasudev@ucmail.uc.edu)
Franck J. Vernerey, Department of Civil, Environmental and Architectural Engineering, University of Colorado, USA (franck.vernerey@colorado.edu)
Gregory J. Wagner, Sandia National Laboratories, USA (gjwagne@sandia.gov)
Chu Wang, Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, New York, USA (wangc9@rpi.edu)
Xiaodong Sheldon Wang, College of Science and Mathematics, Midwestern State University, Texas, USA (sheldon.wang@mwsu.edu)
Xingshi Wang, Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, Troy, New York, USA (wangxs165@gmail.com)
Jie Yang, Department of Mechanical Engineering and Mechanics, Lehigh University, USA (yangchenjie@home.swjtu.edu.cn)
Judy P. Yang, Department of Civil & Environmental Engineering, National Chiao Tung University, Taiwan (jpyang@nctu.edu.tw)

Amir Reza Zamiri, Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, New York, USA (zamira@rpi.edu)

Shahrokh Zeinali-Davarani, Department of Mechanical Engineering, Boston University, USA (zeinalis@bu.edu)

Yongjie Zhang, Department of Mechanical Engineering, Carnegie Mellon University, USA (jessieaz@andrew.cmu.edu)

Lucy Zhang, Department of Mechanical, Aerospace, and Nuclear Engineering, Rensselaer Polytechnic Institute, New York, USA (zhanglucy@rpi.edu)

Yanhang Zhang, Department of Mechanical Engineering, Boston University, USA; Department of Biomedical Engineering, Boston University, USA (yanhang@bu.edu)

Tarek Ismail Zohdi, Department of Mechanical Engineering, University of California, Berkeley, USA (zohdi@me.berkeley.edu)

Yihua Zhou, Department of Mechanical Engineering and Mechanics, Lehigh University, USA (yiz311@lehigh.edu)

3. *Development of meshfree formulations known as reproducing kernel particle methods.* These methods provide exceptional accuracy for the simulation of solids undergoing extremely large deformation and have been implemented in many commercial and laboratory software systems:
- (i) shell elements in DYNA3D, ABAQUS, LS-DYNA, ANSYS, and Argonne National Laboratory (ANL) software;
 - (ii) explicit–implicit methods in US Ballistic Laboratory EPIC-2/EPIC-3 programs, and ANL software;
 - (iii) Lagrangian–Eulerian methods adopted by ANL, Kawasaki, Mitsubishi, Ford Motors, and Grumman;
 - (iv) various meshfree methods implemented by Sandia National Labs, Lawrence Livermore National Lab, General Motors, Ford Motors, Delphi, Ball Aerospace, and Caterpillar;
 - (v) multiscale methods adopted by Goodyear for the design of tires and by Sandia in their TAHOE code for multiscale analysis.

Professor Wing Kam Liu is the recipient of numerous awards and honors that include: the 2012 Gauss–Newton Medal (IACM Congress Medal), the highest award given by IACM; the 2009 ASME Dedicated Service Award; the 2007 ASME Robert Henry Thurston Lecture Award; the 2007 USACM John von Neumann Medal, the highest honor given by USACM; the 2004 Japan Society of Mechanical Engineers (JSME) Computational Mechanics Award; the 2002 IACM Computational Mechanics Award; the 2001 USACM Computational Structural Mechanics Award; the 1995 ASME Gustus L. Larson Memorial Award; the 1985 ASME Pi Tau Sigma Gold Medal; the 1979 ASME Melville Medal (for best paper); the 1989 Thomas J. Jaeger Prize of the International Association for Structural Mechanics; and the 1983 Ralph R. Teetor Educational Award, American Society of Automotive Engineers. In 2001, he is listed by ISI as one of the most highly cited and influential researchers in engineering.

This large number of accolades highlights Wing Liu as a scholar and educator of extraordinary international reputation. This is also underlined by the fact that the present book comprises contributions from North American, Europe, and Asia, and from a very diverse group of people: colleagues, friends, collaborators, and former and current PhD students and post-docs. A wide range of topics is covered in this book: multiscale methods, atomistic simulations, micromechanics, and biomechanics/biophysics. These contributions represent either Wing Kam Liu's own research activities or topics he has taken an interest in over recent years. Moreover, the dedications of the contributing authors show that Wing Liu has represented more than just a scientist to a great number of people, to whom he also serves as friend, supporter, and source of inspiration. We are glad to have the opportunity of editing this book and would like to thank Wiley for its helpful collaboration, the authors for their contributions and making this book a success, and Wing Liu for his inspiring and initiating novel research in computational mechanics.

On behalf of the authors, we congratulate Wing Kam Liu to his 60th birthday and wish him happiness, health, success, and continued intellectual creativity for the years to come.

Shaofan Li and Dong Qian
Houston, Texas
November 2012

Preface



This book is dedicated to Professor Wing Kam Liu (or Wing Liu for those who know him well) on the occasion of his 60th birthday.

In 1976, Professor Wing Kam Liu received a BS degree in Engineering Science from the University of Illinois at Chicago with honors. It was his time at UIC where Wing Liu met Ted Belytschko, then a young assistant professor, and took his graduate course on finite-element methods. After graduation from UIC, Wing Liu was admitted as a graduate assistant at the California Institute of Technology (Caltech) under the supervision of the young Thomas J.R. Hughes, who was beginning his academic career there. During his Caltech years, Wing Liu worked on a number of research topics, including finite-element shell elements, which is known today as the Hughes–Liu element.

Wing Liu received both his MS degree (1977) and PhD degree (1980) in Civil Engineering from Caltech, and he then came back to Chicago to become an assistant professor at Northwest-

ern University, joining Ted Belytschko and kicking off a 30-year collaboration between them. In his 32-year academic career, Professor Liu has made numerous contributions to computational mechanics and micromechanics. Among his most noteworthy contributions are:

1. *Development of multiscale methods that bridge quantum to continuum mechanics.* Using these methods, he has developed software for the analysis and design of nanoparticles in materials, bio-sensing, and drug delivery.
2. *Development of new finite-element techniques.* These include introducing new shell elements, arbitrary Eulerian–Lagrangian methods, and explicit–implicit integration techniques that have significantly enhanced the accuracy and speed in software for crashworthiness and prototype simulations. Wing Liu was also the first to develop nonlinear probabilistic finite-element techniques that made nonlinear stochastic and reliability analyses possible.

Contents

About the Editors	xv
List of Contributors	xvii
Preface	xxi
Part I MULTISCALE SIMULATION THEORY	
1 Atomistic-to-Continuum Coupling Methods for Heat Transfer in Solids	3
<i>Gregory J. Wagner</i>	
1.1 Introduction	3
1.2 The Coupled Temperature Field	5
1.2.1 Spatial Reduction	5
1.2.2 Time Averaging	6
1.3 Coupling the MD and Continuum Energy	7
1.3.1 The Coupled System	7
1.3.2 Continuum Heat Transfer	8
1.3.3 Augmented MD	8
1.4 Examples	9
1.4.1 One-Dimensional Heat Conduction	9
1.4.2 Thermal Response of a Composite System	10
1.5 Coupled Phonon-Electron Heat Transport	12
1.6 Examples: Phonon–Electron Coupling	14
1.6.1 Equilibration of Electron/Phonon Energies	14
1.6.2 Laser Heating of a Carbon Nanotube	15
1.7 Discussion	17
Acknowledgments	18
References	18
2 Accurate Boundary Treatments for Concurrent Multiscale Simulations	21
<i>Shaoqiang Tang</i>	
2.1 Introduction	21
2.2 Time History Kernel Treatment	22
2.2.1 Harmonic Chain	22
2.2.2 Square Lattice	23

2.3	Velocity Interfacial Conditions: Matching the Differential Operator	27
2.4	MBCs: Matching the Dispersion Relation	30
	2.4.1 Harmonic Chain	30
	2.4.2 FCC Lattice	33
2.5	Accurate Boundary Conditions: Matching the Time History Kernel Function	36
2.6	Two-Way Boundary Conditions	39
2.7	Conclusions	41
	Acknowledgments	41
	References	41
3	A Multiscale Crystal Defect Dynamics and Its Applications	43
	<i>Lisheng Liu and Shaofan Li</i>	
3.1	Introduction	43
3.2	Multiscale Crystal Defect Dynamics	44
3.3	How and Why the MCDD Model Works	47
3.4	Multiscale Finite Element Discretization	47
3.5	Numerical Examples	52
3.6	Discussion	54
	Acknowledgments	54
	Appendix	55
	References	57
4	Application of Many-Realization Molecular Dynamics Method to Understand the Physics of Nonequilibrium Processes in Solids	59
	<i>Yao Fu and Albert C. To</i>	
4.1	Chapter Overview and Background	59
4.2	Many-Realization Method	60
4.3	Application of the Many-Realization Method to Shock Analysis	62
4.4	Conclusions	72
	Acknowledgments	74
	References	74
5	Multiscale, Multiphysics Modeling of Electromechanical Coupling in Surface-Dominated Nanostructures	77
	<i>Harold S. Park and Michel Devel</i>	
5.1	Introduction	77
5.2	Atomistic Electromechanical Potential Energy	79
	5.2.1 Atomistic Electrostatic Potential Energy: Gaussian Dipole Method	80
	5.2.2 Finite Element Equilibrium Equations from Total Electromechanical Potential Energy	83
5.3	Bulk Electrostatic Piola–Kirchoff Stress	84
	5.3.1 Cauchy–Born Kinematics	84
	5.3.2 Comparison of Bulk Electrostatic Stress with Molecular Dynamics Electrostatic Force	86
5.4	Surface Electrostatic Stress	87
5.5	One-Dimensional Numerical Examples	89
	5.5.1 Verification of Bulk Electrostatic Stress	89
	5.5.2 Verification of Surface Electrostatic Stress	91

5.6	Conclusions and Future Research	94
	Acknowledgments	95
	References	95
6	Towards a General Purpose Design System for Composites	99
	<i>Jacob Fish</i>	
6.1	Motivation	99
6.2	General Purpose Multiscale Formulation	103
	6.2.1 <i>The Basic Reduced-Order Model</i>	103
	6.2.2 <i>Enhanced Reduced-Order Model</i>	104
6.3	Mechanistic Modeling of Fatigue via Multiple Temporal Scales	106
6.4	Coupling of Mechanical and Environmental Degradation Processes	107
	6.4.1 <i>Mathematical Model</i>	107
	6.4.2 <i>Mathematical Upscaling</i>	109
	6.4.3 <i>Computational Upscaling</i>	110
6.5	Uncertainty Quantification of Nonlinear Model of Micro-Interfaces and Micro-Phases	111
	References	113
Part II	PATIENT-SPECIFIC FLUID-STRUCTURE INTERACTION MODELING, SIMULATION AND DIAGNOSIS	
7	Patient-Specific Computational Fluid Mechanics of Cerebral Arteries with Aneurysm and Stent	119
	<i>Kenji Takizawa, Kathleen Schjodt, Anthony Puntel, Nikolay Kostov, and Tayfun E. Tezduyar</i>	
7.1	Introduction	119
7.2	Mesh Generation	120
7.3	Computational Results	124
	7.3.1 <i>Computational Models</i>	124
	7.3.2 <i>Comparative Study</i>	131
	7.3.3 <i>Evaluation of Zero-Thickness Representation</i>	142
7.4	Concluding Remarks	145
	Acknowledgments	146
	References	146
8	Application of Isogeometric Analysis to Simulate Local Nanoparticulate Drug Delivery in Patient-Specific Coronary Arteries	149
	<i>Shaolie S. Hossain and Yongjie Zhang</i>	
8.1	Introduction	149
8.2	Materials and Methods	151
	8.2.1 <i>Mathematical Modeling</i>	151
	8.2.2 <i>Parameter Selection</i>	156
	8.2.3 <i>Mesh Generation from Medical Imaging Data</i>	158
8.3	Results	159
	8.3.1 <i>Extraction of NP Wall Deposition Data</i>	159
	8.3.2 <i>Drug Distribution in a Normal Artery Wall</i>	160
	8.3.3 <i>Drug Distribution in a Diseased Artery Wall with a Vulnerable Plaque</i>	160

8.4	Conclusions and Future Work	165
	Acknowledgments	166
	References	166
9	Modeling and Rapid Simulation of High-Frequency Scattering Responses of Cellular Groups	169
	<i>Tarek Ismail Zohdi</i>	
9.1	Introduction	169
9.2	Ray Theory: Scope of Use and General Remarks	171
9.3	Ray Theory	173
9.4	Plane Harmonic Electromagnetic Waves	177
	9.4.1 <i>General Plane Waves</i>	177
	9.4.2 <i>Electromagnetic Waves</i>	177
	9.4.3 <i>Optical Energy Propagation</i>	178
	9.4.4 <i>Reflection and Absorption of Energy</i>	179
	9.4.5 <i>Computational Algorithm</i>	183
	9.4.6 <i>Thermal Conversion of Optical Losses</i>	187
9.5	Summary	190
	References	190
10	Electrohydrodynamic Assembly of Nanoparticles for Nanoengineered Biosensors	193
	<i>Jae-Hyun Chung, Hyun-Boo Lee, and Jong-Hoon Kim</i>	
10.1	Introduction for Nanoengineered Biosensors	193
10.2	Electric-Field-Induced Phenomena	193
	10.2.1 <i>Electrophoresis</i>	194
	10.2.2 <i>Dielectrophoresis</i>	195
	10.2.3 <i>Electroosmotic and Electrothermal Flow</i>	198
	10.2.4 <i>Brownian Motion Forces and Drag Forces</i>	199
10.3	Geometry Dependency of Dielectrophoresis	200
10.4	Electric-Field-Guided Assembly of Flexible Molecules in Combination with other Mechanisms	203
	10.4.1 <i>Dielectrophoresis in Combination with Fluid Flow</i>	203
	10.4.2 <i>Dielectrophoresis in Combination with Binding Affinity</i>	203
	10.4.3 <i>Dielectrophoresis in Combination with Capillary Action and Viscosity</i>	203
10.5	Selective Assembly of Nanoparticles	204
	10.5.1 <i>Size-Selective Deposition of Nanoparticles</i>	204
	10.5.2 <i>Electric-Property Sorting of Nanoparticles</i>	205
10.6	Summary and Applications	205
	References	205
11	Advancements in the Immersed Finite-Element Method and Bio-Medical Applications	207
	<i>Lucy Zhang, Xingshi Wang, and Chu Wang</i>	
11.1	Introduction	207
11.2	Formulation	208
	11.2.1 <i>The Immersed Finite Element Method</i>	208
	11.2.2 <i>Semi-Implicit Immersed Finite Element Method</i>	210

11.3	Bio-Medical Applications	211
	11.3.1 <i>Red Blood Cell in Bifurcated Vessels</i>	211
	11.3.2 <i>Human Vocal Folds Vibration during Phonation</i>	214
11.4	Conclusions	217
	References	217
12	Immersed Methods for Compressible Fluid–Solid Interactions	219
	<i>Xiaodong Sheldon Wang</i>	
12.1	Background and Objectives	219
12.2	Results and Challenges	222
	12.2.1 <i>Formulations, Theories, and Results</i>	222
	12.2.2 <i>Stability Analysis</i>	227
	12.2.3 <i>Kernel Functions</i>	228
	12.2.4 <i>A Simple Model Problem</i>	231
	12.2.5 <i>Compressible Fluid Model for General Grids</i>	231
	12.2.6 <i>Multigrid Preconditioner</i>	232
12.3	Conclusion	234
	References	234
Part III FROM CELLULAR STRUCTURE TO TISSUES AND ORGANS		
13	The Role of the Cortical Membrane in Cell Mechanics: Model and Simulation	241
	<i>Louis Foucard, Xavier Espinet, Eduard Benet, and Franck J. Vernerey</i>	
13.1	Introduction	241
13.2	The Physics of the Membrane–Cortex Complex and Its Interactions	243
	13.2.1 <i>The Mechanics of the Membrane–Cortex Complex</i>	243
	13.2.2 <i>Interaction of the Membrane with the Outer Environment</i>	247
13.3	Formulation of the Membrane Mechanics and Fluid–Membrane Interaction	249
	13.3.1 <i>Kinematics of Immersed Membrane</i>	249
	13.3.2 <i>Variational Formulation of the Immersed MCC Problem</i>	251
	13.3.3 <i>Principle of Virtual Power and Conservation of Momentum</i>	253
13.4	The Extended Finite Element and the Grid-Based Particle Methods	255
13.5	Examples	257
	13.5.1 <i>The Equilibrium Shapes of the Red Blood Cell</i>	257
	13.5.2 <i>Cell Endocytosis</i>	259
	13.5.3 <i>Cell Blebbing</i>	260
13.6	Conclusion	262
	Acknowledgments	263
	References	263
14	Role of Elastin in Arterial Mechanics	267
	<i>Yanhang Zhang and Shahrokh Zeinali-Davarani</i>	
14.1	Introduction	267
14.2	The Role of Elastin in Vascular Diseases	268
14.3	Mechanical Behavior of Elastin	269
	14.3.1 <i>Orthotropic Hyperelasticity in Arterial Elastin</i>	269
	14.3.2 <i>Viscoelastic Behavior</i>	271

14.4	Constitutive Modeling of Elastin	272
14.5	Conclusions	276
	Acknowledgments	276
	References	277
15	Characterization of Mechanical Properties of Biological Tissue: Application to the FEM Analysis of the Urinary Bladder	283
	<i>Eugenio Oñate, Facundo J. Bellomo, Virginia Monteiro, Sergio Oller, and Liz G. Nallim</i>	
15.1	Introduction	283
15.2	Inverse Approach for the Material Characterization of Biological Soft Tissues via a Generalized Rule of Mixtures	284
	15.2.1 Constitutive Model for Material Characterization	284
	15.2.2 Definition of the Objective Function and Materials Characterization Procedure	286
	15.2.3 Validation of the Inverse Model for Urinary Bladder Tissue Characterization	287
15.3	FEM Analysis of the Urinary Bladder	289
	15.3.1 Constitutive Model for Tissue Analysis	290
	15.3.2 Validation. Test Inflation of a Quasi-incompressible Rubber Sphere	292
	15.3.3 Mechanical Simulation of Human Urinary Bladder	293
	15.3.4 Study of Urine–Bladder Interaction	295
15.4	Conclusions	298
	Acknowledgments	298
	References	298
16	Structure Design of Vascular Stents	301
	<i>Yaling Liu, Jie Yang, Yihua Zhou, and Jia Hu</i>	
16.1	Introduction	301
16.2	Ideal Vascular Stents	303
16.3	Design Parameters that Affect the Properties of Stents	304
	16.3.1 Expansion Method	305
	16.3.2 Stent Materials	305
	16.3.3 Structure of Stents	306
	16.3.4 Effect of Design Parameters on Stent Properties	308
16.4	Main Methods for Vascular Stent Design	308
16.5	Vascular Stent Design Method Perspective	316
	References	316
17	Applications of Meshfree Methods in Explicit Fracture and Medical Modeling	319
	<i>Daniel C. Simkins, Jr.</i>	
17.1	Introduction	319
17.2	Explicit Crack Representation	319
	17.2.1 Two-Dimensional Cracks	320
	17.2.2 Three-Dimensional Cracks in Thin Shells	323
	17.2.3 Material Model Requirements	323
	17.2.4 Crack Examples	323
17.3	Meshfree Modeling in Medicine	327
	Acknowledgments	331
	References	331

18	Design of Dynamic and Fatigue-Strength-Enhanced Orthopedic Implants	333
	<i>Sagar Bhamare, Seetha Ramaiah Mannava, Leonora Felon, David Kirschman, Vijay Vasudevan, and Dong Qian</i>	
18.1	Introduction	333
18.2	Fatigue Life Analysis of Orthopedic Implants	335
	18.2.1 <i>Fatigue Life Testing for Implants</i>	335
	18.2.2 <i>Fatigue Life Prediction</i>	337
18.3	LSP Process	338
18.4	LSP Modeling and Simulation	339
	18.4.1 <i>Pressure Pulse Model</i>	339
	18.4.2 <i>Constitutive Model</i>	340
	18.4.3 <i>Solution Procedure</i>	341
18.5	Application Example	342
	18.5.1 <i>Implant Rod Design</i>	342
	18.5.2 <i>Residual Stresses</i>	342
	18.5.3 <i>Fatigue Tests and Life Predictions</i>	344
18.6	Summary	348
	Acknowledgments	348
	References	349
Part IV BIO-MECHANICS AND MATERIALS OF BONES AND COLLAGENS		
19	Archetype Blending Continuum Theory and Compact Bone Mechanics	353
	<i>Khalil I. Elkhodary, Michael Steven Greene, and Devin O'Connor</i>	
19.1	Introduction	353
	19.1.1 <i>A Short Look at the Hierarchical Structure of Bone</i>	354
	19.1.2 <i>A Background of Generalized Continuum Mechanics</i>	355
	19.1.3 <i>Notes on the Archetype Blending Continuum Theory</i>	356
19.2	ABC Formulation	358
	19.2.1 <i>Physical Postulates and the Resulting Kinematics</i>	358
	19.2.2 <i>ABC Variational Formulation</i>	359
19.3	Constitutive Modeling in ABC	361
	19.3.1 <i>General Concept</i>	361
	19.3.2 <i>Blending Laws for Cortical Bone Modeling</i>	363
19.4	The ABC Computational Model	367
19.5	Results and Discussion	368
	19.5.1 <i>Propagating Strain Inhomogeneities across Osteons</i>	368
	19.5.2 <i>Normal and Shear Stresses in Osteons</i>	369
	19.5.3 <i>Rotation and Displacement Fields in Osteons</i>	370
	19.5.4 <i>Damping in Cement Lines</i>	372
	19.5.5 <i>Qualitative Look at Strain Gradients in Osteons</i>	372
19.6	Conclusion	373
	Acknowledgments	374
	References	374
20	Image-Based Multiscale Modeling of Porous Bone Materials	377
	<i>Judy P. Yang, Sheng-Wei Chi, and Jiun-Shyan Chen</i>	
20.1	Overview	377
20.2	Homogenization of Porous Microstructures	379