Introduction to Computational Nanomechanics

A comprehensive guide on computational nanomechanics discussing basic theoretical concepts and computer modelings in areas such as computational physics, materials, mechanics, and engineering as well as several other interdisciplinary avenues. This book makes the underlying theory accessible to readers without specialized training or extensive background in quantum physics, statistical mechanics, or theoretical chemistry. It combines a careful treatment of theoretical concepts with a detailed tutorial on computer softwares and computing implementations, including multiscale simulation and computational statistical theory. Multidisciplinary perspectives are provided, yielding a deep insight on the applications of computational nanomechanics across diverse engineering fields. The book can serve as a practical guide with step-by-step discussions of coding, example problems, and case studies. This book will be essential reading for students new to the subject, as well as an excellent reference for researchers and developers.

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Multiscale and Statistical Simulations

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CAMBRIDGE
UNIVERSITY PRESS

Shaftesbury Road, Cambridge CB2 8EA, United Kingdom

One Liberty Plaza, 20th Floor, New York, NY 10006, USA

477 Williamstown Road, Port Melbourne, VIC 3207, Australia

314–321, 3rd Floor, Plot 3, Splendor Forum, Jasola District Centre, New Delhi – 110025, India

103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment, a department of the University of Cambridge.

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www.cambridge.org
Information on this title: www.cambridge.org/9781107011151

DOI: 10.1017/9780511894770

First published 2022

Printed in the United Kingdom by TJ Books Limited, Padstow, Cornwall

A catalogue record for this publication is available from the British Library

ISBN 978-1-107-01115-1 Hardback

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Preface

This book grew from the lecture notes of the graduate course on Introduction to Computational Nanomechanics at the University of California–Berkeley, which I started teaching in Spring 2011.

Most of the materials are compiled and organized from various textbooks or research papers in quantum mechanics, molecular dynamics, computational statistical mechanics, and the like. However, the contents are edited and streamlined, and the texts are rephrased so that first-year engineering graduate students with different backgrounds but without a formal training in graduate-level physics and chemistry can easily understand them. In fact, the main motivation of the book is to teach computational nanomechanics and computational statistical mechanics to students from various disciplines of engineering, biology, and mathematical sciences, who do not have a formal training in quantum physics and statistical mechanics. Because of continuing developments in nanoscience and nanotechnology and their applications to the broader field of engineering, the needs for in-depth knowledge of nanoscience, especially computational nanoscience, have become more and more urgent and demanding. Usually, conventional wisdom says that acquiring such knowledge would require a career change, which demands so much time and effort that many engineering students or researchers are too intimidated.

There are several books on computational nanomechanics available. To distinguish the present book from the others, I would like to focus more on computational statistical mechanics, multiscale simulation, and its applications to solve engineering problems – a subject that is still in the stage of infancy.

My academic background is not quantum physics or computational chemistry, but applied and computational mechanics, which is a subfield of engineering science or applied physics. I always felt that perhaps this was a disadvantage for me in writing a book on computational nanomechanics; on the other hand, I may be in a unique position to understand how the mind of an engineer works, so that I may have a different perspective to write the book in such a way that most engineers will feel more comfortable to read it. It is only this thought that keeps me thinking that this is a useful endeavor.

One of the main features of the book is that it includes many segments of actual computation scripts and computer codes. It provides step-by-step tutorials to show how to conduct a computer simulation of a first-principle calculation or a molecular dynamics calculation. Most of these scripts are collected from various online

resources, as well as private communications and sharings from our research collaborators. Because the computer codes have been migrated from different sources and different versions, we are not able to acknowledge the original sources or developers, and for that we sincerely apologize to the original developers. While we are deeply indebted to these original developers, we are hoping that they also hold same spirits for sharing these information with readers, and especially younger researchers and students. Lastly, in order to help readers have hands-on experience in computer implementation on some of numerical computation examples discussed in this book, computing resource files have been posted on the following website: http://nanomechanics.berkeley.edu/introduction-to-computationalnanomechanics/.

The readers are free to download these resource files.

Shaofan Li

Acknowledgments

My coauthor, Dr. Jun Li, has been working with me on first-principles modeling and simulations of flexoelectricity since 2018. She has provided many inputs and contributed a great deal in the writing of this book. Without her participation and dedication, I would not have been able to finish the book. Finally, I would like to acknowledge and thank the friends, former students, and fellow researchers in computational nanomechanics, who have all helped me gain a better understanding of this topic. In particular, I would like to thank Dr. Shingo Urata, Dr. Lisheng Liu, Dr. Xiaowei Zeng, Dr. Bo Ren, Dr. Houfu Fan, Dr. Tong Qi, Dr. Hiroyuki Miniky, Dr. Dandan Lyu, Dr. Hengameh Shams, Dr. Qingsong Tu, Mr. Qi Zheng, Mr. Caglar Tamur, Dr. Yuxi Xie, Dr. Xin Lai, Dr. Kaiyue Wang, and Dr. Donghoon Kim, among others, who have contributed to the creation and development of this book.