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Molecular Dynamics Simulations in Statistical Physics: Theory and Applications

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To the memory of my mother and father

Preface

Computer simulations are used very often to understand and solve practical problems in the area of statistical physics and biophysics. With proper knowledge of classical mechanics, thermodynamics, and statistical physics, you will be able to understand and judge the content of this book.

This book aims to be a recipe for computer simulations with molecular dynamics techniques in statistical physics, where the main emphases are the macromolecular systems. Numerical methods introduced in the form of computer algorithms can be implemented in computers using any desired computer programing language, such as Fortran 90, C/C++, and others. This book applies some of the discussed numerical methods and their algorithms in the existing computer programing software of macromolecular systems, such as the CHARMM program.

In this book, you will find out some advanced concepts of computer simulation techniques used in statistical physics and a particular understanding of biological and physical systems. It discusses the molecular dynamics approach in details to help understand its use in statistical physics problems.

Chapters 1, 2, and 3 introduce the principles of classical mechanics, thermodynamics, and statistical physics, which are necessary concepts to know to better understand real problems in different fields, such as physics, chemistry, and biology, when we use the computer simulations for solving them, while Chap. 4 introduces the use of statistical thermodynamics in understanding biological phenomena.

In Chap. 5, the main theory used for understanding many useful techniques in a computer simulation, such as calculations by means of molecular dynamics simulations of the absolute free energy, solvation free energy, and binding free energy, which have a broad area of applications in physics, chemistry, and biology, is discussed.

Chapter 6 then introduces molecular dynamics techniques, such as describing the equations of motion in different statistical ensembles of interest to mimic real experimental conditions, while Chap. 7 presents molecular mechanics and represents the primary methods for parameterization of the force fields; in particular, it discusses traditional and automated force field parameterization methods and presents the perspectives on the force field developments.

Chapter 8 further discusses different methods used to determine the frequency spectrum of the motions in a macromolecular system, namely, the normal modes, principal component analysis, and the time-lagged auto-encoder machine learning approach, and an improved modified version of the artificial neural network, called Bootstrapping Swarm Artificial Neural Network. Besides, it introduces an approach of how to derive the equations of motion in the reduced essential subspace of the slow collective variables using the harmonic bath coupling of these variables with the environmental fast degrees of freedom of the system.

Chapter 9 introduces some elements of the information theory and discusses the connection between information theory measures and statistical thermodynamics.

Chapter 10 subsequently discusses some technical aspects of the use of molecular dynamics method in simulations of macromolecular systems. In particular, it describes the periodic boundary condition, treatment of the long-range interactions, spherical cutoffs, and equilibration of the molecular dynamics simulations.

Chapter 11 introduces numerical techniques used to solve molecular dynamics equations of motion using Liouville's formalism and Trotter factorization scheme. Besides, the stability of numerical schemes will be discussed by applying to real physical systems for which the analytical solutions are known.

Finally, in Chap. 12, generalized ensemble molecular dynamics simulation methods used to improve the sampling of lower-energy configurations are discussed. In particular, this chapter introduces the multicanonical sampling, Tsallis ensemble, Swarm particle intelligence molecular dynamics, and replica exchange.

This book is aimed to graduate students and research scientists working in the fields of theoretical and computational biophysics, physics, and chemistry. Also, the book can be used by graduate students of other branches, such as applied mathematics, computer sciences, and bioinformatics.

Skopje, North Macedonia Hiqmet Kamberaj
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About the Author

Hiqmet Kamberaj is an Associate Professor at International Balkan University and the Dean of the Faculty of Engineering. He completed his Ph.D. in Computational Physics in 2005 from Manchester Metropolitan University and his post-doctoral studies from the University of Minnesota, Arizona State University, and the National Institute for Nanotechnology, University of Alberta, Edmonton, Alberta. He received his Bachelor of Science in Physics in 1996 from the University of Tirana and his Master of Science in Physics from the University of Siegen in 2000.

He has published around 20 articles and book chapters in reputed journals and has been serving as Editor in Chief, Editorial Board Member, and Ad Hoc Reviewer of Repute. His articles focus on understanding the structure, dynamics, and thermodynamics of macromolecular systems using the laws of physics and biochemistry, and applied mathematics.

He loves teaching and preparing lecture notes for his students and especially enjoys preparing resumes for his students who are taking the first steps of their careers.

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