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Rugged Free Energy Landscapes

Common Computational Approaches to Spin Glasses, Structural Glasses and Biological Macromolecules

Springer

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Preface

This volume on spin glasses, structural glasses and biological macromolecules collects pedagogically written lecture notes of internationally renowned experts from eight countries, who work on different physical problems but employ similar theoretical concepts and computational methods. The research into at first sight quite different physical phenomena, therefore, faces related problems, whose origin can be traced back to the difficulties of numerical simulations of systems with rugged free-energy landscapes. Many of the original publications presuppose quite specialized "common" knowledge, usually readily accessible only to the experts in each of these fields. Moreover, they are typically published in quite different sets of scientific journals. The main objective of these Lecture Notes is, therefore, to provide the necessary background material in a coherent fashion and thereby to initialize knowledge transfer of advanced methodologies across the boundaries of the disciplines. It can be anticipated that future successful computer simulation studies of static and dynamic properties of the three systems considered here as well as the further development of improved numerical algorithms will greatly profit from an interaction among researchers in these different fields.

More specifically, the merits and drawbacks of the various variants of generalized ensemble methods as employed in computational studies of glassy systems and biomolecules as well as the complicated interplay of different algorithms in combined methods are discussed from rather different viewpoints in this volume. For investigations of spin and structural glasses, the Lecture Notes should have an impact on a better understanding of their similarities in dynamical and non-equilibrium properties, which in turn are intimately related to the rugged free-energy landscape mapped out by means of equilibrium methods. And it can be hoped that the already existing expertise in the physics of glassy systems will give conceptual guidance to similar studies of biological macromolecules, such as peptides and proteins.

The contents of this volume are organized into four parts. The first three parts cover introductory material and reviews of recent research results for spin glasses, structural glasses and biological macromolecules with emphasis

on the protein folding problem. The joint theme of these chapters is rugged free-energy landscapes and computational methods to deal with this multiple-minima problem efficiently. The fourth part, finally, focuses on a detailed exposition of recent, quite general algorithmic developments that alleviate the computational problems and can be put to good use in specific applications in each of the fields considered in the first three parts.

The idea for such a volume came to us about 2 years ago at the occasion of a CECAM workshop in Lyon, France, where about 30 talks on the above topics were presented. The interdisciplinary character of the workshop was indeed very stimulating, and it became clear that an up-to-date volume like this emphasizing the close interrelations between the three fields and at the same time bridging the gap between introductory material and ongoing state-of-the-art research would be highly desirable.

Leipzig, *Wolfhard Janke*
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Contents

Part III Protein Folding

Part IV Algorithmic Developments