

Statistical Mechanics:

Algorithms and Computations

Werner Krauth



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Statistical Mechanics

Algorithms and Computations

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Preface

This book is meant for students and researchers ready to plunge into statistical physics, or into computing, or both. It has grown out of my research experience, and out of courses that I have had the good fortune to give, over the years, to beginning graduate students at the Ecole Normale Supérieure and the Universities of Paris VI and VII, and also to summer school students in Drakensberg, South Africa, undergraduates in Salem, Germany, theorists and experimentalists in Lausanne, Switzerland, young physicists in Shanghai, China, among others. Hundreds of students from many different walks of life, with quite different backgrounds, listened to lectures and tried to understand, made comments, corrected me, and in short helped shape what has now been written up, for their benefit, and for the benefit of new readers that I hope to attract to this exciting, interdisciplinary field. Many of the students sat down afterwards, by themselves or in groups, to implement short programs, or to solve other problems. With programming assignments, lack of experience with computers was rarely a problem: there were always more knowledgeable students around who would help others with the first steps in computer programming. Mastering technical coding problems should also only be a secondary problem for readers of this book: all programs here have been stripped to the bare minimum. None exceed a few dozen lines of code.

We shall focus on the concepts of classical and quantum statistical physics and of computing: the meaning of sampling, random variables, ergodicity, equidistribution, pressure, temperature, quantum statistical mechanics, the path integral, enumerations, cluster algorithms, and the connections between algorithmic complexity and analytic solutions, to name but a few. These concepts built the backbone of my courses, and now form the tissue of the book. I hope that the simple language and the concrete settings chosen throughout the chapters take away none of the beauty, and only add to the clarity, of the difficult and profound subject of statistical physics.

I also hope that readers will feel challenged to implement many of the programs. Writing and debugging computer code, even for the naive programs, remains a difficult task, especially in the beginning, but it is certainly a successful strategy for learning, and for approaching the deep understanding that we must reach before we can translate the lessons of the past into our own research ideas.

This book is accompanied by a compact disc containing more than one hundred pseudocode programs and close to 300 figures, line drawings,

and tables contained in the book. Readers are free to use this material for lectures and presentations, but must ask for permission if they want to include it in their own publications. For all questions, please contact me at www.lps.ens.fr/~krauth. (This website will also keep a list of misprints.) Readers of the book may want to get in contact with each other, and some may feel challenged to translate the pseudocode programs into one of the popular computer languages; I will be happy to assist initiatives in this direction, and to announce them on the above website.