Preface

The material presented in this book was born out of a series of lectures at a Summer School held at Figueira da Foz (Portugal) in 1987. Since then, the field of computational physics has seen an enormous growth and stormy development.

Many new applications and application areas have been found. In the 1980s, we could not foresee this but hoped that the Monte Carlo method would find such widespread acceptance. We were thus very glad to bring the work forward to a second edition correcting some misprints. Since then and over the years and editions of this book, many chapters have been added accounting for the development of new methods and algorithms. However, the basics have remained stable over the years and still serve as an entry point for researchers who would like to apply the Monte Carlo method and perhaps want to develop new ideas. Appending these basics with chapters on newly developed methods has evolved this book a bit into the direction of a textbook giving an introduction and at the same time covering a very broad spectrum. The first part of the book explains the theoretical foundations of the Monte Carlo method as applied to statistical physics. Chapter 3 guides the reader to practical work by formulating simple exercises and giving hints to solve them. Hence, it is a kind of "primer" for the beginner, who can learn the technique by working through these two chapters in a few weeks of intense study. Alternatively, this material can be used as text for a short course in university teaching covering in one term. The following chapters describe some more sophisticated and advanced techniques, e.g., Chap. 4 describes cluster algorithms and reweighting techniques, Chap. 5 describes the basic aspects of quantum Monte Carlo methods, and Chap. 6 (newly added to the 5th edition) describes recent developments in the last decade, such as "expanded ensemble" methods to sample the energy density of states, e.g., the Wang–Landau algorithm, as well as methods to sample rare events, such as "transition path sampling". These chapters then should be useful even for the more experienced practitioner. However, no attempt is made to cover all existing applications of Monte Carlo methods to statistical physics in an encyclopedic style – such an attempt would make this book almost unreadable and unhandy. While the "classic" applications of Monte Carlo methods in the 1970s and 1980s of the last century now are simple examples that a student can work out on his laptop as an exercise, this is not true for the recent developments described in the last chapter,

of course, which often need heavy investment of computer time. Hence, no attempt could as yet be made to enrich the last chapters with exercises as well.

We are very grateful for the many comments, suggestions, and the pointing out of misprints that have been brought to our attention. We would like to thank the many colleagues with whom we had the pleasure to engage with into discussions and that in some way or the other have shaped our thinking and thus have indirectly influenced this work.

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