Preface

You have decided to become an expert in computer simulations, congratulations! This is a good decision, because computational and simulation methods become more and more important in all areas of science, humanities, economy, engineering and mathematics. This book will help you a great deal in learning the most important basics which you need during all phases of a simulation research project, from the phases of program design, implementation, and debugging, through running the simulations, organizing the data and analyzing the results, to the final phase where you want to present and publish your results.

Note that nowadays thousands of different problems exist which are being investigated by computer simulations. One studies, for example, the diffusion of chemicals in soils, the folding of proteins in cells, the communication of neurons in the brain, the deformation of cars in accidents, the behavior of brokers working at the stock market, the evolution of the weather during the next days or weeks, the turbulent behavior of flowing water in a turbine, the movement of electrons in semiconductors, the patterns of words in languages, or the traffic of pedestrians in crowded shopping malls, to name only a few. Consequently, there are many algorithms to treat the variety of problems, for example, finite differences, finite elements, integration methods, matrix inversion, eigenvalue determination, equation solvers, Molecular dynamics simulations, Monte Carlo methods, density functional approaches, graph algorithms, optimization methods, and so on. Which methods are suitable for your problems depends heavily on the problems you want to solve. Since there are way too many algorithms available for all these different problems, and because everybody needs usually a different one, these special-purpose algorithms are *not* covered in this book.

This book instead covers methods, techniques and algorithms, which

you *always* have to apply, independent of the actual simulation research project you are considering. Here, *practical* aspects of conducting research via computer simulations are discussed. An overview is given towards the end of this preface. After reading this book, you only need some additional information about the specific project your are considering, usually provided in scientific papers, and maybe you need a second special-purpose book which you have to get. Then you are ready to start!

The book addresses people who have no or little experience with computer simulations. This book is in particular suited for students who want to start a project, like a PhD thesis, in the field of computer simulations. But also researchers who have conducted already some simulation projects may find a lot of the advanced material helpful. It is assumed that the reader is familiar with an operating system such as UNIX (e.g. Linux), a high-level programming language such as C, JAVA, Fortran or Pascal and has some experience with at least tiny software projects.

Throughout the book, because of the limited space, usually only short introductions to the specific areas are given, as "ready-to-use recipes". The material usually is presented here in a learning-by-example manner. Nevertheless, the material is extensive enough to provide a fundamental set of tools to perform all standard tasks when creating and performing simulations. In addition, references to more specialized literature are cited, allowing specific subjects to be studied more extensively. Most examples of code are in C/C++. Many examples, also solutions to exercises, are available on the CD included with the book. This is indicated by a small `GET SOURCE CODE` box in the text. Also some freely available documentation is contained on the CD. For details, see the appendix.

GET SOURCE CODE
DIR: `c-programming` FILE(S): `first.c`

Next, I give you some idea, how the book was realized. In fact, the work on this book started when I was doing simulations for obtaining my first university degree. I had to develop new algorithms and implement them. I had to do many large-scale simulations on a parallel computing cluster. The data had to be analyzed, usually in many different ways, and over-and-over again when new data became available. Finally, the results had to be presented and summarized in a scientific paper. These basic steps remained my main occupation during my PhD and during my first post-doc projects. I became more and more experienced and refined my approaches. I also improved my ways to work by reading books about software engineering, algorithms, data structures and data analysis, as well as by learning to

use many programs. After the first-post doc years, I began to supervise students. Hence, I started to pass on my knowledge, trying to help other people to avoid many pitfalls and to devise highly efficient programs. Some of my experiences found their way to the last chapter of the book of Heiko Rieger and myself with the title "Optimization Algorithms in Physics". That chapter is in fact a very short version of the present book. Thus, it served as seed of the this book and some material of the old chapter appears occasionally here.[1] During the years, I supervised more and more students, and even gave a university course on the practical aspects of computer simulations. This course contained a lot of new material compared to the book chapter and in fact it served as a seed for the present book. Nevertheless, the material I used for supervising students was still collected from several different sources, often not quite compatible with each other. I started to feel that it would help my work, and also increase the efficiency, if I wrote a full book about practical aspects of computer simulations, which should contain "all" needed material comprehensively. After two more years, I received an email from *World Scientific*, where my course web page was noticed. They asked me whether I would like to write a book, based on the course. Now it was not difficult to come to the decision indeed to realize the book. You are now holding the result in your hands.

Note that this book contains a very personal view of which tools are considered useful. Very often, I present several independent tools, such as tools for editing, compiling and analyzing programs rather than one all-purpose environment which usually contains a framework just integrating these basic tools. Nevertheless, most of the tools introduced are standard programs and available on all computer systems (for Microsoft operating systems they sometimes have other names).

Here, I give an overview over the contents of the book. First, a short introduction to C programming is given. Also related topics like macros, *make files* and shell scripts are touched. In the second chapter, the main ideas of software engineering are explained and several hints allowing the construction of efficient and reliable code are stated. In Chap. 3, a short primer on object-oriented software development is presented. In particular, it is shown that this kind of programming style can be achieved with standard procedural languages such as C as well, but also how C++ can be used. Next, basic types of algorithms and advanced data structures are explained.

[1] Taken from A.K. Hartmann and H. Rieger, *Optimization Algorithms in Physics*, pp. 293–357, 2002, Copyright Wiley-VCH Verlag GmbH & Co. KGaA. Reproduced with permission.

These can be used as auxiliary tools to create highly-professional, efficient simulation programs. In Chap. 5, three very useful debugging tools are presented, which will help you to hunt down bugs in your programs quickly. In the subsequent chapter, the benefit of using libraries like the *Standard Template Library* and the *GNU Scientific Library* is explained and it is shown how you can build your own libraries. In Chap. 7, aspects of probability theory, random-number generation, data analysis, plotting data and curve fitting are covered. In the last chapter, an introduction to information retrieval and literature search in the Internet and to the preparation of presentations and publications is given.

I am indebted to all my colleagues for countless hours of joyful collaborations, which laid the foundations of this book. I am very grateful to Angelika Sievers for thoroughly reading all chapters of the book while checking for typos, language and grammar mistakes. Finally, I would like to thank Björn Ahrens, Luis Apolo, Bernd Burghardt, Niels Hoelzel, Magnus Jungsbluth, Reinhard Leidl, Oliver Melchert, Axel Schulz, Bruno Sciolla and Stefan Wolfsheimer for critically reading manuscript chapters and for giving me many useful comments which helped me to improve the book and to remove many typos.

Alexander K. Hartmann
Oldenburg, November 2008