Preface

This volume provides an overview of some of the basics of the underlying physical theories, the mathematical concepts, the numerical tools and the methods with which the dynamics of condensed matter is treated on several length and associated time scales, with a focus on particle based methods. These methods form the basis of a research area which is generally termed "computational multiscale physics" (CMP) or "computational materials science" (CMS), meaning the modeling and simulation of condensed matter in the fluid or solid state with the aid of efficient algorithms implemented on computers.

The presented methods and theories in this book range from the atomistic quantum scale (nanometers), the microscopic scale (from nano- to micrometers) and the intermediate mesoscopic scale (micrometers), to the scale of macroscopic structures (centimeters and meters). The order of chapters roughly follows this classification of scales and each chapter starts with an introductory overview of some the physical basics of condensed matter modeling on the respective scale.

Presented topics include quantum mechanical ab initio methods in Hilbert space which are frequently used to predict the electronic and/or atomic structures of different materials, described as many particle systems in statistical thermodynamics. These methods are very restricted in the number of treated particles. Semi-empirical techniques such as the tight-binding method and yet more empirical methods such as classical molecular dynamics and Monte Carlo simulations are discussed as well. Applications of these methods in equilibrium and non-equilibrium solid state physics (shock wave physics being one particularly interesting application) as well as in soft matter physics, e.g. polymers. We also discuss classical field theory which is the physical basis of methods such as the finite element method for solving partial differential equations in Sobolev spaces (a special class of Hilbert spaces), usually used in engineering applications of fluid dynamics and with macroscopic structural problems.

With respect to the above said this book offers primarily orientation in the large field of computational multiscale physics by putting together several

numerical methods in a unified fashion with a particular emphasis on explaining the underlying physical theories. These theories may be considered as statements of established "truths" of nature and are used as a general basis for model building, independent of the application of any particular numerical technique. A good understanding of the physics behind each numerical technique is essential for making useful choices of algorithms. In this attempt, the book is necessarily limited as one can neither hope to discuss exhaustively all aspects of physical theories that are important for a thorough understanding of certain numerical methods, nor can one hope to discuss all aspects of computer simulation. However, by focusing on the *fundamental principles* which form the common theoretical basis of many different computational methods. I have attempted to provide a systematic overview which may serve as a sound introduction into several research areas, so that researchers and students can quickly step on from this ground level to more detailed, advanced, and complex problems, but with a thorough understanding of the guiding principles. The selection of examples, illustrating some methods is inevitably biased by the author's own research interests.

Many references to the basic *primary* literature are provided where possible in order to provide the interested reader with several starting points for his or her own research. I apologize in advance with all colleagues and researchers that I may have missed to mention. For those readers, who do not have ready access to primary literature, e.g. through university library loan services, recent references are provided at the end of some chapters, including easily accessible, less technical volumes. Some exercises are occasionally included in the main text and some problems are provided at the end of some chapters in order to show some tricks of the trade with certain methods or to illustrate further some theoretical considerations. Several example applications for numerical techniques and references to research topics of current interest are provided. Boxes summarize certain topics in succinct form in the main text and can be used as a convenient source of reference.

To make this book yet more valuable for those readers interested in learning how to write their own simulation codes, I have also included several guidelines for designing and implementing programs from my own experince in software industry in Chap. 2. Additionally, more explicit instructions are provided in Chap. 6 for writing a basic functioning molecular dynamics program. Thus, not only the theoretical basics and the essential algorithms of several research areas in computational multiscale physics are provided but also some explicit code samples which may be used as a guide for writing own simulation programs.

There is no doubt that computer simulation as an interdisciplinary tool for solving complex scientific problems has become indispensable in modern research both for scientists at universities and engineers in industrial laboratories. Numerical predictions combine elements of theories and models of physics, mathematics, chemistry, computer science, professional code development, materials and engineering science and even biology. Thus, multiscale

physics has a strong interdisciplinary character which is why a thorough understanding of the essentials of various scientific fields is a prerequisite for understanding the recent progress achieved in this area of research. The diversity of basic theories and numerical methods is not easy to overview and to understand for students entering the field of computer simulation. Even for scientists active in this research area it is not an easy task to survey all recent developments even in their own field of expertise.

The number of scientists and engineers using computer simulation as a general tool is steadily increasing. Non-experts entering this field will probably merely want to use commercial software for solving complex problems and they will not be primarily interested in techniques or theoretical "dead freight". Yet, I hope to convince those readers who consider themselves just users of ready-made software packages that it is very interesting to understand some of the common physical and mathematical principles on which these programs are based and, yet more important, that a thorough understanding of the functioning of a simulation code may enhance considerably the efficiency with which such programs are used.

The presented material has emerged from my research experience as a principal investigator and managing project director in scientific research projects both in industrial as well as institutional research in the fields of computer science, materials science[1], polymer physics and genome research. Some of the material covered in this book was originally presented in several national and international conferences and workshops and is presented here in an extended version. Because of the rapid progress in computational methods and modeling strategies in different areas of condensed matter research today and because of the lively interest in these topics that I experienced among students and colleagues over the past years, it became evident that there has been a demand for a book which provides a unified overview of many important concepts and which focuses on the underlying basic theories in the field of CMS.

The fundamental basics in most areas of computational modeling will not change in the near future. Thus, working in the field of computational physics, it is important to realize, that mostly those things are important to be learned and understood which are invariant against general proclivities, software versions, or computer languages. In this sense, this book also offers a basic introduction into physical and numerical model building in a context, in which these topics are probably not conveyed in standard university courses.

This book addresses to advanced students, primarily on the graduate or advanced undergraduate level who want to enter the field of computer simulations. It may also be helpful for researchers and engineers in physics, chemistry, polymer science and materials science who are active in computer simulation in industrial laboratories and in universities, and who are interested in a presentation of some of the fundamental mathematical and physical principles

[1] see e.g.: http://www.mmm-tools.de

underlying the different numerical methods that are used in materials science on different length and time scales.

The level of expertise that is presupposed of the reader in oder to be able to follow the text is first of all a certain amount of scientific maturity, with the precise direction not being overly important. Some physical background knowledge at least in classical mechanics and some exposure to a minimum amount of the modern abstract mathematical notation of set theory and functions on sets is helpful but not essential. This notation is introduced and explained in Part I of the book, particularly in Chap 3. The same holds for the theory and notation of tensors and manifolds which are important mathematical tools for a succinct and precise formulation of physical theories as found in advanced treatises on theoretical physics.

A word about the organization of the book is in order. In Part I many important mathematical and physical basics that are needed in the formulation of theories are summarized. Also some important facts about computer science and a general overview of length scales in the natural sciences are included.

Chapters 1 and 2 are introductory in style. The current status of computer applications in the natural sciences as well as modeling strategies and the development of a notion of "algorithm" and "computability" are discussed from a historical perspective.

In Chap. 3 the most important mathematical and physical basics for applying different theories and models in computational materials science are introduced. The choice of topics covered here is biased by the author's own interests. It is hoped that this chapter provides a sound mathematical background of many abstract concepts prevalently used in physical theories.

Finally, Chap. 4 provides a basic introduction into numerical simulation techniques, from the key algorithms for integrating partial or ordinary differential equations on a computer, to some software engineering techniques that are helpful when writing own simulation programs.

The chapters in Part II follow the length scales from bottom up starting with a presentation of methods on the atomistic scale in Chap. 5 taking into account the electronic degrees of freedom. The most basic methods are ab initio self-consistent Hartree-Fock methods, which are very common in quantum chemistry for obtaining the ground state geometry of small molecules. Starting from an initial guess of the basis wave function, the Schrödinger equation is reduced to a one-particle wave function for one electron in the averaged (mean) potential of all other electrons for which the initial wave functions are used. Therefore, this method is also called mean-field approach. Inserting the results repeatedly into the eigenvalue problem of the Schrödinger equation, it is solved self-consistently until convergence of the solution occurs. A good guess for the initial form of the basis wave functions is provided by using the Slater determinant which correctly includes the symmetry property of the wave function.

It is important to understand that even so-called "ab initio" methods rely on some fundamental approximations. The most important one is the adiabatic Born-Oppenheimer approximation which assumes that the heavy atomic nuclei are in essence stationary compared to the fast moving light electrons, and thus, the wave function can be separated into a product of a core wave function and an electron wave function which can be treated separately. Density Functional Theory (DFT) is discussed as well as half-empirical methods (Tight-Binding, Car-Parinello) and empirical methods which use coarse-grained potentials.

Chapter 6 provides an overview of coarse-grained methods on the microscopic scale, mostly covering the Molecular Dynamics and Monte Carlo methods. Instructions of how to write and organize a basic Molecular Dynamics program are included. Examples from polymer physics and solid state physics illustrate these two methods which are abundant on the microscopic length scale.

Chapter 7 treats some methods abundant on the meso and macroscale and provides some examples. The meso- and macroscale is the scale where fundamental research – usually based on the particle concept – is not dominating the field of materials research any more. Instead, on this scale one enters the area of engineering applications, making ingenious use of fluid dynamics concepts and relying fundamentally on the continuum approximation, which works excellent for many practical purposes. The basics of elasticity theory, continuum fluid theory, as well as Monte Carlo methods and geometric models with applications in solid state physics are presented. The finite element method, along with smooth particle hydrodynamics is well established for applications on this scale and both methods have been incorporated in many commercial program packages, which allow for simulating the materials response to external loading, making use of a large variety of material constitutive models. The meso-/macroscale is a length scale with probably the largest variety of structural properties of solid and liquid systems, due to an interplay between energetic effects (which dominate on small scales) and entropic effects, which come into play on intermediate length scales where materials can acquire many different conformations.

Finally, Chap. 8 provides a short overview of the most pressing problems that might be worthy being addressed with multiscale methods in the near future.

It is my pleasant duty to acknowledge the encouragement, interest and help that I had from colleagues and students when writing this book. In this respect a special vote of thanks is due to my former colleague Dr. Martin Kühn with whom I had endless and very fruitful discussions on the foundations of some research areas in physics and mathematics while working on the manuscript during the year 2006. He also helped improving parts of the manuscript by very useful suggestions.

I am particularly indebted to Prof. Dr. Alexander Blumen of the University of Freiburg, who has always provided support and encouragement in a very

friendly and helpful manner for all aspects of our joint and my own research in Freiburg.

I also owe thanks to Prof. Dr. Klaus Thoma, director of the Fraunhofer Ernst-Mach-Institute for High-Speed Dynamics (EMI) in Freiburg, for his very kind continuous support of my independent research on the application of multiscale methods in shock-wave, solid state, and polymer physics. Along with him, I had the honour and pleasure to lead and manage a large nationwide project ("MMM-Tools") during the years 2003-2005, devoted explicitly to the development of multiscale methods and efficient software applications in materials research.

Julian Schneider helped me with preparing some data and figures on polymer simulations in Chap. 6 and also read parts of the manuscript, and Kai Grass helped developing a mesoscopic particle model for the description of brittle failure in materials upon shock-loading which is dicussed in Chap. 7.

Last but not least I wish to thank my family for their love, enduring patience and great understanding while I was working on the manuscript. It was our precious time that I had to steal in order to finish this book.

Freiburg, Germany, July 2007 *Martin O. Steinhauser*