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Preface

Computer simulation is an indispensible research tool for modeling, understanding, and predicting nanoscale phenomena. There is a huge gap between the complexity of the programs and algorithms used in computational physics courses and and those used in research for computer simulations of nanoscale systems. The advanced computer codes used by researchers are often too complicated for students who want to develop their own codes, want to understand the essential details of computer simulations, or want to improve existing programs.

The aim of this book is to provide a comprehensive program library and description of advanced algorithms to help students and researchers learn novel methods and develop their own approaches. An important contribution of this book is that it is accompanied by an algorithm library in Fortran 90 that implements the computational approaches described in the text.

The physical problems are solved at various levels of sophistication using methods based on classical molecular dynamics, tight binding, density functional approaches, or fully correlated wave functions. Various basis functions including finite differences, Lagrange functions, plane waves, and Gaussians are introduced to solve bound state and scattering problems and to describe electronic structure and transport properties of materials. Different methods of solving the same problem are introduced and compared.

The book is divided into two parts. In the first part we concentrate on one-dimensional problems. The solution of these problems is obviously simpler and this part serves as an introduction to the second, more advanced, part, in which we describe simulations in three-dimensional problems. The first part can be used in undergraduate computational physics education. The second part is more appropriate for graduate and higher-level undergraduate classes.

The problems in the first part are sufficiently simple that the essential parts of the codes can be presented and explained in the text. The second part contains more elaborate codes, often requiring hundreds of lines and sets of different algorithms. Here only the main structure of the codes is explained. We do not try to teach computer programming, as there are excellent books available for that purpose. The codes are written to be simple and easy to follow, sacrificing speed and efficiency for clarity. The reader is encouraged to rewrite these codes to tailor them to his or her own needs.

The computer codes and examples used in this book are available from the book's website; see www.cambridge.org/9781107001701. The codes are grouped corresponding to the sections of the book where they appear. A short description of how to use the code and example inputs and outputs is provided.

We are continuing work on upgrading the codes and refreshing the program library with new examples and novel algorithms.

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