

Preface

This book is based on the Computational Physics course that has been developed and taught by the authors at Purdue for more than a decade. The goal of this course is to introduce students to some basic numerical techniques and then apply these techniques to a number of *modern* topics, that is, problems of current interest to physicists. Students with some experience in differential and integral calculus can readily grasp rather sophisticated computational techniques. These students can use computers as tools with which to attack and solve problems that they would not ordinarily encounter in the undergraduate curriculum. We have used this approach to try to convey the excitement of physics, with a variety of problems of current interest.

While there are many texts with the terms “computers” and “physics” in their titles, most of the books in this area tend to focus heavily on numerical methods rather than physics. Since our goal is to teach a course on *physics*, rather than numerical methods, these books are not a good match for our course. While there are a few books that emphasize the physics that can be done with numerical methods, they are either too advanced for use by undergraduates, or (more commonly) they fail to deal with the types of problems that can profit most from a numerical approach. In too many cases they tend to simply treat the standard problems, which are already dealt with in many traditional texts using analytic methods. Hence the basic motivation for creating this book.

The material for our book is taken from a wide variety of “primary” sources, as will become clear from the references at the end of each chapter. In many cases we started with papers from the recent physics literature and then distilled them to produce problems suitable for an undergraduate class. While it is necessary for this book to introduce a variety of numerical methods of interest to physicists, the overriding emphasis is on the physics that can be done with these methods. The majority of the problems described in this book cannot be solved with purely analytic techniques. A computational approach is required in most cases, and we have tried to use the computer to make the *physics* as clear and as interesting as possible.

As readers scan through this new edition, they will notice a number of changes. Perhaps the most important is that there are now two authors. Besides simply sharing the workload of preparing the new edition, this additional expertise has allowed us to add many new topics (and improve old ones!). In fact, we have added much new material on subjects ranging from diffusion on fractals and cellular automata, to the physics of musical instruments (a new chapter) and a new algorithm for doing time-dependent quantum mechanical problems.

This book has also been reorganized in several ways. The first edition gave programming examples in the *True Basic* language. Now, in this new edition the reliance on the programming language *True Basic* has been removed. We recognize that present-day students will likely be using many different languages, so we have chosen to employ a very general pseudocode to illustrate the algorithms. This

x Preface

pseudocode can easily be translated into virtually any language, and hence support the work of students in a wide variety of programming languages. However, for those students who prefer to see programs or routines in a “real” programming language, the *True Basic* programs from the first edition are still available at our website,¹ www.physics.purdue.edu/~giordano/comp-phys.html. Our plan is to add more programs, in other languages, to this website in the future, so that it can serve as a useful resource for students (and teachers). Another change in this new edition is that we have moved much of the discussion of the algorithms themselves into the appendices, and have added considerably to the depth and rigor of these discussions. It is our hope that the appendices can serve as reference material for students as they work their way through the physics that is covered in the chapters. This separation also allows the chapters to focus even more on the physics of the various topics.

How to Use This Book.

The first edition contained more than could easily be covered in a single course. The second edition contains even more, so it is clearly not possible to cover it all in one semester. The first few chapters rely mainly on elementary mechanics, and can be appreciated with a background at the freshman level. This material can be augmented with selected topics from later chapters (such as on random processes in Chapter 7 and molecular dynamics in Chapter 9) to produce a full-semester course. There is also ample material for a course aimed at advanced undergraduates and beginning graduate students. For example, the material on random processes (Chapter 7) and phase transitions (Chapter 8) can be added to the work on quantum mechanics (Chapter 10) to fill most of a semester at this level. A third way to use the material in this book is for an interdisciplinary course, in which case the chapters on waves (Chapter 6), musical instruments (Chapter 11), and interdisciplinary topics (Chapter 12) could form the core of a course.

The first edition would not have been possible without the help of many people, and we would like to thank them again. The support of Arnold Tubis and the Department of Physics at Purdue, along with that of the National Science Foundation, made our course, and hence this book, possible. Many graduate students helped us teach early versions of this course, including Miguel Castro, Chris Parks, Jan Spitz, Stuart Burnett, Todd Jacobs, and Dan Lawrence. Of course, the undergraduate students who have willingly submitted to the course have provided much useful feedback; there are too many to mention them all here, although Mike Pennington deserves a special thanks. Many colleagues have provided essential advice and encouragement on the manuscript, including Todd Jacobs, Mark Haugan, Paul Muzikar, along with the reviewers Wolfgang Christian, Alejandro Garcia, Jan Tobochnik, and Rodney L. Varley, who were very polite and constructive. The support of the first edition editors Ray Henderson and Alison Reeves was much valued, while the final impetus to actually begin this book was provided by the well-timed encouragement of Earl Prohofskey and Betsy Beasley.

¹The URL listed for the first edition, www.physics.purdue.edu/~ng/comp-phys.html, will take you to this new website.

The second edition owes much to our many colleagues who have sent us suggestions and new ideas for the new edition. In particular, we would like to thank James Behrens, Bob Delaney, Denis Donnelly, Eamin Jamshidi, Michael Oczkowski, Steve Turcotte, and Kobus Visser for alerting us to errors in the first edition, Aaron Montgomery for spotting (and correcting) a mistake in a draft of the second edition, and Eduardo Cuansing, Harvey Gould and Jan Tobochnik for their various contributions and general support. We also greatly appreciate the many constructive comments and suggestions from reviewers Gus Hart, James MacDonald, Micha Tomkiewicz, Thomas Vojta, and Matt Wood concerning drafts of the second edition. And of course, we are grateful to our Editors at Prentice-Hall, Erik Fahlgren and Christian Botting, for patiently guiding (and prodding) us through the preparation of this new edition.

In closing we would like to reaffirm that our goal has been to write a book that uses computational methods to do interesting *physics*. While numerical methods can be fun, they are *not* our primary purpose. We hope that this book helps the student in all of us learn about and enjoy doing physics.

Nicholas J. Giordano and Hisao Nakanishi