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Simon Širca  
Martin Horvat

# Computational Methods for Physicists

Compendium for Students

 Springer

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*Simon Širca and Martin Horvat*

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# **Computational Methods for Physicists**

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ISSN 1868-4513 e-ISSN 1868-4521

ISBN 978-3-642-32477-2 e-ISBN 978-3-642-32478-9

Springer Heidelberg New York Dordrecht London

Library of Congress Control Number: 2012951441

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*Dedicated to our parents*

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# Preface

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This book evolved from short written homework instructions for the course in Computational Physics at the Department of Physics, University of Ljubljana. The feedback received from the students was used to gradually supplement the instructions by oral presentations in the classroom and additional material on the web. The heritage of this course, established and initially taught for a number of years by Professor Kodre, represented a basis onto which we attempted to span an even richer manifold, and to better elucidate the “exercises” from the mathematical, physical, as well as programming and computational viewpoints. The somewhat spartan instructions thus evolved into a much more general textbook which is intended primarily for third- and fourth-year physics students, and for Ph.D. students as an aid for all courses with a mathematical physics tinge. The book might also appeal to mathematics students. It was one of our local goals to modestly interweave physics and mathematics studies, and this is why the book steers between mathematical rigidity and more profane perspectives of numerical methods, while it tries to preserve the colorful content of the field of mathematical physics.

We were driven by the realization that physics students are often insufficiently prepared to face various obstacles they encounter in numerical solution or modeling of physical problems. Only a handful of them truly know how something can “actually be computed” or how their work can be efficiently controlled and its results reliably checked. Everyone can solve the matrix system  $Ax = b$ , but almost no one has an idea how to estimate the error and relate this estimate to the possible true error. They use explicit integrators of differential equations indiscriminately until they try to look closely at solutions of a problem as simple as  $\dot{x} = -x$ . The direness of the situation is compounded by many commercial tools giving a false impression that all problems can be solved by a single keystroke. In parts of the text where basic approaches are discussed, we insist on seemingly ballast numerical details while, on the other hand, we did wish to offer at least some “serious” methods and illustrate them by manageable examples. The book swings back and forth between these extremes: it tries to be neither fully elementary nor encyclopedically complete, but at any rate representative—at least for the first-time reader.

The book is structured exactly with such gradations in mind: additional, “non-compulsory” chapters are marked with stars  $\star$  and can be read by particularly motivated students or used as reference. Similarly, the  $\odot$  symbols denote simpler tasks in the end-of-chapter problems, while more demanding ones are marked by the symbols  $\oplus$ . The purpose of the appendices is not merely to remove the superfluous contents from the main text, but to enhance programming efficiency (above all, Appendices B, C, E, I, and J). The sour apples we force our reader to bite are the lack of detailed derivations and references to formulas placed in remote parts of the text, although we tried to design the chapters as self-contained units. This style requires more concentration and consultation with literature on the reader’s part, but makes the text more concise. In turn, the book does call for an inspired course tutor. In a typical one-semester course, she may hand-pick and fine-tune a dozen or so end-of-chapter problems and supply the necessary background, while the students may peruse the book as a convenient point of departure for work.

The end-of-chapter problems should resonate well with the majority of physics students. We scooped up topics from most varied disciplines and tried to embed them into the framework of the book. Chapters are concluded by relatively long lists of references, with the intent that the book will be useful also as a stepping stone for further study and as a decent vademecum.

In spite of all care, errors may have crept in. We shall be grateful to all readers turning our

attention to any error they might spot, no matter how relevant. The Errata will be maintained at the book's web-page <http://cmp.fmf.uni-lj.si>, which also contains the data files needed in some of the problems.

We wish to express our gratitude to Professor Claus Ascheron, Senior Editor at Springer, for his effort in preparation and advancement of this book, as well as to Donatas Akmanavičius and his team for its meticulous production at VTeX.

The original text of the Slovenian edition was scrutinized by two physicists (Professors Alojz Kodre and Tomaž Prosen) as well as four mathematicians (Associate Professors Emil Žagar, Marjetka Krajnc, Gašper Jaklič, and Professor Valery Romanovski, who carefully examined the section on Gröbner bases). We thank them; from the navigation between the Scylla and Charibdis of these reviewers we emerged as better sailors and arrived happily, after years of roaming the stormy seas, to our Ithaca.

**Simon Širca**  
**Martin Horvat**  
**Ljubljana, Slovenia**

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