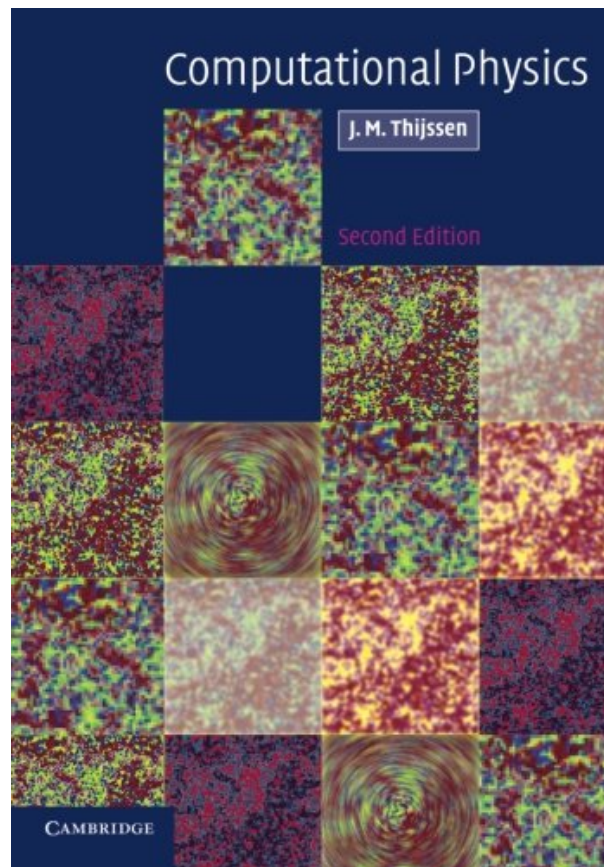
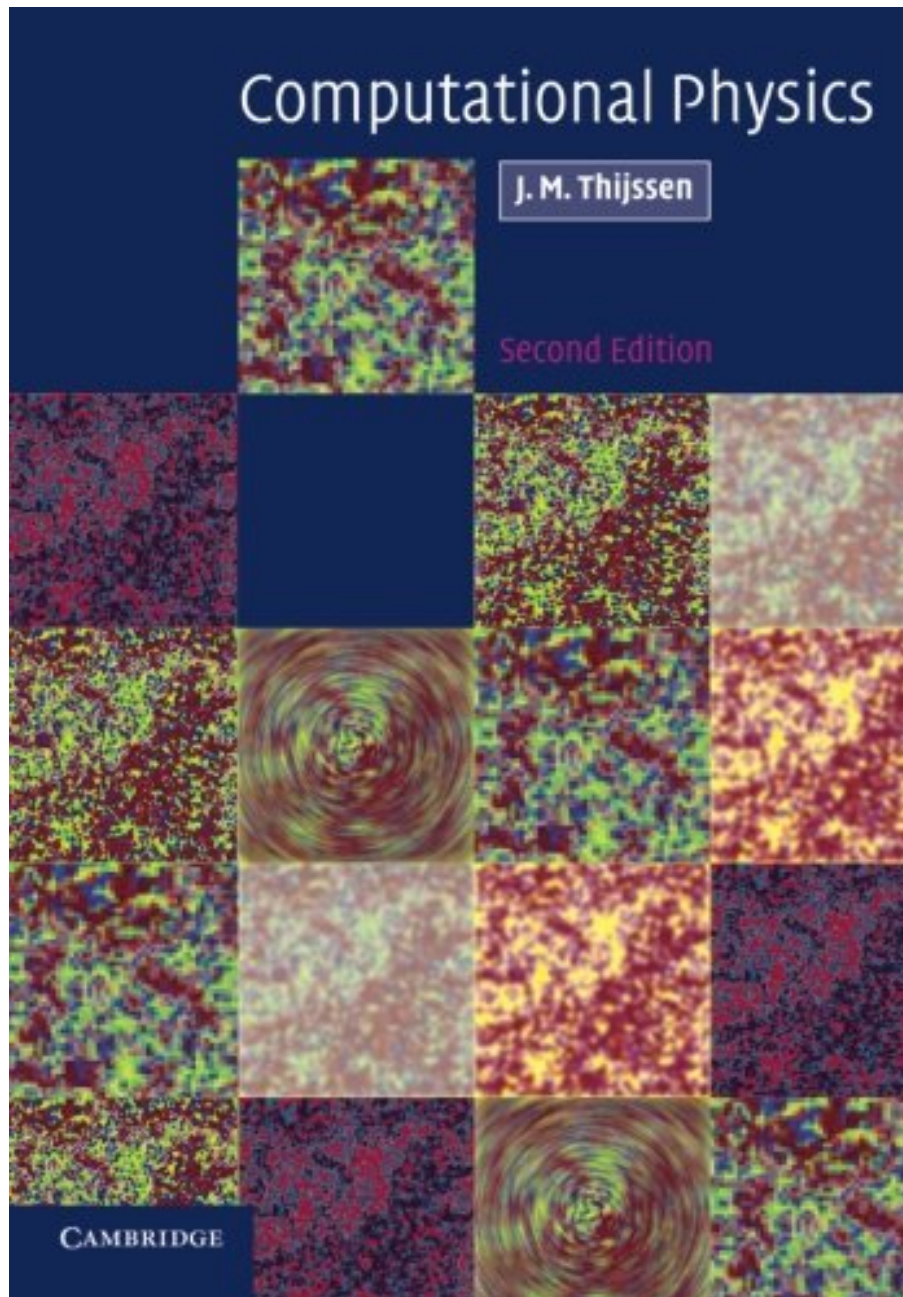


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"... I find this book very useful since it provides a thorough discussion of the computational methods used in physics combined with an extensive presentation of the underlying physics ... On the one hand an experienced researcher can easily transfer the obtained knowledge from this book to a particular research topic, while on the other hand a newcomer in the field will benefit from the presentation of the subject from first principles."

Lampros Nikolopoulos, Contemporary Physics

About the Author

Jos Thijssen is a lecturer at the Kavli Institute of Nanoscience at Delft University of Technology.

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First published in 2007, this second edition describes the computational methods used in theoretical physics. New sections were added to cover finite element methods and lattice Boltzmann simulation, density functional theory, quantum molecular dynamics, Monte Carlo simulation, and diagonalisation of one-dimensional quantum systems. It covers many different areas of physics research and different computational methodologies, including computational methods such as Monte Carlo and molecular dynamics, various electronic structure methodologies, methods for solving partial differential equations, and lattice gauge theory. Throughout the book the relations between the methods used in different fields of physics are emphasised. Several new programs are described and can be downloaded from www.cambridge.org/9781107677135. The book requires a background in elementary programming, numerical analysis, and field theory, as well as undergraduate knowledge of condensed matter theory and statistical physics. It will be of interest to graduate students and researchers in theoretical, computational and experimental physics.

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Most helpful customer reviews

24 of 26 people found the following review helpful.

Finally, a good one!

By Rafael F. Angulo

This book by J. M. Thijssen is a rare gem. You note this as you browse the index. Quantum scattering, variational methods for the Schrödinger equation, the Hartree-Fock method, density functional theory, classical and quantum molecular dynamics and Monte Carlo methods and transfer matrix methods. Even a solid chapter on lattice field theory! The book isn't child's play (like most books on computational physics),

but a beautifully written text covering both physical and computational issues, superficially but concisely. A neat selection of references guides readers to comprehensive, modern literature. The right balance of tricks and theory puts the readers few steps away from developing their own code. I don't award the fifth star because software engineering and object orientation issues are ignored.

18 of 19 people found the following review helpful.

Good book for the price

By Newton Ooi

This book was assigned in a class I took on the computer modeling of materials. The text itself was slightly above my understanding; but that's fine, I just was not prepared for it. The problem is that there are many exercises that require the reader to download software from the author's web site, and use it to perform calculations. Many times the software did not work as intended, and so the professor had to spend time correcting the code, or writing his own version. And of course there were the usual problems of installing the code properly, compiling it, and executing it. This idea would have worked much better if the necessary code was put onto a CD-ROM that came packaged with the book. For the software problems I dock one star out of five.

The introduction states that this text is intended for graduate students in physics, chemistry, materials science, or electrical engineering, and who have taken classes in numerical analysis. I think a more appropriate wording is that this text is for someone versed in all of these listed fields. There is extensive use of thermodynamics, symmetry and crystal structure, linear algebra, statistical mechanics, quantum mechanics, etc... This book should not be used as an introductory guide to computational physics or related fields. The necessary prerequisite knowledge is quite extensive.

The intro should specify at least 2 college classes in computer programming as a prerequisite for this book. The programming assignments included at the end of each chapter are quite challenging, and should not be attempted by someone without previous experience in writing mathematical codes. This here lies another problem with the approach taken by this book. Most science and engineering majors will take 1-2 courses in programming as part of their university education, but these classes often emphasize business applications such as reading / writing to a text file, creating and using databases, formatting of screen output, linked lists, etc... These skills are not very useful in writing a code to do computations. For the latter, needed skills include parsing data, recognizing patterns, using built-in functions, importing and using algorithms from online libraries. utilizing large matrices and vectors, etc...

What the author should have done for each computational homework problem is to write out the solution (code) himself, add in the documentation, and then removed the code while leaving the documentation intact. The student can then use the documentation to craft his/her own solution.

For the difficulty of the computing problems, and of the text in general, I dock another star.

Therefore, I rate this book 3 out of 5 stars.

9 of 10 people found the following review helpful.

The best computational physics book available

By D. Holland

This is a very decent book on computational physics, focusing primarily on condensed matter. It's up there with Allen and Tildesley's "Computer Simulation of Liquids", though with a broader selection of subjects and more suited to physicists.

There are inevitable errors, some of which would take a bit of effort to fix were it not for the error web page

the author maintains.

Many problems in condensed matter are tackled, always with a view toward implementing an actual numerical investigation (this may sound like a given, but several other texts seem to shy away from actually using a computer, exploiting some variant of 'computational' in the title as an excuse to write yet another redundant physics text that is only cursorily computational). Often, nice snippets of pseudocode are presented, along with suggestions for numerical control parameters to use and the corresponding numerical results obtained - so one can try things out and check the answer. Indeed, the book is best used if one sets about to write code to solve problems, both in the main text and in the exercises at the chapter ends. As is often the case, however, getting a piece of new code to behave correctly can be a bit of a pain, which becomes easier only with experience.

In a real sense, the text helps bring some physics to life, and one is rewarded, I think, with a clearer understanding, and some powerful tools at one's disposal.

Though it doesn't have any real competitor, there is room for a second edition: along with correcting errors, several subjects could do with a bit more discussion or even extensive treatment, and other things could profitably be included, e.g., a DFT implementation of Car-Parrinello quantum atomic dynamics.

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