Numerical Methods in Physics with Python

Bringing together idiomatic Python programming, foundational numerical methods, and physics applications, this is an ideal standalone textbook for courses on computational physics. All the frequently used numerical methods in physics are explained, including foundational techniques and hidden gems on topics such as linear algebra, differential equations, root-finding, interpolation, and integration. The second edition of this introductory book features several new codes and 140 new problems (many on physics applications), as well as new sections on the singular-value decomposition, derivative-free optimization, Bayesian linear regression, neural networks, and partial differential equations. The last section in each chapter is an in-depth project, tackling physics problems that cannot be solved without the use of a computer. Written primarily for students studying computational physics, this textbook brings the non-specialist quickly up to speed with Python before looking in detail at the numerical methods often used in the subject.

Alex Gezerlis is Professor of Physics at the University of Guelph. Before moving to Canada, he worked in Germany, the United States, and Greece. He has received several research awards, grants, and allocations on supercomputing facilities. He has taught undergraduate and graduate courses on computational methods, as well as courses on quantum field theory, subatomic physics, and science communication.

Praise for the Second Edition

"Gezerlis' book *Numerical Methods in Physics* with Python is a beautiful example of how an established subject can be brought to the next level by making it very accessible and by introducing several insightful and interdisciplinary applications. This second edition considerably extends the set of exercises, resulting in an extremely useful resource for both students and teachers. Strongly recommended!"

Sonia Bacca, *Johannes Gutenberg-Universität Mainz*

"This new edition of *Numerical Methods*... is another great example of Gezerlis' passion for teaching and for doing so carefully and precisely. Especially welcome, in my view, are the addition of problems at the end of each chapter and the discussion of singular value decomposition (SVD) and Bayesian methods. The SVD is one of the crown jewels of linear algebra which modern students interested in machine learning will surely find beneficial. To physics, computer science, or engineering students mesmerized by the fast Fourier transform, Gezerlis' excellent explanation of it in Chapter 6 is likely to shed some light on the underlying divide-and-conquer algorithm, which is an essential classic."

Joaquin Drut, *University of North Carolina at Chapel Hill*

"A fantastic addition as an introductory textbook for computational physics. The book is timely, and the author made thoughtful and in my view many wise choices. The book is comprehensive and yet accessible to undergraduate students."

Shiwei Zhang, *Flatiron Institute and College of William & Mary*

Praise for the First Edition

"I enthusiastically recommend *Numerical Methods in Physics with Python* by Professor Gezerlis to any advanced undergraduate or graduate student who would like to acquire a solid understanding of the basic numerical methods used in physics. The methods are demonstrated with Python, a relatively compact, accessible computer language, allowing the reader to focus on understanding how the methods work rather than on how to program them. Each chapter offers a self-contained, clear, and engaging presentation of the relevant numerical methods, and captivates the reader with well-motivated physics examples and interesting physics projects. Written by a leading expert in computational physics, this outstanding textbook is unique in that it focuses on teaching basic numerical methods while also including a number of modern numerical techniques that are usually not covered in computational physics textbooks."

Yoram Alhassid, *Yale University*

"In *Numerical Methods in Physics with Python* by Gezerlis, one finds a resource that has been sorely missing! As the usage of Python has become widespread, it is too often the case that students take libraries, functions, and codes and apply them without a solid understanding of what is truly being done 'under the hood' and why. Gezerlis' book fills this gap with clarity and rigor by covering a broad number of topics relevant for physics, describing the underlying techniques and implementing them in detail. It should be an important resource for anyone applying numerical techniques to study physics."

Luis Lehner, *Perimeter Institute*

"Gezerlis' text takes a venerable subject – numerical techniques in physics – and brings it up to date and makes it accessible to modern undergraduate curricula through a popular, open-source programming language. Although the focus remains squarely on numerical techniques, each new lesson is motivated by topics commonly encountered in physics and concludes with a practical hands-on project to help cement the students' understanding. The net result is a textbook which fills an important and unique niche in pedagogy and scope, as well as a valuable reference for advanced students and practicing scientists."

Brian Metzger, *Columbia University*

Numerical Methods in Physics with Python

Second Edition

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CAMBRIDGE
UNIVERSITY PRESS

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103 Penang Road, #05–06/07, Visioncrest Commercial, Singapore 238467

Cambridge University Press is part of Cambridge University Press & Assessment,
a department of the University of Cambridge.

We share the University's mission to contribute to society through the pursuit of
education, learning and research at the highest international levels of excellence.

www.cambridge.org
Information on this title: www.cambridge.org/9781009303866

DOI: 10.1017/9781009303897

First published 2020
Second edition published 2023

A catalogue record for this publication is available from the British Library.

ISBN 978-1-009-30385-9 Hardback
ISBN 978-1-009-30386-6 Paperback

Additional resources for this publication at www.cambridge.org/gezerlis2
and www.numphyspy.org

To Marcos, ψυχή βαθιά

My soul, rather than yearn for life immortal,
press into service every shift at your disposal.

Pindar

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Preface

> The health of the eye seems to demand a horizon.
> We are never tired, so long as we can see far enough.
>
> Ralph Waldo Emerson

This is a textbook for advanced undergraduate (or beginning graduate) courses on Computational Physics. To explain what this means, I first go over what this book is *not*.

First, this is not a text that focuses mainly on physics applications and basic programming, only bringing up numerical methods as the need arises. It's true that such an approach would have the benefit of giving rise to beautiful visualizations and helping students gain confidence in using computers to study science. The disadvantage of this approach is that it tends to rely on external libraries, i.e., "black boxes". To make an analogy with non-computational physics, we teach students calculus before seeing how it helps us do physics. In other words, an instructor would not claim that derivatives are important but already well-studied, so we'll just employ a package that takes care of them. That being said, a physics-applications-first approach may be appropriate for a more introductory course (the type with a textbook that has the answers in the back) or perhaps as a computational addendum to an existing text on mechanics, electromagnetism, and so on.

Second, this is not a text addressing a small subset of modern computational methods. Depending on the instructor's interests and expertise, computational courses sometimes specialize on a single theme, such as: simulations (e.g., molecular dynamics or Monte Carlo), data analysis (e.g., uncertainty quantification), or partial differential equations (e.g., continuum dynamics). Such a targeted approach has the advantage of being intimately connected to research, at the cost of assuming students have picked up the necessary foundational material from elsewhere. To return to the analogy with non-computational physics, a first course on electromagnetism would never skip over things like basic electrostatics to get directly to, say, the Yang–Mills Lagrangian just because non-abelian gauge theory is more "current". Even so, an approach that focuses on modern computational technology is relevant to a more advanced course: once students have mastered the foundations, they can turn to state-of-the-art methods that tackle research problems.

The present text attempts to strike a happy medium: a broad spectrum of numerical methods is studied in detail and then applied to questions from undergraduate physics, via idiomatic implementations in the Python programming language. When selecting and discussing topics, I have prioritized pedagogy over novelty; this is reflected in the chapter titles, which are pretty standard. Of course, my views on what is pedagogically superior are mine alone, so the end result also happens to be original in some respects. Below, I touch upon some of the main features of this book, with a view to orienting the reader.

- **Idiomatic Python:** the book employs Python 3, which is a popular, open-source programming language. A pedagogical choice I have made is to start out with standard Python, use it for a few chapters, and only then turn to the NumPy library; I have found that this helps students who are new to programming in Python effectively distinguish between lists and NumPy arrays. The first chapter includes a discussion of modern programming idioms, which allow me to write shorter codes in the following chapters, thereby emphasizing the numerical method over programming details. This is somewhat counterintuitive: teaching more "advanced" programming than is usual in computational-physics books allows the programming to recede into the background. In other words, not having to fight with the programming language every step of the way makes it *easier* to focus on the physics (or the math).
- **Modern numerical-analysis techniques:** I devote an entire chapter to questions of numerical precision and roundoff error; I hope that the lessons learned there will pay off when studying the following chapters, which typically focus more on approximation-error themes. While this is not a volume on numerical analysis, it does contain a bit more on applied math than is typical: in addition to standard topics, this also includes modern techniques that haven't made it to computational-physics books before (e.g., automatic differentiation or interpolation at Chebyshev points). Similarly, the section on errors in linear algebra glances toward monographs on matrix perturbation theory. To paraphrase Forman Acton [2], the idea here is to ensure that the next generation does not think that an obligatory decimal point is slightly demeaning.
- **Methods "from scratch":** chapters typically start with a pedagogical discussion of a crude algorithm and then advance to more complex methods, in several cases also covering state-of-the-art techniques (when they do not require elaborate bookkeeping). Considerable effort is expended toward motivating and explaining each technique as it is being introduced. Similarly, the chapters are ordered in such a way that the presentation is cumulative. Thus, the book attempts to discuss things "from scratch", i.e., without referring to specialized background or more advanced references; physicists do not expect lemmas and theorems, but do expect to be convinced.[1] Throughout the text, the phrases "it can be shown"[2] and "stated without proof" are actively avoided, so this book may also be used in a flipped classroom, perhaps even for self-study. As part of this approach, I frequently cover things like convergence properties, operation counts, and the error scaling of different numerical methods. When space constraints made it impossible to reach for *simplex munditiis* in explaining a given method, I quietly omitted that method. This is intended as a "first book" on the subject, which should enable students to confidently move on to more advanced expositions.
- **Methods implemented:** while the equations and figures help explain why a method should work, the insight that can be gleaned from an existing implementation of a given algorithm is crucial. I have worked hard to ensure that these code listings are embedded in the main discussion, not tossed aside at the end of the chapter or in an online supplement. Even so, each implementation is typically given its own subsection, in order to

[1] *Nullius in verba*, the motto of the Royal Society, comes to mind. The idea, though not the wording, can clearly be traced to Heraclitus' fragment 50: "Listen, not to me, but to reason".
[2] An instance of *proof by omission*, but still better than "it can be easily shown" (*proof by intimidation*).

help instructors who are pressed for time in their selection of material. Since I wanted to keep the example programs easy to talk about, they are quite short, never longer than a page. In an attempt to avoid the use of black boxes, I list and discuss implementations of methods that are sometimes considered advanced (e.g., the QR eigenvalue method or the fast Fourier transform). While high-quality libraries like NumPy and SciPy contain implementations of such methods, the point of a book like this one is precisely to teach students how and why a given method works. The programs provided (whose filenames also appear in the book's index) can function as templates for further code development on the student's part, e.g., when solving the end-of-chapter problems.

- **Clear separation between numerical method and physics problem:** each chapter focuses on a given numerical theme. The first section always discusses physics scenarios that touch upon the relevant tools; these "motivational" topics are part of the standard undergrad physics curriculum, ranging from classical mechanics, through electromagnetism and statistical mechanics, to quantum mechanics. The bulk of the chapter then focuses on several numerical methods and their implementation, typically without bringing up physics examples. The last numbered section in each chapter is a Project: in addition to involving topics that were introduced in earlier sections (or chapters), these physics projects allow students to carry out calculations they wouldn't attempt without the help of a computer. These projects also provide a first taste of "programming-in-the-large". As a result of this design choice, the book may also be useful to beginning physics students or even students in other areas of science and engineering (with a more limited physics background). Even the primary audience may benefit from the structure of the text in the future, when tackling different physics questions. In the same spirit, the physics-oriented problems in each chapter's problem set are labelled with [$\mathcal{P}$]; these are placed near the end, presupposing the maturity developed while working on the earlier problems. (Since most problems involve some coding, the ones that are purely analytical are labelled with [$\mathcal{A}$], into the bargain.)
- **Second edition includes six new sections on:**
  - the singular-value decomposition (section 4.5),
  - derivative-free optimization (sections 5.5.2 and 5.6.5),
  - maximum-likelihood and Bayesian approaches to linear regression (section 6.6),
  - non-linear fitting via the Gauss–Newton method and neural networks (section 6.7),
  - finite-difference approaches to the diffusion equation (section 8.5.2).

  Six original codes are associated with these sections. Section 6.6 may be of special benefit to readers interested in experimental physics. I found that brief yet meaty introductions to these ideas are useful to physics students, at both the undergraduate and graduate levels. As always, the point was to avoid the dreaded phrase "it turns out that", i.e., the use of (analytical or programming) black boxes. In addition to the totally new material, using the book in a classroom setting has inspired a very large number of other modifications throughout the volume, ranging from minor tweaks (e.g., now explicitly citing problem numbers in the main text) to complete rewrites of selected first-edition sections. From start to finish, I have tried to navigate between Scylla (familiar notation obscuring conceptual subtleties) and Charybdis (too many strange-looking symbols).

- **Second edition includes 140 new problems on:** (a) extensions of techniques introduced in the main text, (b) topics that would otherwise take too many pages to discuss (e.g., problems 5.38, 5.39, and 5.40 on constrained minimization), and (c) a large number of physical applications: I have now included problems on standard themes (e.g., problem 7.65 on the Ising model in two dimensions, problem 8.58 on molecular dynamics for the Lennard–Jones potential, or problem 8.59 on the scattering of a wave packet from a barrier) as well as on topics that I have not encountered in other computational-physics textbooks (e.g., problem 6.67 on credible intervals for a relativistic particle's mass or problem 7.63 on the dimensional regularization of loop integrals). Sometimes a given physical theme carries over across chapters, for example: the Roche potential is visualized in problem 1.17, it is then extremized in problem 5.50 to find the Lagrange points, the volume of the Roche lobe is computed via quadrature in problem 7.56, and the Arenstorf orbit is arrived at by solving differential equations in problem 8.46.
  A word on solutions: standard practice is that computational-physics textbook authors either produce no solutions to the problems or provide solutions only to instructors teaching for-credit courses out of the textbook. I have followed the latter route, but I'm also providing (online) a subset of the solutions to all readers, as a self-study resource.
- **Topic sequence for different courses:** like many textbooks, this one contains more material than can be covered in a single semester. Here are two sample courses:
  - *Advanced undergraduate course:* sections 1.1–1.5, 2.1–2.4.3, 2.5.2, 3.1–3.3, 1.6, 4.1, 4.2.1–4.2.3, 4.3, 4.4.1, 5.1–5.2, 5.4, 5.5.2, 6.1–6.2.2, 6.5, 7.1–7.3, 7.5, 7.7.1–7.7.4, 8.1–8.3.1, 8.4.1, 8.5. Labs focus on Python programming; lectures mainly address numerical methods; physics content limited to motivation and homework assignments.
  - *Beginning graduate course:* appendix B, sections 2.1–2.5, 3.4, 4.1–4.6, 5.1, 5.3–5.6, 6.1, 6.2.2–6.2.3, 6.4–6.8, 7.1, 7.4–7.8, 8.1–8.4, 8.6. Python and an undergrad numerical course are prerequisites. Increased focus on analytical manipulations; programming limited to homework; lectures' physics content determined by a student poll.

Alas, adding 150 pages of new material for the second edition ran the risk of making this volume too expensive. With that in mind, I abridged sections 4.2 and 4.6, placing the original versions in the online supplement at `www.numphyspy.org`. This book continues to be dear to my heart; I hope the reader gets to share some of my excitement for the subject.

On the Epigraphs

I have translated 14 of the quotes appearing as epigraphs myself; in the remaining instances the original was in English. All 17 quotes are not protected by copyright. The sources are: Dedication: Pindar, *Pythian Odes*, 3.61–62 (~474 BCE), Preface: Ralph Waldo Emerson, *Nature*, Chapter III (1836 CE), Chapter 1: Immanuel Kant, *Lectures VI*, Philosophical Encyclopedia (~1780 CE), Chapter 2: Georg Wilhelm Friedrich Hegel, *The Phenomenology of Spirit*, Paragraph 74 (1807 CE), Chapter 3: Emily Dickinson, *Poem F372/J341* (1862 CE), Chapter 4: Vergil, *Georgics*, Book II, Line 412 (~29 BCE), Chapter 5: Karl

Kraus, *The Last Days of Mankind*, Act I, Scene 22 (~1918 CE), Chapter 6: Gabriel Lippmann, quoted in Henri Poincaré, *Calcul des probabilités*, Second edn, Section 108 (1912 CE), Chapter 7: Thucydides, *History of the Peloponnesian War*, Book IV, Paragraph 40 (~420 BCE), Chapter 8: Sophocles, *Oedipus Tyrannus*, Line 486 (~429 BCE), Postscript: Socrates, quoted in Diogenes Laërtius, *Lives and Opinions of Eminent Philosophers*, Book 2 (~220 CE), Appendix A: Aristotle, *Metaphysics* Book III (B), 1001a1 (~330 BCE), Appendix B: Thomas Aquinas, *Commentary on Aristotle's Metaphysics*, Book IV (Γ), Lesson 1, Chapter 2, Commentary (1270 CE), Appendix C: Parmenides, *Fragment 5* (~475 BCE), (Online) Appendix D: Callimachus, *Fragment 465* (~250 BCE), Bibliography: Michel Eyquem de Montaigne, *Essay III.13*, On Experience (1588 CE), Index: James Joyce, *Ulysses*, Episode 16, Eumaeus (1922 CE).

Acknowledgments

My understanding of numerical methods has benefited tremendously from reading many books and papers. In the bibliography I mention only the works I consulted while writing.

I have learned a lot from my graduate students, my collaborators, as well as members of the wider nuclear physics, cold-atom, and astrophysics communities. This textbook is a pedagogical endeavor but it has unavoidably been influenced by my research, which is supported by the Natural Sciences and Engineering Research Council of Canada and the Canada Foundation for Innovation.

I would like to thank my Editor at Cambridge University Press, Vince Higgs, for his sagacious advice. Margaret Patterson did an excellent job copyediting both editions of the book, while Suresh Kumar helped with advanced LaTeX tricks. I am grateful to the anonymous reviewers for the positive feedback and suggestions for additions.

I wish to acknowledge the students taking the classes I taught; their occasional vacant looks resulted in my adding more explanatory material, whereas their (infrequent, even at 8:30 am) yawns made me shorten some sections. Eric Poisson made wide-ranging comments on the lecture notes that turned into the first edition. Aman Agarwal, Eli Bendersky, Liliana Caballero, Ryan Curry, Victoria Leaker, Benjamin Morling, Tristan Pitre and Sangeet-Pal Pannu spotted issues with individual sections or problems. Buried in this book are conceptual distinctions that attempt to preempt misconceptions which are both natural and widespread; I have enjoyed working with Martin Williams on spin-off journal articles.

"What makes us who we are is our choice of good or bad, not our opinion about it" (Aristotle, *Nicomachean Ethics*, 1112a3); Marcos Gezerlis made sure I approached technical subtleties with a similar outlook. Marcos was instrumental in expanding the new material into its current form, immediately picking up on the lacunae in early drafts; I knew I could stop writing when he reached the desired state of staring at nothing in particular while muttering "I understand now". I am indebted to my family (especially Myrsine and Ariadne), *inter multa alia*, for orienting me toward the subjective universal. While several people have helped me refine this book, any remaining poor choices are my responsibility.