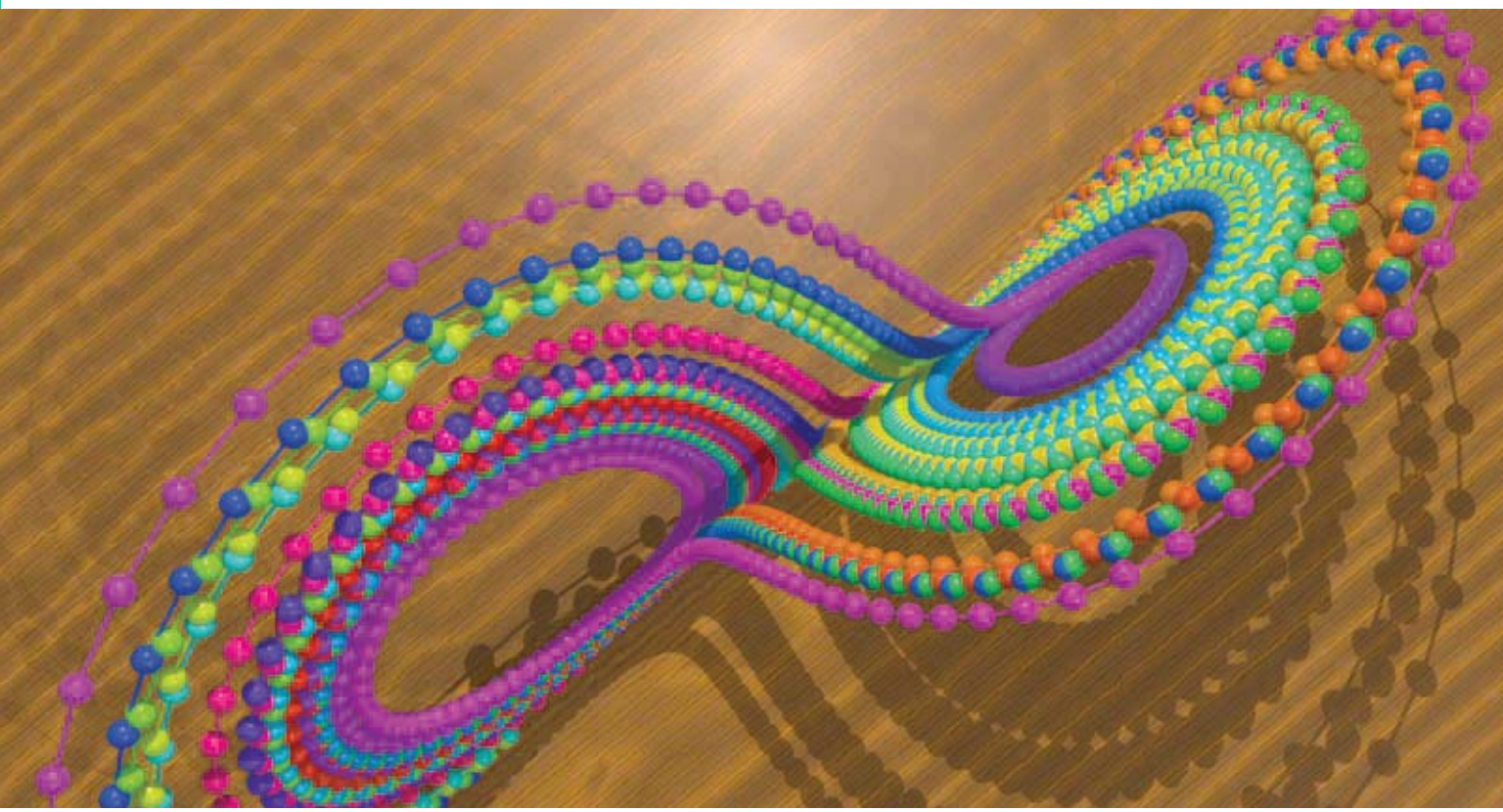
Computational Modeling

AND VISUALIZATION OF PHYSICAL SYSTEMS WITH PYTHON

JAY WANG



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To my Father and Mother,
who taught me that knowledge is to be revered.

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Preface

Computer modeling has had a significant impact on the way we do science and physics, both in research and in teaching. We are able to study problems of all scales from atoms to galaxies, and of complexities that would be impossible without computer modeling. Computation has even led to an entirely new field of science, chaos. In many ways, computational modeling has become the third pillar of physics alongside experimentation and theory.

In this book, we introduce computational modeling and visualization of physical systems that are commonly found in physics and related areas. Our first and foremost goal is to introduce a framework that integrates model building, algorithm development, and data visualization for problem solving via scientific computing. Through carefully selected problems, methods, and projects, the student is guided to learning and discovery by actively doing rather than just knowing physics. By constructing models and algorithms, programming and testing them, and analyzing the results, we will gain insight, ask new questions, tweak the model as necessary, and change the parameters to test what-if scenarios analogous to turning knobs in a virtual experiment. Another goal is to broaden the scope and depth of problems that may be studied with computational modeling. Many fundamental physical systems, despite their apparent simplicity, are beyond reach without computer simulation. Take projectile motion with air resistance and quantum free fall, for example. Though the problems can be expressed in basic calculus, they are unsolvable analytically in closed-form solutions. Computer modeling enables us to not only solve these problems, but also comparatively study the differences and similarities of their behavior in classical and quantum mechanical realms. We also aim to integrate applied computational tools and methods with effective visualization techniques in the simulations, including in situ data graphing and real-time animation within standard and open-source frameworks.

We take a problem-centric approach to the presentation of the material. For most problems, we include sufficient background information or essential relations to make them self-contained as much as possible, as well as to indicate their general importance and relevance. To streamline the text, many of the details are given in appendices or exercises, allowing readers of diverse backgrounds to skip ahead or study the detail at their own pace. We have also created a Digital Online Companion (DOC) for in-depth and advanced topics. Following the description of a problem, we discuss model building, the appropriate computational methods and tools, and visualization techniques to the simulations. Most results are represented in graphical form directly from the simulation programs for analysis and discussion.

Graphical representation of data and effective visualization techniques, including real-time animations of three-dimensional objects, are standard parts of our simulations because they are essential to help interpret and analyze the results, especially in time-dependent studies. They also bring the simulations alive, making them more dynamic, instructive, and exciting.

The tight integration of advanced graphics and visualization into the simulations is made possible with standard, easy-to-use, open-source packages such as Matplotlib, SciPy, and VPython. These packages only require us to manipulate an object's attributes such as the physical position of a particle, so we can avoid low-level graphics programming and focus on modeling and proper techniques in using these tools. Except for schematic illustrations, most graphical representations and animations are created using techniques in the actual codes contained in the book. However, many programs are written such that the integrated graphics can be decoupled

(disabled), replaced with either Matplotlib output or results written to a file, without affecting the calculations.

Because coding is essential to understanding an algorithm or to gaining insight to a physical process, and the most effective way to learn to code is by studying examples, the reader is guided in the process of building over ninety fully working sample programs, with detailed explanations for most of them. Many of the coded algorithms form part of basic building blocks in scientific computing. The associated tools and methods, whether well-known or otherwise still being currently researched, share common elements found in computational research of more complex problems. Through building fully working programs complete with graphical output, the student not only will learn how to write codes for computation, but their finished product is suitable for demonstration as well.

We use Python as the default programming language to show concrete, working examples and to take several advantages it offers: being easy to learn and use, readable, flexible, and powerful. One can think of Python as the modern equivalent of BASIC, but with a large and growing body of open source libraries for common tasks in scientific computing such as those mentioned earlier. Even newcomers to Python can learn from examples and grow quickly, writing functional programs and being productive in about two to three weeks. However, the choice of a programming language can be highly personal. Readers with programming background in other languages should find most Python codes to be expressive, pseudocode-like, and readily adaptable.

Sample systems are drawn from across the fundamental areas of physical science including mechanical, electromagnetic, quantum, and statistical systems. Representative problems within a given topic or theme are organized by chapter. Most chapters start with an animated simulation related to the central topic and end with a brief summary. The chapters and topics are organized as follows. After a brief introduction in Chapter 1 to our approach to modeling and basic programming elements, we discuss methods of solving ordinary differential equations (ODEs) in Chapter 2 as it constitutes the beginning of our framework. Thematic studies begin with the familiar example of projectile motion with air resistance (Chapter 3), followed by planetary and few-body motion including exoplanet modeling (Chapter 4), and nonlinear dynamics and classical chaos (Chapter 5). We study waves and oscillations in Chapter 6 and electromagnetic fields in Chapter 7. In Chapters 8 and 9, we present simulations of time-dependent and time-independent quantum mechanics, respectively. We consider simple random systems in Chapter 10 and statistical and thermal dynamics in Chapter 11. Finally, we investigate classical and quantum scattering in Chapter 12.

To effectively study these topics, the student should be familiar with basic calculus and introductory mechanics for mechanical systems (Chapters 2 through 6). For quantum and thermal systems (Chapters 8, 9, and 11), some familiarity with concepts typically covered in a modern physics course such as the wave function, expectation value, eigenstates, and entropy, will be helpful. We also assume the student to have some programming background, as familiarity with Python is a plus but not required. Past experience has shown that students unfamiliar with Python can successfully learn from examples and become productive quickly. By the time Chapter 3 is finished, most students will have grasped the essential programming elements needed to carry on.

Most of the introductory topics are aimed at the undergraduate level (up to Chapter 7). Starting from Chapter 5 and increasingly toward Chapter 12, we include advanced and more in-depth topics in the DOC content. These topics are geared at upper undergraduate or graduate levels, including quantum chaos, particle transport, Bose-Einstein condensation, quantum transitions, inelastic scattering and atomic reactions.

Moreover, we put a special emphasis on the simulation of quantum systems, expanding the coverage over three chapters (Chapters 8, 9, and 12). Ideally, these topics are better studied after a first course in quantum mechanics. However, some sections should be accessible even without a quantum course, such as Sections 8.1 through 8.3 and Section 9.1, for which a basic

understanding of wave motion should be sufficient. Our motivation for including these topics is due to the fact that, unlike classical mechanics, quantum mechanics has far fewer analytically solvable problems and is less intuitive and less visual compared to classical motion. These factors cause considerable difficulties to students' understanding in introductory quantum mechanics. By simulating and visualizing the behavior of quantum systems such as the quantum oscillator or free fall, we are in a position to help effectively address some of the difficulties, pre- or postquantum class. We regularly use computer simulations to augment and enhance traditional physics classes such as quantum mechanics.

Although some chapters are interrelated, most from Chapter 3 on can be independently studied. Figure 1 shows the major dependencies of the chapters where the primary numerical methods (under the chapter number) are discussed, which are used in subsequent chapters. As the book progresses, most chapters are dependent on two previous chapters or less, except Chapters 9 and 12, which are dependent on five. There are several methods spanning multiple chapters, including ODE solvers (discussed in Chapter 2) for most time-dependent simulations in Chapters 3 through 9 and Chapter 11; the finite element method introduced in Chapter 6 and extended in Chapters 7 and 9; and other methods such as root finding (Chapter 3). In many cases, the reader may skip the methodology section without much disruption. For instance, the fast Fourier transform (FFT) discussed in Chapter 5 of DOC is lightly used in Chapter 6 to analyze fundamental oscillation frequencies, but heavily used in Chapter 8 for evolving quantum systems and for extracting momentum distributions. In both instances, the reader initially unfamiliar with FFT can still work through the simulations without worrying about the technical details of FFT, using it as a supplied library. The reader may come back and review it later for a fuller understanding if desired.

The instructor can pick what sections to cover within a given chapter in most cases. For example, the instructor may skip some sections on ODE solvers to save time (see Introduction in Chapter 2). However, this may be limited due to progression in methodology or conceptual

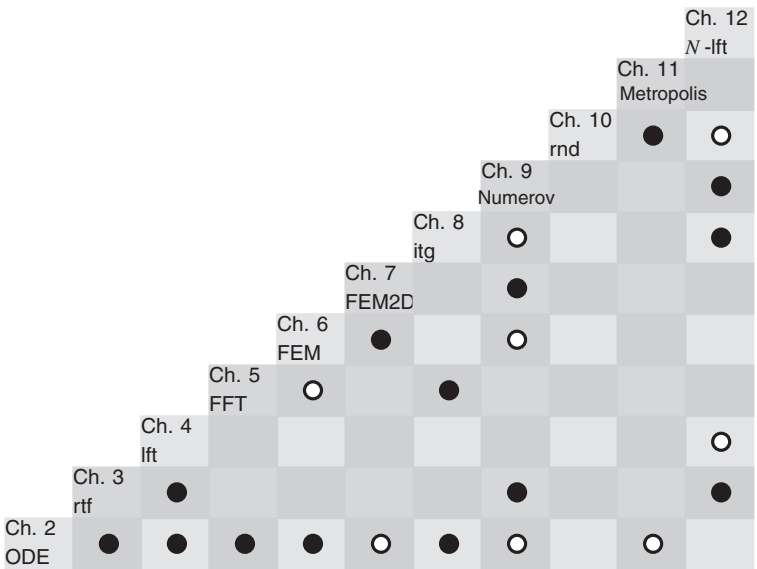

FIGURE 1 Major chapter dependencies at a glance. Open circles indicate minor or Digital Online Companion only dependencies. The abbreviations are: FEM—finite element method; FFT—fast Fourier transform; itg—numerical integration; lft—leapfrog with time-transformation; ODE—ordinary differential equations; rnd—random numbers; and rtf—root finding.

buildup. In such situations, indicated in the narrative and aided by Figure 1, the instructor may choose to discuss the prerequisite section lightly and leave further investigation to a project. Carefully constructed and tested projects given at the end of each chapter are an integral resource enabling the students to extend the models, make predictions, test them, analyze and present the results in project reports. Many in-depth projects, some found in the DOC, are designed for two-person teams to encourage peer learning and collaboration. There are also numerous exercises for the purpose of analytical derivations and proofs or simple programming tasks.

Throughout, references to the DOC content are indicated by the "S:" prefix, including the completely merged index. The DOC content and other electronic resources such as programs, data files, solution manual to select exercises, feedback and contact information, and installation instruction and files can be found at:

`http://www.wiley.com/college/wang` and
`https://github.com/com-py/compy/`

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J Wang
Dartmouth, Massachusetts
www.faculty.umassd.edu/j.wang/

List of Programs

We have built many programs in this book. The following table summarizes these programs and dependencies. Standard libraries such as Matplotlib (2D), NumPy, and SciPy are omitted. Library abbreviations are: fft—fast Fourier transform (`fft.py`, Chapter 5); fem—finite element method (`fem.py`, Chapter 9); fileio—file input/output (`fileio.py`, Chapter 9); itg—numerical integration (`integral.py`, Chapter 8); ode—ordinary differential equation (`ode.py`, Chapter 2); rtf—root finders (`rootfinder.py`, Chapter 3); and vpm—VPython Modules (`vpm.py`, Chapter 6). In addition, we also note the use of 3D and animation libraries: Axes3D—Matplotlib 3D plotting; am—Matplotlib animation; and vp—VPython.

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