A Physicist’s Guide
to Mathematica®
SECOND EDITION

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To
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Sandra, Teresa
Harriette, Frances
## Contents

Preface to the Second Edition xiii  
Preface to the First Edition xv  

I  Mathematica with Physics 1  

1  The First Encounter 3  
1.1. The First Ten Minutes 3  
1.2. A Touch of Physics 6  
1.2.1. Numerical Calculations 6  
1.2.2. Symbolic Calculations 6  
1.2.3. Graphics 6  
1.3. Online Help 7  
1.4. Warning Messages 9  
1.5. Packages 10  
1.6. Notebook Interfaces 12  
1.6.1. Notebooks 12  
1.6.2. Entering Greek Letters 12  
1.6.3. Getting Help 13  
1.6.4. Preparing Input 14  
1.6.5. Starting and Aborting Calculations 15  
1.7. Problems 15  

2  Interactive Use of Mathematica 19  
2.1. Numerical Capabilities 19  
2.1.1. Arithmetic Operations 19  
2.1.2. Spaces and Parentheses 20  
2.1.3. Common Mathematical Constants 20  
2.1.4. Some Mathematical Functions 21  
2.1.5. Cases and Brackets 22  
2.1.6. Ways to Refer to Previous Results 22  
2.1.7. Standard Computations 23  
2.1.8. Exact versus Approximate Values 24  
2.1.9. Machine Precision versus Arbitrary Precision 25  
2.1.10. Special Functions 27  
2.1.11. Matrices 27  
2.1.12. Double Square Brackets 29
2.1.13. Linear Least-Squares Fit 30
2.1.14. Complex Numbers 32
2.1.15. Random Numbers 32
2.1.16. Numerical Solution of Polynomial Equations 33
2.1.17. Numerical Integration 34
2.1.18. Numerical Solution of Differential Equations 39
2.1.19. Iterators 43
2.1.20. Exercises 44

2.2. Symbolic Capabilities 58
2.2.1. Transforming Algebraic Expressions 58
2.2.2. Transforming Trigonometric Expressions 61
2.2.3. Transforming Expressions Involving Special Functions 64
2.2.4. Using Assumptions 64
2.2.5. Obtaining Parts of Algebraic Expressions 67
2.2.6. Units, Conversion of Units, and Physical Constants 69
2.2.7. Assignments and Transformation Rules 72
2.2.8. Equation Solving 76
2.2.9. Differentiation 80
2.2.10. Integration 86
2.2.11. Sums 90
2.2.12. Power Series 94
2.2.13. Limits 96
2.2.14. Solving Differential Equations 97
2.2.15. Immediate versus Delayed Assignments and Transformation Rules 99
2.2.16. Defining Functions 100
2.2.17. Relational and Logical Operators 105
2.2.18. Fourier Transforms 108
2.2.19. Evaluating Subexpressions 112
2.2.20. Exercises 114

2.3. Graphical Capabilities 144
2.3.1. Two-Dimensional Graphics 144
2.3.2. Three-Dimensional Graphics 174
2.3.3. Interactive Manipulation of Graphics 179
2.3.4. Animation 182
2.3.5. Exercise 189

2.4. Lists 226
2.4.1. Defining Lists 226
2.4.2. Generating and Displaying Lists 227
2.4.3. Counting List Elements 229
2.4.4. Obtaining List and Sublist Elements 232
2.4.5. Changing List and Sublist Elements 236
2.4.6. Rearranging Lists 237
2.4.7. Restructuring Lists 238
2.4.8. Combining Lists 241
2.4.9. Operating on Lists 243
2.4.10. Using Lists in Computations 244
2.4.11. Analyzing Data 255
2.4.12. Exercises 268

2.5. Special Characters, Two-Dimensional Forms, and Format Types 287
2.5.1. Special Characters 288
2.5.2. Two-Dimensional Forms 296
2.5.3. Input and Output Forms 306
2.5.4. Exercises 309

2.6. Problems 314

3 Programming in Mathematica 329

3.1. Expressions 329
  3.1.1. Atoms 329
  3.1.2. Internal Representation 331
  3.1.3. Manipulation 334
  3.1.4. Exercises 352

3.2. Patterns 360
  3.2.1. Blanks 361
  3.2.2. Naming Patterns 362
  3.2.3. Restricting Patterns 363
  3.2.4. Structural Equivalence 370
  3.2.5. Attributes 371
  3.2.6. Defaults 373
  3.2.7. Alternative or Repeated Patterns 376
  3.2.8. Multiple Blanks 377
  3.2.9. Exercises 378

3.3. Functions 386
  3.3.1. Pure Functions 386
  3.3.2. Selecting a Definition 392
  3.3.3. Recursive Functions and Dynamic Programming 394
  3.3.4. Functional Iterations 398
  3.3.5. Protection 402
  3.3.6. Upvalues and Downvalues 404
  3.3.7. Exercises 408

3.4. Procedures 414
  3.4.1. Local Symbols 415
  3.4.2. Conditionals 417
  3.4.3. Loops 423
  3.4.4. Named Optional Arguments 428
  3.4.5. An Example: Motion of a Particle in One Dimension 435
  3.4.6. Exercises 446

3.5. Graphics 452
  3.5.1. Graphics Objects 452
Contents

5.3. Charged Particle in Crossed Electric and Magnetic Fields 602
  5.3.1. The Problem 602
  5.3.2. Physics of the Problem 602
  5.3.3. Solution with Mathematica 603
5.4. Problems 607

6 Quantum Physics 611
  6.1. Blackbody Radiation 611
    6.1.1. The Problem 611
    6.1.2. Physics of the Problem 611
    6.1.3. Solution with Mathematica 612
  6.2. Wave Packets 616
    6.2.1. The Problem 616
    6.2.2. Physics of the Problem 616
    6.2.3. Solution with Mathematica 617
  6.3. Particle in a One-Dimensional Box 622
    6.3.1. The Problem 622
    6.3.2. Physics of the Problem 622
    6.3.3. Solution with Mathematica 624
  6.4. The Square Well Potential 626
    6.4.1. The Problem 626
    6.4.2. Physics of the Problem 626
    6.4.3. Solution with Mathematica 629
  6.5. Angular Momentum 639
    6.5.1. The Problem 639
    6.5.2. Physics of the Problem 639
    6.5.3. Solution with Mathematica 644
  6.6. The Kronig–Penney Model 647
    6.6.1. The Problem 647
    6.6.2. Physics of the Problem 647
    6.6.3. Solution with Mathematica 648
  6.7. Problems 650

Appendices

A The Last Ten Minutes 653
B Operator Input Forms 655
C Solutions to Exercises 659
D Solutions to Problems 703

References 709

Index 713
Eleven years have elapsed since the publication of the first edition of this book in 1997. Then Mathematica 3.0 had less than 1200 built-in functions and other objects; now Mathematica 6.0, a major upgrade, has over 2200 of them. Also, Mathematica 6.0 features innovations such as real-time update of dynamic output, interface for interactive parameter manipulation, interactive graphics drawing and editing, load-on-demand curated data, and syntax coloring. Eleven years ago, Mathematica was well-known for its steep learning curve; the curve is no longer steep as we can now learn Mathematica from established courses and reader-friendly books rather than from only the definitive but formidable and encyclopedic reference, The Mathematica Book [Wol03].

The second edition of this book is compatible with Mathematica 6.0 and introduces a number of its new and best features. This new edition expands the material covered in many sections of the first edition; it includes new sections on data analysis, interactive graphics drawing, and interactive graphics manipulation; and it has a 146% increase in the number of end-of-section exercises and end-of-chapter problems. A compact disc accompanies the book and contains all of its Mathematica input and output. An online Instructor’s Solutions Manual is available to qualified adopters of the text.

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For corrections and updates, please visit the author’s webpage at www.humboldt.edu/~ptt1/APGTM_Updates.html, or locate the book’s webpage at http://elsevierdirect.com/companions/9780126831924 and then click the update link. If you encounter difficulties with or have questions about any inputs and outputs in the book, inspect them—with Mathematica 6—in the notebooks on the accompanying compact disc. If the issues are not resolved, send the inputs to the kernel and examine the outputs. Offerings of comments, suggestions, and bug reports are gratefully accepted at Patrick.Tam@humboldt.edu.

Patrick T. Tam
Preface to the First Edition

Traditionally, the upper-division theoretical physics courses teach the formalisms of the theories, the analytical technique of problem-solving, and the physical interpretation of the mathematical solutions. Problems of historical significance, pedagogical value, or if possible, recent research interest are chosen as examples. The analytical methods consist mainly of working with models, making approximations, and considering special or limiting cases. The student must master the analytical skills, because they can be used to solve many problems in physics and, even in cases where solutions cannot be found, can be used to extract a great deal of information about the problems. As the computer has become readily available, these courses should also emphasize computational skills, since they are necessary for solving many important, real, or “fun” problems in physics. The student ought to use the computer to complement and reinforce the analytical skills with the computational skills in problem-solving and, whenever possible, use the computer to visualize the results and observe the effects of varying the parameters of the problem in order to develop a greater intuitive understanding of the underlying physics.

The pendulum in classical mechanics serves as an example to elucidate these ideas. The plane pendulum is used as a model. It consists of a particle under the action of gravity and constrained to move in a vertical circle by a massless rigid rod. For small angular deviations, the equation of motion can be linearized and solved easily. For finite angular oscillations, the motion is nonlinear. Yet it can still be studied analytically in terms of the energy integral and the phase diagram. The period of motion is expressed in terms of an elliptic integral. The integral can be expanded in a power series, and for small angular oscillations the expansion converges rapidly. However, numerical methods and computer programming are necessary for determining the motion of a damped, driven pendulum. The student can use the computer to explore and simulate the motion of the pendulum with different sets of values for the parameters in order to gain a deeper intuitive understanding of the chaotic dynamics of the pendulum.

Normally, physics juniors and seniors have taken a course in a low-level language such as FORTRAN or Pascal and possibly also a course in numerical analysis. Nevertheless, attempts to introduce numerical methods and computer programming into the upper-division theoretical physics courses have been largely unsuccessful. Mastering the symbols and syntactic rules of these low-level languages is straightforward; but programming with them requires too many lines of complicated and convoluted code in order to solve interesting problems. Consequently, rather than enhancing the student’s problem-solving skills and physical intuition, it merely adds a frustrating and ultimately nonproductive burden to the student already struggling in a crowded curriculum.

Mathematica, a system developed recently for doing mathematics by computer, promises to empower the student to solve a wide range of problems including those that are important, real, or “fun,” and to provide an environment for the student to develop intuition and a deeper
understanding of physics. In addition to numerical calculations, *Mathematica* performs symbolic as well as graphical calculations and animates two- and three-dimensional graphics. The numerical capabilities broaden the problem-solving skills of the student; the symbolic capabilities relieve the student from the tedium and errors of “busy” or long-winded derivations; the graphical capabilities and the capabilities for “instant replay” with various parameter values for the problem enable the student to deepen his or her intuitive understanding of physics. These astounding interactive capabilities are sufficiently powerful for handling most problems and are surprisingly easy to learn and use. For complex and demanding problems, *Mathematica* also features a high-level programming language that can make use of more than a thousand built-in functions and that embraces many programming styles such as functional, rule-based, and procedural programming. Furthermore, to provide an integrated technical computing environment, the Macintosh and Windows versions for *Mathematica* support documents called “notebooks.” A notebook is a “live textbook.” It is a file containing ordinary text, *Mathematica* input and output, and graphics. *Mathematica*, together with the user-friendly Macintosh and Windows interfaces, is likely to revolutionize not only how but also what we teach in the upper-division theoretical physics courses.

**Purpose**

The primary purpose of this book is to teach upper-division and graduate physics students as well as professional physicists how to master *Mathematica*, using examples and approaches that are motivating to them. This book does not replace Stephen Wolfram’s *Mathematica: A System for Doing Mathematics by Computer* [Wol91] for *Mathematica* version 2 or *The Mathematica Book* [Wol96] for version 3. The encyclopedic nature of these excellent references is formidable, indeed overwhelming, for novices. My guidebook prepares the reader for easy access to Wolfram’s indispensable references. My book also shows that *Mathematica* can be a powerful and wonderful tool for learning, teaching, and doing physics.

**Uses**

This book can serve as the text for an upper-division course on *Mathematica* for physics majors. Augmented with chemistry examples, it can also be the text for a course on *Mathematica* for chemistry majors. (For the last several years, a colleague in the chemistry department and I have team-taught a *Mathematica* course for both chemistry and physics majors.) Part I, “Mathematica with Physics,” provides sufficient material for a two-unit, one-semester course. A three-unit, one-semester course can cover Part I, sample Part II, “Physics with Mathematica,” require a polished *Mathematica* notebook from each student reporting a project, and include supplementary material on introductory numerical analysis discussed in many texts (see [KM90], [DeV94], [Gar94], and [Pat94]). Exposure to numerical analysis allows the student to appreciate the limitations (i.e., the accuracy and stability) of numerical algorithms and understand the differences between numerical and symbolic functions, for example, between NSolve and Solve, NIntegrate and Integrate, as well as NDSolve and DSolve. Experience suggests that a three-hour-per-week laboratory is essential to the success of both the two- and three-unit courses. For the degree requirement, either course is an appropriate addition
to, if not replacement for, the existing course in a low-level language such as C, Pascal, or FORTRAN.

If a course on *Mathematica* is not an option, a workshop merits consideration. A two-day workshop can cover Chapter 1, “The First Encounter,” and Chapter 2, “Interactive Use of *Mathematica*,” and a one-week workshop can also include Chapter 3, “Programming in *Mathematica*.” Of course, further digestion of the material may be necessary after one of these accelerated workshops.

For students who are *Mathematica* neophytes, this book can also be a supplemental text for upper-division theoretical physics courses on mechanics, electricity and magnetism, and quantum physics. For *Mathematica* to enrich rather than encroach upon the curriculum, it must be introduced and integrated into these courses gradually and patiently throughout the junior and senior years, beginning with the interactive capabilities. While the interactive capabilities of *Mathematica* are quite impressive, in order to realize its full power the student must grasp its structure and master it as a programming language. Be forewarned that learning these advanced features as part of the regular courses, while possible, is difficult. A dedicated *Mathematica* course is usually a more gentle, efficient, and effective way to learn this computer algebra system.

Finally, the book can be used as a self-paced tutorial for advanced physics students and professional physicists who would like to learn *Mathematica* on their own. While the sections in Part I should be studied consecutively, those in Part II, each focusing on a particular physics problem, are independent of each other and can be read in any order. The reader may find the solutions to exercises and problems in Appendices D and E helpful.

**Organization**

Part I gives a practical, physics-oriented, and self-contained introduction to *Mathematica*. Chapter 1 shows the beginner how to get started with *Mathematica* and discusses the notebook front end. Chapter 2 introduces the numerical, symbolic, and graphical capabilities of *Mathematica*. Although these features of *Mathematica* are dazzling, *Mathematica*’s real power rests on its programming capabilities. While Chapter 2 considers many elements of *Mathematica*’s programming language, Chapter 3 treats in depth five key programming elements: expressions, patterns, functions, procedures, and graphics. It also examines three programming styles: procedural, functional, and rule-based. It shows how a proper choice of algorithm and style for a problem results in a correct, clear, efficient, and elegant program. This chapter concludes with a discussion of writing packages. Examples and practice problems, many from physics, are included in Chapters 2 and 3.

Part II considers the application of *Mathematica* to physics. Chapters 4 through 6 illustrate the solution with *Mathematica* of physics problems in mechanics, electricity and magnetism, and quantum physics. Each chapter presents several examples of varying difficulty and sophistication within a subject area. Each example contains three sections: The Problem, Physics of the Problem, and Solution with *Mathematica*. Experience has taught that the Physics of the Problem section is essential because the mesmerizing power of *Mathematica* can distract the student from the central focus, which is, of course, physics. Additional problems are included as exercises in each chapter.
Appendix A relates the latest news on Mathematica version 3.0 before this book goes to press. Appendix B tabulates many of Mathematica’s operator input forms together with the corresponding full forms and examples. Appendix C provides information about the books, journals, conferences, and electronic archives and forums on Mathematica. Appendices D and E give solutions to selected exercises and problems.

Suggestions
The reader should study this book at a computer with a Mathematica notebook opened, key in the commands, and try out the examples on the computer. Although all of the code in this book is included on an accompanying diskette, directly keying in the code greatly enhances the learning process. The reader should also try to work out as many as possible of the exercises at the end of the sections and the practice problems at the end of the chapters. The more challenging ones are marked with an asterisk, and those requiring considerable effort are marked with two asterisks.

Prerequisites
The prerequisites for this book are calculus through elementary differential equations, introductory linear algebra, and calculus-based physics with modern physics. Some of the physics in Chapters 5 and 6 may be accessible only to seniors. Basic Macintosh or Windows skills are assumed.

Computer Systems
This book, compatible with Mathematica versions 3.0 and 2.2, is to be used with Macintosh and Microsoft-Windows-based IBM-compatible computers. While the front end or the user interface is optimized for each kind of computer system, the kernel, which is the computational engine of Mathematica, is the same across all platforms. As over 95% of this book is about the kernel, the book can also be used, with the omission of the obviously Macintosh- or Windows-specific comments, for all computer systems supporting Mathematica, such as NeXT computers and UNIX workstations.

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