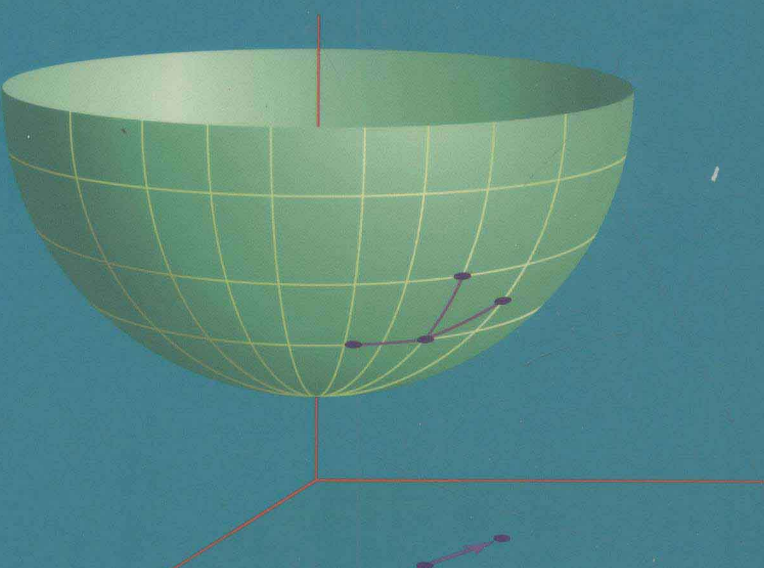
SADRI HASSANI

MATHEMATICAL METHODS Using *Mathematica*®

FOR STUDENTS OF PHYSICS AND RELATED FIELDS



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MATHEMATICAL METHODS USING *MATHEMATICA*®

For Students of Physics and Related Fields

Sadri Hassani

With 93 Illustrations and a CD-ROM

Springer

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COVER ILLUSTRATION: Gradient or differentiation with respect to distance is shown in two dimensions; the surface represents a function of *x* and *y*; the gradient is a vector *in the xy-plane*.

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To my wife, Sarah,

and to my children,

Dane Arash and Daisy Bita

Preface

Over two years have passed since the publication of *Mathematical Methods*, my undergraduate textbook to which the present book was to be a companion. The initial motivation for writing this book was to take some examples from *Mathematical Methods* in which to illustrate the use of a symbolic language such as *Mathematica*®. However, after writing the first few pages, I realized very quickly that, for the book to be most effective, I had to go beyond the presentation of examples. I had to talk about the theory of numerical integration, discrete differentiation, solution of differential equations, and a number of other topics; thus the delay in the publication of the book.

As a result, the book has become a *self-contained* introduction to the use of computer algebra—specifically, *Mathematica*—for undergraduates in physics and related fields. Although many of the examples discussed here are taken from *Mathematical Methods*, no prior knowledge of the content of that book is essential for learning the *techniques* of computer algebra. Of course, a deeper understanding of the underlying physical ideas requires reading the relevant sections of *Mathematical Methods* or a book like it. For those interested in the underlying theories of the examples being discussed, I have placed the appropriate page (or section) numbers in the margin.

I have to emphasize that the book does not discuss programming in *Mathematica*. Nor does it teach all the principles and techniques of the most elegant utilization of *Mathematica*. The book can best be described as "learning the essentials of *Mathematica* through examples from undergraduate physics." In other words, *Mathematica* commands and techniques are introduced as the need arises.

I believe that some understanding of the theory behind the numerical calculations is important, especially if it can invoke some *Mathematica* usage. Therefore, I have included an entire chapter on the theory of the numerical solutions of differential equations, and a rather lengthy discussion on the theory behind numerical integration. In both discussions I make use of *Mathematica* to enhance the understanding of the theories.

After introducing the essential *Mathematica* commands in Chapter 1, I introduce vectors—using the calculation of electric fields and potentials of discrete charge distributions—and matrices—using the calculation of normal modes of mass-spring systems—in Chapter 2 as they are used in *Mathematica.* Chapter 3 discusses numerical integration and a variety of its applications in different physical settings such as the evaluation of electric, magnetic, and gravitational fields of various sources. Infinite series and finite sums are the subject of Chapter 4, in which the theory of numerical integration is used as a nice example of the use of summation in *Mathematica.* Chapter 5 is devoted entirely to a theoretical treatment of the numerical solution of differential equations, discussing such techniques as the Euler methods, the Runge–Kutta method, and the use of discrete differentiation in solving eigenvalue problems. In Chapter 6, I have chosen some examples from classical and quantum mechanics to illustrate how *Mathematica* solves ordinary differential equations.

This book can be used in conjunction with any undergraduate mathematical physics book. Many problems are inherently interesting but cannot be solved analytically. Once the student learns the theory and formal mathematics behind a concept and solves a number of simple and ideal examples analytically, he or she ought to be exposed to problems arising from real-world applications. *Mathematica* (or any other computer-algebra software) can be of tremendous help in treating such problems and exhibiting their solutions graphically (or otherwise). However, *Mathematica* has its greatest impact on the process of learning only if the student has completed the preliminary stage of deeply understanding the analytical methods of solution.

This is hardly the place to enter into the controversy surrounding the role of content and memorization in learning. However, as an educator witnessing the alarming rate at which calculators and computer-algebra software are substituting the learning of physics and mathematics, I feel obligated to emphasize the distinction between the *real utility* of technology and its *advertised glamour.* Technology can be a great tool of learning and teaching once students acquire a certain degree of mathematical maturity. And this maturity can be obtained only through a rigorous training in conventional mathematics that emphasizes content at all levels of a student's education.

The neglect of content—such as the multiplication table at the elementary level, and algebraic/trigonometric identities at the high school level—can have a detrimental effect on the mathematical and analytical ability of the pupil's mind. If the educators sequentially postpone the "memorization" of the multiplication table, algebraic and trigonometric identities, and differentiation and integration rules, arguing that such "facts" are always available on calculators and computers, then students will develop the skill of "pushing buttons" beautifully but will be incapable of doing the simplest integration. Some educators argue that lack of ability to multiply, integrate, or simplify an algebraic expression is not a drawback as long as there are calculators to do the job. To this I have to respond that heavy reliance on calculating machines does to the mind what heavy reliance on vehicular machines does to the body: it makes the mind lazy and inactive. Our minds need raw data—in the form of numbers and symbols in conjunction with the rules that manipulate them—to develop. A mind without data is like a symphony without notes, an opera without lyrics, a poem without words. I sincerely hope that the readers and users of this book will take this advice to heart.

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Note to the Reader

I should point out from the very beginning that, as powerful as *Mathematica* is, it is only a tool. And a tool is more useful if its user has thought through the details of the task for which the tool is designed. Just as one needs to master multiplication—both conceptually (where and how it is used) and factually (the multiplication table)—before a calculator can be of any use, so does one need to master algebra, calculus, trigonometry, differential equations, etc., before *Mathematica* can be of any help. In short, *Mathematica* cannot think for you.

Mathematica, like any other calculational tool, is only as smart as its user can make it!

Once you have learned the concepts behind the equations and *know how to set up a specific problem*, *Mathematica* can be of great help in solving that problem for you. This book, of course, is not written to help you set up the problems; for that, you have to refer to your physics or engineering books. The purpose of this book is to familiarize you with the simple—but powerful—techniques of calculation used to solve problems that are otherwise insoluble. I have taken many examples from your undergraduate courses and have used a multitude of *Mathematica* techniques to solve those problems.

I encourage you to explore the CD-ROM that comes with the book. Not only does it contain all the codes used in the book, but it also gives many explanations and tips at each step of the solution of a problem. The CD-ROM is compatible with both *Mathematica* 3.0 and *Mathematica* 4.0.

Contents

1

Mathematica in a Nutshell

Mathematica® is a high-level computer language that can perform symbolic, numerical, and graphical manipulation of mathematical expressions. In this chapter we shall learn many of the essential *Mathematica* commands.

1.1 Running *Mathematica*

Installing and running *Mathematica* differ from one computer system to another. However, the heart of *Mathematica*, where the calculations are performed, is the same in all systems. *Mathematica* has two major components, the **kernel** and the **front end**. The front end is the window in which you type in your commands. These windows are generally part of **notebooks**, which are *Mathematica*'s interface with the kernel. The kernel is where the commands are processed. It could reside in the computer where the front end resides, or it could be in a remote computer.

of **kernels**, front ends, and notebooks

Mathematica is launched by double-clicking on its icon—or any other shortcut your computer system recognizes. Almost all front ends now incorporate notebooks, and I assume that the reader is communicating with *Mathematica* through this medium. The window of a notebook looks like any other window. After typing in your command, hold down the `Shift` key while hitting the `Return` key to execute that command. In Macintosh, the numeric `Enter` key will also do the job.

Shift+Return or numeric **Enter** tells *Mathematica* to start.

When you enter a command, *Mathematica* usually precedes it with an input sign such as `In[1]:=`; and when it gives out the result of the calculation, the output sign `Out[1]=` appears in front of the answer. The input and output numbers change as the session progresses. This is a convenient way of keeping track of all inputs and outputs for cross referencing. Thus, if you type `2+2` and enter the result, *Mathematica* turns it into `In[1]:= 2+2` and gives the result as `Out[1]=` 4.

In the remaining part of this chapter (and indeed throughout the book), we are going to discuss most of the commands an average user of *Mathematica* will need. Nevertheless, for the important details omitted in this book, the reader is urged to make frequent use of the definitive *Mathematica Book* [Wolf 96] as well as the `Help` menu, which includes the online version of the *Mathematica Book.*

1.2 Numerical Calculations

Mathematica recognizes two types of numerical calculations: integer and floating point. When the input of a mathematical expression is in integer form, *Mathematica*—unless asked specifically—does not approximate the final answer in decimal format. Consider asking *Mathematica* to add 11/3 to 217/43, by typing in

Mathematica calculates integer expressions exactly.

```
11/3 + 217/43
```

and pressing the numeric `Enter` key. *Mathematica* will give the answer as $\frac{1124}{129}$. On the other hand, if you type in

```
11./3 + 217/43
```

you will get the answer 8.71318. The difference between the two inputs is the occurrence of the floating (or decimal) point. In the second input *Mathematica* treats `11.` and all the other numbers in the expression as real numbers and manipulates them as such.

When *Mathematica* encounters expressions involving integers, it evaluates them and often gives the exact result. For example, for 5^{100}, *Mathematica* gives an exact 70-digit answer:

In[2]:= `5^100`

Out[2]= 78886090522101180541172856528278622967320643510902300477027893066406 25

use of `// N`

One can always get an approximate decimal answer by ending the input with `// N`

In[3]:= `5^100 // N`

Out[3]= 7.88861×10^{69}

An alternative way of getting approximations is to use `N[expr,n]`, which returns the numerical value of `expr` to `n` significant figures. Here is how to find the numerical value of π to any desired significant figures. Simply replace 40 with some other (positive) integer:

use of **N[,]**

```
In[4]:= N[Pi,40]
```

Out[4]= 3.141592653589793238462643383279502884197

The example above illustrates how *Mathematica* denotes the constant π. Other mathematical constants also have their own notations:

`Pi`	$\pi = 3.14159$
`E`	$e = 2.71828$
`I`	$i = \sqrt{-1}$
`Infinity`	∞
`Degree`	$\pi/180$: as in 30 Degrees

Mathematica understands the usual mathematical functions with two caveats:

Functions begin with capital letters; arguments are enclosed in square brackets.

- All *Mathematica* functions begin with a capital letter.
- The arguments are enclosed in square brackets.

Here is a list of some common functions:

`Sqrt[x]`	$\sqrt{x}$	`Sin[x], ArcSin[x]`	sine, its inverse
`Exp[x]`	e^x	`Cos[x], ArcCos[x]`	cosine, its inverse
`Abs[x]`	absolute value	`Tan[x], ArcTan[x]`	tangent, its inverse
`n!`	the factorial	`Cot[x], ArcCot[x]`	cotangent, its inverse
`Log[x]`	natural log	`Log[b,x]`	log to base b

By default, the arguments of the trigonometric functions are treated as radians. You can, however, use degrees:

Arguments of the trigonometric functions are treated as radians.

```
In[5]:= Sin[Pi/3]-Cos[45 Degree]
```

Out[5]= $-\frac{1}{\sqrt{2}} + \frac{\sqrt{3}}{2}$

Note that *Mathematica* returns the *exact* result. This is because no floating point appeared in the arguments of the functions. Changing `3` to `3.` or `45` to `45.` returns `0.158919`. Similarly, `Sqrt[2]` will return $\sqrt{2}$, but

```
In[6]:= N[Sqrt[2],45]
```

Out[6]= 1.41421356237309504880168872420969807856967188

Reusing the existing expressions

Mathematica has a very useful shortcut for reusing the existing expressions.

`%`	the last result generated
`%%`	the next-to-last result generated
`%n`	the result on output line `Out[n]`

Typing in `%^2` squares the last result generated and returns its value. Similarly, `Sqrt[%6]` takes the square root of the result on output line `Out[6]`.

1.3 Algebraic and Trigonometric Calculations

The most powerful aspect of *Mathematica* is its ability to handle symbolic mathematics, including all the manipulations one encounters in algebra. The following is a partial list of algebraic expressions frequently encountered in calculations.

`Expand[expr]`	multiply products and powers in *expr*
`Factor[expr]`	write *expr* as products of minimal factors
`Simplify[expr]`	simplify *expr* (standard)
`FullSimplify[expr]`	simplify *expr* (comprehensive)
`PowerExpand[expr]`	transform $(xy)^p$ to $x^p y^p$; useful for changing $\sqrt{a^2}$ to a

Mathematica allows a convenient method of substituting values for a quantity in an expression:

`expr /. x -> value`	replace x by *value* in *expr*
`expr /. {x -> xval, y -> yval}`	perform several replacements

Here is an example of the use of some of the above:

```
In[1]:= x^2-2x+1 /. x -> 2 + y
```

Out[1]= $1 - 2(2 + y) + (2 + y)^2$

```
In[2]:= Expand[%]
```