COMPUTATIONAL PHYSICS

Fortran Version

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Preface

Computation is an integral part of modern science and the ability to exploit effectively the power offered by computers is therefore essential to a working physicist. The proper application of a computer to modeling physical systems is far more than blind "number crunching," and the successful computational physicist draws on a balanced mix of analytically soluble examples, physical intuition, and numerical work to solve problems that are otherwise intractable.

Unfortunately, the ability "to compute" is seldom cultivated by the standard university-level physics curriculum, as it requires an integration of three disciplines (physics, numerical analysis, and computer programming) covered in disjoint courses. Few physics students finish their undergraduate education knowing how to compute; those that do usually learn a limited set of techniques in the course of independent work, such as a research project or a senior thesis.

The material in this book is aimed at refining computational skills in advanced undergraduate or beginning graduate students by providing direct experience in using a computer to model physical systems. Its scope includes the minimum set of numerical techniques needed to "do physics" on a computer. Each of these is developed in the text, often heuristically, and is then applied to solve non-trivial problems in classical, quantum, and statistical physics. These latter have been chosen to enrich or extend the standard undergraduate physics curriculum, and so have considerable intrinsic interest, quite independent of the computational principles they illustrate.

This book should not be thought of as setting out a rigid or definitive curriculum. I have restricted its scope to calculations that satisfy simultaneously the criteria of illustrating a widely applicable numerical technique, of being tractable on a microcomputer, and of having some particular physics interest. Several important numerical techniques have therefore been omitted, spline interpolation and the Fast Fourier Transform among them. *Computational Physics* is perhaps best thought of as establishing an environment offering opportunities for further exploration. There are many possible extensions and embellishments of the material presented; using one's imagination along these lines is one of the more rewarding parts of working through the book.

Computational Physics is primarily a physics text. For maximum benefit, the student should have taken, or be taking, undergraduate courses in classical mechanics, quantum mechanics, statistical mechanics, and advanced calculus or the mathematical methods of physics. This is *not* a text on numerical analysis, as there has been no attempt at rigor or completeness in any of the expositions of numerical techniques. However, a prior course in that subject is probably not essential; the discussions of numerical techniques should be accessible to a student with the physics background outlined above, perhaps with some reference to any one of the excellent texts on numerical analysis (for example, [Ac70], [Bu81], or [Sh84]). This is also *not* a text on computer programming. Although I have tried to follow the principles of good programming throughout (see Appendix B), there has been no attempt to teach programming *per se*. Indeed, techniques for organizing and writing code are somewhat peripheral to the main goals of the book. Some familiarity with programming, at least to the extent of a one-semester introductory course in any of the standard high-level languages (BASIC, FORTRAN, PASCAL, C), is therefore essential.

The choice of language invariably invokes strong feelings among scientists who use computers. Any language is, after all, only a means of expressing the concepts underlying a program. The contents of this book are therefore relevant no matter what language one works in. However, *some* language had to be chosen to implement the programs, and I have selected the Microsoft dialect of BASIC standard on the IBM PC/XT/AT computers for this purpose. The BASIC language has many well-known deficiencies, foremost among them being a lack of local subroutine variables and an awkwardness in expressing structured code. Nevertheless, I believe that these are more than balanced by the simplicity of the language and the widespread fluency in it, BASIC's almost universal availability on the microcomputers most likely to be used with this book, the existence of both BASIC interpreters convenient for writing and debugging programs and of compilers for producing rapidly executing finished programs, and the powerful graphics and I/O statements in this language. I expect that readers familiar with some other high-level language can learn enough BASIC "on the fly" to be able to use this book. A synopsis of the language is contained in Appendix A to help in this regard, and further information can be found in readily available manuals. The reader may, of course, elect to write the programs suggested in the text in any convenient language.

This book arose out of the Advanced Computational Physics Laboratory taught to third- and fourth-year undergraduate Physics majors

at Caltech during the Winter and Spring of 1984. The content and presentation have benefitted greatly from the many inspired suggestions of M.-C. Chu, V. Pönisch, R. Williams, and D. Meredith. Mrs. Meredith was also of great assistance in producing the final form of the manuscript and programs. I also wish to thank my wife, Laurie, for her extraordinary patience, understanding, and support during my two-year involvement in this project.

Steven E. Koonin
Pasadena
May, 1985

Preface to the FORTRAN Edition

At the request of the readers of the BASIC edition of *Computational Physics* we offer this FORTRAN version. Although we stand by our original choice of BASIC for the reasons cited in the preface to the BASIC edition it is clear that many of our readers strongly prefer FORTRAN, and so we gladly oblige. The text of the book is essentially unchanged, but all of the codes have been translated into standard FORTRAN-77 and will run (with some modification) on a variety of machines. Although the programs will run significantly faster on mainframe computers than on PC's, we have not increased the scope or complexity of the calculations. Results, therefore, are still produced in "real time", and the codes remain suitable for interactive use.

Another development since the BASIC edition is the publication of an excellent new text on numerical analysis (*Numerical Recipes* [Pr86]) which provides detailed discussions and code for state-of-the-art algorithms. We highly recommend it as a companion to this text.

The FORTRAN versions of the code were written with the help of T. Berke (who designed the menu), G. Buzzell, and J. Farley. We have also profited from the suggestions of many colleagues who have generously tested the new codes or pointed out errors in the BASIC edition. We gratefully acknowledge a grant from the University of New Hampshire DISCovery Computer Aided Instruction Program which provided the initial impetus for the translation. Lastly, our thanks go to E. Wood for typesetting the text in TEX.

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Pasadena, CA
August, 1989

Dawn C. Meredith
Durham, NH

How to Use This Book

This book is organized into chapters, each containing a text section, an example, and a project. Each text section is a brief discussion of one or several related numerical techniques, often illustrated with simple mathematical examples. Throughout the text are a number of exercises, in which the student's understanding of the material is solidified or extended by an analytical derivation or through the writing and running of a simple program. These exercises are indicated by the symbol ■.

Also located throughout the text are tables of numerical errors. Note that the values listed in these tables were taken from runs using BASIC code on an IBM-PC. When the machine precision dominates the error, your values obtained with FORTRAN code may differ.

The example and project in each chapter are applications of the numerical techniques to particular physical problems. Each includes a brief exposition of the physics, followed by a discussion of how the numerical techniques are to be applied. The examples and projects differ only in that the student is expected to use (and perhaps modify) the program that is given for the former in Appendix B, while the book provides guidance in writing programs to treat the latter through a series of steps, also indicated by the symbol ■. However, programs for the projects have also been included in Appendix C; these can serve as models for the student's own program or as a means of investigating the physics without having to write a major program "from scratch". A number of suggested studies accompany each example and project; these guide the student in exploiting the programs and understanding the physical principles and numerical techniques involved.

The programs for both the examples and projects are available on IBM-PC and MACINTOSH formatted diskettes. (An order form is located in the back of the book.) The codes are suitable for running on any computer that has a FORTRAN-77 standard compiler. Detailed instructions for revising and running the codes are given in Appendix A.

A "laboratory" format has proved to be one effective mode of presenting this material in a university setting. Students are quite able to work through the text on their own, with the instructor being available for consultation and to monitor progress through brief personal interviews on each chapter. Three chapters in ten weeks (60 hours) of instruction

has proved to be a reasonable pace, with students typically writing two of the projects during this time, and using the "canned" codes to work through the physics of the remaining project and the examples. The eight chapters in this book should therefore be more than sufficient for a one-semester course. Alternatively, this book can be used to provide supplementary material for the usual courses in classical, quantum, and statistical mechanics. Many of the examples and projects are vivid illustrations of basic concepts in these subjects and are therefore suitable for classroom demonstrations or independent study.

Contents

The problem with computers is that they only give answers
—attributed to P. Picasso

Chapter 1

Basic Mathematical Operations

Three numerical operations — differentiation, quadrature, and the finding of roots — are central to most computer modeling of physical systems. Suppose that we have the ability to calculate the value of a function, $f(x)$, at any value of the independent variable x. In differentiation, we seek one of the derivatives of f at a given value of x. Quadrature, roughly the inverse of differentiation, requires us to calculate the definite integral of f between two specified limits (we reserve the term "integration" for the process of solving ordinary differential equations, as discussed in Chapter 2), while in root finding we seek the values of x (there may be several) at which f vanishes.

If f is known analytically, it is almost always possible, with enough fortitude, to derive explicit formulas for the derivatives of f, and it is often possible to do so for its definite integral as well. However, it is often the case that an analytical method cannot be used, even though we can evaluate $f(x)$ itself. This might be either because some very complicated numerical procedure is required to evaluate f and we have no suitable analytical formula upon which to apply the rules of differentiation and quadrature, or, even worse, because the way we can generate f provides us with its values at only a set of discrete abscissae. In these situations, we must employ approximate formulas expressing the derivatives and integral in terms of the values of f we can compute. Moreover, the roots of all but the simplest functions cannot be found analytically, and numerical methods are therefore essential.

This chapter deals with the computer realization of these three basic operations. The central technique is to approximate f by a simple function (such as first- or second-degree polynomial) upon which these

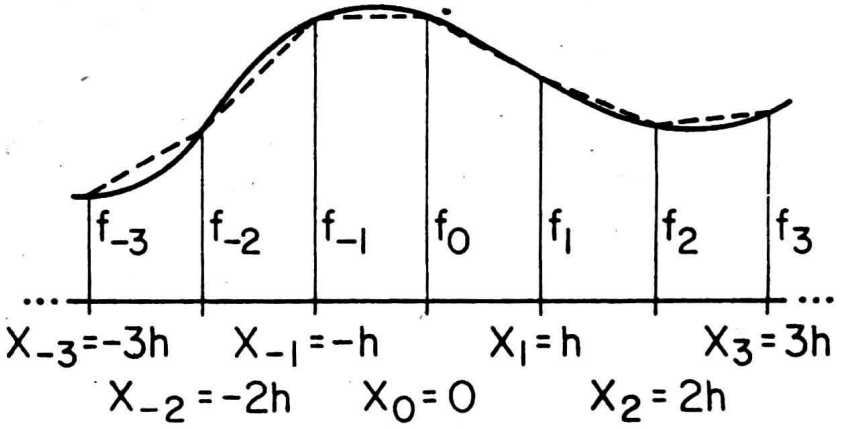

Figure 1.1 Values of f on an equally-spaced lattice. Dashed lines show the linear interpolation.

operations can be performed easily. We will derive only the simplest and most commonly used formulas; fuller treatments can be found in many textbooks on numerical analysis.

1.1 Numerical differentiation

Let us suppose that we are interested in the derivative at $x = 0$, $f'(0)$. (The formulas we will derive can be generalized simply to arbitrary x by translation.) Let us also suppose that we know f on an equally-spaced lattice of x values,

$$f_n = f(x_n)\,; \quad x_n = nh \; (n = 0, \pm 1, \pm 2, \ldots)\,,$$

and that our goal is to compute an approximate value of $f'(0)$ in terms of the f_n (see Figure 1.1).

We begin by using a Taylor series to expand f in the neighborhood of $x = 0$:

$$f(x) = f_0 + xf' + \frac{x^2}{2!}f'' + \frac{x^3}{3!}f''' + \ldots\,, \tag{1.1}$$

where all derivatives are evaluated at $x = 0$. It is then simple to verify that

$$f_{\pm 1} \equiv f(x = \pm h) = f_0 \pm hf' + \frac{h^2}{2}f'' \pm \frac{h^3}{6}f''' + \mathcal{O}(h^4)\,, \tag{1.2a}$$

$$f_{\pm 2} \equiv f(x = \pm 2h) = f_0 \pm 2hf' + 2h^2 f'' \pm \frac{4h^3}{3}f''' + \mathcal{O}(h^4)\,, \tag{1.2b}$$

where $\mathcal{O}(h^4)$ means terms of order h^4 or higher. To estimate the size of such terms, we can assume that f and its derivatives are all of the same order of magnitude, as is the case for many functions of physical relevance.

Upon subtracting f_{-1} from f_1 as given by (1.2a), we find, after a slight rearrangement,

$$f' = \frac{f_1 - f_{-1}}{2h} - \frac{h^2}{6} f''' + \mathcal{O}(h^4) . \tag{1.3a}$$

The term involving f''' vanishes as h becomes small and is the dominant error associated with the finite difference approximation that retains only the first term:

$$f' \approx \frac{f_1 - f_{-1}}{2h} . \tag{1.3b}$$

This "3-point" formula would be exact if f were a second-degree polynomial in the 3-point interval $[-h, +h]$, because the third- and all higher-order derivatives would then vanish. Hence, the essence of Eq. (1.3b) is the assumption that a quadratic polynomial interpolation of f through the three points $x = \pm h$, 0 is valid.

Equation (1.3b) is a very natural result, reminiscent of the formulas used to define the derivative in elementary calculus. The error term (of order h^2) can, in principle, be made as small as is desired by using smaller and smaller values of h. Note also that the symmetric difference about $x = 0$ is used, as it is more accurate (by one order in h) than the forward or backward difference formulas:

$$f' \approx \frac{f_1 - f_0}{h} + \mathcal{O}(h) ; \tag{1.4a}$$

$$f' \approx \frac{f_0 - f_{-1}}{h} + \mathcal{O}(h) . \tag{1.4b}$$

These "2-point" formulas are based on the assumption that f is well approximated by a linear function over the intervals between $x = 0$ and $x = \pm h$.

As a concrete example, consider evaluating $f'(x = 1)$ when $f(x) = \sin x$. The exact answer is, of course, $\cos 1 = 0.540302$. The following FORTRAN program evaluates Eq. (1.3b) in this case for the value of h input:

```
C chap1a.for
      X=1.
      EXACT=COS(X)
```

```
10      PRINT *, 'ENTER VALUE OF H (.LE. 0 TO STOP)'
        READ *,  H
        IF (H .LE. 0) STOP
        FPRIME=(SIN(X+H)-SIN(X-H))/(2*H)
        DIFF=EXACT-FPRIME
        PRINT 20,H,DIFF
20      FORMAT (' H=',E15.8,5X,'ERROR=',E15.8)
        GOTO 10
        END
```

(If you are a beginner in FORTRAN, note the way the value of H is requested from the keyboard, the fact that the code will stop if a non-positive value of H is entered, the natural way in which variable names are chosen and the mathematical formula (1.3b) is transcribed using the SIN function in the sixth line, the way in which the number of significant digits is specified when the result is to be output to the screen in line 20, and the jump in program control at the end of the program.)

Results generated with this program, as well as with similar ones evaluating the forward and backward difference formulas Eqs. (1.4a,b), are shown in Table 1.1. (All of the tables of errors presented in the text were generated from BASIC programs; the numbers may vary from those obtained from FORTRAN code, especially when numerical roundoff dominates.) Note that the result improves as we decrease h, but only up to a point, after which it becomes worse. This is because arithmetic in the computer is performed with only a limited precision (5–6 decimal digits for a single precision BASIC variable), so that when the difference in the numerator of the approximations is formed, it is subject to large "round-off" errors if h is small and f_1 and f_{-1} differ very little. For example, if $h = 10^{-6}$, then

$$f_1 = \sin(1.000001) = 0.841472\,; \quad f_{-1} = \sin(0.999999) = 0.841470\,,$$

so that $f_1 - f_{-1} = 0.000002$ to six significant digits. When substituted into (1.3b) we find $f' \approx 1.000000$, a very poor result. However, if we do the arithmetic with 10 significant digits, then

$$f_1 = 0.8414715251\,; \quad f_{-1} = 0.8414704445\,,$$

which gives a respectable $f' \approx 0.540300$ in Eq. (1.3b). In this sense, numerical differentiation is an intrinsically unstable process (no well-defined limit as $h \to 0$), and so must be carried out with caution.