Numerical Recipes
in Fortran 77

The Art of Scientific Computing

Second Edition

Volume 1 of
Fortran Numerical Recipes

William H. Press

Harvard-Smithsonian Center for Astrophysics

Saul A. Teukolsky

Department of Physics, Cornell University

William T. Vetterling

Polaroid Corporation

Brian P. Flannery

EXXON Research and Engineering Company

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Contents

Contents of Volume 2: Numerical Recipes in Fortran 90

Plan of the Two-Volume Edition

Fortran, long the epitome of stability, is once again a language in flux. Fortran 90 is not just the long-awaited updating of traditional Fortran 77 to modern computing practices, but also demonstrates Fortran's decisive bid to be the language of choice for parallel programming on multiprocessor computers.

At the same time, Fortran 90 is completely backwards-compatible with all Fortran 77 code. So, users with legacy code, or who choose to use only older language constructs, will still get the benefit of updated and actively maintained compilers.

As we, the authors of *Numerical Recipes*, watched the gestation and birth of Fortran 90 by its governing standards committee (an interesting process described by a leading Committee member, Michael Metcalf, in the Foreword to our Volume 2), it became clear to us that the right moment for moving Numerical Recipes from Fortran 77 to Fortran 90 was sooner, rather than later.

On the other hand, it was equally clear that Fortran-77-style programming — no matter whether with Fortran 77 or Fortran 90 compilers — is, and will continue for a long time to be, the "mother tongue" of a large population of active scientists, engineers, and other users of numerical computation. This is not a user base that we would willingly or knowingly abandon.

The solution was immediately clear: a two-volume edition of the Fortran *Numerical Recipes* consisting of Volume 1 (this one, a corrected reprinting of the previous one-volume edition), now retitled *Numerical Recipes in Fortran 77*, and a completely new Volume 2, titled *Numerical Recipes in Fortran 90: The Art of* Parallel *Scientific Computing*. Volume 2 begins with three chapters (21, 22, and 23) that extend the narrative of the first volume to the new subjects of Fortran 90 language features, parallel programming methodology, and the implementation of certain useful utility functions in Fortran 90. Then, in exact correspondence with Volume 1's Chapters 1–20, are new chapters B1–B20, devoted principally to the listing and explanation of new Fortran 90 routines. With a few exceptions, each Fortran 77 routine in Volume 1 has a corresponding new Fortran 90 version in Volume 2. (The exceptions are a few new capabilities, notably in random number generation and in multigrid PDE solvers, that are unique to Volume 2's Fortran 90.) Otherwise, there is no duplication between the volumes. The detailed explanation of the algorithms in this Volume 1 is intended to apply to, and be essential for, both volumes.

In other words: **You can use this Volume 1 without having Volume 2, but you can't use Volume 2 without Volume 1.** We think that there is much to be gained by having and using *both* volumes: Fortran 90's parallel language constructions are not only useful for present and future multiprocessor machines; they also allow for the elegant and concise formulation of many algorithms on ordinary single-processor computers. We think that essentially *all* Fortran programmers will want gradually to migrate into Fortran 90 and into a mode of "thinking parallel." We have written Volume 2 specifically to help with this important transition.

Volume 2's discussion of parallel programming is focused on those issues of direct relevance to the Fortran 90 programmer. Some more general aspects of parallel programming, such as communication costs, synchronization of multiple processers, etc., are touched on only briefly. We provide references to the extensive literature on these more specialized topics.

A special note to C programmers: Right now, there is no effort at producing a parallel version of C that is comparable to Fortran 90 in maturity, acceptance, and stability. We think, therefore, that C programmers will be well served by using Volume 2, either in conjuction with this Volume 1 or else in conjunction with the sister volume *Numerical Recipes in C: The Art of Scientific Computing*, for an educational excursion into Fortran 90, its parallel programming constructions, and the numerical algorithms that capitalize on them. C and C++ programming have not been far from our minds as we have written this two-volume version. We think you will find that time spent in absorbing the principal lessons of Volume 2's Chapters 21–23 will be amply repaid in the future, as C and C++ eventually develop standard parallel extensions.

Preface to the Second Edition

Our aim in writing the original edition of *Numerical Recipes* was to provide a book that combined general discussion, analytical mathematics, algorithmics, and actual working programs. The success of the first edition puts us now in a difficult, though hardly unenviable, position. We wanted, then and now, to write a book that is informal, fearlessly editorial, unesoteric, and above all useful. There is a danger that, if we are not careful, we might produce a second edition that is weighty, balanced, scholarly, and boring.

It is a mixed blessing that we know more now than we did six years ago. Then, we were making educated guesses, based on existing literature and our own research, about which numerical techniques were the most important and robust. Now, we have the benefit of direct feedback from a large reader community. Letters to our alter-ego enterprise, Numerical Recipes Software, are in the thousands per year. (Please, *don't telephone* us.) Our post office box has become a magnet for letters pointing out that we have omitted some particular technique, well known to be important in a particular field of science or engineering. We value such letters, and digest them carefully, especially when they point us to specific references in the literature.

The inevitable result of this input is that this Second Edition of *Numerical Recipes* is substantially larger than its predecessor, in fact about 50% larger both in words and number of included programs (the latter now numbering well over 300). "Don't let the book grow in size," is the advice that we received from several wise colleagues. We have tried to follow the intended spirit of that advice, even as we violate the letter of it. We have not lengthened, or increased in difficulty, the book's principal discussions of mainstream topics. Many new topics are presented at this same accessible level. Some topics, both from the earlier edition and new to this one, are now set in smaller type that labels them as being "advanced." The reader who ignores such advanced sections completely will not, we think, find any lack of continuity in the shorter volume that results.

Here are some highlights of the new material in this Second Edition:

- a new chapter on integral equations and inverse methods
- a detailed treatment of multigrid methods for solving elliptic partial differential equations
- routines for band diagonal linear systems
- improved routines for linear algebra on sparse matrices
- Cholesky and QR decomposition
- orthogonal polynomials and Gaussian quadratures for arbitrary weight functions
- methods for calculating numerical derivatives
- Padé approximants, and rational Chebyshev approximation
- Bessel functions, and modified Bessel functions, of fractional order; and several other new special functions
- improved random number routines
- quasi-random sequences
- routines for adaptive and recursive Monte Carlo integration in high-dimensional spaces
- globally convergent methods for sets of nonlinear equations

- simulated annealing minimization for continuous control spaces
- fast Fourier transform (FFT) for real data in two and three dimensions
- fast Fourier transform (FFT) using external storage
- improved fast cosine transform routines
- wavelet transforms
- Fourier integrals with upper and lower limits
- spectral analysis on unevenly sampled data
- Savitzky-Golay smoothing filters
- fitting straight line data with errors in both coordinates
- a two-dimensional Kolmogorov-Smirnoff test
- the statistical bootstrap method
- embedded Runge-Kutta-Fehlberg methods for differential equations
- high-order methods for stiff differential equations
- a new chapter on "less-numerical" algorithms, including Huffman and arithmetic coding, arbitrary precision arithmetic, and several other topics.

Consult the Preface to the First Edition, following, or the Table of Contents, for a list of the more "basic" subjects treated.

Acknowledgments

It is not possible for us to list by name here all the readers who have made useful suggestions; we are grateful for these. In the text, we attempt to give specific attribution for ideas that appear to be original, and not known in the literature. We apologize in advance for any omissions.

Some readers and colleagues have been particularly generous in providing us with ideas, comments, suggestions, and programs for this Second Edition. We especially want to thank George Rybicki, Philip Pinto, Peter Lepage, Robert Lupton, Douglas Eardley, Ramesh Narayan, David Spergel, Alan Oppenheim, Sallie Baliunas, Scott Tremaine, Glennys Farrar, Steven Block, John Peacock, Thomas Loredo, Matthew Choptuik, Gregory Cook, L. Samuel Finn, P. Deuflhard, Harold Lewis, Peter Weinberger, David Syer, Richard Ferch, Steven Ebstein, and William Gould. We have been helped by Nancy Lee Snyder's mastery of a complicated TEX manuscript. We express appreciation to our editors Lauren Cowles and Alan Harvey at Cambridge University Press, and to our production editor Russell Hahn. We remain, of course, grateful to the individuals acknowledged in the Preface to the First Edition.

Special acknowledgment is due to programming consultant Seth Finkelstein, who influenced many of the routines in this book, and wrote or rewrote many more routines in its C-language twin and the companion Example books. Our project has benefited enormously from Seth's talent for detecting, and following the trail of, even very slight anomalies (often compiler bugs, but occasionally our errors), and from his good programming sense.

We prepared this book for publication on DEC and Sun workstations running the UNIX operating system, and on a 486/33 PC compatible running MS-DOS 5.0/Windows 3.0. (See §1.0 for a list of additional computers used in program tests.) We enthusiastically recommend the principal software used: GNU Emacs, TEX, Perl, Adobe Illustrator, and PostScript. Also used were a variety of FORTRAN compilers — too numerous (and sometimes too buggy) for individual

acknowledgment. It is a sobering fact that our standard test suite (exercising all the routines in this book) has uncovered compiler bugs in a large majority of the compilers tried. When possible, we work with developers to see that such bugs get fixed; we encourage interested compiler developers to contact us about such arrangements.

WHP and SAT acknowledge the continued support of the U.S. National Science Foundation for their research on computational methods. D.A.R.P.A. support is acknowledged for §13.10 on wavelets.

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William H. Press
Saul A. Teukolsky
William T. Vetterling
Brian P. Flannery

Preface to the First Edition

We call this book *Numerical Recipes* for several reasons. In one sense, this book is indeed a "cookbook" on numerical computation. However there is an important distinction between a cookbook and a restaurant menu. The latter presents choices among complete dishes in each of which the individual flavors are blended and disguised. The former — and this book — reveals the individual ingredients and explains how they are prepared and combined.

Another purpose of the title is to connote an eclectic mixture of presentational techniques. This book is unique, we think, in offering, for each topic considered, a certain amount of general discussion, a certain amount of analytical mathematics, a certain amount of discussion of algorithmics, and (most important) actual implementations of these ideas in the form of working computer routines. Our task has been to find the right balance among these ingredients for each topic. You will find that for some topics we have tilted quite far to the analytic side; this where we have felt there to be gaps in the "standard" mathematical training. For other topics, where the mathematical prerequisites are universally held, we have tilted towards more in-depth discussion of the nature of the computational algorithms, or towards practical questions of implementation.

We admit, therefore, to some unevenness in the "level" of this book. About half of it is suitable for an advanced undergraduate course on numerical computation for science or engineering majors. The other half ranges from the level of a graduate course to that of a professional reference. Most cookbooks have, after all, recipes at varying levels of complexity. An attractive feature of this approach, we think, is that the reader can use the book at increasing levels of sophistication as his/her experience grows. Even inexperienced readers should be able to use our most advanced routines as black boxes. Having done so, we hope that these readers will subsequently go back and learn what secrets are inside.

If there is a single dominant theme in this book, it is that practical methods of numerical computation can be simultaneously efficient, clever, and — important — clear. The alternative viewpoint, that efficient computational methods must necessarily be so arcane and complex as to be useful only in "black box" form, we firmly reject.

Our purpose in this book is thus to open up a large number of computational black boxes to your scrutiny. We want to teach you to take apart these black boxes and to put them back together again, modifying them to suit your specific needs. We assume that you are mathematically literate, i.e., that you have the normal mathematical preparation associated with an undergraduate degree in a physical science, or engineering, or economics, or a quantitative social science. We assume that you know how to program a computer. We do not assume that you have any prior formal knowledge of numerical analysis or numerical methods.

The scope of *Numerical Recipes* is supposed to be "everything up to, but not including, partial differential equations." We honor this in the breach: First, we *do* have one introductory chapter on methods for partial differential equations (Chapter 19). Second, we obviously cannot include *everything* else. All the so-called "standard" topics of a numerical analysis course have been included in this book:

linear equations (Chapter 2), interpolation and extrapolation (Chaper 3), integration (Chaper 4), nonlinear root-finding (Chapter 9), eigensystems (Chapter 11), and ordinary differential equations (Chapter 16). Most of these topics have been taken beyond their standard treatments into some advanced material which we have felt to be particularly important or useful.

Some other subjects that we cover in detail are not usually found in the standard numerical analysis texts. These include the evaluation of functions and of particular special functions of higher mathematics (Chapters 5 and 6); random numbers and Monte Carlo methods (Chapter 7); sorting (Chapter 8); optimization, including multidimensional methods (Chapter 10); Fourier transform methods, including FFT methods and other spectral methods (Chapters 12 and 13); two chapters on the statistical description and modeling of data (Chapters 14 and 15); and two-point boundary value problems, both shooting and relaxation methods (Chapter 17).

The programs in this book are included in ANSI-standard `FORTRAN`-77. Versions of the book in `C`, `Pascal`, and `BASIC` are available separately. We have more to say about the `FORTRAN` language, and the computational environment assumed by our routines, in §1.1 (Introduction).

Acknowledgments

Many colleagues have been generous in giving us the benefit of their numerical and computational experience, in providing us with programs, in commenting on the manuscript, or in general encouragement. We particularly wish to thank George Rybicki, Douglas Eardley, Philip Marcus, Stuart Shapiro, Paul Horowitz, Bruce Musicus, Irwin Shapiro, Stephen Wolfram, Henry Abarbanel, Larry Smarr, Richard Muller, John Bahcall, and A.G.W. Cameron.

We also wish to acknowledge two individuals whom we have never met: Forman Acton, whose 1970 textbook *Numerical Methods that Work* (New York: Harper and Row) has surely left its stylistic mark on us; and Donald Knuth, both for his series of books on *The Art of Computer Programming* (Reading, MA: Addison-Wesley), and for TEX, the computer typesetting language which immensely aided production of this book.

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William H. Press
Brian P. Flannery
Saul A. Teukolsky
William T. Vetterling