Computer Software Reviews

Numerical Recipes in Fortran 90: The Art of Scientific Computing, Second Edition, Volume 2. (3 CD-ROMs and Manual) By William H. Press, Saul A. Teukolsky, William T. Vetterling, and Brian P. Flannery. Cambridge University Press: New York, 1996.

This is the latest version of a remarkable collection of programs for a wide range of computations. Each of the CD-ROMs assembles all the code from all the previous *Numerical Recipes* books, including programs in Fortran (both Fortran 77 and Fortran 90), in C (both ANSI and K&R versions), in Pascal, and in BASIC (both MS BASIC and TrueBASIC), as well as programs translated from Pascal into Modula 2 and from Fortran into Common Lisp, plus additional features described below. Included with each package is a license to use all those codes that are copyrighted on a single PC-compatible (under DOS, Microsoft Windows 3.1 or 95, or OS/2) computer, on a Macintosh-compatible computer, or on a UNIX computer.

A CD-ROM drive is of course necessary for the CD-ROM versions, and a Macintosh or UNIX computer must be compatible with ISO-9660 File Access. It takes too much time to use the computer's File Search facility to find by name one of the ca. 30000 files on a CD-ROM. Instead file searching is made feasible through HMTL index files that can be opened and viewed with a Web browser, such as Netscape Navigator or Microsoft Explorer. These index files then link directly to open and view the program chosen. Without a browser it is necessary to read the text versions of the index files or to search down through the folders/directories to find the desired program. This is not so difficult, despite the large number of files, because they are organized into folders/directories according to operating system, language, and purpose. It should be noted that the documentation for the programs in Common Lisp is provided as Postscript files, which can be viewed with Ghostscript, freeware that is available from the Web through access instructions included.

There is a wide variety of additional features. The CD-ROMs contain the complete SLATEC Mathematical Library, a comprehensive collection of over 1400 mathematical and statistical routines in Fortran. Other collections of programs in C are the files from the book *A Numerical Library in C for Scientists and Engineers* by H. T. Lau (CRC Press) and from the books *C Tools* and *More C Tools* by Louis Baker (McGraw-Hill). There are links to a large collection of numerical methods on the World-Wide Web, to the publisher (Cambridge University Press), and to a collection of "Murphy's Laws", all readily accessible with a Web browser. Also included are the relevant licensing information and a small number of troubleshooting tips. Inexplicably, the CD-ROMs include the complete works of William Shakespeare, in text versions and also in hypercard format for Macintosh, which requires decompression.

A useful feature that takes advantage of the storage capacity of a CD-ROM is a set of 20 files, each with 1.7 million (2^{24}) random bytes, readable with a program in C (which I do not have), along with a program for testing randomness. A colleague has verified that a bug in an earlier random number generator has been fixed.

For chemists and chemical physicists the most useful programs may be the ones in Fortran or C, which include an extensive set of routines for solution of linear algebraic equations, interpolation and extrapolation, integration of functions, evaluation of functions, special functions, random numbers, sorting, root finding and sets of nonlinear equations, minimization or maximization of functions, eigensystems, fast Fourier transform, Fourier and spectral applications, statistical description of data, modeling of data, integration of ordinary differential equations, two-point boundary value problems, integral equations, and partial differential equations. There is no program among the Numerical Recipes files for finding eigenvalues and eigenvectors of a general (nonsymmetric) matrix, but one is available in the SLATEC Library. Most of the algorithms are presented as subroutines associated with a driver program that provides an example of how the algorithm can be used. It is very helpful to have a pattern that can be adapted.

Once found, a program must be compiled before it can be executed, but no compiler for any language is provided with this collection. To compile, the program must be opened, copied, and pasted into an edit document of the compiler, or else copied onto the working computer disk and opened under the edit routine. I was unable to compile directly from the CD-ROM, but this may be a quirk of my compiler. Anyway, it is usually necessary to edit a program before compiling, and of course it is not permissible to write changes to the CD.

All of the Fortran 77 programs that I tested on my Macintosh Quadra 630 worked well. Among these were the following: fitting a function to a polynomial, finding roots of nonlinear equations, numerical integration by Simpson's Rule, power-series expansion, evaluation of the exponential integral and of factorial, solution of simultaneous equations by Gaussian elimination, and Runge−Kutta integration of a system of ordinary differential equations. Adapting them to my computer was not always easy. The compiler that I used was Absoft MS Fortran, Version 2.2, dating from 1986, and I had difficulties with input/output, with transferring numerical arguments to function subroutines, and with transferring array parameters to subroutines. Such difficulties were not always easy to overcome, since it was necessary to trace the course of the program, locate the source of difficulty, and edit the program to include a remedy.

The book that accompanied the package was useless in the absence of a Fortran 90 compiler. The advantage of the Fortran 90 modernization is that it gains from parallel programming, which is particularly applicable to the handling of arrays (vectors, matrices). The book compares the Fortran 90 version to the Fortran 77 one but cannot be used alone. Instead it is essential to consult either the first (1986) or second (1992) edition of *Numerical Recipes in FORTRAN: The Art of Scientific Computing*, by the same authors and publisher. This is an excellent description of the programs, of how they work, and of when and how to use them. Comparable books are available for the program in C, in BASIC, and in Pascal, which were adapted from the original ones in Fortran.

Floating-point calculations are performed at 32-bit single precision, or with a roundoff error of ca. 1 part in 10^8. Double-precision arithmetic is possible, but programs must be edited to convert all floating-point variables, including the constants. There are instructions for conversion of Fortran programs in the accompanying book, and there is a utility file that serves as a tool to facilitate the conversions, but I did not attempt it. The instructions for its use are buried in a help file that had been included with the original diskette version and that is designated as having little applicability to the CD-ROM version.

In summary, this is an immense but accessible compilation of programs for carrying out a wide range of computations, probably far more than most chemists or chemical physicists will ever need. It will never be as popular as the molecular-orbital or molecular-mechanics packages that have become so useful to chemists. Nor does it have the versatility of the Mathematica software. Moreover, I would judge that the major impediment to its use is that there is very little on-line instruction.

CD-ROM with Windows, DOS, or Macintosh single screen license $89.95 + shipping; CD-ROM with UNIX single screen license $149.95 + shipping; Fortran 90 and Fortran 77 Diskette (IBM, 3-1/2 inch/1.44M) $39.95 + shipping; book *Numerical Recipes in Fortran 90: The Art of Parallel Scientific Computing* $44.95 + shipping.

Charles L. Perrin, *University of California at San Diego*

JA965936F

S0002-7863(96)05936-7