NUMERICAL EVALUATION OF SPECIAL FUNCTIONS

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ABSTRACT. Higher transcendental functions continue to play varied and important roles in investigations by engineers, mathematicians, scientists and statisticians. The purpose of this paper is to assist in locating useful approximations and software for the numerical generation of these functions, and to offer some suggestions for future developments in this field.

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Preface

The article printed in this report will appear in Walter Gautschi (ed.), *Mathematics of Computation 1943–1993: A Half-Century of Computational Mathematics*, Proceedings of Symposia in Applied Mathematics, American Mathematical Society, Providence, Rhode Island 02940. This report is intended for limited distribution only until the primary publication appears in print.

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Additional copies of this report have been made for distribution to Digital Library of Mathematical Functions Project Participants (editors, associate editors, authors, validators, and support staff). No changes have been made in the body of the report. The exact bibliographic reference for the published article is [LO94]. A revision is in preparation and will be provided to DLMF Project Participants when ready. It will include references that have appeared in the literature since 1993.

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This report has been updated through 1999, resulting in an approximate 15% increase in the number of references and a modest expansion of the classification scheme in §4 and §5. The software packages, libraries and systems, described in §3 and cross-referenced in §4 and §5, were re-examined. Maple and Mathematica (§3.4.3 and §3.4.5) were found to have added considerable support for special functions, and three new libraries (§3.2.1, §3.2.3 and §3.3.3) were included. For the Web version, see http://math.nist.gov/nesf.

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1. Introduction

When automatic computers began to appear in the 1950s various confident, and often incorrect, predictions were made concerning the impact of these devices on applied mathematics, science and engineering. One of these predictions was that the need for special functions, or higher transcendental functions (as they are also known), would disappear entirely. This was based on the observation that the main use of these functions in those days was to approximate the solutions of classical partial differential equations: with automatic computers it would become possible to solve these equations by direct numerical methods. This observation is indeed correct; nevertheless, a perusal of current computational journals in the sciences reveals a persistent need for numerical algorithms to generate Airy functions, Bessel functions, Coulomb wave functions, error functions and exponential integrals—to name but a few of the classical special functions. Equally significantly, the National Bureau of Standards' Handbook of Mathematical Functions [AS64][1] continues to be one of the best-selling mathematical books of all time[2].

The purpose of the present paper is to provide some assistance to those mathematicians, engineers, scientists, and statisticians who discover that they need to generate numerical values of the special functions in the course of solving their problems. "Generate" is the operative word here: we are thinking primarily of either software or numerical approximations that can be programmed fairly easily. Numerical tables are not covered in this survey. Furthermore, for the most part we shall concentrate on the functions themselves; only in certain cases do we include, for example, zeros, inverse functions or indefinite integrals. Elementary functions, also, are excluded[3]. Lastly, we believe that the majority of readers would prefer us to emphasize the more useful algorithms rather than make an attempt to be encyclopedic: algorithms or approximations that have clearly been superseded are omitted.

We identify three stages in the development of computational procedures for the special functions:

1. Derivation of relevant mathematical properties.
2. Development of numerical approximations and algorithms.
3. Construction and testing of robust software.

Included in Stage (i) are asymptotic expansions, continued fractions, difference and differential equations, functional identities, integral representations, and Taylor-series expansions. Included in Stage (ii) are expansions in series of Chebyshev polynomials ("Chebyshev series"), minimax polynomial and rational approximations, Padé approximations, numerical quadrature, and numerical solution of difference and differential equations. **In this paper the emphasis will be on Stages (ii) and (iii), but in §2 we supply some general references for Stage (i).**

[1] An explanation of the scheme used for acronyms of references is given on p. 21.

[2] In 1988 the National Bureau of Standards became the National Institute of Standards and Technology.

[3] Methods for constructing and testing algorithms for generating elementary functions are surveyed in [CW80]. See also [Bai93, Bre76, Bre78a, Bre78b, Cod93a, LCY65, MY91, Smi89, Smi91, Ziv91].

In §3 we make a general survey of software libraries and packages[4] that include collections of special functions.

In §§4 and 5 the functions are treated individually. We list software that is already available and readily programmable numerical approximations. In §6 we also include references to articles (or books) that may be useful for the testing or comparison of existing software, or in the construction of new libraries. We do not attempt what would be a herculean task of testing and comparing everything that is available. Our philosophy in this survey has to be that of *caveat emptor*: no algorithm, approximation or package that we mention should be relied upon to produce accurate output in the absence of evidence of independent and systematic checks.

As in the progress of other branches of numerical analysis, procedures used to evaluate special functions are influenced heavily by the computing equipment available at the time. In the era of desk-calculating machines the medium was a printed table of numerical values of the wanted function, or functions, generally for equispaced values of the arguments. Nontabular values were calculated by means of Lagrange's interpolation formula or central-difference interpolation formulas [Fox56]. In other words, local polynomial approximations were employed. These interpolation procedures were reasonably successful for functions of a single variable, but two-dimensional interpolation on desk-calculating machines was often a laborious computation that was prone to error. The daunting task that faced a (human) computer is summed up in the following quotation from the Introduction to Karl Pearson's tables of the incomplete gamma function [Pea22]:

"As a matter of fact, supposing the use of a machine, which every modern computer has at his command, no interpolation suggested ought to take more than an hour's work and many much less. If the user of these tables groans under that hour, let him compute *de novo* a function value, say $I(6.86877, 47.1813)$ —including of course $\Gamma(48.1813)$—to seven-figure accuracy, and when he has completed the task, we believe his feelings towards those who have provided him with these tables will be very sensibly modified."

With electronic computers, the number of arithmetic operations that could be contemplated for the generation of a single function value increased considerably. In consequence, high-degree global approximations appeared for functions of a single variable in the form of minimax polynomial or rational approximations, or truncated Chebyshev-series expansions; see, for example, [Cle62, HCL$^+$68] and [Luk77b].

Chebyshev series in two dimensions also became feasible [CP66, Luk71a, Luk71b, Luk72a]. However, because of their more complicated asymptotic behavior, special functions of two variables cannot be covered comprehensively simply by use of polynomial or rational approximations or Chebyshev series. The situation is cloudier still when the variables or parameters are complex, or of course when they are more than two in number. For this reason, to achieve maximum speed, a comprehensive software package for generating a function of two (or more) variables typically employs several different algorithms in addition to, or quite commonly in place of, polynomial or rational approximations or Chebyshev series. The construction and testing of such a package invariably entails prodigious effort.

[4]Certain company products are identified in the text. In no case does such identification imply recommendation or endorsement by the National Institute of Standards and Technology, nor does it imply that the products are necessarily the best available for the purpose.

Computers continue to increase in sophistication and power; in consequence we should expect further changes in the algorithms used to generate the special functions. So far, the potential offered by the introduction of vector and parallel computing machines has not been exploited to any great extent. It might well lead to simplifications in the algorithms needed for many functions, as well as to an increase in execution speeds. We refer again to this possibility in the concluding section (§7).

In assembling the bibliography of this paper we have been assisted by the references collected and classified by the late Dr. L. W. Fullerton in his 1980 Bell Laboratories report [Ful80], by access to Dr. N. M. Temme's private collection of references, and by GAMS, the Guide to Available Mathematical Software prepared by the National Institute of Science and Technology [BHKS90]. Accessible at http://gams.nist.gov/, GAMS is a convenient, free source for documentation and nonproprietary source code.

We have searched through issues of the following journals of the past twenty-five years for relevant references:

Applied Statistics (Appl. Statist.), *Association for Computing Machinery Transactions on Mathematical Software* (ACM Trans. Math. Software), *BIT*, *Collected Algorithms from the Association for Computing Machinery* (CALGO), *Communications of the Association for Computing Machinery* (Comm. ACM), *Computer Physics Communications* (Comput. Phys. Comm.), *Computing*, *Journal of Computational and Applied Mathematics* (J. Comput. Appl. Math.), *Journal of Computational Physics* (J. Comput. Phys.), *Mathematical Reviews* (Math. Rev.), *Mathematics of Computation* (Math. Comp.), *Numerische Mathematik* (Numer. Math.), *U.S.S.R. Computational Mathematics and Mathematical Physics* (U.S.S.R. Comput. Math. and Math. Phys.)[5], *Zeitschrift für Angewandte Mathematik und Physik* (Z. Angew. Math. Phys.), *Zentralblatt für Mathematik und ihre Grenzgebiete* (Zbl.).

However, because of the sheer volume and diversity of publications on special functions it is almost inevitable that we have overlooked some useful algorithms and important articles. In this event we tender, in advance, our apologies to the authors.

2. Mathematical Developments

Comprehensive compendia of mathematical properties of the special functions are provided by the National Bureau of Standards' Handbook of Mathematical Functions [AS64], published originally in 1964, and the 3-volume set that resulted from the Bateman Manuscript Project [EMOT53a, EMOT53b, EMOT55], published in 1953 and 1955. These references employ the same notation for the special functions, and we shall follow them. The NBS Handbook has been reprinted many times by the U. S. Government Printing Office and has also been issued in whole, or in part, by other publishers including Dover Publications, Moscow Nauka, Verlag Harri Deutsch and Wiley-Interscience.

The forerunner of [AS64] is the book of Jahnke and Emde [JE45], published originally in 1909, and still in print[6]. It continues to be useful, especially for its collection of graphs. Other useful compendia include those of Magnus, Oberhettinger and Soni [MOS66], and (from the standpoint of hypergeometric functions)

[5] In 1991 this journal was retitled *Computational Mathematics and Mathematical Physics*.

[6] A more recent edition, with F. Lösch added as author [JEL60], is no longer in print.

Luke [Luk69a]. For an introductory compendium, see the recent "atlas" of Spanier and Oldham [SO87].

Books and articles that include descriptions or surveys of general methods for computing special functions include [Bre78b, DKK81, Gau75, HCL+68, Luk69b, Luk77b, PT84, PTVF92, Tem78, vdLT84].

Other books and articles that provide indepth coverage of pertinent topics include:

[Ask89, survey of compendia], [BG81a, BG81b, Padé approximations], [BH75, asymptotic approximations], [Bre91, continued fractions, Padé approximations], [BvI93, Padé approximations], [Cod70, polynomial and rational approximations], [Fik68, polynomial and rational approximations], [FP68, Chebyshev polynomials], [JT80, continued fractions], [Kar91, power series], [KG80, statistical computations], [Luk75, supplement to **AS64**—especially for functions of hypergeometric type], [Mor80, power series], [Olv74, asymptotic approximations], [Riv90, Chebyshev polynomials], [Tem77, integral representations], [Tem85, asymptotic approximations], [Wim84, recurrence relations], [Won89, asymptotic approximations].

3. Packages, Libraries and Systems

This section reviews a selection of mathematical software with respect to its support for the numerical evaluation of special functions[7]. In some cases only a descriptive overview is given while in others cross-references by individual function are given in the subsequent sections §4 and §5. The cross-referenced packages, libraries and systems are marked with a ♣. We used the following criteria in assigning the ♣ marks:

First, a marked item must be readily accessible. Often this means it is commercial software that is purchased or leased for a fee but we also include software that is distributed, usually over computer networks, by journals and research institutions.

Second, a marked item must have a significant following in North America. (In most cases the unmarked software is used widely elsewhere.)

Third, a marked item must be reasonably comprehensive in its coverage of special functions.

3.1. **Software Packages.**

In this paper *software package* will mean a set of subroutines, or just a single subroutine, that addresses a subfield of numerical mathematics. There are three important series of software packages that include special functions. These packages are research contributions written in a variety of programming languages.

3.1.1. ♣ *ACM Algorithms.*

These were published in the *Communications of the ACM*, Volumes 3–18 (1960–75) and since then in the *ACM Transactions on Mathematical Software* (*TOMS*). The transition between the two journals took place with Algorithm 493 in Volume 1, Number 2 of *TOMS*. Algol was required originally but Fortran and other languages were allowed after it became clear that this condition was too restrictive. The current ACM Algorithms Policy appears at http://www.acm.org/calgo/AlgPolicy.html; also see [Kro91]. The policy requires ACM Algorithms to be self-contained, adequately documented through comments

[7]General reviews of mathematical software appeared regularly from 1988 to 1994 in the Computers and Mathematics column of the *Notices of the American Mathematical Society*. An index is given in [DW95].

in the code, and reasonably portable from one machine to another. A test program with sample output is also required. The policy provides for addenda to previously published algorithms. All ACM Algorithms that appear in *TOMS* are refereed. The ACM Algorithms Policy has been in effect, with little change, since 1975.

ACM Algorithms are accessible at http://www.acm.org/calgo/. For indexing purposes, each is assigned a symbol from a modification of the SHARE classification system; cf. [ACM] or [ACM64]. Cumulative indexes by SHARE classification for 1960–1980, 1981–1986 and 1987–1988 appear in [ACM]. Algorithm 620 [Ham85, HM90b, RH84] provides a data base and Fortran program for preparing a cumulative index by SHARE classification. This data base is updated periodically by the ACM.

3.1.2. ♣ *AS Algorithms.* A section for statistical subroutines in *Applied Statistics* was established in 1968 to "encourage the development of a published literature on statistical computing" as the specialized needs of statistical computing were "only partly met" by the algorithm sections of other journals [AS68]. The current version of detailed instructions and other information for authors of AS Algorithms, first published in 1968, can be found in [RWGH87]. All submissions adhere to a standard format and are refereed. A test program is required for the referee's use. Addenda to previously published algorithms are accepted and are subjected to the same refereeing process as original algorithms. An index appears at the end of every volume. A cumulative index of the first 251 AS Algorithms (1968–1989, with addenda) appears in [HM90a], organized according to the GAMS scheme [BHK91]. Corrected and improved versions of selected AS Algorithms appear in [GH85]. Instructions for obtaining AS Algorithms on computer diskette can be found in issues of *Applied Statistics* starting in 1993.

3.1.3. ♣ *CPC Programs.* The journal *Computer Physics Communications* was begun in 1969 to "facilitate the exchange of physics programs and of relevant information about the use of computers in the physics community". It publishes descriptions of CPC Programs and, in addition, general papers on the computational aspects of physics and physical chemistry. Programs and their descriptions are refereed.

Program descriptions consist of a Program Summary (a concise description in a standard format with keywords) and a Long Write-Up (a detailed description of the underlying physics and algorithms). A test program is required for each CPC Program, and each CPC Program is required to be well documented and as portable and self-contained as possible. An index of CPC Programs is printed at the end of every volume. Two cumulative indexes without Program Summaries [CPC87, CPC90] and one with Program Summaries [CPC84] exist. A more attractive alternative is the up-to-date cumulative index, with Program Summaries, that is accessible by electronic mail[8]. All these indexes are organized according to a physics-oriented classification scheme.

CPC Programs can be ordered individually or by subscription service. Ordering instructions and an order form are printed in the back of every issue of *Computer Physics Communications.*

[8]To get started with the cumulative index, send the message "get cpc intro cpcindex" to `listral@earn-relay.ac.uk`, or see the instructions printed in every issue of *Computer Physics Communications.*

3.2. **Intermediate Libraries.** Under this heading we place software that is in some sense intermediate between software packages, which embody original research contributions, and comprehensive libraries (§3.3 below). The libraries we consider here provide support only for mathematical functions. Furthermore, they are largely restricted to codification of existing algorithms with all their advantages—and limitations.

3.2.1. ♣ *Atlas for Computing Mathematical Functions* [Tho97]. The purpose of this book with CD-ROM is to provide C or Fortran 90 source code for most of the functions included in the *NBS Handbook of Mathematical Functions* [AS64]. It claims "most of the functions are computed ... to an accuracy of at least 10 decimal digits." The functions are computed for real variables only.

3.2.2. ♣ *C Mathematical Function Handbook* [Bak92]. This volume with diskette is keyed to the *NBS Handbook of Mathematical Functions* [AS64]. Most chapters of the *NBS Handbook* have a counterpart here in which brief introductory material is followed by C code listings. A complex arithmetic package is included since C supports only real and integer arithmetic. The author advocates the use of C because it "is rapidly becoming the *lingua franca* of the computer world" and "algorithms written in C should be very portable". He has written two other books on C programming for technical applications.

3.2.3. ♣ *Computation of Special Functions* [ZJ96]. This book with included diskette provides Fortran 77 code for most of the functions in the *NBS Handbook of Mathematical Functions* [AS64]. For many of the functions, codes are supplied for complex as well as real arguments. In some cases complex parameters are supported also.

3.2.4. ♣ *Mathematical Function Library for Microsoft Fortran or C* [ULI90]. These volumes exist to "provide users with a comprehensive set of mathematical function routines to assist them in solving their mathematical problems on IBM PC/XT/AT or compatibles." Each consists of a looseleaf manual with diskettes. The documentation for each function gives usage instructions, input range, accuracy, definition of the function, algorithm, sample program and sample results. The functions are evaluated only for real arguments. The diskettes contain a compiled library in microprocessor assembly code for use with Microsoft compilers and the Fortran or C source code for use with other compilers.

3.2.5. ♣ *Methods and Programs for Mathematical Functions* [Mos89]. This volume with separate diskette of C programs presents a selection of special functions with real arguments and integer or real parameters. The programs are designed for double precision, and tables of test results included for every function typically show absolute or relative errors (whichever is appropriate) of the order of 10^{-16}. Where polynomial or rational approximations are used, the expansion coefficients were generated in multiple precision using C programs that are given in the book. The programs have been collected under the heading "cephes" and are downloadable free-of-charge from Netlib; see http://gams.nist.gov/serve.cgi/Package/CEPHES/.

3.3. **Comprehensive Libraries.** When new algorithms are developed they tend to appear first as subroutines in software packages (§3.1 above). Later they may be assimilated into more complete software products such as intermediate libraries (§3.2 above). Even more useful are *comprehensive libraries* that integrate evaluation of special functions with other essential elements of numerical computing and offer

additional advantages such as uniform documentation, style of usage, and handling of error conditions. Corrections and improvements, particularly in orienting the programming toward particular computer architectures, are often made.

3.3.1. *CERN Library.* The European Laboratory for Particle Physics maintains a comprehensive software library [CER93], mostly in Fortran but with a few routines in assembly language, in support of high-energy physics research. The coverage of special functions includes the error function of real and complex argument; the Dawson and Fresnel integrals; exponential, sine, cosine and arctangent integrals; the gamma and digamma functions of real and complex argument; incomplete gamma function; real dilogarithm and complex generalized polylogarithms; Bessel functions of real argument and orders 0, $\pm\frac{1}{4}$, $\pm\frac{1}{3}$, $\pm\frac{1}{2}$, $\pm\frac{2}{3}$, $\pm\frac{3}{4}$ and 1; Bessel functions of real order and real or complex argument; Bessel functions of complex order and argument; zeros of the Bessel functions J and Y and of their derivatives; Coulomb wave functions of complex order, argument and parameter; complete and incomplete elliptic integrals; Jacobi's elliptic functions (real and complex); Jacobi's theta functions (real); Bose-Einstein and Fermi-Dirac integrals ; Legendre and associated Legendre functions; conical functions of the first kind; Struve functions. The library is distributed, with some restrictions, to organizations outside CERN.

3.3.2. ♣ *IMSL Library.* International Mathematical and Statistical Libraries was incorporated in 1970 "with the intent of providing high-quality, supported Fortran subroutine libraries in mathematics and statistics" [Air84]. In its first ten years it produced libraries tailored to twelve different computer lines, providing an alternative to manufacturer-supplied libraries. Currently the company offers a wide range of products for large-scale scientific computing. At the center of its product line is the IMSL numerical subroutine library for mathematics and statistics, which includes an extensive coverage of real and complex special functions [IMS91] ; this reference includes a GAMS index [BHK91] and a KWIC (keyword in context) index. The library is optimized, vectorized and parallelized where appropriate, depending on the target computer architecture, but it contains no vector or parallel support for special functions.

A subset of the IMSL library is offered also as a C library. This is an essential component of a powerful interactive system (§3.4 below) which has the capability of providing graphical and numerical computing with very large data sets. Optionally, Maple (§3.4.3 below) can be incorporated to provide for symbolic computing.

3.3.3. ♣ *Mathematical Software for the P.C. and Work Stations* [WNO94]. This book describes a library for scientific computing that was developed originally more than 30 years ago in Japan. It has become a standard component of computer centers in Japanese universities and remains important because its developers have continually provided modifications to keep abreast of advances in computers and numerical analysis. Its coverage of special functions includes Bessel, gamma, incomplete gamma and error functions; exponential, Fresnel and complete elliptic integrals; and classical orthogonal polynomials. The Bessel and gamma functions are supported for complex as well as real arguments. The library routines are provided on a diskette that comes with the book.

3.3.4. ♣ *NAG Library.* An overview of the development, structure and contents of the NAG Fortran library [NAG99] is given in [FP84]. After originating as a

cooperative project among several British computing centers in 1970 with the purpose of providing "a balanced, general-purpose numerical algorithms library," the Numerical Algorithms Group formed a not-for-profit company in 1976 to provide for the wider distribution of the library. The library is organized around the ACM modification of the SHARE classification system (see §3.1.1 above) and is available for a wide cross-section of computing systems. A KWIC (keyword in context) index and an index in the GAMS classification scheme [BHK91] are provided in the library documentation.

Subsets of the full library are available in Ada, Algol 68, C, Fortran 90 and Pascal. NAG is actively developing and marketing an interactive system (§3.4 below) that integrates most of the numerical power of the full NAG library with online symbolic and graphical capabilities.

3.3.5. *NSWC Library.* In 1976 the Naval Surface Warfare Center, Dahlgren, Virginia, began development of "a [Fortran] library of general purpose subroutines that would provide a basic computational ability in a variety of mathematical activities" [Mor93]. The design goals stressed reliability, transportability, efficiency, ease of use, and generality. In 1993 the library contained 576 user-level subroutines, including ones in real arithmetic for the error function and its inverse; Dawson's integral and Fresnel integrals; exponential, sine and cosine integrals; gamma, psi and polygamma functions; dilogarithm; incomplete gamma function and its inverse; incomplete beta function; complete and incomplete elliptic integrals; Jacobi's and Weierstrass' elliptic functions; Bessel functions of real argument and order. It also contained Airy functions and complete elliptic integrals of complex argument, and Bessel functions of complex argument and integer or complex order.

3.3.6. *NUMAL Library.* In 1973 the Mathematisch Centrum, Amsterdam, introduced this library of numerical procedures in Algol-60 with " the aim ... to provide Algol-60 programmers with a high-level numerical library which contains a set of validated numerical procedures together with supporting documentation" [Hem81]. In 1979 it contained approximately 430 subroutines, including ones for the exponential, sine and cosine integrals; gamma function; incomplete gamma and beta functions; error and inverse error functions; Fresnel integrals; modified and unmodified Bessel functions of integer, half-integer or real order; Airy functions. All subroutines are for real variables.

3.3.7. ♣ *Numerical Recipes.* This partly pedagogical series of books offers "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" [PTVF92]. Besides being listed fully in the text, the computer routines are available for purchase under a variety of licensing arrangements, one of which is tailored to the needs of classroom instructors. Example books with test programs and diskettes are available also. Standard fields of numerical computation are covered, with approximation of functions and evaluation of special functions included. Except for the hypergeometric function, the software applies to real variables only. The book is published in four versions with the software coded in Basic, C, Fortran or Pascal; another volume for Basic is [Spr91].

3.3.8. *NUMPAC Library.* The Nagoya University Mathematical Package is used widely in Japan. It is a comprehensive Fortran library oriented toward Japanese computers, including vector supercomputers. Coverage includes Airy functions; error and inverse error functions; Dawson and Fresnel integrals; exponential, sine and cosine integrals; complex gamma function; digamma function; dilogarithm; Riemann's zeta function; Bessel functions of integer or real order and real or complex argument; zeros and integrals of Bessel functions; complete and incomplete elliptic integrals; Jacobi's elliptic functions; incomplete beta and gamma functions; Legendre polynomials and associated Legendre functions; classical orthogonal polynomials; Struve functions; Abramowitz, Debye and elliptic theta functions; solutions of the Blasius and Thomas-Fermi equations. Information can be obtained in Japanese and partially in English at http://numpac.fuis.fukui-u.ac.jp/.

3.3.9. *PORT Library.* This library [FHS78b, Fox84] is mentioned here because it provides a framework [FHS78a] for constructing portable Fortran libraries that has proven its utility. The framework supplies computer arithmetic parameters via Fortran function calls. Algorithms are coded so as to be valid for a range of values of the arithmetic parameters; actual values are substituted at run time. The PORT framework is used, for example, in the SLATEC library (§3.3.10 below). It is particularly valuable in the special function routines because of their sensitivity to precision, underflow and overflow. The PORT framework is available as ACM Algorithm 528 (§3.1.1 above).

3.3.10. *Scientific Desk Library.* C. Abaci offers the following products: (i) the Scientific Desk Library, a Fortran-based collection of numerical software; (ii) the Scientific Desk Analysis System, an interactive system (§3.4 below); (iii) software produced by others, including the ACM algorithms (§3.1.1 above). The library is available in object code for personal computers under a variety of Fortran compilers and in Fortran source code for other computers. The Analysis System, which is strongly oriented toward statistics, simplifies the programming burden and provides for simple graphical output. C. Abaci distributes the SPECFUN collection [Cod93b] of Fortran programs for special functions and the ELEFUNT, INTFUNT and CELEFUNT tests [Cod93a, CW80] for elementary functions. Inquire at *C. Abaci, Inc., P. O. Box 2626, Raleigh, NC 27602.*

3.3.11. ♣ *SLATEC Library.* The acronym stands for Sandia, Los Alamos, Air Force Weapons Laboratory Technical Exchange Committee[9], formed in 1974 to "foster the exchange of technical information among the three computing departments". In 1977 a subcommittee undertook the development of a complete, noncommercial Fortran library for numerical supercomputing [Buz84]. The primary motivation was that the suppliers of commercial libraries regarded the supercomputing market as too small. The library subcommittee admitted subsequently five additional U. S. Government agencies (the Lawrence Livermore, Oak Ridge and Sandia Livermore National Laboratories, the National Energy Supercomputer Center at Lawrence Livermore, and the National Institute of Standards and Technology). SLATEC Version 1.0 appeared in 1981. Version 4.0, the third major revision and expansion, was released in December 1992. The initial coverage of special functions coincided with FNLIB [Ful77], FUNPACK [Cod75, Cod84a] and AMOSLIB [AD79]. Subroutines from [ADW77a, ADW77b, Amo80a, Amo83a, Amo83b, Amo86, CN81, LS81, OS83]

[9]The Air Force Weapons Laboratory has been renamed the Phillips Laboratory.

were added later. Available from *Energy Science and Technology Center, P. O. Box 1020, Oak Ridge, TN 37831* and from http://gams.nist.gov/.

3.4. **Interactive Systems.** The software packages and libraries considered in the preceding three sections are used in conjunction with standard programming languages. These languages are not fully interactive. A program needs to be written, compiled and linked to libraries before it can be executed, and after the results are examined the cycle may need to be repeated to correct errors or change parameters. An *interactive system* provides a powerful set of commands which the user can enter at the keyboard. The response to each command is displayed immediately. The burden of programming and the compile-link-execute cycle is reduced. Programming in an interactive system serves a new purpose: to extend or customize the command set.

A striking characteristic of interactive systems is their ability to integrate nonnumerical tasks with numerical computation. Graphical and symbolic computing work best in an interactive environment, and one or both are combined powerfully with numerical computing in commercially available interactive systems. The trend toward increased integration of these computational components is being recognized by recent developments of the IMSL, NAG and Scientific Desk libraries (§§3.3.2, 3.3.4 and 3.3.10 above).

A particular type of interactive system with a special capability for the numerical evaluation of special functions is the *computer algebra system*, developed to provide symbolic processing of mathematical formulas and intended, primarily, to assist in mathematical developments. These systems contain basic mathematical information that enables them to manipulate algebraic expressions, make substitutions, differentiate and integrate functions, solve algebraic, transcendental and differential equations, manipulate power series, and the like. Some knowledge of mathematical properties of special functions is built in, and more can be added by programming extensions to the command set. Numerical approximations are to be avoided, in keeping with the primary purpose of supporting exact mathematical developments, but floating-point computation is provided as a secondary capability. This often comes with a bonus when compared to the usual programming languages which simply use the hardware computer arithmetic: the precision can be set arbitrarily.

The rationale for arbitrary precision is not entirely clear. It is clear that exact rational arithmetic is essential in computer algebra applications. Perhaps multiple-precision floating-point, being relatively easy to implement, is considered a worthwhile additional capability. Also, evaluation of symbolic expressions may require high precision because of numerical sensitivity. Whatever the reason, for occasional usage of arbitrary-precision floating-point, computer algebra systems are well worth considering.

3.4.1. *HiQ* (*Apple Macintosh, Sun*). This system [Bim93] approaches the goal of reducing the need to write programs by making concentrated use of the graphical user interface (the image displays and controls associated with the computer screen). The system opens with a blank worksheet (in a window on the screen) and an array of icons. Each icon corresponds to a particular kind of task.

For example, one icon is called the "expression evaluator". When activated by the mouse, this icon presents a window with three areas. An algebraic expression is entered into the input area in a conventional programming-language syntax (like Fortran). This expression can contain numbers, symbols representing numbers, and

symbols representing built-in HiQ functions. The symbols representing numbers are assigned numerical values in the options area as constants or finite arithmetical sequences. Output icons are generated in the output area when the "run button" (another icon) is "pushed" by clicking the mouse. The output icons, when activated, display tables and graphs of the computed data.

Other tasks that can be performed by similar sequences of manipulations with icons are numerical integration, optimization, data fitting, finding roots of polynomials and nonlinear functions of one variable, and solving nonlinear systems, integral equations, and initial-value and boundary-value problems in ordinary differential equations.

Special functions included in HiQ are Airy functions; beta, gamma, log gamma, psi, incomplete beta, incomplete gamma, and complementary incomplete gamma functions; Kelvin functions; Bessel functions of integer and half-integer order; Struve and Weber parabolic cylinder functions; hypergeometric function and series; confluent hypergeometric function and series; Riemann zeta function. Although HiQ performs complex arithmetic, most if not all the special functions are evaluated for real arguments only.

3.4.2. *Macsyma.* Macsyma [Sym92] is a computer algebra system that supports symbolic, graphical and numerical computing on personal computers, scientific workstations and mainframes. Its built-in capabilities can be extended by programming in either Lisp or an Algol-like procedural language.

Macsyma avoids numerical approximations unless floating-point numbers are introduced, either explicitly or as the result of special commands. Floating-point numbers are represented internally in machine single precision, machine double precision, or software arbitrary precision. When arbitrary precision is being used there is a precision specifier. Operand precisions are adjusted, if necessary, to the specified operational precision by truncating or extending with zero digits before arithmetic operations are performed. The precision specifier can be changed at any time.

Macsyma supports the numerical evaluation of elliptic, error, gamma, polygamma, polylogarithmic and zeta functions; Airy, Bessel and Legendre functions; complete elliptic integrals and the exponential integral; classical orthogonal polynomials. Only the gamma, polygamma and Riemann zeta functions are computable in arbitrary precision. Some of the other functions are restricted to single precision. Complex arguments are allowed for the error, gamma and Bessel functions.

3.4.3. ♣ *Maple.* Maple 6 is a computer algebra system containing symbolic, numerical and graphical capabilities; see http://www.maplesoft.com/. It contains extensive support for special functions, and is available for personal computers, Unix workstations and vector supercomputers. The normal mode of operation is interactive. A Pascal-like programming language, called the Maple language, is provided also. Much of the Maple system is programmed in this language. This part, called the Maple Library, can be viewed on the screen or printed, and serves as useful supplementary documentation or as a guide for the preparation of additional library modules. The core of Maple, written in the C programming language, is not normally accessible to users.

Because of its emphasis on symbolic computing, Maple avoids any evaluation which would introduce an inexact result unless the user specifically requests it. Expressions are evaluated symbolically, with numbers rendered as rational fractions

with arbitrarily long numerators and denominators or represented as symbols. The user can request floating-point evaluation to arbitrary precision. For mathematical functions, Maple detects certain special values and can make appropriate substitutions. Otherwise the functions are left as symbolic representations until the user explicitly requests their evaluation in floating-point format. These evaluations, if they can be done at all, are to the precision specified by the user.

3.4.4. *Mathcad* (*PC with Microsoft Windows*). This system [Mat93a] is oriented toward the engineering professions but is useful also in educational, mathematical, scientific and statistical applications. Mathcad can be regarded as an editor and calculator that can be used to create complete documents. These documents can include graphics, ordinary text, and mathematical text resulting from input commands and their associated numerical or symbolic output. Commands are selected from an extensive array of icons (similar to HiQ, §3.4.1 above) or they can be activated by appropriate keystrokes. Numerical commands support real and complex computations with scalars, vectors and matrices; numerical differentiation and integration ; solution of algebraic equations; constrained and unconstrained minimization; Fourier transforms; statistical operations. Symbolic commands are supported by a subset of Maple (§3.4.3 above). Coverage of special functions includes error, gamma and polylogarithmic functions; sine, cosine and Fresnel integrals; Bessel functions of integer order. Except for the gamma function, all arguments must be real.

3.4.5. ♣ *Mathematica.* Mathematica [Wol99] is a computer algebra system for symbolic, graphical and numerical computing on personal computers, scientific workstations, and larger computers. It has extensive support for special functions. A highly developed user interface, available on some of this hardware, integrates Mathematica output with ordinary text for the preparation of complete documents entirely within the Mathematica system. A programming language, based on pattern matching, is included and can be used for extending the capabilities of the system.

As with other computer algebra systems, Mathematica uses floating-point numbers only when requested explicitly. If numbers are introduced with no more significant figures than the precision of the machine floating-point system, and if the machine underflow and overflow limits are not exceeded, then computations proceed in hardware floating-point arithmetic. On the other hand, numbers that are not machine-representable are stored in a software floating-point format. Each such number is tagged with its own precision, and computations are performed in software floating-point arithmetic. The precision of nonmachine numbers is arbitrary but the internal representation is set to the highest justifiable precision. This is determined by the number of significant figures in an input number and by the precision of the operands or arguments in arithmetic operations and function evaluations. If numbers in a hardware computation underflow or overflow, then the software arithmetic takes over automatically.

3.4.6. *Matlab.* This system [Mat92] uses matrix notation to provide a built-in set of commands for standard algorithms of numerical computation. A graphics capability is included also. Additional commands can be coded in concise procedures using Matlab notation. Symbolic computing is supported through a recently introduced option using Maple (§3.4.3 above). Matlab runs on a broad range of computers from personal computers and scientific workstations to vector supercomputers. One

of its strengths is that it treats complex arithmetic as the natural extension of real arithmetic: variables do not have a fixed real or complex type as in Fortran. Nevertheless, Matlab's coverage of complex functions is limited. It supports Bessel functions of real order and complex argument z but warns in the online help system that the functions "may produce inaccurate results" for large order and $|z|$. Built-in special functions for real arguments and parameters include error and inverse error functions; gamma function; incomplete gamma and beta functions; Bessel functions I, J, K and Y; complete elliptic integrals; Jacobi's elliptic functions.

4. Functions of One Variable

In the references that follow an indication is made of the programming language where applicable. Also, special note is made of references that include surveys. Libraries and interactive systems are listed separately.

In the subsections of §4 and §5, a library or interactive system is listed only if it employs an algorithm tailored to the restrictions of the subsection. For example, NAG is listed in §4.1.1 and §4.1.2 because it has separate capabilities for Airy functions of real and complex argument. Mathematica is listed only in §4.1.2 because it does not use a restricted algorithm for real arguments. Because these distinctions are sometimes difficult to infer from software documentation and even, when available, from source code, they should be regarded only as a guide, both in §4 and §5.

4.1. **Airy Functions.** This section includes Scorer's functions.

4.1.1. *Real Arguments.* [Mac94a], [Mac96a, Fortran], [Ném92], [Pri75, Fortran], [RS81]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**.

4.1.2. *Complex Arguments.* [Amo86, Fortran], [CJR92, Fortran]. Libraries: **NAG**, **SLATEC**. Systems: **Maple**, **Mathematica**.

4.1.3. *Articles.* [CCF83], [Gor69], [Lee80], [LO93], [Moo81], [SAG79], [VRZG96].

4.2. **Error Functions, Dawson's Integral, Fresnel Integrals, Goodwin-Staton Integral.**

4.2.1. *Error Functions of Real Argument.* [Ada69, Algol], [Cle62], [CMW63, Algol], [Cod69], [Cod90a, Fortran], [CT85, Fortran], [Hil73, Fortran], [Luk69b], [Luk75], [Ném92], [Sch78], [SL81], [SZ70, Fortran], [Tem94b, Pascal]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**.

4.2.2. *Inverse Error Functions of Real Argument.* [BEJ76], [Cun69, Fortran], [HD73, Algol]. Libraries: [Mos89], [ULI90], [WNO94], **IMSL**, **NAG**.

4.2.3. *Integrals of the Error Function.* [Gau77a, Fortran], [Woo67]. Libraries: [Bak92]. Systems: **Maple**.

4.2.4. *Dawson's Integral of Real Argument.* [CPT70], [Hum64], [Let97], [Ném92], [Ryb89, Fortran]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**.

4.2.5. *Fresnel Integrals of Real Argument.* [Bul67, Algol], [Boe60], [Cod68], [Hea85], [LG64, Algol], [Luk69b], [Luk75], [Ném65], [Sny93, Fortran]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**.

4.2.6. *Complex Arguments.* [Gau69a, Algol], [Luk69b], [Lyn93, Fortran], [PW90a, Fortran], [SZ81, Fortran]. Libraries: [Bak92], [ZJ96], **IMSL**, **NAG**. Systems: **Maple**, **Mathematica**.

4.2.7. *Goodwin-Staton Integral.* [Mac96a, Fortran].

4.2.8. *Articles.* [BR71], [Cod90b, includes survey], [Col87a], [Fle68], [Gau70], [Gau77b], [Hen79], [HR72], [Let98], [LW90], [LW91], [McC74], [Mor83], [MR71], [PW90b], [Str68], [vdLT84], [Wei94a, includes survey], [Wei94b].

4.3. Exponential Integrals, Logarithmic Integral, Sine and Cosine Integrals.

4.3.1. *Exponential Integrals of Real Argument.* [Amo80a, Fortran], [Cle62], [CMW63, Algol], [CT69], [Gau73, Algol], [Luk69b], [Luk76], [Pac70, Fortran], [SZ76, Fortran]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**.

4.3.2. *Logarithmic Integral of Real Argument.* Libraries: [Bak92], [Tho97], [ULI90], **IMSL**, **SLATEC**. Systems: **Maple**.

4.3.3. *Sine and Cosine Integrals and Hyperbolic Sine and Cosine Integrals of Real Argument.* [Bul67, Algol], [Luk69b], [Mac96b, Fortran]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**.

4.3.4. *Complex Arguments.* [Amo90a, Fortran], [Luk69b]. Libraries: [Bak92], [ZJ96]. Systems: **Maple**, **Mathematica**.

4.3.5. *Articles.* [Amo80b], [Amo90b], [CT68], [TM68], [vdLT84].

4.4. Gamma, Psi, and Polygamma Functions.

4.4.1. *Gamma Function of Real Argument.* [BZ92], [CH67], [Cle62], [CMW63, Algol], [CT85, Fortran], [FS67, Algol], [Luk69b], [Luk75], [Mac89, Fortran], [Ném92], [Tem94b, Pascal]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**.

4.4.2. *Psi and Polygamma Functions of Real Argument.* [Amo83b, Fortran], [Bow84, Fortran], [CST73], [Luk69b], [Luk75]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [ZJ96], **IMSL**, **NAG**, **SLATEC**.

4.4.3. *Complex Arguments.* [BD80, Fortran], [Köl72a, Fortran], [Kon96, C], [Kuk72a, Fortran], [Luk69b]. Libraries: [Bak92], [WNO94], [ZJ96], **IMSL**, **SLATEC**. Systems: **Maple**, **Mathematica**.

4.4.4. *Articles.* [AB87b], [Bri95], [Cha80], [Cod91, includes survey], [FW80], [Kat78], [Krä90], [Kuk72b], [Luk70a], [McC81], [Ng75, includes survey], [Spo94], [vdLT84].

4.5. Landau Density and Distribution Functions.

4.5.1. *Real Variables.* [KS84d, Fortran], [Sch74, Fortran].

4.6. Polylogarithms, Clausen Integral.

4.6.1. *Dilogarithms.* [GZ75, Fortran], [Luk75]. Libraries: [Bak92], [Mos89], [Tho97], **IMSL**, **SLATEC**. Systems: **Maple**.

4.6.2. *Higher Polylogarithms.* Libraries: [Bak92], [Tho97]. Systems: **Maple**, **Mathematica**.

4.6.3. *Clausen Integral.* [Köl95], [Mac96a, Fortran]. Libraries: [Tho97].

4.6.4. *Articles.* [GT81], [JL72], [Mor79], [OPP95].

4.7. **Zeta Function.**

4.7.1. *Real Arguments.* [CHT71], [Luk69b], [Mar65, Algol], [PB72]. Libraries: [Bak92], [Mos89], [Tho97].

4.7.2. *Complex Arguments.* [BD80, Fortran], [YKK88, Fortran]. Systems: **Maple**, **Mathematica**.

4.7.3. *Articles.* [AB89], [EKK85], [Ker80, includes survey].

4.8. **Additional Functions of One Variable.**

4.8.1. *Lambert Function (W–Function).* [BBC95, Fortran]. Systems: **Maple**, **Mathematica**.

4.8.2. *Articles.* [BCB95].

5. Functions of Two or More Variables

As in §4, an indication is made of the programming language where applicable and special note is made of references that include surveys. Libraries and interactive systems are listed separately, and similar remarks apply about the inclusiveness of the subsections.

5.1. **Bessel Functions.** All of the following subsections apply to the ordinary Bessel functions (J and Y) and the modified Bessel functions (I and K).

5.1.1. *Orders 0 and 1, Real Arguments.* [Bla74], [BS92, Fortran], [Cle62], [Hil81, Fortran], [Luk69b], [Luk75], [WBR82]. Libraries: [Bak92], [Mos89], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**.

5.1.2. *Integer or Half-Integer Orders, Real Arguments.* This subsection includes spherical Bessel functions. [AM61], [AM78, Fortran], [BZ95, Fortran], [Col80, Fortran], [Hil81, Fortran], [MM90], [PB82], [RF93, Fortran], [SFR97, Fortran]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **Numerical Recipes**.

5.1.3. *Real Orders, Real Arguments.* [ADW77a, Fortran], [Bar82b, Fortran], [Cam79, Fortran], [Cod83, Fortran], [CP66], [Luk69b], [Luk71a], [Luk71b], [Luk72a], [Luk75], [Mat93b, Fortran], [Ném92], [Pie84b, Fortran], [Tem75, Algol], [Tem76, Algol]. Libraries: [Mos89], [ULI90], [WNO94], [ZJ96], **IMSL**, **Numerical Recipes**, **SLATEC**.

5.1.4. *Integer or Half-Integer Orders, Complex Arguments.* This subsection includes Kelvin functions. [BKN88a, Fortran], [BKN88b, Fortran], [Bur63], [CM83], [dT93], [Mas83, Fortran], [Ném92]. Libraries: [Bak92], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**.

5.1.5. *Imaginary Orders, Real Arguments.* [PA99].

5.1.6. *Real Orders, Complex Arguments.* This subsection includes Hankel functions. [Amo86, Fortran], [Cam81, Fortran], [Luk69b], [Luk75], [TB87, Fortran]. Libraries: [ZJ96], **IMSL**, **NAG**, **SLATEC**.

5.1.7. *Complex Orders, Complex Arguments.* [TB85, Fortran]. Systems: **Maple**, **Mathematica**.

5.1.8. *Integrals of Bessel Functions.* [Amo83a, Fortran], [And82a, Fortran], [BEJ78], [Cha83, Fortran], [Feu91, Fortran], [GP64], [Lem97, Fortran], [Mac96a, Fortran], [Ném92], [PB84, Fortran], [Pie82, Fortran], [SZ79, Fortran], [Tal83, Fortran], [Wie99, Fortran]. Libraries: [Bak92], [ZJ96], **SLATEC**.

5.1.9. *Zeros of Bessel Functions.* [Cam84, Fortran], [KRVZ98, Fortran], [Let96], [Ném92], [Pie84a], [Pie90, Fortran], [Tem79, Algol], [VRS+95, Fortran]. Libraries: [Bak92], [ZJ96].

5.1.10. *Articles—Functions.* [Ach86], [ADW77b], [Amo74], [Bar81a], [BGV93], [BL96], [Cam80], [CF87], [CMF77], [Cod80, includes survey], [Col87b], [CS89, includes survey], [Gau91b], [GB87], [GS78], [Hit68], [Jab94], [KS84b], [Luk72b], [Luk77b], [Mac94b], [Mat93b], [Nes84], [OS72], [Rem73], [SJ96], [TB86], [VGK+91], [Wal84], [WC90], [WFQ92], [YM97], [YN74], [Yos92], [ZB95], [ZB97], [Zha95], [Zha96a], [Zha96b].

5.1.11. *Articles—Integrals.* [Amo83c], [And82b], [BFST86], [BGV93], [BP96], [Cam95], [Can81], [Chr90], [Cof91], [Cor72], [DK90], [Ehr95], [Gab79], [Gab80], [GM81], [Gue94], [Han85], [IKJ95], [Joh75], [Lew91], [Lin72], [LK73], [LPM81], [LS95], [Luc95], [Lun85], [MDS92], [Moo83], [OFM78], [PB82], [PB83], [PB85, includes survey], [PDL93], [Puo88], [SBK92], [Sec99], [Sid97], [Sie77], [vVNZ94], [ZK95].

5.1.12. *Articles—Zeros.* [CH70a], [IKF91], [IKF+93], [KS84a], [KS84c], [KS85a], [KS85b], [KS85c], [KS87], [Let96], [Mac97], [MF86], [Seg98], [Sko85], [VGRZ97], [VRS+97], [ZGRV96].

5.2. **Coulomb Wave Functions.**

5.2.1. *Real Arguments and Parameters.* [Bar76, Fortran], [Bar81b, Fortran], [Bar82b, Fortran], [BDG+72, Fortran], [BS80, Fortran], [CH70b], [CT94, Fortran], [HN97b, Fortran], [NT84, Fortran], [Sea82, Fortran], [She74]. Libraries: [Bak92], [Tho97].

5.2.2. *Complex Arguments and Parameters.* [TB85, Fortran], [TR69, Fortran].

5.2.3. *Articles.* [AS92], [Bar81a], [Bar82a], [Bar82c], [Gau69b], [HN97a], [Köl72b, includes survey], [MBF94], [Nes84], [Pex70], [SG72], [TB86].

5.3. **Elliptic Integrals and Functions.** An important recent change in the old subject of elliptic integrals is a renormalization of the definitions of the integrals. This is due to B. C. Carlson: references will be found in §5.3.5.

5.3.1. *Complete Elliptic Integrals.* [Bel88], [Bul65a, Algol], [Bul65b, Algol], [Bul69b, Algol], [Cod65a], [Cod65b], [DR94a, Fortran], [Luk69b], [MH73, Algol]. Libraries: [Bak92], [Mos89], [ULI90], [WNO94], [ZJ96], **IMSL**, **Numerical Recipes**. Systems: **Maple**, **Mathematica**.

5.3.2. *Incomplete Elliptic Integrals.* [Bul65a, Algol], [Bul69b, Algol], [Car87, Fortran], [Car88, Fortran], [CN81, Fortran], [Luk69b], [PT90, Fortran]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**. Systems: **Maple**, **Mathematica**.

5.3.3. *Jacobi's Elliptic Functions.* This subsection includes the theta functions. [Bul65a, Algol]. Libraries: [Bak92], [Tho97], [Mos89], [ULI90], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**. Systems: **Maple** (includes inverse functions), **Mathematica** (includes inverse functions).

5.3.4. *Weierstrass' Elliptic Functions.* This subsection includes modular functions. [Eck76], [Eck77], [Eck80, Fortran]. Libraries: [Bak92], [ULI90], **IMSL**. Systems: **Maple**, **Mathematica**.

5.3.5. *Articles.* [ACJP85, includes survey], [Bul69a], [Car65], [Car77a], [Car77b], [Car79], [Car87], [Car88], [Car89], [Car91], [Car92], [Car95], [CGL90], [Cri89], [DR94b], [FGG82], [FI94], [FL67], [Kin88], [Lee90], [Lee92], [Luk68], [Luk69b], [Luk70b], [LY88], [MH73, Algol], [Mid75], [Mor99], [NC66], [PDK96], [Sal89], [War60].

5.4. **Fermi-Dirac, Bose-Einstein, and Debye Integrals.** This section includes the Lerch transcendent.

5.4.1. *Real Parameter and Argument.* [BDM81, Fortran], [CT67], [FR86, Fortran], [Goa95, Fortran], [Mac96a, Fortran], [Mac98, Fortran], [NDT69]. Libraries: [Bak92], [Tho97].

5.4.2. *Complex Argument and/or Parameters.* Systems: **Maple**, **Mathematica**.

5.4.3. *Articles.* [Bui91], [Gau93a], [Gau93c], [LS91], [MN97], [NM93], [Pas88], [Pas91], [Pic89], [Sag91a], [Sag91b].

5.5. **Hypergeometric and Confluent Hypergeometric Functions.**

5.5.1. *Hypergeometric Functions.* [For97, Fortran], [Hsu93, Fortran]. Libraries: [Bak92], [Kha97], [Mos89], [Tho97], [ULI90], [ZJ96], **Numerical Recipes**. Systems: **Mathematica**.

5.5.2. *Confluent Hypergeometric Functions.* [BS80, Fortran], [NPB92a, Fortran], [NT84, Fortran], [Tem83, Algol], [Yos95]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [ZJ96], **SLATEC**. Systems: **Maple**, **Mathematica**.

5.5.3. *Other Hypergeometric Functions.* [CM84, Pascal], [Ném92, Fortran], [PBN93], [RP96, Fortran]. Libraries: [Bak92], [Mos89]. Systems: **Maple**, **Mathematica**.

5.5.4. *Articles.* [AB91], [BMOF92], [CG89], [CLM97], [dIVPM95], [Kal92], [Luk75], [Luk77a], [MF94], [Mor96], [Ném92], [NPB92b], [Pas95], [Wim74].

5.6. **Incomplete Bessel Functions, Incomplete Beta Function.** This section includes F–, t– and von Mises' distribution functions.

5.6.1. *Incomplete Bessel Functions.* [Hil77, Fortran].

5.6.2. *Incomplete Beta Function.* [CS97, Fortran], [DM92, Fortran], [Dor68, Algol], [Gau64, Algol], [Hil70a, Algol], [Lev69, Fortran], [MB73a, Fortran], [Mor69, Algol], [Phi90, Basic]. Libraries: [Bak92], [Tho97], [Mos89], [ULI90], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**. Systems: **Maple**, **Mathematica**.

5.6.3. *Inverse Incomplete Beta Function.* [AS93a, Fortran], [Hil70b, Algol], [MB73b]. Libraries: [Mos89], [ULI90], **IMSL**, **NAG**. Systems: **Maple**, **Mathematica**.

5.6.4. *Articles.* [AS93b], [DJ67], [OM68], [Tem92b].

5.7. **Incomplete Gamma Functions, Generalized Exponential Integrals.** These functions are essentially equivalent; thus $E_p(z) = z^{p-1}\Gamma(1-p, z)$. This section includes the chi-square distribution function.

5.7.1. *Real z and Integer or Half-Integer p.* [Amo80a, Fortran], [FO94], [SP75, Fortran], [SZ74, Fortran]. Libraries: [Mos89], [Tho97], [ULI90], [ZJ96], **IMSL**, **SLATEC**. Systems: **Maple**.

5.7.2. *Real z and Real p.* [CLM90a, Fortran], [CLM90b, Fortran], [DM87, Fortran], [Ful72, Fortran], [Gau79a, Fortran], [Moo82, Fortran], [She88, Fortran], [Tem94b, Pascal]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [WNO94], [ZJ96], **IMSL**, **NAG**, **Numerical Recipes**, **SLATEC**. Systems: **Maple**.

5.7.3. *Complex z and Real or Complex p.* Systems: **Maple**, **Mathematica**.

5.7.4. *Inverse Function.* [DM87, Fortran], [Phi88, Fortran]. Libraries: [Mos89], [ULI90], **IMSL**, **NAG**. Systems: **Maple**, **Mathematica**.

5.7.5. *Articles.* [AB87a], [Amo80b], [Bar61], [CLM87], [CLM88], [CLM90c], [ČP98], [DM86], [Gau79b], [Gau99], [JT85], [LDP93], [Luk75], [Mar82], [Tem85], [Tem87], [Tem92a], [Tem94a], [Tem95].

5.8. **Legendre Functions and Associated Legendre Functions.** This section includes the conical and toroidal functions. See also hypergeometric functions (§5.5) and orthogonal polynomials (§5.10).

5.8.1. *Real Argument and Parameters.* [Bra73, Fortran], [Del79, Fortran], [Gau65, Algol], [GS97, Fortran], [GS98, Fortran], [LS81, Fortran], [OS83, Fortran]. Libraries: [Bak92], [Tho97], [ZJ96], **Numerical Recipes**, **SLATEC**.

5.8.2. *Conical Functions.* [Köl81]. Libraries: [Bak92]. [Tho97].

5.8.3. *Complex Argument and/or Parameters.* [GS98, Fortran]. Libraries: [Bak92]. Systems: **Maple**, **Mathematica**.

5.8.4. *Articles.* [CM78], [CM79], [EWB84], [Fet70], [Hun95], [LW95], [SOL81].

5.9. **Mathieu, Lamé, and Spheroidal Wave Functions.**

5.9.1. *Characteristic Values of Mathieu's Equation.* [Cle69, Fortran], [Del73, Algol], [Lee79, Fortran], [RL80, Fortran], [Shi93a, Fortran]. Libraries: [Bak92], [ZJ96], **IMSL**. Systems: **Mathematica**.

5.9.2. *Mathieu Functions.* [Cle69, Fortran], [Del73, Algol], [RL80, Fortran], [Shi93a, Fortran]. Libraries: [Bak92], [ZJ96], **IMSL**. Systems: **Mathematica**.

5.9.3. *Spheroidal Wave Functions.* [BC83a, Fortran], [BC83b, Fortran], [KBH70, Fortran], [KvB70, Fortran], [vBBH70, Fortran]. Libraries: [Bak92], [Tho97], [ZJ96].

5.9.4. *Articles.* [ADK+84], [ADKL89], [ADKL91], [Alh96, includes survey], [ATZ83], [Bla46], [Cal88], [Can71], [DNM96], [DR98], [Egl84], [EP69], [Hod70], [LF94], [Liu96], [Pal69], [Shi93b], [SM75], [TP83], [vBBHK72], [VGK+92].

5.10. **Orthogonal Polynomials.** See also hypergeometric functions (§5.5), Legendre functions (§5.8), and Weber parabolic cylinder functions (§5.13).

5.10.1. *Classical Polynomials (Chebyshev, Hermite, Jacobi, Laguerre, Legendre etc.), Real Arguments.* [LPT80, Fortran], [Sim64, Algol], [Wit68, Fortran]. Libraries: [Bak92], [Tho97], [ULI90], [WNO94], [ZJ96].

5.10.2. *Classical Polynomials, Complex Arguments.* Systems: **Maple**, **Mathematica**.

5.10.3. *Other Orthogonal Polynomials.* [Bis91, Maple], [Coo68, Fortran], [EK92], [Gau94, Fortran], [Öpi87, Fortran].

5.10.4. *Articles.* [BEGG91], [BR91], [Chi92], [Cra94], [CS93], [FG91], [FG92], [Gau82], [Gau85], [Gau90], [Gau91a], [Gau93b], [GZ95], [Luk75], [PA92], [Ren96], [Upo92], [WMC97].

5.11. **Polylogarithms (Generalized).**

5.11.1. *Real Variables.* [KMR70, Algol]. Systems: **Mathematica**.

5.11.2. *Articles.* [Bar74], [Pas95].

5.12. **Struve and Anger-Weber Functions.**

5.12.1. *Struve Functions or Integrals of Struve Functions.* [Luk69b], [Luk75], [Mac93], [Mac96a, Fortran], [New84]. Libraries: [Bak92], [Mos89], [Tho97], [ULI90], [ZJ96]. Systems: **Maple**, **Mathematica**.

5.12.2. *Anger-Weber Functions.* Libraries: [Tho97]. Systems: **Maple**.

5.12.3. *Integrals of Anger-Weber Functions.* Libraries: [Bak92].

5.12.4. *Articles.* [Zan75].

5.13. **Weber Parabolic Cylinder Functions.** See also confluent hypergeometric functions (§5.5).

5.13.1. *Real Arguments and Parameters.* [SG98, Fortran], [Tau92, Fortran]. Libraries: [Bak92], [Tho97], [ZJ96].

5.13.2. *Complex Arguments, Real Parameters.* [BN89]. Libraries: [ZJ96]. Systems: **Maple**.

5.13.3. *Articles.* [LR74], [MMV81], [RL76], [SGA81].

5.14. **Zeta Function (Generalized).**

5.14.1. *Real arguments.* [AB89]. Libraries: [Bak92], [Mos89]. Systems: **Maple**, **Mathematica**.

5.14.2. *Articles.* [CHT71], [Cra98], [Moi88].

5.15. **Additional Functions of Two or More Variables.**

5.15.1. *3j, 6j, 9j Symbols (Clebsch-Gordan Coefficients).* [Kae95, Pascal]. Libraries: [Tho97]. Systems: **Mathematica**.

5.15.2. *Articles.* [RBMW59].

6. Testing and Library Construction

In this section we list articles and books that provide general observations on the testing of software and/or the construction of software libraries for the special functions. For information on individual libraries see §3.

[Cod74], [Cod76], [Cod82], [Cod84b], [Cod85], [CS91], [Eva74, especially pp. 275–301 and 357–435], [Ful77], [Gaf88], [Kuk71], [LMS73a], [LMS73b], [Mos89], [PTVF92, example books], [Ric83], [Sch76], [SL73].

7. Future Trends

Great progress has been made in recent years in the construction of software for generating the special functions, yet enormous gaps remain for functions having variable parameters in addition to the argument. This is especially true when the variables are complex. In this concluding section we offer some general suggestions concerning future work in this area.

First, because of the sheer magnitude of the effort required, there should be a perceived physical or other applied need before a decision is made to embark on the construction of extensive new software for functions of two or more variables. At present there are simply too many gaps to fill to be able to indulge in the luxury of arbitrary selection. Moreover, great care should be exercised in the choice of actual functions to be generated. For example, neither the Airy function $\mathrm{Bi}(z)$ nor the Bessel function of the second kind $Y_\nu(z)$ has a useful role when the argument z is not real; compare [Olv74, Chapters 7 and 11].

Second, coverage of a chosen region should be dictated by uniform accuracy requirements (in an appropriate measure), not by the limitations of the methods that happen to be used. At the very least it is frustrating for users to discover that the precision yielded by a package varies widely, or worse still disappears altogether, in parts of the claimed regions of coverage.

Third, the potential offered by the ongoing increase in power of computers should be exploited with a view to reducing the number and complexity of algorithms to be used. This includes, for example, the use of parallel or vector methods for summing series [Kar91] or solving differential or difference equations [LO93].

Fourth—and here we are looking further into the future—the use of systems of computer arithmetic other than floating-point should be considered. The floating-point system has two disadvantages which become especially annoying and time-consuming in the construction of special-function software. One is that the associated error measure, relative precision, is quite inappropriate in the neighborhoods of zeros. The other stems from failure due to overflow or underflow: here the usual remedy of rescaling can be difficult to apply, owing to the extremely varied asymptotic behavior of functions of several variables. A system of computer arithmetic that is capable of overcoming both problems in an elegant manner is the so-called level-index system [COT89].

Lastly, any new algorithm or package should be documented fully. It should also be subjected to exhaustive testing procedures, and these, too, need to be documented. Indeed, the proposed testing procedures should be considered at an early stage in the planning of the main algorithms[10]. There are so many pitfalls in the

[10] For example, it is better to avoid the use of Wronskian and Casoratian relations in the main computing package, if possible, in order to reserve these identities for consistency checks.

construction of algorithms for the special functions that the use of undocumented or insufficiently tested packages is a risky proposition[11].

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A Note on the Reference Acronyms

In the references that follow, the acronyms within the identifying square brackets follow the AMS BibTeX scheme. Initial letters pertain to the author(s) or editor(s). These are followed by two digits representing the year of publication; a letter may also be appended to distinguish between publications in the same year, e.g. [AB87a], [AB87b]. In the case of papers or books with more than four authors, initial letters from the names of the first three authors are used, followed by a $^+$ sign, e.g. [ADK$^+$84]. **It is also important to note that the references are listed according to the alphabetical order of the acronyms and not according to the alphabetical order of the authors' names**.

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