27
11/21/79
246715

ORNL/CSD/TM-93

UCC-ND

**NUCLEAR
DIVISION**

**UNION
CARBIDE**

MASTER

**Information and Advice on the
Numerical Software Available
for the Fusion Energy Program
at Oak Ridge**

P. W. Gaffney

OPERATED BY
UNION CARBIDE CORPORATION
FOR THE UNITED STATES
DEPARTMENT OF ENERGY

PROPERTY OF THE DEPARTMENT OF THE UNITED STATES

Contract No. W-7405-eng-26

COMPUTER SCIENCES DIVISION

INFORMATION AND ADVICE ON THE NUMERICAL SOFTWARE
AVAILABLE FOR THE FUSION ENERGY PROGRAM AT OAK RIDGE

P. W. Gaffney

Sponsor: R. A. Dory
Originator: P. W. Gaffney

Date Published - November 1979

NOTICE

This document contains information of a preliminary nature.
It is subject to revision or correction and therefore does
not represent a final report.

UNION CARBIDE CORPORATION, NUCLEAR DIVISION
Operating the
Oak Ridge Gaseous Diffusion Plant . Oak Ridge National Laboratory
Oak Ridge Y-12 Plant . Paducah Gaseous Diffusion Plant
for the
DEPARTMENT OF ENERGY

DISCLAIMER

This document contains information of a preliminary nature. It is subject to revision or correction and therefore does not represent a final report. The information contained herein is not to be used for any purpose other than that for which it was prepared. The information contained herein is not to be used for any purpose other than that for which it was prepared. The information contained herein is not to be used for any purpose other than that for which it was prepared.

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

500

iii

RELEASE DATE: September 1979

TABLE OF CONTENTS

ACKNOWLEDGMENTS	vii
ABSTRACT	1
I. INTRODUCTION	3
II. PROBLEM AREAS	7
III. SOFTWARE CONTENTS	9
IV. ABBREVIATIONS USED	11
V. SOFTWARE	13
APPENDIX A: Availability of Software	69
APPENDIX B: The NASTI Database	73
APPENDIX C: SANDIA Special Function Routines	79
APPENDIX D: The Contents of MP	83

ACKNOWLEDGMENTS

I wish to thank Richard Hicks and Bill van Rij for making several suggestions which have led to improvements in this report. Moreover, I also extend my thanks to Janice Hughes for her patience and diligence throughout the typing of this report.

Support for this work was provided by the Fusion Energy Division and the Computing Applications Department, Computer Sciences Division.

ABSTRACT

The purpose of this report is to describe some of the numerical routines that have been retained for the Fusion Energy program at Oak Ridge.

The report is organized by problem area. Each area contains a list of relevant numerical routines. These routines are described in detail and, where appropriate, we give advice on their correct use. Furthermore, we have ranked the subroutine libraries NAG, IMSL, and HARWELL according to how satisfactory their routines are for that particular area.

In an Appendix we provide information on how to access the routines and the subroutine libraries described in this report. Moreover, we describe a growing online data base which contains a condensed version of the information in this report.

I. INTRODUCTION

The purpose of this report is to describe some of the mathematical software that has been obtained for the Fusion Energy program at Oak Ridge. However, because we provide state-of-the-art numerical support for this program, the report is of necessity incomplete.

The report is designed in such a way that a computer user may conveniently obtain information and advice on the use of the numerical routines. Thus, in Section V, each routine has been placed in a particular problem area. A list of the 21 problem areas that are covered by this report is given in Section II. At the beginning of each problem area, we list the major subroutine libraries which include software that we recommend for that particular area. The subroutine libraries that we have considered are NAG, IMSL and HARWELL, and the order in which they are presented within each problem area reflects the author's recommendations.

In addition to the software contained in the above subroutine libraries, there exists a wide variety of numerical routines for the problem areas covered by this report. However, some of these routines fail to meet our requirement of being state-of-the-art. Therefore, for some problem areas there are few routines that we can recommend; and in this case we rely upon the above subroutine libraries to provide the appropriate codes. When state-of-the-art software exists at Oak Ridge, we have endeavored to include a description of it in this report. However, since the phrase "state-of-the-art" is open to interpretation, some people may

BLANK PAGE

disagree with the author's selection of routines. Furthermore, since this report currently contains information on only 79 routines, it follows that we have not described all state-of-the-art software in Oak Ridge. To inform users of new software and to minimize the number of quality routines that are omitted from the report, we intend to provide updates at regular intervals.

The description of the additional software is presented in the form:

*** Name of Software ***	Origin
Software Description.	

We have not attempted to rank this software. However, in most cases we have included in the description some advice on the use of the software. Usually, this advice is given on the basis of our experience with the software.

In Appendix A, we describe the availability of the software to computer users at Oak Ridge. In Appendix B, we describe a growing online data base, called NASTI (Numerical Analysis Software Tutorial Inquirer), which is designed to inform computer users of some of the state-of-the-art mathematical routines that exist at Oak Ridge. The information contained in this report is available in a condensed form in NASTI.

In Appendix C we give a list of the subroutines in the Sandia Mathematical Subroutine Library that may be used for approximating special functions. In Appendix D, we present the contents of

Richard Brent's multiple precision package. We believe that this package will be very useful to computer users.

We have prepared this report using TEDI.^{*} In this way the report can be easily updated and copies may be readily obtained. To ensure that users are referring to the most recent issue of this report, we have provided at the front of the report a release date for each update. When updates are made, the release date will change accordingly and a copy of the new report will be available on microfiche from the author.

---

^{*}This is a text editor/formatter developed by Clair Neilson, Los Alamos Scientific Laboratory.

II. PROBLEM AREAS

<u>SECTION</u>	<u>SUBJECT</u>	<u>PAGE</u>
1	COMPLEX ARITHMETIC	14
2	ZEROS OF POLYNOMIALS	15
3	ROOTS OF ONE OR MORE TRANSCENDENTAL EQUATIONS	16
4	SUMMATION OF SERIES	18
5	QUADRATURE	19
6	ORDINARY DIFFERENTIAL EQUATIONS	21
7	PARTIAL DIFFERENTIAL EQUATIONS	27
8	NUMERICAL DIFFERENTIATION	36
9	INTEGRAL EQUATIONS	37
10	INTERPOLATION	39
11	CURVE AND SURFACE FITTING	42
12	MINIMIZING OR MAXIMIZING A FUNCTION	43
13	MATRIX OPERATIONS	48
14	EIGENVALUES AND EIGENVECTORS	49
15	DETERMINANTS	51
16	SIMULTANEOUS LINEAR EQUATIONS	52
17	STATISTICS	60
18	APPROXIMATION OF SPECIAL FUNCTIONS	61
19	MULTIPLE PRECISION ROUTINES	64
20	SOFTWARE TOOLS	65
21	MESH GENERATORS	67

III. SOFTWARE CONTENTS

<u>TITLE</u>	<u>PAGE</u>	<u>TITLE</u>	<u>PAGE</u>
A02AAF	14	FFTPAK	18
A02ABF	14	FMIN	45
A02ACF	14	FUNPACK	61
ADAPT	42	GEAR	23
BICUBIC	40	GEARB	23
BLKTRI	29	GEARBD	23
BRENT1	16	GEARBI	23
BRNANL	66	GEARBIL	23
BT	55	GEARIB	23
BTMS	55	GEARS	23
CHFD	58	GERK	21
COLGDE	24	GMA	57
DAVE	65	GMAS	57
D04AAF	36	HYBRD1	17
D05AAF	37	IDBVIP	42
D05ABF	37	IDSFFT	42
DE	22	LANSO	50
DECOMP	52	LANSOI	50
DEROOT	22	LAWSON-HANSON CODES	58
EISPACK	49	LINPACK	53
EPISODE	24	LMDER1	43
EPISODEB	24	LMDIP1	44

<u>TITLE</u>	<u>PAGE</u>	<u>TITLE</u>	<u>PAGE</u>
LZ	50	PWSSSP	29
MA28	53	QAGS	19
MOL1D	32	QAINF	19
MP	64	QUANC8	20
MUGPK1	34	RKF45	21
ODE	22	SEVAL	39
ODERT	22	SOLVE	52
PASVA3	25	SPLINE	39
PDECOL	34	SUPORT	24
PDEONE	31	SYD	58
PFORT	65	TB06A	40
POIS	29	TG03A	40
POLISH	65	TILE	67
PRAXIS	45	VF02AD	45
PWSCRT	27	YSMPN	55
PWSCSP	28	YSMPS	55
PWSCYL	28	ZEROIN	16
PWSPLR	28		

IV. ABBREVIATIONS USED

<u>Abbreviation</u>	<u>Meaning and Information</u>
ACH.LLL	Alan C. Hindmarsh, Lawrence Livermore Laboratory.
FMM	"Computer Methods for Mathematical Computations" by G. E. Forsythe, M. Malcolm and C. B. Moler. Published by Prentice-Hall.
HARWELL	Harwell Subroutine Library.
IMSL	International Mathematical and Statistical Libraries.
MINPACK1	A subroutine package for optimization. The package is being constructed at the Argonne National Laboratory by B. S. Garbow, K. E. Hillstom and J. J. More.
NAG	Numerical Algorithms Group.
NCAR	National Center for Atmospheric Research.
QUADPACK	A subroutine package for numerical integration. The package is being constructed in a joint project by the "Technische Universität Wien" (H. J. Stetter and C. W. Uberhuber, Vienna, Austria) and the "Katholieke Universiteit Leuven" (A. Piessens and E. de Doncker, Leuven, Belgium).
S.G.	"Computer Solution of Ordinary Differential Equations" by L. F. Shampine and M. K. Gordon published by W. H. Freeman and Company.
S.S.	"Efficient FORTRAN Subprograms for the Solution of Elliptic Partial Differential Equations," by P. Swarztrauber and R. Sweet, NCAR Technical Note/IA-109, July 1975.
TOMS	ACM Transactions on Mathematical Software.

V. SOFTWARE

BLANK PAGE

1. COMPLEX ARITHMETIC

NAG

The A02 chapter of the NAG subroutine library contains three subroutines for arithmetic operations involving complex numbers.

They are:

A02AAF   Evaluates the square root of a complex number.

A02ABF   Evaluates the modulus of a complex number.

AC2ACF   Divides one complex number by a second complex number.

These routines were originally written for use by the NAG library routines which compute eigensystems of real and complex matrices. However, they may be of general use to programmers using complex numbers.

2. ZEROS OF POLYNOMIALS

IMSL

HARWELL

NAG

The appropriate routines in the above libraries are recommended.

3. ROOTS OF ONE OR MORE TRANSCENDENTAL EQUATIONS

NAG

HARWELL

IMSL

*** ZEROIN *** FMM (R. Brent)

This is a function subprogram for computing a real zero of a single function. That is, find x such that

$$f(x) = 0 .$$

The numerical method that is used is a combination of bisection, inverse quadratic interpolation and the secant method. ZEROIN is reliable, fast and accurate. Therefore, it is highly recommended.

*** BRENT1 *** MINPACK1

This subroutine tries to find a solution to a system of N nonlinear equations in N unknowns. That is, BRENT1 tries to find $x_1, \dots, x_N$ such that

$$f_1(x_1, \dots, x_N) = 0$$

$$f_2(x_1, \dots, x_N) = 0$$

$$\vdots$$

$$f_N(x_1, \dots, x_N) = 0 .$$

The numerical method that is used is due to R. Brent. This routine is not as reliable as the following routine HYBRD1. However, on those problems for which it is successful BRENT1 works extremely well and is very fast.

Interested users are referred to the paper, "Numerical Solution of Nonlinear Equations" by Jorge J. More and Michael Y. Cosnard, which was published in TOMS, March 1979, Vol. 5, No. 1, pp. 64-85.

*** HYBRD1 *** MINPACK1

This subroutine tries to find a solution to a system of N nonlinear equations in N unknowns by a modification of the Powell method. The routine is reliable and accurate, and it has worked successfully on a large number of problems. Thus it is recommended without hesitation.

4. SUMMATION OF SERIES

NAG

HARWELL

IMSL

*** FETPAK *** NCAR

A package of Fortran subroutines for the Fast Fourier Transform of (Real or Complex) periodic sequences and other symmetric sequences.

5. QUADRATURE

NAG

HARWELL

IMSL

Adaptive quadrature routines should be used with a great deal of caution. In particular if the integrand $f(x)$ possesses a derivative which is unbounded, then an adaptive quadrature routine may prove too expensive and may produce an inaccurate answer. In general any properties of $f(x)$ should be fully exploited by the integration routine. This often means that adaptive routines are excluded from consideration.

*** QAGS, QAINF *** (from QUADPACK)

QAGS and QAINF are two subroutines for automatic integration. Specifically, QAGS calculates an approximation to the integral

$$\int_a^b f(x) dx$$

where a and b are finite numbers, and QAINF calculates an approximation to integrals of the form

$$\int_a^\infty f(x) dx, \quad \int_{-\infty}^b f(x) dx, \quad \int_{-\infty}^\infty f(x) dx.$$

The subroutines are globally adaptive, and they each use a non-linear extrapolation technique that is based on the epsilon algorithm. Because of their robustness, they are capable of

integrating functions which have jump discontinuities and singularities. QAGS and QAINF have worked very well on a wide selection of test problems, and they have proved to be economical in function evaluations, accurate and fast.

The routines QAGS and QAINF are part of the integration package called Q'ADPACK which is being developed jointly at the 'Technische Universitat Wien' in Austria and the 'Katholieke Universiteit Leuven' in Belgium.

*** QUANC8 *** FMM (J. Lyness)

This is an adaptive quadrature routine which tries to approximate the integral

$$\int_a^b f(x)dx$$

to within a user specified tolerance. The limits a and b must be finite. The numerical method that is used is an adaptive Newton Cote's 8-panel rule. Because QUANC8 endeavors to be reliable and because of the adaptive technique that it employs, it is possible that a large number of function evaluations may be used to obtain the required accuracy.

6. ORDINARY DIFFERENTIAL EQUATIONS

NAG

IMSL

Initial Value Problems

The following codes integrate a system of n first order ordinary differential equations:

$$\frac{dy_i}{dt} = f_i(t, y_1, \dots, y_n) \quad i=1, \dots, n$$

given initial values of $y_1, \dots, y_n$. The codes differ in the numerical methods that are used to approximate the solution of the differential equations. Therefore, some advice is given on the types of problems that each code is suitable for.

*** RKF45 *** FMM

This code uses the Runge-Kutta-Fehlberg (4-5) method with stepsize control.

If the functions $f_i(t, y_1, \dots, y_n)$, $i=1, \dots, n$ are not too expensive to evaluate, and if fairly modest accuracy is requested (for example less than 8 significant digits), then RKF45 is appropriate.

*** GERK *** L. F. Shampine and H. A. Watts

Uses the Runge-Kutta-Fehlberg (4-5) method with stepsize control and global error assessment.

GERK provides a reliable and efficient estimate of the global error, that is, the difference between the solution of the problem posed and the numerical result returned by the code. Therefore,

if it is important to have a readily available estimate of the actual global error committed (for example in those cases where the differential equations may be mathematically unstable), then GERK should be used.

*** DE, ODE *** S.G

Uses a variable order Adams method to dynamically adapt the order of integration to the problem. The main difference between DE and ODE is in the number of differential equations that each can integrate. DE has been coded to integrate up to 20 first order differential equations, whereas ODE has no such restriction.

If the functions $f_i(t, y_1, \dots, y_n)$, $i=1, \dots, n$ are expensive to evaluate, and if high accuracy is required, then DE or ODE is appropriate. If the equations are stiff, then subroutine GEAR should be used. However, for non-stiff problems DE (or ODE) is recommended in preference to using GEAR with the non-stiff option.

*** DEROOT, ODERT *** S.G

These codes use the same numerical method as DE and ODE to solve the differential equations. In addition DEROOT and ODERT have been designed to compute a root of the user-specified nonlinear scalar equation

$$g(t, y_1, \dots, y_n) = 0 \quad .$$

They should be used only when the application calls for a root-finding feature which depends upon the solution of the initial value problem. The main difference between DEROOT and ODERT is that DEROOT has been coded to integrate up to 20 first

order differential equations whereas the maximum number of equations that ODERT will integrate is user supplied.

*** GEAR *** ACH.LLL

Uses variable order Adams method and backward differentiation formulas. It is particularly suitable for stiff systems but it can be used for non-stiff systems. However, DE (or ODE) is preferable for non-stiff problems. When the differential equations are stiff, the methods used by GEAR require the Jacobian matrix:

$$\begin{bmatrix} \frac{\partial f_i}{\partial y_j} \end{bmatrix}$$

The user may supply this matrix or alternatively it can be approximated by the routines in GEAR.

GEARB: Single precision version for banded Jacobian matrices.

GEARBD: Double precision version of GEARB.

GEARBI: Useful for ordinary differential equations which arise from the method of lines solution of two- or three-dimensional P.D.E.'s.

GEARBIL: Large Core version of GEARBI.

GEARIB: Often a system of ODE's is not given explicitly, but is given in an implicit form, e.g., $A(y,t)\dot{y} = g(y,t)$, where A is an $n \times n$ matrix. The variant GEARIB was written to solve this class of problems, where the matrices A and $\partial g / \partial y$ are banded.

GEARS: A variant which is useful for problems which involve a general sparse Jacobian matrix.

EPISODE: A package of routines which use variable step size formulas. These routines differ from those in the GEAR package in that the latter are based on fixed step size formulas, with step changes achieved by interpolation. For problems that require frequent and drastic step size changes, EPISODE is likely to be more efficient than GEAR.

EPISODEB: The only variant, so far, of EPISODE. It is intended for banded Jacobian matrices.

*** **COLODE** *** B. L. Hulme and S. L. Daniel

Uses collocation methods to solve stiff ordinary differential equations. Because of high overhead, COLODE is generally inefficient for non-stiff problems.

Boundary Value Problems

*** **SUPPORT** *** M. R. Scott and H. A. Watts

This code solves a linear two-point boundary value problem of the form

$$\begin{bmatrix} \frac{dy_1}{dx} \\ \vdots \\ \frac{dy_n}{dx} \end{bmatrix} = \begin{bmatrix} F_{1,1}(x) & F_{1,2}(x) & \cdots & F_{1,n}(x) \\ \vdots & \vdots & \ddots & \vdots \\ F_{n,1}(x) & F_{n,2}(x) & \cdots & F_{n,n}(x) \end{bmatrix} \begin{bmatrix} y_1(x) \\ \vdots \\ y_n(x) \end{bmatrix} + \begin{bmatrix} g_1(x) \\ \vdots \\ g_n(x) \end{bmatrix}$$

subject to the boundary conditions

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,n} \\ \vdots & \vdots & \vdots \\ a_{n-k,1} & a_{n-k,2} & a_{n-k,n} \end{bmatrix} \begin{bmatrix} y_1(a) \\ \vdots \\ y_{n-k}(a) \\ \vdots \\ y_n(a) \end{bmatrix} = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_{n-k} \end{bmatrix} \quad 1 \leq k \leq n-1$$

and

$$\begin{bmatrix} b_{1,1} & b_{1,2} & b_{1,n} \\ \vdots & \vdots & \vdots \\ b_{k,1} & b_{k,2} & b_{k,n} \end{bmatrix} \begin{bmatrix} y_1(b) \\ \vdots \\ y_k(b) \\ \vdots \\ y_n(b) \end{bmatrix} = \begin{bmatrix} \beta_1 \\ \vdots \\ \beta_k \end{bmatrix}$$

where the matrix $A = [a_{i,j}]$ is of rank $n-k$ and the matrix $B = [b_{i,j}]$ is of rank k .

SUPPORT uses the method of superposition together with orthonormalization. This results in a very reliable and efficient code for solving linear differential equations. The code is primarily intended for solving problems which may be classified as mathematically unstable, that is, problems with exponentially growing solutions.

*** PASVA3 *** M. Lentini and V. Pereyra

This code solves nonlinear two-point boundary value problems of the form

$$\frac{dy_1}{dx} = f_1(x, y_1, \dots, y_n)$$

$$\frac{dy_2}{dx} = f_2(x, y_1, \dots, y_n) \quad a \leq x \leq b$$

$$\vdots \quad \vdots \quad \vdots$$

$$\frac{dy_n}{dx} = f_n(x, y_1, \dots, y_n)$$

subject to

$$g_1(y_1(a), \dots, y_n(a), y_1(b), \dots, y_n(b)) = 0$$

$$g_2(y_1(a), \dots, y_n(a), y_1(b), \dots, y_n(b)) = 0$$

$$\vdots$$

$$g_n(y_1(a), \dots, y_n(a), y_1(b), \dots, y_n(b)) = 0 \quad .$$

It uses a variable order finite difference method combined with deferred corrections. Adaptive meshes are automatically produced in order to detect and resolve mild boundary layers and other sharp gradient situations.

7. PARTIAL DIFFERENTIAL EQUATIONS

NAG

The Mark 7 edition of the NAG library has a new chapter devoted to this important problem area. At present it contains only four routines. However, later editions of the library promise to substantially increase the contents of this chapter.

Elliptic

The following seven codes comprise a suite of Fortran subroutines for the solution of Elliptic Partial Differential Equations. They were written by Paul Swartztrauber and Roland Sweet at the National Center for Atmospheric Research in Boulder, Colorado. The codes are very efficient and reliable and regarded as state-of-the-art software.

*** 1. PWSCRT *** S. S.

Solves the Helmholtz equation in cartesian coordinates:

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} + \lambda u = f(x,y) \quad .$$

*** 2. PWSPLR *** S. S.

Solves the Helmholtz equation in polar coordinates:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} + \lambda u = f(r, \theta) \quad .$$

*** 3. PWSCYL *** S. S.

Solves the modified Helmholtz equation in cylindrical coordinates:

$$\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{\partial^2 u}{\partial z^2} + \frac{\lambda}{r^2} u = f(r, z) \quad .$$

This two-dimensional modified Helmholtz equation results from the Fourier transform of the three-dimensional Poisson equation.

*** 4. PWSCSP *** S. S.

Solves the modified Helmholtz equation in spherical coordinates assuming axisymmetry (no dependence on longitude):

$$\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial u}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial u}{\partial \theta} \right) + \frac{\lambda}{r^2 \sin^2 \theta} u = f(\theta, r)$$

where θ is colatitude and r is the radial coordinate.

This two-dimensional modified Helmholtz equation results from the Fourier transform of the three-dimensional Poisson equation.

*** 5. PWSSSP *** S. S.

Solves the Helmholtz equation in spherical coordinates and on the surface of the unit sphere (radius of 1):

$$\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} (\sin\theta \frac{\partial u}{\partial\theta}) + \frac{1}{\sin^2\theta} \frac{\partial^2 u}{\partial\phi^2} + \lambda u = f(\theta, \lambda)$$

where θ is colatitude and λ is longitude.

*** 6. POIS *** S. S.

May be used to solve finite difference approximations to an equation of the form:

$$a(x) \frac{\partial^2 u}{\partial x^2} + b(x) \frac{\partial u}{\partial x} + c(x)u + \frac{\partial^2 u}{\partial y^2} = g(x, y)$$

*** 7. BLKTRI *** S. S.

May be used to solve finite difference approximations to the general separable equation:

$$a(x) \frac{\partial^2 u}{\partial x^2} + b(x) \frac{\partial u}{\partial x} + c(x)u + d(y) \frac{\partial^2 u}{\partial y^2} + e(y) \frac{\partial u}{\partial y} + f(y)u = g(x, y) \quad .$$

Whenever possible POIS should be used in preference to BLKTRI.

Elliptic, Parabolic and Hyperbolic

The following three pieces of software, namely PDEONE, MOL1D, and PDECOL, are each designed for solving coupled systems of nonlinear partial differential equations of the form:

$$\frac{\partial \underline{u}}{\partial t} = \underline{f}(t, x, \underline{u}, \underline{u}_x, \underline{u}_{xx}) \quad a \leq x \leq b \quad t \geq t_0$$

where $\underline{u}$ is a vector of solution components

$$\underline{u} = (u_1, u_2, \dots, u_{n-1}, u_n) ,$$

each of which is a function of the scalar quantities t and x . The quantities $\underline{u}_x$ and $\underline{u}_{xx}$ are the corresponding vectors of partial derivatives

$$\underline{u}_x = \left(\frac{\partial u_1}{\partial x}, \frac{\partial u_2}{\partial x}, \dots, \frac{\partial u_{n-1}}{\partial x}, \frac{\partial u_n}{\partial x} \right)$$

$$\underline{u}_{xx} = \left(\frac{\partial^2 u_1}{\partial x^2}, \frac{\partial^2 u_2}{\partial x^2}, \dots, \frac{\partial^2 u_{n-1}}{\partial x^2}, \frac{\partial^2 u_n}{\partial x^2} \right)$$

and $\underline{f}$ is, in general, a nonlinear function of the variables x , $\underline{u}$, $\underline{u}_x$ and $\underline{u}_{xx}$, with n components, that is

$$\underline{f} = (f_1, f_2, \dots, f_{n-1}, f_n) .$$

The associated boundary conditions must be of the form

$$\underline{b}(\underline{u}, \underline{u}_x) = \underline{g}(t) ,$$

where $\underline{b}$ and $\underline{g}$ are vector valued functions with n components. The initial conditions assume that each solution component u_j is a known function of x at $t = t_0$, that is

$$u_j(t_0, x) = \phi_j(x) \quad j = 1, \dots, n$$

where $\phi_j(x)$ is a known function of x .

The numerical method that is used by PDEONE, MOL1D and PDECOL is the method of lines. In this method the system of partial differential equations is converted into a system of first order ordinary differential equations, which is then solved using a sophisticated ODE integrator. The main difference between PDEONE, MOL1D and PDECOL is the technique that is used to convert the PDE's into a system of ODE's. The codes that are likely to be more useful are PDECOL and MOL1D. The main reason for this is because the user has to interface an appropriate ODE integrator with PDEONE whereas the integrator is built into the packages PDECOL and MOL1D.

*** PDEONE *** R. F. Sincovec and N. K. Madsen

This is an interface subroutine which uses centered finite difference approximations to convert one-dimensional systems of partial differential equations into a system of first order ordinary differential equations. The routine is intended to be

used in conjunction with an appropriate ODE integrator. A suitable code for this purpose is GEARB.

The spatial differencing that is employed in PDEONE is more suitable for parabolic and elliptic partial differential equations than for hyperbolic ones. Therefore, users should exercise care when using PDEONE for hyperbolic systems.

*** MOL1D *** J. M. Hyman

MOL1D is a package of subroutines for solving a system of initial-boundary-value partial differential equations by the method of lines.

The system of PDE's that can be integrated must be of the form

$$\frac{\partial u}{\partial t} = F(t, x, u, u_x, u_{xx}, h_x)$$

where $\underline{h}$ is a vector

$$\underline{h} = (h_1, h_2, \dots, h_{n-1}, h_n)$$

whose components are functions of t, x, u, u_x and u_{xx} , that is

$$h_j = h_j(t, x, u, u_x, u_{xx}), \quad j = 1, \dots, n.$$

Like the previous subroutine MOL1D uses finite difference approximations to convert the system of PDE's into a system of first order ODE's. However, unlike PDEONE, it allows the user to

choose the spatial discretization that is to be used. The available approximations are:

- (i) Sixth order centered differences.
- (ii) Fourth order centered differences.
- (iii) Second order centered differences.
- (iv) Fast Fourier transform approximation.
- (v) Fast Fourier transform with linear filtering of the higher modes.
- (vi) Second order differences oriented into the characteristics of $u_t = f_x$. Centered differences are used if the characteristics are perpendicular to the x-axis.
- (vii) Fourth order centered differences or unsymmetric third order differences oriented into the characteristics of $u_t = f_x$.
- (viii) Derivative not to be calculated by the package.

Because this flexibility has been incorporated into the code, MOL1D provides the user with the capability of solving a wide variety of different types of PDE's. This includes linear and nonlinear hyperbolic equations with or without discontinuities.

In order to solve the system of first order ordinary differential equations, MOL1D uses GEARB. Therefore, the equations are integrated using either the implicit Adams methods or the backward differentiation formula methods. The user may specify which type of method is to be used. Alternatively the code will automatically select an appropriate method.

MOL1D is a highly sophisticated piece of numerical software. It can accurately solve partial differential equations with a minimum of programming effort. Therefore, its use is highly recommended.

*** PDECOL *** N. K. Madsen and R. F. Sincovec

This is a suite of subroutines for solving a system of partial differential equations by the method of lines. It uses a finite element collocation procedure for converting the system of PDE's into a system of first order ODE's. The basis functions that are used in the collocation procedure are piecewise polynomials whose degree is specified by the user. The resultant system of ODE's is solved using a slightly modified version of GEARIB.

*** MUGPK1 *** A. Brandt

This is the complete set of codes from the ICASE Workshop on Multi-Grid Methods that was held in June 1978, at the NASA-Langley Research Center in Hampton, Virginia. The codes include routines for solving the linear equations that arise from the finite difference approximation to the solution of certain types of partial differential equations. The method that is used to solve the linear equations is called a Multi-Level (or Multi-Grid) adaptive technique. This method may be viewed as one in which the partial differential equation is discretized on a sequence of successively refined grids. The solution of the resulting linear equations from a coarse grid is then used to obtain the solution

on a finer grid. This process is repeated in an automatic way from coarse grid to fine grid and vice versa. The resulting scheme proves to be very efficient for solving the discretized equations. Moreover, since the finer grids may be introduced at any time in the solution process, it follows that the entire scheme may be adaptive. Thus, for example, local grid refinement near singular points or curved boundaries is possible.

In addition to the codes for solving the linear equations MUGPK¹, also contains routines for the grid refinement.

For further information about Multi-Grid methods, see the paper "Multi-Level Adaptive Techniques (MLAT) for Partial Differential Equations: Ideas and Software" by Achi Brandt in the book Mathematical Software III by J. Rice, published by Academic Press in 1977, and/or contact P. W. Gaffney.

8. NUMERICAL DIFFERENTIATION

NAG

*** D04AAF *** NAG

At present there is only one subroutine, namely D04AAF, in the NAG library for numerical differentiation. This is a semi-automatic routine for obtaining approximations to the first 14 derivatives of a real valued function $f(x)$ at a specified point $\hat{x}$. The user must provide a FUNCTION subprogram for computing $f(x)$, and also a step length h which is used in calculating the derivatives. It is because of this last requirement that D04AAF is called a semi-automatic routine.

D04AAF returns a set of approximations $DER(j)$ and corresponding error estimates $EREST(j)$ which hopefully satisfy

$$|DER(j) - f^{(j)}(\hat{x})| \leq EREST(j), \quad j = 1, \dots, n \leq 14,$$

where n is a user-specified upper limit on the number of derivatives required. Users interested in numerical differentiation should consult the fine introduction to the D04 chapter in the NAG subroutine library manual, as well as the references cited therein.

9. INTEGRAL EQUATIONS

NAG

*** D05AAF *** NAG

This routine solves a linear non-singular Fredholm integral equation of the second kind:

$$f(x) - \lambda \int_a^b K(x,s)f(s)ds = g(x), \quad a \leq x \leq b$$

where $f(x)$ is the unknown function to be determined, $g(x)$ and the kernel $K(x,s)$ are known, and $K(x,s)$ is of 'split' type, that is, $K(x,s)$ is of the form

$$K(x,s) = \begin{cases} k_1(x,s) & a \leq s \leq x \\ k_2(x,s) & x < s \leq b \end{cases},$$

where k_1 and k_2 are well behaved functions while K or its derivative with respect to s may be discontinuous. D05AAF will also solve a linear non-singular Volterra integral equation of the second kind:

$$f(x) - \lambda \int_a^x K(x,s)f(s)ds = g(x), \quad a \leq x$$

*** D05ABF *** NAG

This routine solves a linear non-singular Fredholm integral equation of the second kind with a smooth kernel.

Users who wish to solve Integral equations are urged to consult the D05 chapter in the NAG subroutine library manual.

10. INTERPOLATION

NAG

HARWELL

IMSL

*** SPLINE/SEVAL *** FMM

SPLINE is a Fortran subroutine for computing the coefficients of a cubic spline

$$S(x) = y_i + b_i(x-x_i) + c_i(x-x_i)^2 + d_i(x-x_i)^3 \quad \begin{matrix} x_i \leq x \leq x_{i+1} \\ i=1, \dots, n \end{matrix}$$

which passes through $n+1$ given values, that is

$$S(x_j) = y_j, \quad j=1, \dots, n+1.$$

The knots of $s(x)$ are at the data points

$$x_2, x_3, \dots, x_n.$$

This subroutine should be used only when it is sensible to approximate the data by a function which passes through all of the function values.

SEVAL is a Function subprogram for evaluating the cubic spline function $S(x)$ at a specified value of x .

Because $S(x)$ has $n-1$ knots and because these knots must be at the given data points $x_2, x_3, \dots, x_n$, the user cannot relax the continuity properties of $S(x)$. For example, if it is known that the given values $\{y_j\}$ $j=1, \dots, n+1$ are obtained from a function $y(x)$, say, which has a discontinuous first derivative in the range $x_1 \leq x \leq x_{n+1}$, then it is not sensible to approximate $y(x)$ by a cubic spline whose first two derivatives are continuous throughout

$[x_1, x_{n+1}]$. It follows that in some cases the spline provided by SPLINE may be an unsatisfactory approximation to the data.

*** TB06A/TG03A *** Harwell (P. W. Gaffney)

TB06A is a subroutine for computing a spline $R(x)$ of degree $k-1$ which passes through $n+1$ given values, that is

$$R(x_j) = y_j, \quad j = 1, \dots, n+1, \\ 1 \leq k \leq n+1.$$

The knots of $R(x)$ are at the points

$$\eta_1 < \eta_2 < \dots < \eta_{n-k} < \eta_{n+1-k}$$

where

$$x_i < \eta_i < x_{i+k}, \quad i=1, \dots, n+1-k.$$

TB06A should be used only when it is sensible to use an approximating function which passes through all of the given function values.

The advantages of TB06A over, e.g., SPLINE, are that the degree of the spline and the position of the knots may be specified by the user. This allows the user some flexibility in determining the continuity properties of the approximation.

TG03A evaluates a spline of degree $k-1$ and its derivatives $s^{(j)}(x)$, $j=1, \dots, n \leq k-1$, at a specified value of x .

*** BICUBIC *** UCC-ND (P. W. Gaffney)

This is a package of subroutines for computing a bicubic spline function which interpolates values of a function u :

41

$$u_{ij} = u(x_i, y_j) \quad \begin{array}{l} i=1, \dots, n \\ j=1, \dots, m \end{array}$$

on a rectangular grid.

The routines implement the 1962 algorithm of de Boor for computing the coefficients of the spline.

The bicubic spline that is computed has knots at the interior grid points

$$x_2, x_3, \dots, x_{n-2}, x_{n-1}$$

and

$$y_2, y_3, \dots, y_{m-2}, y_{m-1} \quad .$$

Therefore, it suffers from the same limitation as, for example, the one-dimensional spline obtained from SPLINE.

11. CURVE AND SURFACE FITTING

NAG

HARWELL

IMSL

Some of the finest routines that exist at present for curve and surface fitting are in the E02 chapter of the NAG library. These routines are recommended without hesitation. Therefore, users with problems in this area are urged to consult the NAG library before anything else.

*** IDBVIP/IDSEFT ***   Algorithm 526 in TOMS (H. Akima)

This is a subroutine package that implements Akima's method of bivariate interpolation and smooth surface fitting for irregularly distributed data points.

*** ADAPT ***   Algorithm 525 in TOMS (J. R. Rice)

This is a subroutine for approximating a function of one variable, $f(x)$, to within a user-specified smoothness. It uses piecewise polynomials to approximate $f(x)$. The degree of the polynomials and the accuracy required of the approximation are supplied by the user. ADAPT also requires the user to supply a routine to calculate $f(x)$ and its derivatives. Therefore, ADAPT is unsuitable for discrete data sets.

12. MINIMIZING OR MAXIMIZING A FUNCTION

NAG

HARWELL

Computer users with problems in this area are strongly advised to consult the NAG and Harwell subroutine libraries, before using anything else. The software for this subject in the NAG library covers a wide variety of problems and reflects state-of-the-art methods. The corresponding software in the Harwell library can suffer from portability problems. However, like the NAG library, the software is extremely good and covers a significant range of problems.

*** LMDER1 *** MINPACK1

This subroutine tries to minimize the sum of the squares of m nonlinear equations in n unknowns:

$$\begin{aligned} f_1(x_1, \dots, x_n) &= 0 \\ f_2(x_1, \dots, x_n) &= 0 \\ &\vdots \\ f_m(x_1, \dots, x_n) &= 0 \end{aligned}$$

The user must supply a subroutine for computing the quantities

$$f_i(x_1, \dots, x_n), \quad i=1, \dots, m$$

and the Jacobian matrix

$$JAC = \begin{bmatrix} \frac{\partial f_1}{\partial x_j} \end{bmatrix}.$$

44

The numerical method that is used by LMDER1 is a modification of the Levenberg-Marquardt algorithm. Because this method is iterative, the user must supply an initial estimate of the solution vector. In practice LMDER1 has proved to be relatively insensitive to a poor initial estimate.

The documentation for LMDER1 is perfectly satisfactory and the user interface is excellent. Therefore, LMDER1 can be used with confidence.

*** LMDIF1 *** MINPACK1

This subroutine tries to minimize the sum of squares of m nonlinear equations in n unknowns:

$$\begin{aligned} f_1(x_1, \dots, x_n) &= 0 \\ f_2(x_1, \dots, x_n) &= 0 \\ &\vdots \\ f_m(x_1, \dots, x_n) &= 0 \end{aligned}$$

The user must provide a subroutine which calculates the quantities

$$f_i(x_1, \dots, x_n), \quad i = 1, \dots, m.$$

The Jacobian matrix $\left[\frac{\partial f_i}{\partial x_j} \right]$ is then approximated, in LMDIF1, using finite differences.

Apart from the Jacobian calculation, LMDIF1 is similar to LMDER1. Therefore, it is recommended without reservation.

*** FMIN *** FMM (R. Brent)

This is a function subprogram for computing an approximation to the point x^* , in the interval $a < x < b$, where $f(x)$ attains its minimum.

The numerical method that is used by FMIN is a combination of the golden-section search and successive parabolic interpolation. Therefore convergence to a minimum is guaranteed. However, if the function f is not unimodal, then FMIN may converge to a local minimum which is not necessarily the global minimum.

*** PRAXIS *** R. Brent

This is a subroutine for minimizing a function of N variables

$$f(x_1, x_2, \dots, x_{n-1}, x_n)$$

without calculating derivatives. It is a modified version of Powell's 1964 algorithm, which uses conjugate directions to obtain the minimum. The main modification to Powell's algorithm is to the procedure for obtaining and maintaining linearly independent search directions. In PRAXIS this is accomplished by the principal axis method.

Numerical results indicate that PRAXIS is a very reliable subroutine for computing a minimum of a general function without calculating derivatives.

*** VF02AD *** Harwell (M. J. D. Powell)

This is a modified version of Professor M. J. D. Powell's new routine VMCON for constrained optimization. Specifically VF02AD is a Double Precision Fortran subroutine for calculating

the least value of a function of several variables subject to general constraints on the values of the variables. The objective function is

$$F(x_1, x_2, \dots, x_n)$$

and the constraints are

$$c_i(x_1, x_2, \dots, x_n) = 0 \quad i = 1, 2, \dots, p$$

$$c_i(x_1, x_2, \dots, x_n) \geq 0 \quad i = p+1, \dots, m$$

where the $\{c_i\}$ may be linear or non-linear functions of the variables $x_1, \dots, x_n$.

The user is required to provide initial values for the variables $x_1, \dots, x_n$, and suitable code for evaluating F and c_i and their first derivatives

$$\frac{\partial F}{\partial x_j}, \frac{\partial c_i}{\partial x_j}, \quad i=1, \dots, m \text{ and } j=1, \dots, n \quad .$$

The original VMCON was modified by J. K. Reid et al. so that it would be portable and so that it would have a convenient user interface. With respect to the latter requirement VFC2AD, uses "reverse communication" for obtaining the values of

$$F, c_i, \frac{\partial F}{\partial x_j} \text{ and } \frac{\partial c_i}{\partial x_j}, \quad i=1, \dots, m, j=1, \dots, n \quad .$$

A description of the algorithm is given by M. J. D. Powell in "A Fast Algorithm for Nonlinearly Constrained Optimization Calculations" which is published in the proceedings of the

Biennial Conference on Numerical Analysis, Dundee 1977, by
Springer-Verlag.

13. MATRIX OPERATIONS

NAG

HARWELL

IMSL

In this section we have included routines for the following problems:

Matrix Inversion

Matrix Transformation

and

Matrix Manipulation (for example: Transpose,
Multiplication, Subtraction,
Addition, etc.)

The routines for Matrix Inversion should not be used to solve simultaneous linear equations.

14. EIGENVALUES AND EIGENVECTORS

NAG

IMSL

HARWELL

*** EISPACK ***

This is a collection of subroutines for computing the eigenvalues and/or the eigenvectors of a matrix. The types of matrices that can be handled by EISPACK are

COMPLEX GENERAL

COMPLEX HERMITIAN

REAL GENERAL

REAL SYMMETRIC

REAL SYMMETRIC TRIDIAGONAL

and SPECIAL REAL TRIDIAGONAL .

The subroutines in EISPACK are based on the algorithms published in the Springer-Verlag handbook series by Wilkinson and Reinsch. Therefore, users can be sure that the numerical methods employed by the subroutines are perfectly satisfactory. Moreover, since EISPACK is a product of the NAST (National Activity to Test Software) Project, the contents of EISPACK have been thoroughly tested and reflect quality mathematical software.

The corresponding subroutines in the F02 chapter of the NAG library are also based on the algorithms in the Wilkinson-Reinsch handbook. Moreover, the NAG routines are of the same high quality as those in EISPACK. Therefore, from a convenience point of view,

computer users may prefer to choose the F02 routines. This choice is recommended by the author.

*** LANSO *** UCC-ND (D. S. Scott)

LANSO is a new subroutine for computing a specified number of either the smallest or the largest eigenvalues, and corresponding eigenvectors, of a real symmetric matrix A . It is designed for the case when the matrix A is large. Consequently, for small eigenproblems more appropriate routines are available.

LANSO has been written in such a way that the user may take advantage of any sparsity pattern in the matrix A . Thus, it is particularly efficient for large sparse symmetric matrices.

*** LANSOI *** UCC-ND (D. S. Scott)

This is a subroutine for computing all of the eigenvalues, and corresponding eigenvectors, of a real symmetric matrix that are outside a given interval.

*** LZ *** Algorithm 496 in TOMS (L. Kaufman)

This is a Fortran subroutine for computing the vector x and the constant λ such that the equation

$$Ax = \lambda Bx$$

is satisfied, where A and B are square matrices, which may be complex. The subroutine uses the LZ algorithm for finding x and λ . Therefore, it may be used when either or both matrices are singular.

15. DETERMINANTS

NAG

IMSL

HARWELL

16. SIMULTANEOUS LINEAR EQUATIONS

NAG

HARWELL

IMSL

The routines, in the NAG, Harwell and IMSL libraries, for solving systems of linear equations

$$\underline{Ax} = \underline{b}$$

are among the best currently available. In particular the Harwell subroutine library contains the excellent sparse matrix package MA28.

*** DECOMP/SOLVE *** FMM

This is a pair of subroutines for obtaining the solution of a system of linear equations of the form:

$$\underline{Ax} = \underline{b} ,$$

where A is a real $n \times n$ matrix, $\underline{x}$ is the vector of unknowns,

$$\underline{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

and $\underline{b}$ is a vector of n given components.

Specifically, DECOMP performs Gaussian elimination, with partial pivoting, on the matrix A, and saves the multipliers and pivot information. It also provides an estimate of the condition of the matrix A. The size of this estimate indicates whether it is safe to try to complete the solution using SOLVE.

Using the information obtained from DECOMP, subroutine SOLVE performs forward and back substitution to compute the solution $\underline{x}$ for any right-hand side $\underline{b}$. Both subroutines are excellent for analyzing and calculating the solution to a system of real linear equations when the matrix A does not possess any special structure, for example, A is not banded. If the matrix does possess some structure, then it may be sensible to use a routine that has been designed to take advantage of this structure.

*** LINPACK ***

This is a suite of subroutines for solving various types of linear systems. It contains routines for solving linear equations of the form

$$\underline{Ax} = \underline{b} ,$$

where A can either be a general square matrix or it can be banded, symmetric indefinite, symmetric positive definite, triangular or tridiagonal. There are also routines in LINPACK for rectangular matrices. Thus, linear least squares problems may be solved by using either the QR method or the singular value decomposition.

The subroutines in LINPACK are designed to be reliable, efficient and portable. Therefore, they are highly recommended.

*** MA28 *** Harwell (I. S. Duff)

This is a set of subroutines for the solution of sparse unsymmetric sets of linear equations:

$$\underline{Ax} = \underline{b} .$$

The subroutines are divided into three distinct phases called MA28A, MA28B, and MA28C. MA28 first permutes the matrix A into the block lower triangular form

$$\begin{bmatrix} A_{1,1} & & & & \\ A_{2,1} & A_{2,2} & & & \\ A_{3,1} & A_{3,2} & A_{3,3} & & \\ \vdots & \vdots & \vdots & \ddots & \\ A_{n,1} & A_{n,2} & A_{n,3} & \dots & A_{n,n} \end{bmatrix}$$

where the matrices $A_{i,i}$ are square. Then, it performs Gaussian elimination with pivoting on each diagonal block $A_{i,i}$ to obtain the factorization

$$A_{i,i} = L_i U_i \quad i=1, \dots, n$$

where L_i is a lower triangular matrix whose diagonal elements are equal to one, and U_i is an upper triangular matrix.

The main advantage of permuting A into block lower triangular form is in the solution process. For, if the matrices $A_{i,i}$ are much smaller than A, (which is usually the case), then there is a saving in storage and execution time.

MA28A provides the user with the option of omitting the permutation step and obtaining a full decomposition of the original matrix.

MA28B uses information from a previous call to MA28A to factorize a new matrix which has a similar sparsity pattern.

MA28C solves sets of linear equations of the form

$$\underline{Ax} = \underline{b}$$

or

$$\underline{A^T x} = \underline{b}$$

using the factorization obtained by MA28A or MA28B. The MA28 package is state-of-the-art software for this problem. It is reliable, efficient and fast. Therefore, it is recommended without reservation.

*** YSMPS/YSMPN *** Yale

These are two software packages for solving sparse systems of linear equations:

$$\underline{Ax} = \underline{b} \quad .$$

YSMPS solves the system when A is symmetric.

YSMPN solves the system when A is non-symmetric.

The numerical method that is used is a sparse variant of Gaussian elimination. However, no pivoting is performed for numerical stability.

For symmetric positive definite systems, that is when $A = A^T$ and all the eigenvalues of A are positive, YSMPS will probably be more efficient than MA28. However, for unsymmetric problems and for problems which require some pivoting to maintain stability, users should use MA28 in preference to YSMPS or YSMPN.

*** BT/BTMS *** ACH LLL

This is a pair of subroutines for solving linear equations

$$\underline{Ax} = \underline{b}$$

where the matrix A has the block tridiagonal structure

$$A = \begin{bmatrix} A_1 & B_1 & C_1 & & & \\ C_2 & A_2 & B_2 & & & \\ & C_3 & A_3 & B_3 & & \\ & & \ddots & \ddots & \ddots & \\ & & & C_{n-1} & A_{n-1} & B_{n-1} \\ & & & & B_n & C_n & A_n \end{bmatrix}$$

and each A_i , B_i , C_i is a square matrix of order m .

Matrices of this type frequently occur in the numerical solution of systems of partial differential equations.

BT assumes that the matrix A and the vector $\underline{b}$ can both be stored in core simultaneously. If this is not the case, then the minimal storage version of BT, namely BTMS should be used. This is the main difference between BT and BTMS.

The numerical method that is used is a block Crout LU-decomposition of the matrix A followed by forward and back substitutions. The matrix L is block lower triangular, and the matrix U is block upper triangular with identity matrices on the diagonal. During the computation of the decomposition, partial pivoting is performed to maintain stability.

These routines are written in ANS Fortran. They have proved reliable and efficient, and they are duly recommended for block-tridiagonal systems of linear equations.

*** GMA/GMAS *** Algorithm 527 in TOMS (R. E. Bank)

These are two subroutines which are implementations of the generalized marching algorithm. They may be used to solve linear equations

$$\underline{Ax} = \underline{b}$$

where the matrix A is of the form

$$A = \begin{bmatrix} T + \alpha_1 I & -\beta_2 I & & & -\beta_1 I \\ -\beta_2 I & T + \alpha_2 I & -\beta_3 I & & \\ & \ddots & \ddots & \ddots & \\ & & \beta_{n-1} I & T + \alpha_{n-1} I & -\beta_n I \\ -\beta_1 I & & & -\beta_n I & T + \alpha_n I \end{bmatrix}$$

and T is the nearly tridiagonal matrix

$$T = \begin{bmatrix} \gamma_1 & -\gamma_2 & & & -\sigma_1 \\ -\sigma_2 & \gamma_2 & -\sigma_3 & & \\ & \ddots & \ddots & \ddots & \\ & & -\sigma_{m-1} & \gamma_{m-1} & -\sigma_m \\ -\sigma_1 & & & -\sigma_m & \gamma_m \end{bmatrix}$$

with α_i , β_i , γ_i , and σ_i all scalars.

Linear equations of this form arise from 5-point discretizations of separable or constant coefficient elliptic boundary-value problems on rectangular domains.

GMA is appropriate for the case when the matrix A is positive definite or negative definite.

When the matrix A is positive or negative semidefinite, (that is when all the eigenvalues of A are respectively greater than or equal to zero, or less than or equal to zero), with zero an eigenvalue of multiplicity one, then subroutine GMAS should be used to compute a least squares solution.

*** SVD *** FMM

This is a subroutine for computing the singular value decomposition of a real rectangular matrix. It is a slightly modified version of the corresponding routine in EISPACK.

*** LAWSON-HANSON CODES ***

This is the complete set of main programs and subroutines from the book "Solving Least Squares Problems" by C. L. Lawson and R. J. Hanson. This is a very useful and practical book. The routines are well written and thoroughly documented, and they cover a wide range of problems. Consequently they are recommended for users who analyze and solve linear least squares problems. For the casual user, the appropriate routines in the NAG library or LINPACK collection may prove more satisfactory.

*** CHEB *** Algorithm 495 in TOMS (I. Barrodale and C. Phillips)

This subroutine is designed to compute the Chebyshev solution of an overdetermined system of linear equations:

$$\begin{bmatrix} a_{1,1} & a_{1,2} & a_{1,n} \\ \vdots & \vdots & \vdots \\ a_{n,1} & a_{n,2} & a_{n,n} \\ \vdots & \vdots & \vdots \\ a_{m,1} & a_{m,2} & a_{m,n} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \\ \vdots \\ x_m \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_n \\ \vdots \\ b_m \end{bmatrix}, \quad m \geq n.$$

Specifically, it computes a vector $\mathbf{x}^* = [x_1^*, \dots, x_m^*]^T$ which minimizes the quantity

$$\text{Max.}_{1 \leq i \leq m} |b_i - \sum_{j=1}^n a_{i,j} x_j^*|.$$

The subroutine may be used to solve the Chebyshev data fitting problem:

Given m data points (z_i, y_i) compute a function of the form

$$p(z) = \alpha_1 \phi_1(z) + \alpha_2 \phi_2(z) + \dots + \alpha_n \phi_n(z)$$

such that the quantity

$$\text{Max.}_{1 \leq i \leq m} |y_i - p(z_i)|$$

is minimized.

If the values $y_1, \dots, y_m$ contain only small inherent errors, then the Chebyshev approximation $p(z)$ may provide a more realistic approximation of the data than a least squares or a least-first-power fit.

17. STATISTICS

IMSL

NAG

The IMSL subroutine library offers a wide selection of good software for statistical calculations. At present the NAG library is weak in this area. However, there are plans to increase the number of statistics routines in later versions of the NAG library.

18. APPROXIMATION OF SPECIAL FUNCTIONS

NAG

IMSL

HARWELL

The three subroutine libraries listed above are extremely weak in this area. Furthermore, there is a sad lack of software for special functions throughout the numerical software world. This unfortunate circumstance is likely to persist for some time. Therefore, computer users who wish to compute special functions may have to resort to coding the approximations themselves. This is not such a difficult problem since there already exists some excellent software for approximating functions (see Sections 10 and 11). Therefore, the advice to users who require special function routines is to search the main subroutine libraries, the routines described below, the routines in Appendices C and D, and then, if they have not found the appropriate routine, to consult a Numerical Analyst.

*** FUNPACK ***

FUNPACK is a collection of quality routines for evaluating certain special functions. A list of the functions that may be approximated using FUNPACK is given below. This list highlights the fact that FUNPACK does not contain many routines. Moreover, it does not contain any routines which allow complex values of the independent variable.

Functions That Can be Approximated Using FUNPACK

- 1) Bessel functions of the first kind

$$J_0(x) \text{ and } J_1(x)$$

- 2) Bessel function of the second kind

$$Y_\nu(x) \quad x > 0, \quad 0 \leq \nu < 1$$

sometimes called Weber's function and sometimes denoted by $N_\nu(x)$.

- 3) Modified Bessel functions of the first kind

$$I_0(x) \text{ and } I_1(x) \quad .$$

- 4) Modified Bessel functions of the second kind

$$K_0(x) \text{ and } K_1(x) \quad x \geq 0 \quad .$$

- 5) Dawson's Integral

$$e^{-x^2} \int_0^x e^{t^2} dt \quad .$$

- 6) Complete Elliptic integral of the first kind:

$$\int_0^{\pi/2} (1 - K^2 \sin^2 \phi)^{-1/2} d\phi \quad 0 \leq K^2 < 1$$

- 7) Complete Elliptic integral of the second kind:

$$\int_0^{\pi/2} (1 - K^2 \sin^2 \phi)^{1/2} d\phi \quad 0 \leq K^2 \leq 1$$

8) The exponential integral

$$Ei(x) = \begin{cases} \int_{-\infty}^x \frac{e^t}{t} dt & x > 0 \\ -\int_{-x}^{\infty} \frac{e^{-t}}{t} dt & x < 0 \end{cases}$$

9) The logarithmic derivative of the Gamma function

$$\psi(x) = \frac{\Gamma'(x)}{\Gamma(x)}$$

sometimes called the Psi function.

19. MULTIPLE PRECISION ROUTINES

*** MP ***   Algorithm 524 in TOMS (R. Brent)

MP is a collection of portable Fortran subroutines for performing multiple-precision floating point arithmetic, and for evaluating elementary and special functions in multiple precision. It is extremely useful in applications that call for a higher precision than can be obtained using standard software. MP is state-of-the-art software and is highly recommended.

A list of the contents of MP is given in Appendix D.

20. SOFTWARE TOOLS

Strictly speaking, the information in this section does not pertain to numerical routines. However, because computer programmers should be aware of the tools in this section, we feel justified to include a description of the tools in this report.

*** PFORT *** Bell Laboratories

PFORT is a Fortran program for verifying that a Fortran computer code adheres to a portable subset of the American National Standard (ANS) Fortran (1966). The computer code may consist of a single subprogram, a group of subprograms, a main program, or a main program plus subprograms.

*** DAVE *** University of Colorado

DAVE is a system for analyzing Fortran programs. It is designed to report the presence, or possible presence, of a wide variety of programming errors. In addition it provides information on the usage of all local and global variables, and on the logical flow through a program. DAVE is written in Fortran and is designed for ease of portability.

*** POLISH *** University of Colorado

POLISH is an ANS Fortran program for editing Fortran programs. Specifically, POLISH, will read an ANS Fortran program and generate a copy of the program that is designed to be easy for a user to read. The copy of the original program is edited in such a way that statement labels are ordered, DO loops are

indented and terminate on unique CONTINUE statements, and blank lines and unreferenced labels are removed. Apart from these fixed editing features there are a number of others which may be controlled by the user in an automatic way. Thus, unlike some text editors, POLISH does not require the manual insertion of editing cues.

*** BRNANL ***   University of Colorado

BRNANL is a Fortran program for identifying basic blocks in a Fortran program. Specifically, BRNANL, will read an ANS Fortran program and generate a copy of the program which contains a subroutine call at the head of every basic block. The name and purpose of this subroutine are at the control of the user. Therefore, BRNANL may be used to gather statistics about the performance of a program. For example, the sections of code that are executed in a program may be recorded, the sequence in which statements are executed may be recorded, etc.

21. MESH GENERATORS

*** TILE *** (P. J. Green and R. Sibson)

TILE is a group of ANS Fortran programs for computing the Dirichlet tessellation and the corresponding Delaunay triangulation from a given set of distinct data points. It is useful for finite element calculations, contour plotting, surface fitting, etc.

The main advantages of TILE over similar routines are that it is economical in storage and it is very fast.

APPENDIX A

Availability of Software

The purpose of this appendix is to assist computer users, at Oak Ridge, in obtaining the software that is described in Section V. Figure 1 describes the availability of the subroutine libraries: NAG, IMSL and HARWELL, and the software tools: DAVE, POLISH, BRNANL and PFORT. Figures 2 and 3 describe the commands that are required to invoke this software on the ORNL PDP-10, the FED Y-12 PDP-10 and the IBM 360 computers. In order to use the above software on the NMFEC computers, users are at the moment advised to contact Kirby Fong, telephone: (FTS) 8-532-4205. The remaining subroutines that are described in Section V are available from the author on various mediums. Therefore, for one of these codes and for general numerical advice, computer users should not hesitate to contact Pat Gaffney, telephone: 4-0630.

BLANK PAGE

Figure 1. Availability of Subroutine Libraries and Software Tools

ORNL-DWG 79-2615 FED

PDP - 10 at Y - 12	
NAG	EX YURPGM, REL: NAG/SEA
IMSL	EX YURPGM, @ PUB: IMSL
HARWELL	SEE PAT GAFFNEY, 4-0630
POLISH	DO POLISH YURPGM
BRNANL	DO BRNANL YURPGM
PFORT	DO PFORT YURPGM

PDP - 10 at ORNL	
NAG	EX YURPGM, SYS: NAGSP/SEA
HARWELL	SEE MIKE HEATH 4-5411 or PAT GAFFNEY 4-0630
POLISH	DO POLISH YURPGM
BRNANL	DO BRNANL YURPGM
PFORT	DO PFORT YURPGM

Figure 2. Commands Required to Invoke the Subroutine Libraries and Software Tools

IBM 360 at ORNL and K-25	
NAG (DOUBLE PRECISION)	<pre>// LKED.SYSLIB DD // DD // DD // DD DSN=A.MTH10276.NAGDP,DISP=SHR // LKED.SYSIN DD * /* 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35</pre>
NAG (SINGLE PRECISION) The final letter, F, of the NAG routine must be changed to E	<pre>// LKED.SYSLIB DD // DD // DD // DD DSN=A.MTH10276.NAGSP,DISP=SHR // LKED.SYSIN DD * /* 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35</pre>
IMSL (DOUBLE PRECISION)	<pre>// LKED.SYSLIB DD // DD // DD // DD DSN=A.MTH10276.IMSLDP,DISP=SHR // LKED.SYSIN DD * /* 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35</pre>
HARWELL	<pre>SEE MIKE HEATH 4 5411 or PAT GAFFNEY 4 0630</pre>
DAVE	<pre>// EXEC DAVE // PHASE0.SYSIN DD * =YURPGM /* 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19</pre>
POLISH	<pre>// EXEC POLISH =YURPGM \$ /* 1 2 3 4 5 6 7 8 9 10 11 12 13 14</pre>
BRNANL	<pre>// EXEC BRNANL BRNSUB BRNVAR 1 1 Y =YURPGM \$ /* 1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25 26 27 28 29 30 31 32 33 34 35</pre>
PFORT	<pre>// EXEC PFORT =YURPGM /* 1 2 3 4 5 6 7 8 9 10 11 12 13</pre>

Figure 3. JCL Required to Invoke the Subroutine Libraries and Software Tools

APPENDIX B

The NASTI Database

The purpose of this appendix is to describe a data base which contains information about the subroutines described in this paper. The name of the data base is NASTI which stands for Numerical Analysis Software Tutorial Inquirer. Thus, as the name implies NASTI is an interactive program. It is designed to inform computer users of some of the existing state-of-the-art software for particular problem areas. The areas that are covered by NASTI are listed in Section II of this paper, and in Figure 1 of this appendix. A user's manual for the NASTI data base is available as ORNL/CSD/TM-97. Therefore, we will briefly describe the commands that are necessary to invoke NASTI.

The NASTI data base is managed by the System 1022 Data Base Management System.* Therefore, we will use the nomenclature of this system to describe NASTI.

For each piece of software that is described in NASTI, there are six attributes, namely:

NAME
PURPOSE
PROBLEM
METHOD
ORIGIN
and VERSION .

---

* "System 1022 Data Base Management System," Software House, Cambridge, Massachusetts 02138.

The attribute

PROBLEM

is keyed.

COMPLEX ARITHMETIC
ZEROS OF POLYNOMIALS
ROOTS OF ONE OR MORE TRANSCENDENTAL EQUATIONS
SUMMATION OF SERIES
QUADRATURE
ORDINARY DIFFERENTIAL EQUATIONS
PARTIAL DIFFERENTIAL EQUATIONS
NUMERICAL DIFFERENTIATION
INTEGRAL EQUATIONS
INTERPOLATION
CURVE AND SURFACE FITTING
MINIMIZING OR MAXIMIZING A FUNCTION
MATRIX OPERATIONS
EIGENVALUES AND EIGENVECTORS
DETERMINANTS
SIMULTANEOUS LINEAR EQUATIONS
STATISTICS
APPROXIMATION OF SPECIAL FUNCTIONS
MULTIPLE PRECISION ROUTINES
SOFTWARE TOOLS
MESH GENERATORS

Figure 1. PROBLEM Areas for NASTI

The remaining attributes are said to be unkeyed.

The attribute that is most likely to be useful, for examining the data base is, PROBLEM. Thus, in Figure 1, we give a list of the PROBLEM areas that are allowed by NASTI. A complete description of each attribute is given in the NASTI manual. Therefore, in order to describe how to use NASTI, we now consider a simple example.

EXAMPLE

Suppose that a computer user wishes to solve a partial differential equation. Furthermore, suppose that the user wishes to know some available state-of-the-art routines for this problem area. Then, the following sequence of commands could be used.

1) Log on to the PDP-10 at Y-12 or X-10.

2) Type the following:

R 1022

OPEN NASTI[200,23000] at Y-12

or

OPEN NASTI[6137,463] at X-10

FIND PROBLEM "PARTIAL DIFFERENTIAL EQUATIONS"

The FIND command is designed for very fast retrieval of information from the data base. To accomplish this, it is restricted to the keyed attributes. Therefore, in this case it may be used with PROBLEM.

In the above example all of the records that are connected with the PROBLEM area PARTIAL DIFFERENTIAL EQUATIONS are selected. At this point the user may issue the command:

TYPE Attribute ". . ."

in which case the attribute ". . ." for every record that has been selected, by the FIND command, will be typed at the user's terminal. To avoid having to retype every attribute, the user can issue the command

USE NASTI.TYP[200,23000]   at Y-12

USE NASTI.TYP[6137,463]   at X-10

The file NASTI.TYP is designed so that all of the attributes, for every record that has been selected, will be typed at the user's terminal. If the user requires this information to be sent to a disk file, then the command

USE NASTI.FIL[200,23000]   at Y-12

USE NASTI.FIL[6137,463]   at X-10

will write the information in the file NASTI.OUT. As noted above the FIND command may only be used with the keyed attributes. For the unkeyed attributes the SEARCH command (which must follow a FIND command) may be used. For example the sequence of commands in 2) may be replaced with

R 1022

OPEN NASTI[200,23000]

FIND PROBLEM "PARTIAL DIFFERENTIAL EQUATIONS"

SEARCH PURPOSE CONTAINS "POISSON"

In this case the FIND command selects all of the records for the problem area of partial differential equations. Then, the search command:

SEARCH PURPOSE CONTAINS "POISSON"

selects from this group all of the records whose attribute PURPOSE

contains the word Poisson. The operator CONTAINS may be abbreviated to CT.

The above examples are intended only to introduce users to the NASTI data base. In order to realize the full potential of the 1022 system, users are urged to consult the system 1022 manual.

APPENDIX C

SANDIA Special Function Routines

This appendix contains a list of subroutines, from the Sandia Mathematical Subroutine Library, for the approximation of special functions.

The information contained in this appendix appears in the Sandia report SAND77-1441 entitled: 'Brief Instructions for Using the Sandia Mathematical Subroutine Library (Version 7.2)' by Karen H. Haskell and Randall E. Jones.

Bessel Functions

BESI for $I_\alpha(x)$, where α is any nonnegative number, $x \geq 0$

BESJ for $J_\alpha(x)$, where α is any nonnegative number, $x \geq 0$

BESKN for $K_n(x)$, where n is any nonnegative integer, $x > 0$

BESYN for $Y_n(x)$, where n is any nonnegative integer, $x > 0$.

These routines can also return N member sequences $I_{\alpha+k}(x)$, $J_{\alpha+k}(x)$, $K_{n+k}(x)$, $Y_{n+k}(x)$, $k=0,1,\dots,N-1$.

The Airy functions are also available through the routines

AIRY for $Ai(x)$

DAIRY for $Ai'(x)$

BAIRY for $Bi(x)$

DBAIRY for $Bi'(x)$.

The Hankel functions $H_n^{(1)}(x)$ and $H_n^{(2)}(x)$ can be evaluated by means of

$$H_n^{(1)}(x) = J_n(x) + iY_n(x)$$

$$H_n^{(2)}(x) = J_n(x) - iY_n(x) .$$

BLANK PAGE

All Bessel function routines produce near-maximum accuracy. That is, they are nearly as accurate as the system SIN and COS routines in the oscillatory regions, and nearly as accurate as EXP in the nonoscillatory regions. All routines are easy to call and do not require any working storage. Many of the routines provide scaling options to extend the admissible argument ranges.

Beta Functions

BETALN computes the logarithm of the beta function

$$B(a,b) = \int_0^1 t^{a-1}(1-t)^{b-1} dt, \quad \begin{matrix} a > 0 \\ b > 0 \end{matrix}$$

for positive a and b . This function can also be expressed in terms of gamma functions

$$B(a,b) = \frac{\Gamma(a) \Gamma(b)}{\Gamma(a+b)}$$

but the routine has been constructed to minimize logarithm computation.

BETAIC and BETBIC both compute the incomplete beta function

$$I_x(a,b) = \frac{1}{B(a,b)} \int_0^x t^{a-1}(1-t)^{b-1} dt \quad \begin{matrix} a > 0 \\ x \geq 0 \end{matrix}$$

for nonnegative x , where $I_x(a,b)$ has been normalized by $B(a,b)$ so that $0 \leq I_x \leq 1$. The difference between BETAIC and BETBIC is that N member sequence $I_x(a+k,b)$, indexed on the parameter a , can be computed with BETAIC while N member sequences $I_x(a,b+k)$, indexed on the parameter b , can be computed with BETBIC, $k=0,1,\dots,N-1$.

If absolute accuracy is acceptable, the argument x for $I_x(a,b)$ can be kept less than or equal to $1/2$ by using the identity

$$I_x(a,b) = 1 - I_{1-x}(b,a)$$

when $x > 1/2$. This makes the evaluation several times faster than direct evaluation of $I_x(a,b)$ when $x > 1/2$.

Gamma Functions

GAMFN evaluates the gamma function

$$\Gamma(x) = \int_0^{\infty} e^{-t} t^{x-1} dt, \quad x > 0$$

and its analytic continuation for $x < 0$ for $-169 < x \leq 170$ except at the poles $x=0,-1,-2,\dots$. The gamma function is related to the factorial of x (when x is an integer) by

$$x! = \Gamma(x+1) .$$

However, many applications involve multiplying or dividing gamma functions by other functions which partially cancel the fast growth of $\Gamma(x)$. In these cases logarithms are appropriate and one should use GAMLN for $\ln \Gamma(x)$, $x > 0$ for better scaling which will extend argument ranges.

GAMMAZ evaluates the gamma function for complex arguments z except in the neighborhood of the poles, $z=0,-1,-2,\dots$.

GAMIC and GAMTL compute the incomplete gamma functions

$$\gamma(\alpha, x) = \frac{1}{\Gamma(\alpha)} \int_0^x e^{-t} t^{\alpha-1} dt$$

$$\Gamma(\alpha, x) = \frac{1}{\Gamma(\alpha)} \int_x^\infty e^{-t} t^{\alpha-1} dt$$

$$\begin{matrix} \alpha > 0 \\ x \geq 0 \end{matrix}$$

respectively for positive α and nonnegative x . These functions have been normalized by $\Gamma(\alpha)$ so that $0 \leq \gamma < 1$, $0 < \Gamma \leq 1$ and

$$\gamma(\alpha, x) + \Gamma(\alpha, x) = 1 \quad .$$

APPENDIX D

The Contents of MP (see Section 19)

This appendix contains a list of those subroutines in the multiple precision package MP, which may be useful to computer users. In the list below an "MP number" means a multiple-precision number.

MPABS	Computes absolute value of an MP number
MPADD	Adds two MP numbers
MPADDI	Adds an MP number to an integer
MPADDQ	Adds a rational number to an MP number
MPART1	Computes ARCTAN (1/N) for N .GT. 1 (called by MPPI)
MPASIN	Computes ARCSIN of an MP number
MPATAN	Computes ARCTAN of an MP number
MPBERN	Computes BERNOULLI numbers B ₂ , B ₄ , B ₆ , ...
MPBESJ	Computes Bessel function J(NU,X) for MP X and small integer NU
MPBES2	Routine called by MPBESJ (uses backward recurrence to evaluate J(NU,X))
MPCDM	Converts double-precision to multiple-precision
MPCIM	Converts integer to multiple-precision
MPCLR	Sets some digits of an MP number to zero
MPCMD	Converts an MP number to double-precision real
MPCMDE	Converts an MP number to (double-precision) fraction and (decimal) exponent
MPCMEF	Converts MP number to fraction and (decimal) exponent
MPCMF	Finds fractional part of an MP number
MPCMI	Converts an MP number to an integer
MPCMIM	Converts an MP number to a multiple-precision integer

MPCMPA	Compares absolute values of two MP numbers MPCMPA (X, Y) returns sign (ABS(X)-ABS(Y))
MPCMPI	Compares an MP number with an integer, MPCMPI (X, I) returns SIGN (X-I)
MPCMPR	Compares an MP number with a real, MPCMPR (X, RI) returns SIGN (X-RI)
MPCMR	Converts an MP number to (single-precision) real call MPCMR (X, RZ) means RZ = SNGL(X)
MPCMRE	Converts an MP number to exponent and (single-precision) fraction, i.e., F*10**I
MPCOMP	Compares two MP numbers. MPCOMP (X, Y) returns SIGN (X-Y)
MPCOS	Computes cosine of an MP number
MPCOSH	Computes hyperbolic cosine of an MP number using MPEXP
MPCQM	Converts a rational number to multiple-precision
MPCRM	Converts real to multiple-precision
MPDAW	Computes Dawson's integral, DAW(X) = EXP(-X**2)*(integral from 0 to X of EXP(U**2) DU)
MPDIV	Divides two MP numbers
MPDIVI	Divides an MP number by an integer (much faster than MPDIV)
MPDUMP	Dumps an MP number (useful for debugging)
MPEI	Evaluates exponential integral of an MP number
MPEPS	Computes the (multiple-precision) machine precision
MPERF	Computes error function of an MP number
MPERFC	Computes complementary error function of an MP number
MPERF2	Computes EXP(X*X)*(integral from 0 to X of EXP(-U*U) DU)
MPEUL	Returns Euler's constant (gamma = 0.57721566...) to multiple-precision accuracy
MPEXP	Computes exponential of a multiple-precision number
MPEXP1	Computes EXP(X)-1 for ABS(X) .LT. 1 (called by MPEXP, MPSINH and MPTANH)

MPGAM	Computes gamma function of an MP argument
MPGAMQ	Computes gamma function of a rational argument
MPGCD	Divides two integers by their greatest common divisor
MPHANK	Routine called by MPBESJ (evaluates Hankel's asymptotic series for Bessel functions)
MPIN	Converts fixed-point number read under A1 format to multiple-precision
MPINE	Same as MPIN but result is multiplied by a power of 10 (useful for reading in floating-point numbers)
MPLI	Evaluates logarithmic integral LI(X)
MPLN	Computes natural log of an MP number
MPLNGM	Computes $\text{LN}(\text{GAMMA}(X))$ for positive MP X, using Stirling's approximation
MPLNGS	Computes natural log of an MP number, using the Gauss-Salamin algorithm. Recommended for testing MPLN and MPLNI only.
MPLNI	Computes natural log of an integer
MPLNS	Computes $\text{LN}(1+X)$ for small MP X
MPL235	Computes natural log of an integer whose prime factors are 2, 3 and/or 5 (called by MPLNI)
MPMAX	Computes the maximum of two MP numbers
MPMAXR	Computes the largest positive MP number
MPMIN	Computes the minimum of two MP numbers
MPMINR	Returns the smallest normalized positive MP number
MPMUL	Multiplies two MP numbers
MPMULI	Multiplies an MP number by an integer (faster than MPMUL)
MPMULQ	Multiplies MP number by a rational number
MPNEG	Reverses sign of an MP number
MPOUT	Converts multiple-precision to a form suitable for printing under A1 format (corresponds to F or I formats)

MPOUTE	Similar to MPOUT but gives (decimal) exponent and fraction (corresponds to E format)
MPOUT2	Same as MPOUT but any base from 2 to 16 may be used for output representation
MPPI	Returns PI to multiple-precision accuracy
MPPIGL	Returns PI to multiple-precision accuracy, using Gauss-Legendre method
MPPOLY	Evaluates a polynomial with integer coefficients
MPPWR	Raises MP number to integer power
MPPWR2	Raises nonnegative MP number to MP power
MPQPWR	Raises rational number to rational power
MPREC	Forms reciprocal of MP number
MPROOT	Computes the N-th root of an MP number using Newton's method
MPSIN	Computes sine of an MP number
MPSINH	Computes hyperbolic sine of an MP number
MPSIN1	Computes SIN(X) or COS(X) for ABS(X) .LE. 1
MPSQRT	Computes square root of a nonnegative MP number, using Newton's method
MPSTR	Stores one MP number in another
MPSUB	Subtracts one MP number from another
MPTAN	Computes TAN of an MP number
MPTANH	Computes hyperbolic TAN of an MP number
MPZETA	Computes Riemann zeta function for positive integer arguments