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COMPUTATION OF SPECIAL FUNCTIONS

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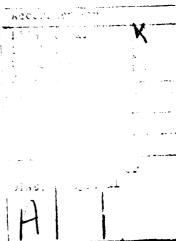
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FOREWORD

A library of subroutines was prepared in machine language for the Naval Ordnance Research Calculator. Many of the subroutines have been rewritten in FORTRAN. Those subroutines in the library which perform operations on polynomials and on matrices have been documented in previous reports. Those subroutines which compute special functions are documented herewith. The manuscript for this report was completed by 7 November 1978.

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ABSTRACT

Documentation is given for some subroutines which compute potentials and other functions. A set of subroutines uses rational approximations to compute Bessel functions of integral order. One subroutine uses the Debye approximation for the efficient computation of Bessel functions of complex argument and complex order. Empirical formulae have been developed to express the limiting boundaries of the modes of computation.

INTRODUCTION

On the Naval Ordnance Research Calculator, programs were coded directly in machine language. It was necessary to provide subroutines for such elementary functions as square root, sine, cosine, exponential, logarithm, and arctangent. With the advent of the FORTRAN compiler, versions of such functions were available from the compiler, and it was no longer considered necessary to provide function routines with each program.

The function name SQRT has been preempted in FORTRAN for the square root. The function name CBRT is used on the Univac 1108 computer for the cube root. A new function routine for the cube root has been prepared for the CDC 6600 computer. It obviates the inefficiency of exponentiation.

Too many problems have arisen with the four-quadrant arctangent function routines of the Control Data Corporation. Among the versions and revisions of the double-precision DATAN2 function routines on Scope 3.3, some have returned nonzero when they should have returned zero, and some have returned zero when they should have returned $+\pi$. Even the single-precision ATAN2 function routine on Scope 3.4 returns completely erroneous values for angles outside of that quadrant which straddles zero. The double-precision DATAN2 function routine on Scope 3.4 returns zero when it should return $+\pi$.

Patches in FORTRAN have been designed by A. H. Morris, Jr. to cure the arctangent function routines in Scope 3.4. These patches convert arguments into absolute values before series expansion and restore signs to the function after series expansion. The patches do not stand alone, because they depend upon the system function routines ABS and ATAN.

New FORTRAN function routines have been prepared for both ATAN2 and DATAN2. When they are included with a program deck, they override the function routines with the same names already in the system. The new FORTRAN function routines use the signs of arguments directly to determine the sign of the function. They stand alone because they make no reference to systems function routines.

The arctangent is a multiple-valued function. If only the projections x, y of a line on the coordinate axes are given, then the angle which the line makes with the x-axis is indeterminate modulo 2π . The accepted convention is to assume that the arctangent satisfies the inequality

$$-\pi < \tan^{-1}\left(\frac{y}{x}\right) \le +\pi \tag{1}$$

Any arctangent function routine must give $+\pi$ when x is negative and y is zero. Otherwise incorrect results will be obtained when real numbers are included in a set of complex numbers, as often happens in mathematical exercises.

In arctangent function routines the addition theorem is used for various centers of expansion and the Maclaurin expansion is used at each center of expansion. An increase in the number of centers permits a decrease in the number of terms. In the CDC version the range of tangents from 0 to 1 is divided into sixteen sectors. A five-term expansion is used from one center to the next higher center. In the new version the range of angle from $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$ is divided into sectors at seven angles for which the tangents are known to especially many digits of accuracy. The series

expansion runs through eight terms or less from the midpoint between one pair of centers to the midpoint between the next higher pair of centers.

Bessel functions are given analytically by absolutely convergent series everywhere in the complex plane, but evaluation of the convergent series by computer is feasible only in a limited range of order and argument. There are asymptotic series which are valid for large argument, but evaluation of the asymptotic series also is feasible only in a limited range of order and argument. The Debye asymptotic approximation can be used to reduce the gap in the range of order and argument to a narrow zone which straddles the line of equal order and argument. The zone which still is not covered by the series can be crossed with the aid of recurrence equations. Evaluation of the Debye series requires a double summation, but the time for evaluation is less than the time which would be required for recurrence from the classical series. Formulae for the Debye approximation have been given by Watson^{1,2} and by Abramowitz and Stegun³, while explicit recurrence equations for the terms of the series have been given by Amos⁶⁻¹⁰.

CUBE ROOT

Analysis

One third of the exponent of x is biased and is attached to 1 to form an initial approximation which is larger than the cube root of x. The initial approximation is diminished by Newton-Raphson iteration until the increment in root is zero or positive from rounding error.

Programming

The cube root of x with sign is computed by Newton-Raphson iteration and is stored in address CBRT.

FOUR-QUADRANT ARCTANGENT

Analysis

Let x, y be the arguments of the arctangent function. The given arguments x, y can be replaced by new arguments u, v through the application of symmetry relations. Let c be a constant which is added to the arctangent of u, v and let h be the center of expansion of the arctangent of u, v.

If x, y satisfy the inequalities

$$|y| \le |x| \qquad \qquad 0 < x \tag{2}$$

then u, v, c are given by the substitutions

$$u \to +x \qquad v \to +y \qquad c \to 0 \tag{3}$$

If x, y satisfy the inequality

$$|x| < |y| \tag{4}$$

then u, v, c are given by the substitutions

$$u \rightarrow + y$$
 $v \rightarrow -x$ $c \rightarrow \pm \frac{1}{2}\pi$ (5)

where the sign of c is the same as the sign of y. If x, y satisfy the inequality

$$|y| \le |x| \qquad x < 0 \tag{6}$$

then u, v, c are given by the substitutions

$$u \rightarrow x$$
 $v \rightarrow y$ $c \rightarrow \pm \pi$ (7)

where the sign of c is the same as the sign of y.

The parameters c and h are adjusted in accordance with the substitutions

$$c \rightarrow c + \theta$$
 $h \rightarrow \tan \theta$ (8)

where θ is that angle among the angles

$$0 \pm \frac{1}{12}\pi \pm \frac{1}{6}\pi \pm \frac{1}{4}\pi (9)$$

which is nearest to $\tan^{-1}(v/u)$, and $\tan\theta$ is the corresponding tangent among the tangents

0
$$\pm (2 - \sqrt{3})$$
 $\pm \frac{1}{\sqrt{3}}$ 1 (10)

Then the Maclaurin expansion is given by the equation

$$\tan^{-1}q = \sum_{m=0}^{\infty} \frac{(-1)^m q^{2m+1}}{(2m+1)}$$
 (11)

for which the parameter q is given by the equation

$$q = \frac{v - hu}{u + hv} \tag{12}$$

and the arctangent function is given by the equation

$$\tan^{-1}\left(\frac{y}{x}\right) = c + \tan^{-1}q \tag{13}$$

Multiple-precision values for the constants c and h are to be found in the following table, which is derived from references 17 and 18.

 $2 - \sqrt{3} = 0.26794919243112270647255365849387236$

 $\frac{1}{\sqrt{2}}$ = 0.57735 02691 89625 76450 91487 80502 04254

 $\frac{1}{12}\pi = 0.26179\,93877\,99149\,43653\,85536\,15273\,29191$

 $\frac{1}{8}\pi = 0.52359877559829887307710723054658382$

 $\frac{1}{4}\pi = 0.78539816339744830961566084581987572$

 $\frac{1}{2}\pi = 1.57079632679489661923132169163975144$

 $\pi = 3.14159\ 26535\ 89793\ 23846\ 26433\ 83279\ 50288$

Multiplication or division of the numbers by small integers can be verified by hand computation.

Programming

FUNCTION ATAN2 (Y, X)

FORTRAN FUNCTION ROUTINE FOR SINGLE PRECISION ARCTANGENT

The variables x, y are given in the arguments X, Y. The four-quadrant arctangent of y/x is returned as the function ATAN2.

DOUBLE FUNCTION DATAN2 (Y, X)

FORTRAN FUNCTION ROUTINE FOR DOUBLE PRECISION ARCTANGENT

The variables x, y are given in the arguments X, Y. The four-quadrant arctangent of y/x is returned as the function DATAN2.

POTENTIAL OF PLATE

Let a plate have unit mass per unit area. Let x, y, z be Cartesian coordinates with origin at the center of the plate, and with z in the direction perpendicular to the plate. Let r be the distance to a point in the field from an element of surface ds on the plate. The potential φ at the field point is given by the equation

$$\varphi = \int \frac{|d\mathbf{s}|}{r} \tag{14}$$

The gradient of the potential is given by the equation

$$-\nabla \varphi = \int \frac{\nabla r \, |d\mathbf{s}|}{r^2} \tag{15}$$

where ∇r is a unit vector in the direction toward the field point. The derivative of φ with respect to z is given by the equation

$$-\frac{\partial \varphi}{\partial z} = -\mathbf{k} \cdot \nabla \varphi = \int \frac{\nabla r \cdot d\mathbf{s}}{r^2} = \omega \tag{16}$$

where ${\bf k}$ is a unit vector in the direction of increasing z, and ω is the solid angle of the plate. The derivative of φ with respect to z also is the potential of a uniformly polarized plate. Since the derivative of a solution of Laplace's equation with respect to a Cartesian coordinate is itself a solution of Laplace's equation, both the potential and the solid angle are solutions of Laplace's equation.

In the definition of a function at a point in the field it is convenient to regard r as the distance from a point on the plate to a point in the field, while in the transformation of integrals it is convenient to regard r as the distance from the point in the field to a point on the plate. In either case the gradients of r differ only in sign.

The field of a unit current along the perimeter of the plate is defined by the equation

$$-\nabla\varphi = \oint \frac{d\mathbf{r} \times \nabla \mathbf{r}}{r^2} \tag{17}$$

while for transformation the field is expressed by the equation

$$-\nabla \varphi = \oint d\mathbf{r} \times \nabla \left(\frac{1}{r}\right) \tag{18}$$

Application of the scalar-vector triple product theorem gives the equation

$$\oint d\mathbf{r} \times \nabla \left(\frac{1}{r}\right) = \oint d\mathbf{r} \times \nabla \left(\frac{1}{r}\right) \cdot \mathbf{I} = \oint d\mathbf{r} \cdot \nabla \left(\frac{1}{r}\right) \times \mathbf{I} \tag{19}$$

where I is the identity tensor. Application of the Stokes theorem gives the equation

$$\oint d\mathbf{r} \cdot \nabla \left(\frac{1}{r}\right) \times \mathbf{I} = \int d\mathbf{s} \cdot \nabla \times \left\{ \nabla \left(\frac{1}{r}\right) \times \mathbf{I} \right\} \tag{20}$$

Application of the vector-vector triple product theorem gives the equation

$$\int d\mathbf{s} \cdot \nabla \times \left\{ \nabla \left(\frac{1}{r} \right) \times \mathbf{I} \right\} = \int \nabla \nabla \left(\frac{1}{r} \right) \cdot d\mathbf{s}$$
 (21)

Since the gradient of the gradient of a scalar function is symmetric, the field is given by the equation

$$-\nabla \varphi = \int \nabla \nabla \left(\frac{1}{r}\right) \cdot d\mathbf{s} \tag{22}$$

Thus the potential of a circuit of unit current is just the solid angle of the circuit.

CIRCULAR DISK

Analysis

Let α be the radius of a disk of unit mass per unit area. Let x, y, z be Cartesian coordinates with z in the direction of the axis of the disk.

The potential and the solid angle of the disk may be expanded in a series of spherical harmonics. Symmetry about the axis of the disk requires that only symmetric harmonics may appear in the series expansion. The coefficients of the spherical harmonics may be derived by reference to special series expansions on the axis of the disk.

Let u be the radial distance from the center of the disk. Then the potential along the axis is given by the equation

$$\varphi = 2\pi \int_0^a \frac{u \, du}{\sqrt{u^2 + z^2}} = 2\pi \{ \sqrt{a^2 + z^2} - z \}$$
 (23)

and the solid angle along the axis is given by the equation

$$\omega = -\frac{\partial \varphi}{\partial z} = 2\pi \left\{ 1 - \frac{z}{\sqrt{a^2 + z^2}} \right\} \tag{24}$$

Let r be the distance from the axis of the disk to the point in the field. Expansion in

series of ascending powers of z and identification of the powers of z with spherical harmonics lead to the equations

$$\varphi = -2\pi |z| - 2\pi a \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{(2n-1)2^{2n} (n!)^2} \left(\frac{\sqrt{r^2+z^2}}{a}\right)^{2n} P_{2n} \left(\frac{z}{\sqrt{r^2+z^2}}\right) (\sqrt{r^2+z^2} < a) (25)$$

$$\omega = \pm 2\pi - 2\pi \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{2^{2n} (n!)^2} \left(\frac{\sqrt{r^2 + z^2}}{a} \right)^{2n+1} P_{2n+1} \left(\frac{z}{\sqrt{r^2 + z^2}} \right) \qquad (\sqrt{r^2 + z^2} < a)$$
 (26)

Expansion in series of descending powers of z and identification of the powers of z with spherical harmonics lead to the equations

$$\varphi = + \pi a \sum_{n=0}^{\infty} \frac{(-1)^n (2n)!}{2^{2n} n! (n+1)!} \left(\frac{a}{\sqrt{r^2 + z^2}} \right)^{2n+1} P_{2n} \left(\frac{z}{\sqrt{r^2 + z^2}} \right) \qquad (\sqrt{r^2 + z^2} > a) (27)$$

$$\omega = + \pi \sum_{n=0}^{\infty} \frac{(-1)^n (2n+1)!}{2^{2n} n! (n+1)!} \left(\frac{a}{\sqrt{r^2 + z^2}} \right)^{2n+2} P_{2n+1} \left(\frac{z}{\sqrt{r^2 + z^2}} \right) \qquad (\sqrt{r^2 + z^2} > a) (28)$$

The convergence of the series deteriorates as the point in the field approaches a sphere of radius a.

Let a line be constructed through the field point and perpendicular to the plane of the disk. Let the intersection between the perpendicular line and the plane of the disk be the center of a circular arc. Let the reference line for azimuth angle be the extension of the line from the center of the arc to the center of the disk. The circular arc intersects the edge of the disk at a point whose radius from the center of the disk makes an angle ϕ with the reference line. Then the radius of the circular arc is given by the expression

$$\sqrt{a^2 + 2ar\cos\phi + r^2} \tag{29}$$

The derivative of the radius with respect to ϕ is given by the expression

$$-\frac{ar\sin\phi}{\sqrt{a^2+2ar\cos\phi+r^2}}\tag{30}$$

The distance of the circular arc from the field point is given by the expression

$$\sqrt{a^2 + 2ar\cos\phi + r^2 + z^2} \tag{31}$$

The potential of the disk is given therefore by the equation

$$\varphi = 2ar \int_0^{\pi} \tan^{-1} \left(\frac{a \sin \phi}{r + a \cos \phi} \right) \frac{\sin \phi \, d\phi}{\sqrt{a^2 + 2ar \cos \phi + r^2 + z^2}} \tag{32}$$

The arctangent can be removed from the integrand through an integration by parts. The interpretation of the arctangent at the limits of integration depends upon whether the center of the arc is inside the perimeter of the disk or outside the perimeter of the disk.

If the center of the arc is inside the perimeter of the disk, then the potential is given by the equation

$$\varphi = -2\pi |z| + 2a \int_0^{\pi} \left(\frac{a + r\cos\phi}{a^2 + 2ar\cos\phi + r^2} \right) \sqrt{a^2 + 2ar\cos\phi + r^2 + z^2} d\phi \quad (r < a) \quad (33)$$

and the solid angle is given by the equation

$$-\frac{\partial \varphi}{\partial z} = \pm 2\pi - 2az \int_0^{\pi} \left(\frac{a + r\cos\phi}{a^2 + 2ar\cos\phi + r^2} \right) \frac{d\phi}{\sqrt{a^2 + 2ar\cos\phi + r^2 + z^2}} \qquad (r < a) (34)$$

If the center of the arc is outside the perimeter of the disk, then the potential is given by the equation

$$\varphi = +2a \int_{0}^{\pi} \left(\frac{a + r \cos \phi}{a^{2} + 2ar \cos \phi + r^{2}} \right) \sqrt{a^{2} + 2ar \cos \phi + r^{2} + z^{2}} d\phi \quad (a < r) (35)$$

and the solid angle is given by the equation

$$-\frac{\partial \varphi}{\partial z} = -2az \int_0^{\pi} \left(\frac{a+r\cos\phi}{a^2+2ar\cos\phi+r^2} \right) \frac{d\phi}{\sqrt{a^2+2ar\cos\phi+r^2+z^2}} \qquad (a < r) (36)$$

A rearrangement of terms leads to the equation

$$\varphi = (a^{2} - r^{2}) \int_{0}^{\pi} \frac{d\phi}{\sqrt{a^{2} + 2ar\cos\phi + r^{2} + z^{2}}} + \int_{0}^{\pi} \sqrt{a^{2} + 2ar\cos\phi + r^{2} + z^{2}} d\phi + (a^{2} - r^{2})z^{2} \int_{0}^{\pi} \frac{d\phi}{(a^{2} + 2ar\cos\phi + r^{2})\sqrt{a^{2} + 2ar\cos\phi + r^{2} + z^{2}}}$$
 (a < r) (37)

and to the equation

$$-\frac{\partial \varphi}{\partial z} = -z \int_0^{\pi} \frac{d\phi}{\sqrt{a^2 + 2ar\cos\phi + r^2 + z^2}}$$
$$-(a^2 - r^2)z \int_0^{\pi} \frac{d\phi}{(a^2 + 2ar\cos\phi + r^2)\sqrt{a^2 + 2ar\cos\phi + r^2 + z^2}} \qquad (a < r) (38)$$

The substitution

$$\cos \phi = 1 - 2\sin^2\frac{1}{2}\phi \tag{39}$$

and replacement of $\frac{1}{2}\phi$ by θ leads to the expression of the integrals in terms of Legendre elliptic integrals. The first and second kinds of elliptic integral are defined by the equations

$$F(\phi, k) = \int_0^{\phi} \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}} \qquad E(\phi, k) = \int_0^{\phi} \sqrt{1 - k^2 \sin^2 \theta} \ d\theta \qquad (40)$$

and the third kind of elliptic integral is defined by the equation

$$\Pi(\phi, \alpha, k) = \int_0^{\phi} \frac{d\theta}{(1 - \alpha^2 \sin^2 \theta) \sqrt{1 - k^2 \sin^2 \theta}}$$
(41)

If the modulus α is defined by the equation

$$\alpha^2 = \frac{4\alpha r}{(a+r)^2} \tag{42}$$

and the modulus k is defined by the equation

$$k^2 = \frac{4ar}{(a+r)^2 + z^2} \tag{43}$$

then the potential is given by the equation

$$\varphi = -2\pi |z| + 2\frac{(a^2 - r^2)}{\sqrt{(a+r)^2 + z^2}} F(\frac{\pi}{2}, k) + 2\sqrt{(a+r)^2 + z^2} E(\frac{\pi}{2}, k)$$
$$+ 2\frac{(a-r)}{(a+r)} \frac{z^2}{\sqrt{(a+r)^2 + z^2}} \Pi(\frac{\pi}{2}, \alpha, k) \qquad (r < a)$$
(44)

and the solid angle is given by the equation

$$-\frac{\partial \varphi}{\partial z} = \pm 2\pi - \frac{2z}{\sqrt{(a+r)^2 + z^2}} F(\frac{\pi}{2}, k) - 2\frac{(a-r)}{(a+r)} \frac{z}{\sqrt{(a+r)^2 + z^2}} \Pi(\frac{\pi}{2}, \alpha, k) \quad (r < a) \quad (45)$$

when the field point is inside the perimeter, while the potential is given by the equation

$$\varphi = +2 \frac{(a^2 - r^2)}{\sqrt{(a+r)^2 + z^2}} F(\frac{\pi}{2}, k) + 2\sqrt{(a+r)^2 + z^2} E(\frac{\pi}{2}, k) + 2\frac{(a-r)}{(a+r)} \frac{z^2}{\sqrt{(a+r)^2 + z^2}} \Pi(\frac{\pi}{2}, \alpha, k) \qquad (a < r)$$
(46)

and the solid angle is given by the equation

$$-\frac{\partial \varphi}{\partial z} = -\frac{2z}{\sqrt{(\alpha+r)^2+z^2}}F(\frac{\pi}{2},k) - 2\frac{(\alpha-r)}{(\alpha+r)}\frac{z}{\sqrt{(\alpha+r)^2+z^2}}\Pi(\frac{\pi}{2},\alpha,k) \qquad (\alpha < r) (47)$$

when the field point is outside the perimeter.

The complete elliptic integral of the third kind is expressed in terms of the incomplete integrals of the first two kinds by formulae on page 228 of Handbook of Elliptic Integrals by Byrd and Friedman⁴. If the angle θ is defined by the equation

$$\theta = \sin^{-1} \sqrt{\frac{\alpha^2 - k^2}{\alpha^2 k'^2}} \tag{48}$$

and the parameter $\Lambda(\theta, k)$ is defined by the equation

$$\Lambda(\boldsymbol{\theta}, \boldsymbol{k}) = \frac{2}{\pi} \left[E(\frac{\pi}{2}, \boldsymbol{k}) F(\boldsymbol{\theta}, \boldsymbol{k}') + F(\frac{\pi}{2}, \boldsymbol{k}) E(\boldsymbol{\theta}, \boldsymbol{k}') - F(\frac{\pi}{2}, \boldsymbol{k}) F(\boldsymbol{\theta}, \boldsymbol{k}') \right]$$
(49)

where the comodulus k' is defined by the equation

$$k'^2 = 1 - k^2 \tag{50}$$

then the complete elliptic integral of the third kind is given by the equation

$$\Pi(\frac{\pi}{2}, \alpha, k) = \frac{\pi}{2} \frac{\alpha \Lambda(\theta, k)}{\sqrt{(\alpha^2 - k^2)(1 - \alpha^2)}}$$
(51)

When the moduli are expressed in terms of the coordinates, then θ is given by the

equation

$$\theta = \tan^{-1} \frac{z}{|a-r|} \tag{52}$$

and the moduli can be combined as expressed by the equation

$$\frac{\alpha}{\sqrt{(\alpha^2-k^2)(1-\alpha^2)}} = \frac{(a+r)}{|a-r|} \frac{\sqrt{(a+r)^2+z^2}}{z}$$
 (53)

Thus the potential and the solid angle are reduced to simple expressions in terms of $\Lambda(\theta, k)$.

Accuracy and efficiency were determined by comparisons between computations by two formulations on a common boundary between their zones of application. Optimization of accuracy and efficiency limits the use of the elliptic integrals to an annular zone between a sphere of radius $\frac{1}{2}a$ and a sphere of radius 2a.

Programming

SUBROUTINE CDSKP (AA, AR, AZ, FP) FORTRAN SUBROUTINE FOR POTENTIAL OF CIRCULAR DISK

The radius a of the disk is given in argument AA, the distance r from the axis of the disk is given in argument AR, and the distance z from the plane of the disk is given in argument AZ. The potential of the disk is stored in function FP.

SUBROUTINE CDSKO (AA, AR, AZ, FO)

FORTRAN SUBROUTINE FOR SOLID ANGLE OF CIRCULAR DISK

The radius α of the disk is given in argument AA, the distance r from the axis of the disk is given in argument AR, and the distance z from the plane of the disk is given in argument AZ. The solid angle of the disk is stored in function FO.

RECTANGULAR PLATE

Analysis

Let 2a be the length of a plate and let 2b be the breadth of the plate. Let x, y, zbe Cartesian coordinates with x in the direction of the length of the plate, with y in the direction of the breadth of the plate, and with z in the direction perpendicular to the plate. Let a line be constructed through the field point and perpendicular to the plane of the plate. The perpendicular line intersects the plane of the plate at a point with coordinates x, y with respect to the center of the plate. Let u, v be the coordinates of a point on the plate with respect to the point of intersection. Then the potential at the field point is given by the equation

$$\varphi(x, y, z) = \int_{-b-y}^{+b-y} \int_{-a-x}^{+a-x} \frac{dudv}{\sqrt{u^2 + v^2 + z^2}}$$
 (54)

Initial integration leads to an inverse hyperbolic function, then final integration is

completed with an integration by parts. Introduction of limits of integration leads to the equation

$$\varphi = (a - x)\sinh^{-1}\frac{(b - y)}{\sqrt{(a - x)^2 + z^2}} + (a - x)\sinh^{-1}\frac{(b + y)}{\sqrt{(a - x)^2 + z^2}}$$

$$+ (a + x)\sinh^{-1}\frac{(b - y)}{\sqrt{(a + x)^2 + z^2}} + (a + x)\sinh^{-1}\frac{(b + y)}{\sqrt{(a + x)^2 + z^2}}$$

$$+ (b - y)\sinh^{-1}\frac{(a - x)}{\sqrt{(b - y)^2 + z^2}} + (b - y)\sinh^{-1}\frac{(a + x)}{\sqrt{(b - y)^2 + z^2}}$$

$$+ (b + y)\sinh^{-1}\frac{(a - x)}{\sqrt{(b + y)^2 + z^2}} + (b + y)\sinh^{-1}\frac{(a + x)}{\sqrt{(b + y)^2 + z^2}}$$

$$- z\tan^{-1}\frac{(a - x)(b - y)}{z\sqrt{(a - x)^2 + (b - y)^2 + z^2}} - z\tan^{-1}\frac{(a - x)(b + y)}{z\sqrt{(a - x)^2 + (b + y)^2 + z^2}}$$

$$- z\tan^{-1}\frac{(a + x)(b - y)}{z\sqrt{(a + x)^2 + (b - y)^2 + z^2}} - z\tan^{-1}\frac{(a + x)(b + y)}{z\sqrt{(a + x)^2 + (b + y)^2 + z^2}}$$
 (55)

Partial differentiation and cancellation of terms gives the components of the gradient of the potential.

Differentiation with respect to x leads to the equation

$$-\frac{\partial \varphi}{\partial x} = \sinh^{-1} \frac{(b-y)}{\sqrt{(a-x)^2 + z^2}} + \sinh^{-1} \frac{(b+y)}{\sqrt{(a-x)^2 + z^2}}$$
$$-\sinh^{-1} \frac{(b-y)}{\sqrt{(a+x)^2 + z^2}} - \sinh^{-1} \frac{(b+y)}{\sqrt{(a+x)^2 + z^2}}$$
(56)

differentiation with respect to y leads to the equation

$$-\frac{\partial \varphi}{\partial y} = \sinh^{-1} \frac{(a-x)}{\sqrt{(b-y)^2 + z^2}} + \sinh^{-1} \frac{(a+x)}{\sqrt{(b-y)^2 + z^2}}$$
$$-\sinh^{-1} \frac{(c-x)}{\sqrt{(b+y)^2 + z^2}} - \sinh^{-1} \frac{(a+x)}{\sqrt{(b+y)^2 + z^2}}$$
(57)

and differentiation with respect to z leads to the equation

$$-\frac{\partial \varphi}{\partial z} = \tan^{-1} \frac{(a-x)(b-y)}{z\sqrt{(a-x)^2 + (b-y)^2 + z^2}} + \tan^{-1} \frac{(a-x)(b+y)}{z\sqrt{(a-x)^2 + (b+y)^2 + z^2}} + \tan^{-1} \frac{(a+x)(b-y)}{z\sqrt{(a+x)^2 + (b+y)^2 + z^2}}$$

$$+ \tan^{-1} \frac{(a+x)(b-y)}{z\sqrt{(a+x)^2 + (b-y)^2 + z^2}} + \tan^{-1} \frac{(a+x)(b+y)}{z\sqrt{(a+x)^2 + (b+y)^2 + z^2}}$$
 (58)

Programming

SUBROUTINE RPLTP (AA, AB, AX, AY, AZ, FP)

FORTRAN SUBROUTINE FOR POTENTIAL OF RECTANGULAR PLATE

The half-length a of the plate is given in argument A, the half-breadth b of the

The half-length a of the plate is given in argument A, the half-breadth b of the plate is given in argument AB, and the Cartesian coordinates x, y, z of the field point are given in the arguments AX, AY, AZ. The potential of the plate is stored in function A is A.

SUBROUTINE RPLTO (AA, AB, AX, AY, AZ, FO)

PODTDAN CUIDDAUTINE EAD CALID ANGLE OF DECTANGULAD DIATE

FORTRAN SUBROUTINE FOR SOLID ANGLE OF RECTANGULAR PLATE

The half-length α of the plate is given in argument AA, the half-breadth b of the plate is given in argument AB, and the Cartesian coordinates x, y, z of the field point are given in the arguments AX, AY, AZ. The solid angle of the plate is stored in function FO.

NONUNIFORM PLATE

Analysis

The potential of the uniform rectangular plate is given by the equation

$$\varphi = \int_{-b-v}^{+b-y} \int_{-a-x}^{+a-x} \frac{du \, dv}{\sqrt{u^2 + v^2 + z^2}}$$
 (59)

and the derivatives of the potential are given by the equations

$$-\frac{\partial \varphi}{\partial x} = -\int_{-b-y}^{+b-y} \int_{-a-x}^{+a-x} \frac{u \, du \, dv}{\{u^2 + v^2 + z^2\}^{\frac{3}{2}}}$$
 (60)

$$-\frac{\partial \varphi}{\partial y} = -\int_{-b-y}^{+b-y} \int_{-a-x}^{+a-x} \frac{v \, du \, dv}{\{u^2 + v^2 + z^2\}^{\frac{3}{2}}}$$
 (61)

$$-\frac{\partial \varphi}{\partial z} = + \int_{-\mathbf{b}-\mathbf{y}}^{+\mathbf{b}-\mathbf{y}} \int_{-\mathbf{a}-\mathbf{x}}^{+\mathbf{a}-\mathbf{x}} \frac{z \, du \, dv}{\{u^2 + v^2 + z^2\}^{\frac{3}{2}}}$$
 (62)

If the surface density of the rectangular plate can be expressed as a polynomial in the powers of x + u and y + v, then the potential of the nonuniform plate and its derivatives are expressible in terms of members of a family of integrals of which the integral

$$\int_{-b-y}^{+b-y} \int_{-a-x}^{+a-x} \frac{(x+u)^m (y+v)^n}{\{u^2+v^2+z^2\}^{\frac{3}{2}}} du dv$$
 (63)

is the m, nth member.

Integrations of lowest degree with respect to u are given by the equations

$$\int \frac{du}{\{u^2 + v^2 + z^2\}^{\frac{3}{2}}} = \frac{u}{(z^2 + v^2)\sqrt{u^2 + v^2 + z^2}}$$
(64)

$$\int \frac{(x+u)du}{\{u^2+v^2+z^2\}^{\frac{3}{2}}} = \frac{xu}{(z^2+v^2)\sqrt{u^2+v^2+z^2}} - \frac{1}{\sqrt{u^2+v^2+z^2}}$$
(65)

$$\int \frac{(x+u)^2 du}{\{u^2+v^2+z^2\}^{\frac{3}{2}}} = \frac{x^2 u}{(z^2+v^2)\sqrt{u^2+v^2+z^2}} - \frac{2x+u}{\sqrt{u^2+v^2+z^2}} + \sinh^{-1}\frac{u}{\sqrt{z^2+v^2}}$$
(66)

Integrations of higher degree are given by the recurrence equation

$$\int \frac{(x+u)^{m}du}{\{u^{2}+v^{2}+z^{2}\}^{\frac{3}{2}}} = \frac{(x+u)^{m-1}}{(m-2)\sqrt{u^{2}+v^{2}+z^{2}}} + \frac{(2m-3)}{(m-2)} x \int \frac{(x+u)^{m-1}du}{\{u^{2}+v^{2}+z^{2}\}^{\frac{3}{2}}} - \frac{(m-1)}{(m-2)} (x^{2}+v^{2}+z^{2}) \int \frac{(x+u)^{m-2}du}{\{u^{2}+v^{2}+z^{2}\}^{\frac{3}{2}}}$$
(67)

Inasmuch as the square of v satisfies the identity

$$x^{2} + v^{2} + z^{2} = x^{2} + y^{2} + z^{2} - 2y(y + v) + (y + v)^{2}$$
 (68)

it follows that the recurrence equation replaces the integrals of lowest degree by the products of power polynomials in $y+\nu$ and the three basic functions

$$\frac{u}{(z^2+v^2)\sqrt{u^2+v^2+z^2}}, \qquad \frac{1}{\sqrt{u^2+v^2+z^2}}, \qquad \sinh^{-1}\frac{u}{\sqrt{z^2+v^2}}$$
(69)

Thus integration with respect to v is completed with the aid of three sets of integrals. The integrations of lowest degree with respect to v for the first set are given by the equations

$$u \int \frac{dv}{(z^2 + v^2)\sqrt{u^2 + v^2 + z^2}} = \frac{1}{z} \tan^{-1} \frac{uv}{z\sqrt{u^2 + v^2 + z^2}}$$
 (70)

$$u \int \frac{(y+v)dv}{(z^2+v^2)\sqrt{u^2+v^2+z^2}} = \frac{y}{z} \tan^{-1} \frac{uv}{z\sqrt{u^2+v^2+z^2}} + \frac{1}{2} \log \frac{\sqrt{u^2+v^2+z^2}-u}{\sqrt{u^2+v^2+z^2}+u}$$
(71)

while the integrals of higher degree are generated by the recurrence equation

$$u \int \frac{(y+v)^{n}dv}{(z^{2}+v^{2})\sqrt{u^{2}+v^{2}+z^{2}}} = u \int \frac{(y+v)^{n-2}dv}{\sqrt{u^{2}+v^{2}+z^{2}}} + 2yu \int \frac{(y+v)^{n-1}dv}{(z^{2}+v^{2})\sqrt{u^{2}+v^{2}+z^{2}}} - (y^{2}+z^{2})u \int \frac{(y+v)^{n-2}dv}{(z^{2}+v^{2})\sqrt{u^{2}+v^{2}+z^{2}}}$$
(72)

This recurrence is cycled in the direction of ascending degree if the arguments satisfy the stability criterion

$$(y^2 + z^2) \le 3(y + v)^2 \tag{73}$$

Otherwise the recurrence is cycled in the direction of descending degree as expressed by the equation

$$u \int \frac{(y+v)^{n}dv}{(z^{2}+v^{2})\sqrt{u^{2}+v^{2}+z^{2}}} = \frac{u}{y^{2}+z^{2}} \int \frac{(y+v)^{n}dv}{\sqrt{u^{2}+v^{2}+z^{2}}} + \frac{2yu}{y^{2}+z^{2}} \int \frac{(y+v)^{n+1}dv}{(z^{2}+v^{2})\sqrt{u^{2}+v^{2}+z^{2}}} - \frac{u}{y^{2}+z^{2}} \int \frac{(y+v)^{n+2}dv}{(z^{2}+v^{2})\sqrt{u^{2}+v^{2}+z^{2}}}$$

$$(74)$$

The integrations of lowest degree with respect to v for the second set are given by the equations

$$\int \frac{dv}{\sqrt{u^2 + v^2 + z^2}} = \sinh^{-1} \frac{v}{\sqrt{u^2 + z^2}}$$
 (75)

$$\int \frac{(y+v)dv}{\sqrt{u^2+v^2+z^2}} = y \sinh^{-1} \frac{v}{\sqrt{u^2+z^2}} + \sqrt{u^2+v^2+z^2}$$
 (76)

while the integrals of higher degree are generated by the recurrence equation

$$\int \frac{(y+v)^n dv}{\sqrt{u^2+v^2+z^2}} = \frac{(y+v)^{n-1}}{n} \sqrt{u^2+v^2+z^2} + \frac{(2n-1)}{n} y \int \frac{(y+v)^{n-1} dv}{\sqrt{u^2+v^2+z^2}} - \frac{(n-1)}{n} (u^2+y^2+z^2) \int \frac{(y+v)^{n-2} dv}{\sqrt{u^2+v^2+z^2}}$$
(77)

This recurrence is cycled in the direction of ascending degree if the arguments satisfy the stability criterion

$$(u^2 + y^2 + z^2) \le 3(y + v)^2 \tag{78}$$

Otherwise the recurrence is cycled in the direction of descending degree as expressed by the equation

$$\int \frac{(y+v)^{n}dv}{\sqrt{u^{2}+v^{2}+z^{2}}} = \frac{(y+v)^{n+1}}{(n+1)(u^{2}+y^{2}+z^{2})} \sqrt{u^{2}+v^{2}+z^{2}} + \frac{(2n+3)y}{(n+1)(u^{2}+y^{2}+z^{2})} \int \frac{(y+v)^{n+1}dv}{\sqrt{u^{2}+v^{2}+z^{2}}} - \frac{(n+2)}{(n+1)(u^{2}+y^{2}+z^{2})} \int \frac{(y+v)^{n+2}dv}{\sqrt{u^{2}+v^{2}+z^{2}}}$$

$$(79)$$

The integration of lowest degree with respect to v for the third set is given by the equation

$$\int \sinh^{-1} \frac{u}{\sqrt{z^2 + v^2}} dv = v \sinh^{-1} \frac{u}{\sqrt{z^2 + v^2}} + u \int \frac{dv}{\sqrt{u^2 + v^2 + z^2}} - z^2 u \int \frac{dv}{(z^2 + v^2)\sqrt{u^2 + v^2 + z^2}} (80)$$

while the integrals of higher degree are generated by the recurrence equation

$$\int (y+v)^{n} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} dv = \frac{(z^{2}+v^{2})(y+v)^{n-1}}{(n+1)} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} + \frac{u}{(n+1)} \int \frac{(y+v)^{n} dv}{\sqrt{u^{2}+v^{2}+z^{2}}} - \frac{yu}{(n+1)} \int \frac{(y+v)^{n-1} dv}{\sqrt{u^{2}+v^{2}+z^{2}}} + \frac{2ny}{(n+1)} \int (y+v)^{n-1} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} dv - \frac{(n-1)}{(n+1)} (y^{2}+z^{2}) \int (y+v)^{n-2} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} dv$$
(81)

This recurrence is cycled in the direction of ascending degree if the arguments satisfy the stability criterion

$$(y^2 + z^2) \le 3(y + v)^2 \tag{82}$$

Otherwise the recurrence is cycled in the direction of descending degree as expressed by the equation

$$\int (y+v)^{n} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} dv = \frac{(z^{2}+v^{2})(y+v)^{n+1}}{(n+1)(y^{2}+z^{2})} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}}$$

$$-\frac{yu}{(n+1)(y^{2}+z^{2})} \int \frac{(y+v)^{n+1}dv}{\sqrt{u^{2}+v^{2}+z^{2}}}$$

$$+\frac{u}{(n+1)(y^{2}+z^{2})} \int \frac{(y+v)^{n+2}dv}{\sqrt{u^{2}+v^{2}+z^{2}}}$$

$$+\frac{2(n+2)y}{(n+1)(y^{2}+z^{2})} \int (y+v)^{n+1} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} dv$$

$$-\frac{(n+3)}{(n+1)(y^{2}+z^{2})} \int (y+v)^{n+2} \sinh^{-1} \frac{u}{\sqrt{z^{2}+v^{2}}} dv \quad (83)$$

The cycling of each recurrence equation in the direction of descending degree is started at the 64th integral in order to achieve full accuracy at the lowest degree. Validity of all formulae for indefinite integrals may be verified directly by differentiation.

Definite integrals are evaluated by an external subroutine which refers to an internal subroutine for the evaluation of indefinite integrals. References are made to the internal subroutine with arguments set equal to the limits of integration. The definite integrals are stored in a matrix. Accuracy of computation can be verified by comparisons

between evaluations by subroutine and high-order numerical integrations, if the value of z is not too small.

If the arguments satisfy the inequality

$$x^2 + y^2 + z^2 \ge 2(a^2 + b^2) \tag{84}$$

then the integrals are evaluated with 16-point Gaussian integration. The m, nth member of the family of integrals,

$$\int_{-b}^{+b} \int_{-a}^{+a} \frac{u^m v^n \, du \, dv}{\{(u-x)^2 + (v-y)^2 + z^2\}^{\frac{3}{2}}} \tag{85}$$

is derived through change of variable from x + u to u and from y + v to v.

Programming

SUBROUTINE RPLTM (AA, AB, NA, NB, AX, AY, AZ, FM)

FORTRAN SUBROUTINE FOR POWER INTEGRATION OVER RECTANGULAR PLATE

The half-length a of the plate is given in argument AA, and the half-breadth b of the plate is given in argument AB. The number of powers m of x+u is given in the argument NA, and the number of powers n of y+v is given in the argument NB. The Cartesian coordinates x, y, z of the field point are given in the arguments AX, AY, AI. The subroutine constructs three arrays of integrals with respect to v, then synthesizes polynomials to complete integration with respect to u. The definite integrals are stored in the $m \times n$ matrix FM. The maximum order of matrix is limited to 32×32 .

SPHERICAL POLAR COORDINATES

Analysis

Let x,y,z be the Cartesian coordinates of a point in space and let i,j,k be unit vectors in the directions of increasing x,y,z. Let r,θ,ϕ be spherical polar coordinates and let $\epsilon_1,\epsilon_2,\epsilon_3$ be unit vectors in the directions of increasing r,θ,ϕ . The Cartesian coordinates are expressed in terms of the spherical polar coordinates by the equations

$$x = r \sin \theta \cos \phi \tag{86}$$

$$y = r \sin \theta \sin \phi \tag{87}$$

$$z = r \cos \theta \tag{88}$$

The spherical polar coordinates are expressed in terms of the Cartesian coordinates

by the equations

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$$r = \sqrt{x^2 + y^2 + z^2} \tag{89}$$

$$\theta = \tan^{-1} \frac{\sqrt{x^2 + y^2}}{z} \tag{90}$$

$$\phi = \tan^{-1} \frac{y}{x} \tag{91}$$

The position vector r is given by the equation

$$\mathbf{r} = r \sin \theta \cos \phi \,\mathbf{i} + r \sin \theta \sin \phi \,\mathbf{j} + r \cos \theta \,\mathbf{k} \tag{92}$$

and the differential element of volume is given by the equation

$$|d\mathbf{r}| = r^2 \sin\theta \, dr \, d\theta \, d\phi \tag{93}$$

The unit vectors $\epsilon_1,\epsilon_2,\epsilon_3$ are expressed in terms of the unit vectors i,j,k by the equations

$$\epsilon_1 = \sin \theta \cos \phi \, \mathbf{i} + \sin \theta \sin \phi \, \mathbf{j} + \cos \theta \, \mathbf{k}$$
 (94)

$$\epsilon_{2} = \cos\theta\cos\phi \,\mathbf{i} + \cos\theta\sin\phi \,\mathbf{j} - \sin\theta \,\mathbf{k} \tag{95}$$

$$\mathbf{\epsilon_3} = -\sin\phi \,\mathbf{i} + \cos\phi \,\mathbf{j} \tag{96}$$

The unit vectors i, j, k are expressed in terms of the unit vectors $\epsilon_1, \epsilon_2, \epsilon_3$ by the equations

$$\mathbf{i} = \sin\theta\cos\phi\,\,\mathbf{\epsilon_1} + \cos\theta\cos\phi\,\,\mathbf{\epsilon_2} - \sin\phi\,\,\mathbf{\epsilon_3} \tag{97}$$

$$\mathbf{j} = \sin\theta \sin\phi \, \mathbf{\epsilon}_1 + \cos\theta \sin\phi \, \mathbf{\epsilon}_2 + \cos\phi \, \mathbf{\epsilon}_3 \tag{98}$$

$$\mathbf{k} = \cos \theta \, \mathbf{\epsilon_1} - \sin \theta \, \mathbf{\epsilon_2} \tag{99}$$

The unit vectors are right-handed and orthogonal. Any vector or tensor invariant can be referred interchangeably to either set of unit vectors. The components of the invariant are derived from the scalar products of the invariant with the unit vectors Let ψ be a function of r, θ, ϕ as expressed by the equation

$$\psi = f(r, \theta, \phi) \tag{100}$$

The gradient $\nabla \psi$ is expressed by the equation

$$\nabla \psi = \epsilon_1 \frac{\partial \psi}{\partial r} + \frac{\epsilon_2}{r} \frac{\partial \psi}{\partial \theta} + \frac{\epsilon_3}{r \sin \theta} \frac{\partial \psi}{\partial \phi}$$
 (101)

The gradient of the gradient $\nabla\nabla\psi$ has the matrix

$$\nabla\nabla\psi = \begin{bmatrix} \frac{\partial^{2}\psi}{\partial r^{2}} & \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial\psi}{\partial\theta}\right) & \frac{\partial}{\partial r} \left(\frac{1}{r\sin\theta} \frac{\partial\psi}{\partial\phi}\right) \\ \frac{\partial}{\partial r} \left(\frac{1}{r} \frac{\partial\psi}{\partial\theta}\right) & \frac{1}{r} \frac{\partial\psi}{\partial r} + \frac{1}{r^{2}} \frac{\partial^{2}\psi}{\partial\theta^{2}} & \frac{\partial}{\partial\theta} \left(\frac{1}{r^{2}\sin\theta} \frac{\partial\psi}{\partial\phi}\right) \\ \frac{\partial}{\partial r} \left(\frac{1}{r\sin\theta} \frac{\partial\psi}{\partial\phi}\right) & \frac{\partial}{\partial\theta} \left(\frac{1}{r^{2}\sin\theta} \frac{\partial\psi}{\partial\phi}\right) & \frac{1}{r} \frac{\partial\psi}{\partial r} + \frac{\cos\theta}{r^{2}\sin\theta} \frac{\partial\psi}{\partial\theta} + \frac{1}{r^{2}\sin^{2}\theta} \frac{\partial^{2}\psi}{\partial\phi^{2}} \end{bmatrix}$$
(102)

The trace of the matrix is the Laplacian,

$$\nabla \cdot \nabla \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2}$$
(103)

Laplace's equation is

$$\nabla \cdot \nabla \psi = 0 \tag{104}$$

It may be solved by the method of separation of variables.

Let ψ be represented by $R\Theta\Phi$ where R is a function of r alone, Θ is a function of θ alone, and Φ is a function of ϕ alone. Substitution in Laplace's equation shows that the factors are solutions of ordinary differential equations which are linked together through arbitrary constants n, m. The constants n, m must be integers in order that the functions shall be cyclical with respect to θ, ϕ .

The equation for R is

$$\frac{1}{r^2R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{n(n+1)}{r^2} = 0 \tag{105}$$

The function R is any linear combination of the functions

$$\frac{1}{r^{n+1}} \tag{106}$$

The first derivatives of the functions are given by the equations

$$\frac{d}{dr}(r^n) = nr^{n-1} \tag{107}$$

$$\frac{d}{dr}\left(\frac{1}{r^{n+1}}\right) = -\frac{(n+1)}{r^{n+2}}\tag{108}$$

and the second derivatives of the functions are given by the equations

$$\frac{d^2}{dr^2}(r^n) = n(n-1)r^{n-2} \tag{109}$$

$$\frac{d^2}{dr^2}\left(\frac{1}{r^{n+1}}\right) = +\frac{(n+1)(n+2)}{r^{n+3}} \tag{110}$$

The equation for 9 is

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$$\frac{1}{\sin\theta} \frac{d}{\theta} \left(\sin\theta \frac{d\theta}{d\theta} \right) + n(n+1) - \frac{m^2}{\sin^2\theta} = 0$$
 (111)

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The function 0 is any linear combination of the functions

$$P_n^m(\cos\theta) \qquad \qquad Q_n^m(\cos\theta) \qquad (112)$$

where $P_n^m(\cos\theta)$ is an associated Legendre function of the first kind and $Q_n^m(\cos\theta)$ is an associated Legendre function of the second kind. The associated functions are defined in terms of the regular functions by the equations

$$P_n^m(\cos\theta) = \sin^m\theta \, \frac{d^m P_n(\cos\theta)}{d(\cos\theta)^m} \tag{113}$$

$$Q_n^m(\cos\theta) = \sin^m\theta \, \frac{d^mQ_n(\cos\theta)}{d(\cos\theta)^m} \tag{114}$$

An analysis of Legendre functions is given in Appendix A. The function $P_n(\cos\theta)$ is expressed by the Rodrigues formula

$$P_n(\cos\theta) = \frac{(-1)^n}{2^n n!} \frac{d^n \sin^{2n}\theta}{d(\cos\theta)^n}$$
 (115)

The function $P_n(\cos \theta)$ is a power polynomial of the *n*th degree in $\cos \theta$. The function $Q_n(\cos \theta)$ is given by the equation

$$Q_{n}(\cos\theta) = \frac{1}{2}P_{n}(\cos\theta)\log\left(\frac{1+\cos\theta}{1-\cos\theta}\right) - W_{n-1}(\cos\theta)$$
 (116)

where $W_{n-1}(\cos\theta)$ is a polynomial of degree n-1 in $\cos\theta$. The functions of the first kind are finite everywhere whereas the functions of the second kind have logarithmic singularities at the poles. When $\sin\theta$ approaches zero the associated functions of the first kind approach zero like $\sin^m\theta$ whereas the associated functions of the second kind approach infinity like $\csc^m\theta$. When $\sin\theta$ is not zero both functions with increasing n approach asymptotic values where the ratio between the amplitude of the second kind and the amplitude of the first kind is $\frac{1}{2}\pi$.

The functions of lowest order are relatively simple and the functions of progressively higher order may be generated from them with the aid of three-term recurrence equations. When an error has been introduced into the recurrence at the kth cycle, it may be represented by a linear combination of P_n^m and Q_n^m such that the error is equal to zero for the (k-1)th cycle but is equal to ϵ for the kth cycle. Application of the recurrence equations to the linear combination of P_n^m and Q_n^m changes progressively the order of each term. If the recurrence is used to generate P_n^m , then the recurrence must be cycled in that direction in which the ratio Q_n^m/P_n^m decreases, or if the recurrence is used to generate Q_n^m , then the recurrence must be cycled in that direction in which the ratio P_n^m/Q_n^m decreases. Otherwise the relative rounding error will not remain bounded.

The functions of lowest order are given by the equations

$$P_0 = 1 \qquad \qquad Q_0 = P_0 Q_0 = \frac{1}{2} \log \left(\frac{1 \cdot \cos \theta}{1 \cdot \cos \theta} \right) \tag{117}$$

$$P_1 = \cos \theta \qquad \qquad Q_1 = P_1 Q_0 - 1 \tag{118}$$

The functions for m = 0 then satisfy the recurrence equations

$$nP_{n-1} - (2n+1)\cos\theta P_n + (n+1)P_{n+1} = 0$$
 (119)

$$nQ_{n-1} - (2n+1)\cos\theta Q_n + (n+1)Q_{n+1} = 0$$
 (120)

Except for the logarithmic singularity in Q_n the regular functions do not differ greatly in magnitude and both recurrences may be cycled in the direction of increasing n. The associated functions satisfy the recurrence equations

$$(n+m)P_{n-1}^{m} - (2n+1)\cos\theta P_{n}^{m} + (n-m+1)P_{n+1}^{m} = 0$$
 (121)

$$(n+m)Q_{n-1}^m - (2n+1)\cos\theta Q_n^m + (n-m+1)Q_{n+1}^m = 0$$
 (122)

The recurrence becomes more sensitive to direction with increase in m and must be cycled toward increasing n for P_n^m but toward decreasing n for Q_n^m . In the case of P_n^m the recurrence is started with the equations

$$P_{m-1}^{m}(\cos\theta) = 0 \tag{123}$$

$$P_m^m(\cos\theta) = \frac{(2m)!}{2^m m!} \sin^m\theta \tag{124}$$

and then the functions are generated at constant m for progressively increasing n. If $\sin\theta$ is very small, and m is very large the value of P_m^m can be below the index range of the computer. Such a situation is avoided when the recurrence is applied to the derivatives of P_n prior to multiplication by the powers of $\sin\theta$.

The functions with common n satisfy the recurrence equations

$$(n+m)(n-m+1)P_n^{m-1} - 2m \frac{\cos \theta}{\sin \theta} P_n^m + P_n^{m-1} = 0$$
 (125)

$$(n+m)(n-m+1)Q_n^{m-1} - 2m \frac{\cos \theta}{\sin \theta} Q_n^m + Q_n^{m+1} = 0$$
 (126)

which must be cycled toward decreasing m for P_n^m but toward increasing m for Q_n^m . In the case of Q_n^m initial values are derived from Q_0, Q_1 , through the use of the recurrence equations

$$nQ_{n+1} - (2n+1)\cos\theta Q_n + (n+1)Q_{n+1} = 0$$
 (127)

$$Q_{n-1}^1 + (2n+1)\sin\theta Q_n - Q_{n+1}^1 = 0 \tag{128}$$

and then the functions are generated at constant n for progressively increasing m. The associated function of the first kind is defined by the equation

$$P_n^m(\cos\theta) = \sin^m\theta \, \frac{d^m P_n(\cos\theta)}{d(\cos\theta)^m} \tag{129}$$

The first derivative of the associated function is given by the equation

$$\frac{dP_n^m}{d\theta} = m \sin^{m-1}\theta \cos\theta \frac{d^m P_n}{d(\cos\theta)^m} - \sin^{m+1}\theta \frac{d^{m+1} P_n}{d(\cos\theta)^{m+1}} \tag{130}$$

and the second derivative of the associated function is given by the equation

$$\frac{d^{2}P_{n}^{m}}{d\theta^{2}} = m(m-1)\sin^{m-2}\theta \frac{d^{m}P_{n}}{d(\cos\theta)^{m}} + \{m-n(n+1)\}\sin^{m}\theta \frac{d^{m}P_{n}}{d(\cos\theta)^{m}} + \sin^{m}\theta\cos\theta \frac{d^{m+1}P_{n}}{d(\cos\theta)^{m+1}} \tag{131}$$

Other derivatives which are important for the computation of space invariants are given by the equation

$$m\frac{d}{d\theta}\left(\frac{P_n^m}{\sin\theta}\right) = m(m-1)\sin^{m-2}\theta\cos\theta \frac{d^m P_n}{d(\cos\theta)^m} - m\sin^m\theta \frac{d^{m+1}P_n}{d(\cos\theta)^{m+1}}$$
(132)

and by the equation

$$-\frac{m^2 P_n^m}{\sin^2 \theta} + \frac{\cos \theta}{\sin \theta} \frac{d P_n^m}{d \theta} = -m(m-1) \sin^{m-2} \theta \frac{d^m P_n}{d(\cos \theta)^m}$$
$$-m \sin^m \theta \frac{d^m P_n}{d(\cos \theta)^m}$$
$$-\sin^m \theta \cos \theta \frac{d^{m+1} P_n}{d(\cos \theta)^{m+1}}$$
(133)

Wherever negative powers of $\sin\theta$ appear in the formulae they are multiplied by zero. The equation for Φ is

$$\frac{1}{\varphi} \frac{d^2 \varphi}{d \varphi^2} + m^2 = 0 \tag{134}$$

The function Φ is any linear combination of the functions

$$\cos m\phi$$
 $\sin m\phi$ (135)

The first derivatives of the functions are given by the equations

$$\frac{d\cos m\phi}{d\phi} = -m\sin m\phi \tag{136}$$

$$\frac{d\sin m\phi}{d\phi} = + m\cos m\phi \tag{137}$$

and the second derivatives of the functions are given by the equations

$$\frac{d^2 \cos m\phi}{d\phi^2} = -m^2 \cos m\phi \tag{138}$$

$$\frac{d^2 \sin m\phi}{d\phi^2} = -m^2 \sin m\phi \tag{139}$$

Let ψ be expressed by the equation

$$\psi = \sum \frac{c_n^m}{r^{n+1}} P_n^m(\cos \theta) e^{im\phi}$$
 (140)

All m derivatives of $P_n(\cos\theta)$ are computed and are stored in an array. Initial summations with respect to n establish five arrays with the elements

$$\sum \frac{c_n^m}{r^{n+1}} \frac{d^m P_n(\cos \theta)}{d(\cos \theta)^m} \tag{141}$$

$$\sum \frac{nc_n^m}{r^{n+1}} \frac{d^m P_n(\cos \theta)}{d(\cos \theta)^m}$$
 (142)

$$\sum \frac{n^2 c_n^m}{r^{n+1}} \frac{d^m P_n(\cos \theta)}{d(\cos \theta)^m} \tag{143}$$

$$\sum \frac{c_n^m}{r^{n+1}} \frac{d^{m+1} P_n(\cos \theta)}{d(\cos \theta)^{m+1}}$$
 (144)

$$\sum \frac{nc_n^m}{r^{n+1}} \frac{d^{m+1}P_n(\cos\theta)}{d(\cos\theta)^{m+1}} \tag{145}$$

Final summations with respect to m consist of complex polynomial evaluations in powers of the argument $\sin\theta~e^{i\phi}$.

Programming

SUBROUTINE SPHPDV (MO, AR, AQ, AF, NC, SC, CC, RP, PF, DF, DD)

FORTRAN SUBROUTINE FOR SPHERICAL POTENTIAL AND ANGULAR DERIVATIVES

The mode of operation is given by MO. The radius r is given in the argument AR, the polar angle θ is given in the argument AQ, and the azimuth angle ϕ is given in the argument AF. The order of the matrices of coefficients is given in argument NC, the matrix of coefficients for $\sin m\phi$ is given in the array SC, and the matrix of coefficients for $\cos m\phi$ is given in the array CC. The matrix of Legendre functions is stored in the array RP. In each matrix the rows are numbered in the direction of increasing n and the columns are numbered in the direction of increasing m. The upper right-hand half of each matrix is padded out with zeros. The potential φ is stored in the function PF if the mode of operation MO is 0. The potential and the first derivatives $\partial \varphi$ $\partial \theta$, $\partial \varphi/\partial \phi$ are stored in the function PF and in the 2-array DF when the mode of operation MO is 1. The potential, the first derivatives, and the second derivatives $\partial^2 \varphi/\partial \theta^2$, $\partial^2 \varphi/\partial \theta \partial \phi$. $\partial^2 \varphi/\partial \theta \partial \phi$ are stored in the function PF, in the 2-array DF, and in the 3-array SD when the mode of operation MO is 2.

FORTRAN SUBROUTINE FOR SPHERICAL POTENTIAL AND SPACE GRADIENTS

The mode of operation is given by MO. The radius r is given in the argument AR, the polar angle θ is given in the argument AQ, and the azimuth angle ϕ is given in the argument AF. The order of the matrices of coefficients is given in the argument NC, the matrix of coefficients for $\sin m\phi$ is given in the array SC, and the matrix of coefficients for $\cos m\phi$ is given in the array CC. The matrix of Legendre functions is stored in the array RP. In each matrix the rows are numbered in the direction of increasing n and the columns are numbered in the direction of increasing m. The upper right-hand half of each matrix is padded out with zeros. The potential φ is stored in the function PF if the mode of operation MO is 0. The potential and the gradient $\nabla \varphi$ are stored in the function PF, and in the 3-array GF when the mode of operation MO is 1. The potential, the gradient, and the gradient of the gradient $\nabla \nabla \varphi$ are stored in the function PF, in the 3-array GF, and in the 9-array DF when the mode of operation MO is 2.

ERROR FUNCTION

Analysis

The error function $\operatorname{erf} z$ is defined by the equation

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \int_0^z e^{-u^2} du \tag{146}$$

The Dawson integral H(z) is defined by the equation

$$H(z) = \int_0^z e^{u^2} du \tag{147}$$

and is expressed in terms of the error function by the equation

$$H(z) = -i\frac{\sqrt{\pi}}{2}\operatorname{erf}(+iz) \tag{148}$$

The conventional Fresnel integrals C(v) and S(v) are defined by the equation

$$C(v) + iS(v) = \int_0^v e^{i\frac{1}{2}\pi u^2} du$$
 (149)

and are expressed in terms of the error function by the equation

$$C(v) + iS(v) = \frac{1+i}{2} \operatorname{erf}\left(\frac{1-i}{2}\sqrt{\pi}v\right)$$
 (150)

Expansion of the exponential function in series and term by term integration leads to the equation

$$\operatorname{erf} z = \frac{2}{\sqrt{\pi}} \sum_{m=0}^{\infty} \frac{(-1)^m z^{2m+1}}{(2m+1)m!}$$
 (151)

which expresses the error function as an absolutely convergent ascending series. The complex Fresnel integral is defined by the equation

$$E(z) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{z} \frac{e^{t}}{t^{\frac{1}{2}}} dt$$
 (152)

where the path of integration lies within that part of the complex plane from which the positive real axis is excluded. The phase of z is limited to the range 0 to 2π , and the phase of $z^{1/2}$ is half the phase of z. There are convergent series, rational approximations, and asymptotic series for the complex Fresnel integral. The convergent series is given by the equation

$$E(z) = -\frac{i}{\sqrt{2}} + \left(\frac{2z}{\pi}\right)^{\frac{1}{2}} \sum_{m=0}^{\infty} \frac{z^m}{(2m+1)m!}$$
 (153)

The substitution $z \to -z^2$ converts the series for Fresnel integral into the series for error function as expressed by the equation

$$\operatorname{erf} z = 1 - i\sqrt{2}E(-z^2) \tag{154}$$

If the argument x + iy satisfies the inequality

$$x^2 + y^2 \le 1 \tag{155}$$

or both of the inequalities

$$1 < x^2 + y^2 < 38 x^2 - y^2 + 0.256 x^2 y^2 \le 0 (156)$$

then the error function is computed with the ascending series.

If the argument x + iy satisfies both of the inequalities

$$1 < x^2 + y^2 < 38 x^2 - y^2 + 0.256 x^2 y^2 > 0 (157)$$

then the error function is computed with the rational approximation of the Fresnel integral. The error function is expressed by the equation

erf
$$z = 1 - \frac{ze^{-z^2}}{\sqrt{\pi}} \sum_{i=1}^{18} \frac{\epsilon_i}{z^2 + \delta_i}$$
 (158)

where the phase of z is limited to the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, and the positions δ_i and the residues ϵ_i are for the approximation of the Fresnel integral by sets of poles.

If the argument x + iy satisfies the inequality

$$x^2 + y^2 \ge 38 \tag{159}$$

then the error function is computed from the asymptotic series. Repeated integration by parts leads to the equation

erf
$$z = 1 - \frac{e^{-z^2} \sum_{m=0}^{N-1} \frac{(-1)^m (2m)!}{2^{2m} m! z^{2m+1}}$$
 (160)

for which the phase of z is limited to the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, and $N \le 38$.

Extension of the range of phase beyond these limits is accomplished with the aid of the equation

$$\operatorname{erf}(z) = \operatorname{erf}(z) \tag{161}$$

which expresses the symmetry of the error function.

Programming

SUBROUTINE CERF (MO, AZ, EF)

FORTRAN SUBROUTINE FOR COMPLEX ERROR FUNCTION

The mode of operation is given in MO. The real and imaginary parts of argument z are given in array AZ. The complex error function is computed by series expansions and rational approximations. If MO = 0, the real and imaginary parts of the function erf z are stored in array EF. If MO = 1, and the phase of z is in the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, the real and imaginary parts of the function $1 - \operatorname{erf} z$ are stored in array EF.

COMPLEX GAMMA FUNCTION

Analysis

The gamma function $\Gamma(z)$ is defined by the equation

$$\Gamma(z) = \frac{e^{-\gamma z}}{z} \prod_{n=1}^{\infty} \left[\frac{e^{\frac{z}{n}}}{1 + \frac{z}{n}} \right]$$
 (162)

where γ is Euler's constant. The gamma function has poles at the negative integers such that the residue of the *n*th pole is $(-1)^n/n!$.

For a small argument the reciprocal of the gamma function is given by the Bourguet convergent series and for a large argument the logarithm of the gamma function is given by the Stirling asymptotic series. Intermediate regions can be spanned by recurrence relations. A rational approximation is not necessary.

The gamma function of an argument with a negative real part is expressed in terms of the gamma function of an argument with a positive real part by the reciprocal equation

$$\Gamma(z)\Gamma(1-z) = \frac{\pi}{\sin \pi z} \tag{163}$$

It is necessary to evaluate series expansions only for arguments with positive real parts.

If the argument x + iy satisfies the inequality

$$x^2 + y^2 \le 1 \tag{164}$$

then the gamma function is derived from an ascending power series. The reciprocal of the gamma function is given by the equation

$$\frac{1}{\Gamma(1+z)} = \sum_{m=0}^{\infty} c_m z^m \tag{165}$$

for which the coefficients c_m are derived in Appendix B.

If the argument x + iy satisfies the inequality

$$x^2 + y^2 \ge 32 \tag{166}$$

then the gamma function is computed from a descending power series. From the equations on page 252 of reference 1, the logarithm of the gamma function is given by the equation

$$\log \Gamma(z) = (z - \frac{1}{2}) \log z - z + \frac{1}{2} \log (2\pi) + \sum_{m=1}^{N} \frac{B_{2m}}{2m(2m-1)z^{2m-1}}$$
 (167)

for which the Bernoulli numbers B_{2m} are derived in Appendix B. Summation of the series is continued until there is no change in sum or until m = 18.

If the argument x + iy satisfies the inequality

$$1 < x^2 + y^2 < 32 \tag{168}$$

then the gamma function is computed with the aid of the difference equation

$$\Gamma(1+z)=z\Gamma(z) \tag{169}$$

If n is the integer which is nearest in value to x and if n satisfies the inequality

$$|z-n|^2 \le 1 \tag{170}$$

then the gamma function is given by the equation

$$\Gamma(z) = (z-1)\cdots(z-n+1)\Gamma(z-n+1) \tag{171}$$

for which $\Gamma(z-n+1)$ is evaluated from the convergent series. If n is the smallest integer which satisfies the inequality

$$|z+n|^2 \ge 32 \tag{172}$$

then the gamma function is given by the equation

$$\Gamma(z) = \frac{\Gamma(z+n)}{z\cdots(z+n-1)} \tag{173}$$

for which $\Gamma(z+n)$ is evaluated from the asymptotic series.

Programming

SUBROUTINE CGAMMA (MO, AZ, FG)

FORTRAN SUBROUTINE FOR COMPLEX GAMMA FUNCTION

The mode of operation is given in MO. The real and imaginary parts of the complex argument z are given in array A.T. The complex gamma function is computed by series expansions and recurrence relations. If MO = 0, the real and imaginary parts of the

complex function $\Gamma(z)$ are stored in array °G. If VO = 1, the real and imaginary parts of the complex function $\log \Gamma(z)$ are stored in array FG.

SUBROUTINE DGAMMA (MO, AI, FG)

FORTRAN SUBROUTINE FOR DOUBLE- PRECISION GAMMA FUNCTION

The mode of operation is given in MO. The real and imaginary parts of the

double-precision argument z are given in array AZ. The complex gamma function is computed by series expansions and recurrence relations. If MO = 0, the real and imaginary parts of the double-precision function $\Gamma(z)$ are stored in array FG. If MO = 1, the real and imaginary parts of the double-precision function $\log \Gamma(z)$ are stored in array FG.

COMPLEX DIGAMMA FUNCTION

Analysis

The digamma function $\Psi(z)$ is defined in terms of the gamma function $\Gamma(z)$ and the derivative of the gamma function $\Gamma'(z)$ by the equation

$$\Psi(z) = \frac{\Gamma'(z)}{\Gamma(z)} \tag{174}$$

For a small argument the reciprocal of the gamma function is given by the Bourguet convergent series and for a large argument the logarithm of the gamma function is given by the Stirling asymptotic series. The derivative of the gamma function is derived by differentiation of the series.

The digamma function of an argument with a negative real part is expressed in terms of the digamma function of an argument with a positive real part by the reciprocal equation

$$\Psi(z) = \Psi(1-z) - \pi \cot \pi z \tag{175}$$

It is necessary to evaluate series expansions only for arguments with positive real parts.

If the argument x + iy satisfies the inequality

$$x^2 + y^2 \le 1 \tag{176}$$

then the digamma function is given by the equation

$$\Psi(1+z) = -\Gamma(1+z) \sum_{m=1}^{\infty} m c_m z^{m-1}$$
 (177)

for which the coefficients c_m are derived in Appendix B.

If the argument x + iy satisfies the inequality

$$x^2 + y^2 \ge 32 \tag{178}$$

then the digamma function is given by the equation

$$\Psi(z) = \log z - \frac{\frac{1}{2}}{z} - \sum_{m=1}^{N} \frac{B_{2m}}{2mz^{2m}}$$
 (179)

for which the Bernoulli numbers B_{2m} are derived in Appendix B. Summation of the series is continued until there is no change in sum or until m = 18.

If the argument x + iy satisfies the inequality

$$1 < x^2 + y^2 < 32 \tag{180}$$

then the digamma function is computed with the aid of a difference equation. If n is

the integer which is nearest in value to x and if n satisfies the inequality

$$|z-n|^2 \le 1 \tag{181}$$

then the digamma function is given by the equation

$$\Psi(z) = \frac{1}{z-1} + \dots + \frac{1}{z-n+1} + \Psi(z-n+1)$$
 (182)

for which $\Psi(z-n+1)$ is evaluated from the convergent series. If n is the smallest integer which satisfies the inequality

$$|z+n|^2 \ge 32 \tag{183}$$

then the digamma function is given by the equation

$$\Psi(z) = -\frac{1}{z} - \dots - \frac{1}{z+n-1} + \Psi(z+n)$$
 (184)

for which $\Psi(z+n)$ is evaluated from the asymptotic series.

Programming

SUBROUTINE CPSI (MO, AZ, PS)

FORTRAN SUBROUTINE FOR COMPLEX DIGAMMA FUNCTION

The mode of operation is given in MO. The real and imaginary parts of the argument z are given in array AZ. The complex digamma function is computed by series expansions and recurrence relations. Calls are made when necessary to Subroutine CGAMMA. If MO = 0, the real and imaginary parts of the function $\Gamma'(z)$ are stored in array PS. If MO = 1, the real and imaginary parts of the function $\Psi(z)$ are stored in array PS.

FIRST ORDINARY BESSEL FUNCTION

Analysis

The ordinary Bessel function of the first kind $J_{m{n}}(z)$ is given by the absolutely convergent series in the equation

$$J_n(z) = \sum_{m=0}^{\infty} \frac{(-1)^m (\frac{1}{2}z)^{n+2m}}{m!(n+m)!}$$
 (185)

The convergent series is used if the order and the argument satisfy the criterion

$$|n| \ge \frac{1}{4}|z|^2 \tag{186}$$

A descending recurrence is used to extend the range of orders to lower orders. The Bessel function is given by the equation

$$J_{n}(z) = \frac{i}{\pi} \left\{ e^{\frac{1}{2}n\pi i} K_{n}(iz) - e^{-\frac{1}{2}n\pi i} K_{n}(-iz) \right\}$$
 (187)

in which the modified Bessel functions of the second kind can be expressed by rational

approximations. Thus the Bessel function is given by the equation

$$J_{n}(z) = \frac{1}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{-iz - \delta_{k}} \right\} \left\{ \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) + i\sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$

$$+ \frac{1}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{+iz - \delta_{k}} \right\} \left\{ \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) - i\sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$
 (188)

where the phase of z is limited to the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, and the positions δ_k and the residues ϵ_k are for the approximation of the modified Bessel function by sets of poles. The rational approximation is used if the argument x+iy satisfies the inequalities

$$(x^2 + y^2)^{\frac{1}{2}} \le 17.5 \qquad -|y| + 0.096 \, x^2 > 0 \tag{189}$$

The rational approximation is available for orders 0 and 1.

The Bessel function is given by the equation

$$J_n(z) = \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} \left\{ P_n(z) \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) - Q_n(z) \sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$
(190)

where $P_n(z)$ is the sum of the even-ordered terms and $Q_n(z)$ is the sum of the odd-ordered terms in the asymptotic series in the equation

$$P_n(z) + i Q_n(z) = \sum_{m=0}^{N-1} \frac{\left\{n^2 - \left(\frac{1}{2}\right)^2\right\} \cdots \left\{n^2 - \left(m - \frac{1}{2}\right)^2\right\}}{m!(-2iz)^m}$$
(191)

with $N \le 36$. The asymptotic series is used if the order and the argument satisfy the criterion

$$|z| \ge 17.5 + \frac{1}{2}n^2 \tag{192}$$

An ascending recurrence is used to extend the range of order to larger orders if the order satisfies the criteria

$$|z| \ge 17.5\tag{193}$$

and

$$\sqrt{2(|z|-17.5)} \le |n| \le \frac{1}{2}|z| - \frac{1}{2}|\mathcal{F}m|z| + \frac{1}{2}|\frac{1}{2}|z| - |\mathcal{F}m|z| \tag{194}$$

Otherwise the ascending series is used with a descending recurrence.

Use of the series expansions is limited to positive orders and to arguments with phase in the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$. Extension of ranges of order and phase is accomplished with the aid of the equations

$$J_{-n}(z) = (-1)^n J_n(z) = J_n(-z)$$
(195)

which express the symmetry of the Bessel function.

Programming

SUBROUTINE BSSLJ (AZ, IN, FJ)

FORTRAN SUBROUTINE FOR ORDINARY BESSEL FUNCTION OF INTEGRAL ORDER

The real and imaginary parts of the argument z are given in array A2, and the

integer order n is given in IN. The ordinary Bessel function of the first kind is computed by series expansions and recurrence relations. The real and imaginary parts of the function $J_n(z)$ are stored in array FJ.

SECOND ORDINARY BESSEL FUNCTION

Analysis

The ordinary Bessel function of the second kind $Y_n(z)$ is given by the absolutely convergent series in the equation

$$Y_{n}(z) = -\frac{1}{\pi} \sum_{m=0}^{n-1} \frac{(n-m-1)!}{m!} \left(\frac{1}{2}z\right)^{-n+2m} + \frac{2}{\pi} \sum_{m=0}^{\infty} \left[\gamma + \log(\frac{1}{2}z) - \frac{1}{2} \sum_{k=1}^{m} \frac{1}{k} - \frac{1}{2} \sum_{k=1}^{n+m} \frac{1}{k} \right] \frac{(-1)^{m}(\frac{1}{2}z)^{n+2m}}{m!(n+m)!}$$
(196)

The convergent series is used if the argument x + iy satisfies the inequality

$$x^2 + y^2 \le 1 \tag{197}$$

or both of the inequalities

$$x^2 + y^2 < 289 - |y| + 0.096 x^2 \le 0 (198)$$

The evaluation of the convergent series for $Y_n(z)$ is continued to convergence of the associated series for $J_n(z)$.

The Bessel functions are given by the equations

$$J_{n}(z) = +\frac{i}{\pi} \left\{ e^{\frac{1}{2}n\pi i} K_{n}(iz) - e^{-\frac{1}{2}n\pi i} K_{n}(-iz) \right\}$$
 (199)

$$Y_{n}(z) = -\frac{1}{\pi} \left\{ e^{\frac{1}{2}n\pi i} K_{n}(iz) + e^{-\frac{1}{2}n\pi i} K_{n}(-iz) \right\}$$
 (200)

in which the modified Bessel functions of the second kind can be expressed by rational approximations. Thus the Bessel functions are given by the equations

$$J_{n}(z) = + \frac{1}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{-iz - \delta_{k}} \right\} \left\{ \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) + i\sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$

$$+ \frac{1}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{+iz - \delta_{k}} \right\} \left\{ \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) - i\sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$

$$Y_{n}(z) = -\frac{i}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{-iz - \delta_{k}} \right\} \left\{ \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) + i\sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$

$$+ \frac{i}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{+iz - \delta_{k}} \right\} \left\{ \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) - i\sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$

$$(202)$$

where the phase of z is limited to the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, and the positions δ_k and the residues ϵ_k are for the approximation of the modified Bessel function by sets of poles.

The rational approximation is used if the argument x + iy satisfies the inequalities

The rational approximation is available for orders 0 and 1.

The Bessel function is given by the equation

$$Y_n(z) = \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} \left\{ P_n(z) \sin(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) + Q_n(z) \cos(z - \frac{1}{2}n\pi - \frac{1}{4}\pi) \right\}$$
(204)

where $P_n(z)$ is the sum of the even-ordered terms and $Q_n(z)$ is the sum of the odd-ordered terms in the asymptotic series in the equation

$$P_{n}(z) + i Q_{n}(z) = \sum_{m=0}^{N-1} \frac{\{n^{2} - (\frac{1}{2})^{2}\} \cdots \{n^{2} - (m - \frac{1}{2})^{2}\}}{m!(-2iz)^{m}}$$
(205)

with $N \leq 36$. The asymptotic series is used if the argument x + iy satisfies the criterion

$$x^2 + y^2 \ge 289 \tag{206}$$

The rational approximation and the asymptotic approximation are used only for arguments with phase in the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$. Extension of phase to other ranges is accomplished with the aid of the equations

$$Y_n(z) = e^{-n\pi i} Y_n(ze^{-\pi i}) + 2i\cos n\pi J_n(ze^{-\pi i})$$
 (207)

$$Y_n(z) = e^{+n\pi i} Y_n(ze^{+\pi i}) - 2i\cos n\pi J_n(ze^{+\pi i})$$
 (208)

where the first equation is used if z is in the second quadrant and the second equation is used if z is in the third quadrant.

The series evaluations are used only for orders zero and one, and an ascending recurrence is used if the order is greater than one. The extension of order to negative orders is achieved with the aid of the equation

$$Y_{-n}(z) = (-1)^n Y_n(z) \tag{209}$$

which expresses the symmetry of the Bessel function

Programming

SUBROUTINE BSSLY (AZ, IN, FY)

FORTRAN SUBROUTINE FOR ORDINARY BESSEL FUNCTION OF INTEGRAL ORDER

The real and imaginary parts of the argument z are given in array $A\mathbb{Z}$, and the integer order n is given in \mathbb{N} . The ordinary Bessel function of the second kind is computed by series expansions, rational approximations, and recurrence relations. The real and imaginary parts of the function $Y_n(z)$ are stored in array \mathbb{N} .

FIRST MODIFIED BESSEL FUNCTION

Analysis

The modified Bessel function of the first kind $I_n(z)$ is given by the absolutely

convergent series in the equation

$$I_n(z) = \sum_{m=0}^{\infty} \frac{(\frac{1}{2}z)^{n+2m}}{m!(n+m)!}$$
 (210)

The convergent series is used if the order and the argument satisfy the criterion

$$|n| \ge \frac{1}{4}|z|^2 \tag{211}$$

A descending recurrence is used to extend the range of order to lower orders. The Bessel function is given by the equations

$$I_n(z) = +\frac{i}{\pi} \left\{ K_n(ze^{\pi i}) - e^{-n\pi i} K_n(z) \right\}$$
 (212)

$$I_{n}(z) = -\frac{i}{\pi} \left\{ K_{n}(ze^{-\pi i}) - e^{n\pi i} K_{n}(z) \right\}$$
 (213)

where the first equation is used if z is in the fourth quadrant and the second equation is used if z is in the first quadrant. The modified Bessel functions of the second kind can be expressed by rational approximations. Thus the Bessel function is given by the equation

$$I_{n}(z) = \frac{e^{z}}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_{k}}{-z - \delta_{k}} \right\} + \frac{e^{-z \pm n\pi i \pm \frac{1}{2}\pi i}}{(2\pi z)^{\frac{1}{2}}} \left\{ 1 - \sum_{k=1}^{14} \frac{\epsilon_{k}}{z - \delta_{k}} \right\}$$
(214)

where the \pm sign is the same as the sign of y, and the positions δ_k and the residues ϵ_k are for the approximation of the modified Bessel function by sets of poles. The rational approximation is used if the argument x+iy satisfies the inequalities

$$(x^2 + y^2)^{\frac{1}{2}} \le 17.5 \qquad -|x| + 0.096 y^2 > 0$$
 (215)

The rational approximation is available for orders 0 and 1.

The Bessel function is given by the asymptotic series in the equation

$$I_n(z) = \frac{e^z}{(2\pi z)^{\frac{1}{2}}} \sum_{m=0}^{N-1} \frac{\{n^2 - (\frac{1}{2})^2\} \cdots \{n^2 - (m - \frac{1}{2})^2\}}{m!(-2z)^m}$$

$$+\frac{e^{-z\pm n\pi i\pm\frac{1}{2}\pi i}\sum_{m=0}^{N-1}\frac{\{n^2-(\frac{1}{2})^2\}\cdots\{n^2-(m-\frac{1}{2})^2\}}{m!(2z)^m}$$
(216)

for which $N \leq 36$. The asymptotic series is used if the order and the argument satisfy the criterion

$$|z| \ge 17.5 + \frac{1}{2}n^2 \tag{217}$$

An ascending recurrence is used to extend the range of order to larger orders if the order satisfies the criteria

$$|\Re e z| \ge 17.5 \tag{218}$$

and

$$\sqrt{2(|z| + 17.5)} \le |n| \le \frac{1}{2}|z| - \frac{1}{2}|\Re e|z| + \frac{1}{2}|\frac{1}{2}|z| - |\Re e|z|$$
 (219)

Otherwise the ascending series is used with a descending recurrence.

Use of the series expansions is limited to positive orders and to arguments with phase in the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$. Extension of ranges of order and phase is accomplished with the aid of the equations

$$I_{-n}(z) = (-1)^n I_n(-z) = I_n(z)$$
(220)

which express the symmetry of the Bessel function.

Programming

SUBROUTINE BSSLI (MO, AZ, IN, FI)

FORTRAN SUBROUTINE FOR MODIFIED BESSEL FUNCTION OF INTEGRAL ORDER

The mode of operation is given in MO. The real and imaginary parts of argument zare given in array AZ, and the integer order n is given in IN. The modified Bessel function of the first kind is computed by series expansions and recurrence relations. If MO = 0, the real and imaginary parts of the function $I_n(z)$ are stored in array Fi. If MO = 1, and the phase of z is in the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, the real and imaginary parts of the function $e^{-z}I_n(z)$ are stored in array FI.

SECOND MODIFIED BESSEL FUNCTION

Analysis

The modified Bessel function of the second kind $K_n(z)$ is given by the absolutely convergent series in the equation

$$K_{n}(z) = \frac{1}{2} \sum_{m=0}^{n-1} \frac{(-1)^{m} (n-m-1)!}{m!} \left(\frac{1}{2}z\right)^{-n+2m} - (-1)^{n} \sum_{m=0}^{\infty} \left[\gamma + \log(\frac{1}{2}z) - \frac{1}{2} \sum_{k=1}^{m} \frac{1}{k} - \frac{1}{2} \sum_{k=1}^{n+m} \frac{1}{k} \right] \frac{(\frac{1}{2}z)^{n+2m}}{m!(n+m)!}$$
(221)

The convergent series is used if the argument x + iy satisfies the inequality

$$x^2 + y^2 \le 1 \tag{222}$$

or both of the inequalities

$$x^2 + y^2 < 289 + x + 0.096 y^2 \le 0$$
 (223)

The evaluation of the convergent series for $K_n(z)$ is continued to convergence of the associated series for $I_n(z)$.

The Bessel function is given by the rational approximation

$$K_n(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} e^{-z} \left\{ 1 + \sum_{k=1}^{14} \frac{\epsilon_k}{z - \delta_k} \right\}$$
 (224)

for which the positions δ_k and the residues ϵ_k are for the approximation of the modified Bessel function by sets of poles. The rational approximation is used if the argument

x + iy satisfies the inequalities

The rational approximation is available for orders 0 and 1.

The Bessel function is given by the asymptotic series in the equation

$$K_{\mathbf{n}}(z) = \left(\frac{\pi}{2z}\right)^{\frac{1}{2}} e^{-z} \sum_{m=0}^{N-1} \frac{\left\{n^2 - \left(\frac{1}{2}\right)^2\right\} \cdots \left\{n^2 - \left(m - \frac{1}{2}\right)^2\right\}}{m! (2z)^m}$$
(226)

for which $N \leq 37$. The asymptotic series is used when the argument x+iy satisfies the inequality

$$x^2 + y^2 \ge 289 \tag{227}$$

The series evaluations are used only for orders zero and one, and an ascending recurrence is used if the order is greater than one. The extension of order to negative orders is achieved with the aid of the equation

$$K_{-n}(z) = K_n(z)$$
 (228)

which is an identity for all orders integer or complex.

Programming

SUBROUTINE BSSLK (MO, AZ, IN, FK)

FORTRAN SUBROUTINE FOR MODIFIED BESSEL FUNCTION OF INTEGRAL ORDER

The mode of operation is given in MO. The real and imaginary parts of the argument z are given in array AZ, and the integer order n is given in IN. The modified Bessel function of the second kind is computed by series expansion, rational approximation, and recurrence relations. If MO = 0, the real and imaginary parts of the function $K_n(z)$ are stored in array FK. If MO = 1, the real and imaginary parts of the function $e^z K_n(z)$ are stored in array FK.

COMPLEX BESSEL FUNCTION

Analysis

Bessel functions of complex order ν and complex argument z are expressed by absolutely convergent series. The Bessel function $J_{\nu}(z)$ is given by the equation

$$J_{\nu}(z) = \sum_{m=0}^{\infty} \frac{(-1)^m (\frac{1}{2}z)^{\nu+2m}}{m! \Gamma(\nu+m+1)}$$
 (229)

and the Weber function $Y_{\nu}(z)$ is given by the equation

$$Y_{\nu}(z) = \frac{J_{\nu}(z)\cos\nu\pi - J_{-\nu}(z)}{\sin\nu\pi}$$
 (230)

If ν is a negative integer -n then all terms with $m \le n$ are zero in the series for $J_{-n}(z)$ because the gamma function of a negative integer is infinite. Thus the Bessel functions

satisfy the equation

$$J_{-n}(z) = (-1)^n J_n(z) \tag{231}$$

and the Weber function is given by the equation

$$Y_n(z) = \lim_{\nu \to n} Y_{\nu}(z) \tag{232}$$

The Weber function $Y_n(z)$ must be expressed by a special series.

If z is replaced by $e^{\pm ni}z$ in the convergent series then $J_{\nu}(z)$ is replaced by $e^{\pm \nu ni}J_{\nu}(z)$. The phase of z is limited to the range from $-\pi$ to $+\pi$ in the evaluation of $J_{\nu}(z)$, but the factors $e^{\pm \nu ni}$ may be applied to $J_{\nu}(z)$ in order to extend the range of the phase of z outside the range from $-\pi$ to $+\pi$. If ν is real the absolute magnitude of $e^{\pm \nu ni}$ is unity, but if ν has any imaginary part, then the magnitude of $e^{\pm \nu ni}$ may be small or large according to the sign of the imaginary part of ν .

The ratio between the absolute value of the mth term and the absolute value of the (m-1)th term is given by the expression

$$\frac{|\frac{1}{2}z'|^2}{m[\nu+m]} \tag{233}$$

The ratio is unity wherever the terms in the series have a minimum or a maximum. If ν is negative and real, the terms of the convergent series may increase, decrease, increase, and decrease with increasing order m. The value of m for a unit ratio between terms is estimated by the equation

$$m = \frac{+|\nu| \pm \sqrt{|\nu|^2 - |z|^2}}{2} \qquad (m > \nu) (234)$$

and by the equation

$$m = \frac{-\nu \pm \sqrt{\nu^2 + |z|^2}}{2} \qquad (m > \nu) (235)$$

The requirement that m be real and positive limits the number of minima to one and the number of maxima to two unless |z| > |v|.

If ν is positive and real, the terms of the convergent series may increase before they finally decrease with increasing order m. The value of m for a unit ratio between terms is established by the equation

$$m = \frac{-|\nu| \pm \sqrt{|\nu|^2 + |z|^2}}{2} \tag{236}$$

The requirement that m be positive limits the number of maxima to one. When ν is complex the values of m become the roots of a quartic equation.

The absolute rounding error in the convergent series is determined by the relative rounding error in the largest term of the series. In order to control the relative rounding error in the series itself it is necessary to limit the evaluation of the series to conditions where the terms diminish after the first term. The full accuracy of the computer is guaranteed only if the order and the argument satisfy the criterion

$$\frac{\left|\frac{1}{2}z\right|^2}{|\nu|} \le 1\tag{237}$$

A practical accuracy of computation still may be achieved if this criterion is relaxed.

especially when the order is negative or the argument is imaginary.

The Bessel function is given by the equation

$$J_{\nu}(z) = \left(\frac{2}{\pi z}\right)^{\frac{1}{2}} \left\{ P_{\nu}(z)\cos(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi) - Q_{\nu}(z)\sin(z - \frac{1}{2}\nu\pi - \frac{1}{4}\pi) \right\}$$
(238)

where the function $P_{\nu}(z)$ is the sum of the even-ordered terms and the function $Q_{\nu}(z)$ is the sum of the odd-ordered terms in the asymptotic series

$$P_{\nu}(z) + i Q_{\nu}(z) = \sum_{m=0}^{N-1} \frac{\Gamma(\nu + m + \frac{1}{2})}{m! \Gamma(\nu - m + \frac{1}{2})(-2iz)^m}$$
(239)

The ratio of gamma functions is computed from the product

$$\frac{\Gamma(\nu + m + \frac{1}{2})}{\Gamma(\nu - m + \frac{1}{2})} = \prod_{k=1}^{m} \{\nu^2 - (k - \frac{1}{2})^2\}$$
 (240)

If ν is half an odd integer the series terminates after a finite number of terms.

If z is replaced by $e^{\frac{i2\pi i}{2}z}$ in the asymptotic series, then the terms of the series are reversed in sign, whereas the actual value of $J_{\nu}(z)$ may be smaller or larger according to the sign of the imaginary part of ν . This failure of the asymptotic series is related to the Stokes phenomenon. Its effect is diminished if use of the asymptotic series is limited to arguments with phase in the range $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$, whence the asymptotic series is corrected by the factor $e^{\pm\nu\pi i}$ when the actual phase is outside the range from $-\frac{1}{2}\pi$ to $+\frac{1}{2}\pi$.

If ν is real the terms of the asymptotic series may increase, decrease, and increase with increasing order m. The ratio between the absolute value of the mth term and the absolute value of the (m-1)th term is given by the expression

$$\frac{|\nu^2 - (m - \frac{1}{2})^2|}{m|2z|} \tag{241}$$

The ratio is unity wherever the terms in the series have a minimum or a maximum. When ν is real, the value of m for a unit ratio between terms is estimated by the equation

$$m - \frac{1}{2} = -|z| \pm \sqrt{|z|^2 - |z| + |\nu|^2}$$
 $(m - \frac{1}{2} \le \nu)$ (242)

and by the equation

$$m - \frac{1}{2} = + |z| \pm \sqrt{|z|^2 + |z| + |\nu|^2}$$
 $(m - \frac{1}{2} \ge |\nu|)$ (243)

The requirement that m be real and positive limits the number of minima to one and the number of maxima to one unless $|\nu| \le \frac{1}{2}$ and |z| satisfies the inequality

$$\frac{1 - \sqrt{1 - 4|\nu|^2}}{2} \le |z| \le \frac{1 + \sqrt{1 - 4|\nu|^2}}{2} \tag{244}$$

When ν is complex the values of m become the roots of a quartic equation.

The absolute rounding error of the asymptotic series is determined by the relative rounding error in the largest term of the series, while the absolute truncation error of the series is determined by the magnitude of the smallest term of the series. In order to control the relative rounding error in the series it is necessary to limit the evaluation of the series to conditions where the terms diminish after the first term. The full accuracy of the computer is guaranteed only if the order and the argument

satisfy the criterion

$$\frac{\frac{1}{2}|\nu|^2}{|z|} \le 1 \tag{245}$$

In order to control the truncation error in the series it is necessary to limit the evaluation of the series to conditions where the smallest term is on the order of rounding error. For the CDC 6600 computer the argument must satisfy the criterion $|z| \ge 17.5$.

The criteria for full accuracy severely restrict the range of order and argument in which the classical series may be applied.

Required for the Debye approximation are polynomials $u_m(t)$ which are expressed by the equation

$$u_m(t) = \sum_{k=0}^{m} c_{mk} t^{m+2k}$$
 (246)

for which the coefficients are given by the Amos^{6–10} recurrence equations. The evaluation of the coefficients is started with the equation

$$c_{00} = 1 \tag{247}$$

and is continued with the equation

$$c_{mk} = \left[\frac{\frac{1}{8}}{n_{L} + 2k} + \frac{m + 2k - 1}{2}\right] c_{m-1,k} - \left[\frac{\frac{5}{8}}{m + 2k} + \frac{m + 2k - 3}{2}\right] c_{m-1,k-1}$$
(248)

A parameter γ is defined by the equations

$$\tanh \gamma = \sqrt{1 - \frac{z^2}{\nu^2}}$$
 (249)

and

$$\gamma = -\log \frac{\frac{z}{\nu}}{1 + \sqrt{1 - \frac{z^2}{\nu^2}}}$$

$$(250)$$

Let functions s_1 and s_2 be defined by the equations

$$s_1 = \frac{e^{+\nu(\tanh \gamma - \gamma)}}{\sqrt{+2\pi\nu \tanh \gamma}} \sum_{m=0}^{N} \frac{u_m(\coth \gamma)}{(+\nu)^m}.$$
 (251)

$$s_{1} = \frac{e^{+\nu(\tanh\gamma-\gamma)}}{\sqrt{+2\pi\nu\tanh\gamma}} \sum_{m=0}^{N} \frac{u_{m}(\coth\gamma)}{(+\nu)^{m}}$$

$$s_{2} = \frac{e^{-\nu(\tanh\gamma-\gamma)}}{\sqrt{-2\pi\nu\tanh\gamma}} \sum_{m=0}^{N} \frac{u_{m}(\coth\gamma)}{(-\nu)^{m}}$$
(251)

Thus s_2 is obtained from s_1 by a reversal of the sign of ν . Both functions are the product of a factor and a series. The factor contains two radicals and a logarithm. while the series is asymptotic. Let s_1 be the Debye approximation with a positive sign assigned to the radical

$$\sqrt{1 - \frac{z^2}{\nu^2}} \tag{253}$$

and let s_2 be the Debye approximation with a negative sign assigned to this radical.

Reversal of the sign of the radical replaces the argument of the logarithm by its reciprocal and reverses the sign of the logarithm. Reversal of the sign of the radical replaces the exponential function by its reciprocal. Thus where s_1 is large, s_2 is small, and vice versa.

The radical is zero at branch points in the complex ν -plane where $\nu = \pm z$. In the vicinity of each branch point the logarithm may be expanded in powers of the binomials

$$1 - \frac{z}{v}$$
 or $1 + \frac{z}{v}$ (254)

Cancellation of the lowest order terms and omission of the highest order terms lead to the approximation

$$\sqrt{1 - \frac{z^2}{\nu^2} + \log \frac{\frac{z}{\nu}}{1 + \sqrt{1 - \frac{z^2}{\nu^2}}} \sim -\frac{1}{3} \left(1 - \frac{z^2}{\nu^2}\right)^{\frac{3}{2}}$$
 (255)

Three nodal lines emanate from each branch point. On each nodal line,

$$|s_1| = |s_2|$$
 or $|e^{\pm 2\pi\nu i}s_1| = |s_2|$ (256)

For the exponential functions in the approximations to have the same absolute values it is necessary for their arguments to be pure imaginary. For the approximation of the argument to be pure imaginary the order must be given by one of the equations

$$\nu - z = A \nu^{\frac{1}{3}} e^{\frac{1}{3}\pi i}$$
 $(\nu \sim + z)$ (257)

$$\nu + z = A \nu^{\frac{1}{3}} e^{\frac{1}{3}\pi i}$$
 $(\nu \sim -z)$ (258)

where A is a real parameter. Thus the nodal lines emanate from the branch points in the directions of the three roots of 1 with respect to a line which makes an angle with the real axis equal to one third of the angle which z makes with the real axis. As z rotates the nodal lines rotate at one third the rate of rotation of z.

On the positive side of the imaginary axis computation shows that the Bessel function is given by s_1 alone along the nodal lines which emanate to the right of z, but the Bessel function is given by $s_1 + s_2$ along the nodal line which emanates to the left. The boundary between the regions where s_1 alone is used and where $s_1 + s_2$ must be used presumably is intermediate between nodal lines, where s_2 is so much smaller than s_1 that the difference in formulation is immaterial.

On the negative side of the imaginary axis computation shows that the Bessel function is given by the sum

$$+ s_1 + s_2 + e^{\pm 2\pi\nu i} s_1 \tag{259}$$

on the left of an hyperbola and is given by the sum

$$+ s_1 + s_2 - e^{\pm 2\pi\nu i} s_1$$
 (260)

on the right of the hyperbola. In these formulae the \pm sign is — in a region counterclockwise from an outward extension of -z and is + in a region clockwise from the extension of -z. The boundary of the region where $e^{\pm 2\pi\nu i}s_1$ must be included presumably is on a line midway between nodal lines, where $e^{\pm 2\pi\nu i}s_1$ is so much smaller than $s_1 + s_2$ that the difference in formulation is immaterial.

For a large value of ν on the positive side of the imaginary axis the signs of radicals are positive and the logarithm requires no correction, but in other regions corrections are required because the radicals and logarithm are evaluated on the assumption that their arguments range from a value just more than $-\pi$ through the value $\pm \pi$. The conditions for correction are determined from Argand diagrams in the complex ν -plane.

Let z and ν be expressed in terms of their components by the equations

$$z = x + iy v = \lambda + i\mu (261)$$

Let λ diminish from $+\infty$ with the other components constant. Then the trace of ν is a straight line parallel to the real axis and the trace of $1/\nu$ is a circle of radius $1/2\mu$ which starts at the origin and has a center offset along the imaginary axis to a distance $-1/2\mu$. Multiplication by z amplifies and rotates the circle. The ratio z/ν is a circle which intersects the origin and is rotated through an angle equal to the phase of z. The trace of the square z^2/ν^2 is a cardioid which is rotated through an angle equal to twice the phase of z.

The sign of the radical

$$\sqrt{1-\frac{z^2}{\nu^2}}\tag{262}$$

is positive for large $|\nu|$ but must be reversed whenever its argument crosses the negative real axis. Let the argument be expressed by the equation

$$1 - \frac{z^2}{\nu^2} = -r^2 \tag{263}$$

where r is a real variable. Solution gives the equation

$$\frac{z}{\nu} = \pm \sqrt{1 + r^2} \tag{264}$$

For the ratio $z^{'}\nu$ to be real it is necessary for the components to be related in accordance with the equation

$$\frac{y}{x} = \frac{\mu}{\lambda} \tag{265}$$

Then the ratio z/ν is given by the equation

$$\frac{z}{\nu} = + \frac{y}{\mu} = \pm \sqrt{1 + r^2}$$
 (266)

The argument crosses the negative real axis therefore on the line where ν is congruent to z and $\mu' \otimes {}^iy'$.

The argument of the logarithm is

$$\frac{z}{\nu}$$

$$1 + \sqrt{1 + \frac{z^2}{\nu^2}}$$
(267)

Even when $|\nu|$ is large, the argument crosses the negative real axis when μ and ν are

opposite in sign. Let the argument be expressed by the equation

$$\frac{\frac{z}{\nu}}{1 + \sqrt{1 - \frac{z^2}{\nu^2}}} = -\frac{1}{r} \tag{268}$$

where r is a positive real value. Solution gives the equation

$$\frac{z}{\nu} = -\frac{2r}{1+r^2} \tag{269}$$

This function of r ranges from zero through a minimum and back to zero as r ranges from 0 to ∞ . The minimum is located where the derivative with respect to r is zero. The minimum value is -1. For the ratio z/ν to be real it is necessary for the components to be related in accordance with the equation

$$\frac{y}{x} = \frac{\mu}{\lambda} \tag{270}$$

Then the ratio z/ν is given by the equation

$$\frac{z}{\nu} = +\frac{y}{\mu} = -\frac{2r}{1+r^2} \tag{271}$$

The argument crosses the negative real axis therefore on the line where ν is congruent to z and μ , y have opposite signs with $|\mu| > |y|$. At the crossing the logarithm is corrected by $\mp 2\pi i$.

The sign of the radical

$$\frac{1}{\sqrt{\nu\sqrt{1-\frac{z^2}{\nu^2}}}} = \frac{1}{(\nu^2-z^2)^{\frac{1}{4}}}$$
 (272)

is positive for large $|\nu|$ but must be reversed whenever its argument crosses the negative real axis. Let the argument be expressed by the equation

$$v^2 - z^2 = -r^2 \tag{273}$$

where r is a real variable. For the argument to be real it is necessary for the components to be related in accordance with the equation

$$\lambda \mu = xy \tag{274}$$

Then the argument v^2 z^2 is given by the equation

$$\nu^2 - z^2 = \frac{x^2 y^2}{\mu^2} - \mu^2 - x^2 + y^2 \tag{275}$$

The argument is positive only if $|\mu| < |y|$ whence its square root can be real. The trace of the condition for correction is an hyperbola with the equation

$$\lambda = \frac{xy}{\mu} \tag{276}$$

Whether a correction is necessary depends upon the sign of the radical

$$\sqrt{1-\frac{z^2}{\nu^2}}\tag{277}$$

The correction is necessary only if the radical has a direction opposite to the complex conjugate of ν . The condition for the correction is not met when the sign of the radical has been reversed.

The Debye approximation is not useful inside a boundary where the smallest term of the series would be greater than rounding error. Exploratory computations have shown that the limiting boundary for large argument and order is a cubic parabola. An empirical criterion which defines the limiting boundary for accurate evaluation is given by the equation

$$A|z|^{2} \frac{\left|1 - \frac{\nu}{z}\right|^{3} \left|1 + \frac{\nu}{z}\right|^{3}}{\left|1 - \frac{\nu}{z}\right|^{4} + \left|1 + \frac{\nu}{z}\right|^{4}} \ge 1$$
 (278)

where the constant $A \sim 0.004$. This criterion matches the true boundary for extreme arguments and does not deviate significantly from the true boundary at intermediate arguments. If the criterion is not met for a given value of ν , then unit increments are added to ν until the criterion is met.

Inasmuch as each term of the Debye series is itself a polynomial it has a number of roots equal to its degree. In order to avoid a premature termination of the series, the polynomials are evaluated both with the complex arguments and with their absolute values until the summation of the absolute values of the terms remains stationary.

Values of the order and the argument which are outside the range of the classical series still can be reached by an application of recurrence equations which are started within the range of the classical series. The Bessel functions and the Weber functions satisfy the recurrence equations

$$J_{\nu-1}(z) + J_{\nu+1}(z) = \frac{2\nu}{z} J_{\nu}(z)$$
 (279)

$$Y_{\nu-1}(z) + Y_{\nu+1}(z) = \frac{2\nu}{z} Y_{\nu}(z)$$
 (280)

and the recurrence relation

$$J_{\nu}(z)Y_{\nu+1}(z) - J_{\nu+1}(z)Y_{\nu}(z) = -\frac{2}{\pi z}$$
 (281)

Let ϵ_{μ} be the rounding error which has been introduced in the μ th cycle of iteration. The persisting error in the ν th cycle is given by the expression

$$-\frac{\pi}{2}z\left\{Y_{\mu+1}(z)J_{\nu}(z)-J_{\mu+1}(z)Y_{\nu}(z)\right\}\epsilon_{\mu} \tag{282}$$

for a descending recurrence, and by the expression

$$+\frac{\pi}{2}z\left\{Y_{\mu-1}(z)J_{\nu}(z)-J_{\mu-1}(z)Y_{\nu}(z)\right\}\epsilon_{\mu} \tag{283}$$

for an ascending recurrence. In the computation of $J_{\nu}(z)$ the recurrence must be cycled in whichever direction $|Y_{\nu}(z)|$ diminishes relative to $|J_{\nu}(z)|$.

The recurrence is applied actually to $\Gamma(\nu+1)(\frac{1}{2}z)^{-\nu}J_{\nu}(z)$ when the convergent series is the origin of $J_{\nu}(z)$ in order to keep the recurrence within the index range of the computer. The recurrence is applied actually to $(\pi z/2)^{1/2}J_{\nu}(z)$ when the asymptotic series is the origin of $J_{\nu}(z)$ in order to improve the efficiency of computation.

The convergent approximation is used when $|z| \le 17.5$. There are two modes of computation with the convergent approximation. In the first mode the convergent series is used for orders with large positive real parts, and descending recurrence is used to bring the order down to orders with less positive real parts. In the second mode the convergent series is used for orders with large negative real parts, and ascending recurrence is used to bring the order up to orders with less negative real parts. The relative error in either recurrence increases until the order crosses a nodal line, then the error remains constant thereafter.

Boundaries between modes are located where the errors are the same for both modes. The ideal boundaries between modes are represented by complicated surfaces in the four-dimensional space of order and argument. Information about the location of boundaries is derived from comparisons between single-precision and double-precision computations. The boundaries can be perceived only dimly in the computations because of random fluctuations in rounding error. Within the random fluctuations the boundaries can be simulated by surfaces with polygonal sections.

In the first mode of computation, recurrence is started with that order with a positive real part which satisfies the criterion

$$|\nu| \ge \left|\frac{1}{2}z\right|^2 \tag{284}$$

In the second mode of computation, recurrence is started with that order with a negative real part which satisfies the criterion

$$\Re e \ \nu \ge -\frac{5}{4}(|z| - |\Im m \ \nu|) \tag{285}$$

The first mode is used in preference to the second mode when the order and argument satisfy both of the criteria

$$\Re v = \frac{5}{4} \left(z + \frac{1}{2} \Im m v - \Im m z - \frac{1}{2} \Im m v \right)$$
 (286)

and

The second secon

$$\Re e \, \nu < \frac{5}{4} |z| = \frac{5}{8} \frac{6}{5} z - \Im m \, \nu - \Im m \, z - \frac{5}{8} \frac{6}{5} z - \Im m \, \nu - \Im m \, z$$
 (287)

The two criteria combine to give polygonal sections on planes of constant z in accordance with the computations.

The Debye approximation is used when $z \to 17.5$. A zone in the ν -plane from which the Debye approximation is excluded can be traversed by descending recurrence when the zone is on the positive side of the imaginary axis. Only part of the zone can be traversed by descending recurrence when the zone is on the negative side of the imaginary axis. An ascending recurrence with the Debye approximation gives too much error. Within the zone of exclusion it is possible to use the convergent approximation. Insofar as the descending recurrence starts with equally accurate initial values for either the Debye approximation or the convergent approximation, the error during descending recurrence is the same for both approximations. The same boundaries apply between descending recurrence from the Debye approximation and ascending recurrence from the convergent approximation. The Bessel function is computed with a combination of Debye approximation with descending recurrence and convergent

approximation with ascending recurrence.

The relative error is not uniform over the complex ν -plane. Wherever the Bessel function approaches zero the relative error approaches infinity. The relative error is large over a nodal line where the Bessel function is small. When z is real, the Bessel function can be computed with full machine accuracy. When z is rotated out of the real axis a zone of rounding error appears and grows. The zone of rounding error straddles the negative real axis. Eventually the zone of exclusion cuts off the zone of rounding error.

Programming

SUBROUTINE CBSSLJ (AZ, CN, FJ)

FORTRAN SUBROUTINE FOR COMPLEX BESSEL FUNCTION OF FIRST KIND

The real and imaginary parts of the complex argument z are given in array $\mathbb{A}\mathbb{C}$, and the real and imaginary parts of the complex order ν are given in array \mathbb{C} . The complex Bessel function is computed with series expansions and recurrence relations.

Calls are made to Subroutine CGAMMA. The real and imaginary parts of the complex function $J_{\nu}(z)$ are stored in array FJ.

SUBROUTINE DBSSLJ (AZ, CN, FJ)

FORTRAN SUBROUTINE FOR DOUBLE-PRECISION BESSEL FUNCTION OF FIRST KIND

The real and imaginary parts of the double-precision argument z are given in array AZ, and the real and imaginary parts of the double-precision order ν are given in array C1. The double-precision Bessel function is computed with series expansions and recurrence relations. Calls are made to Subroutine DGAMMA. The real and imaginary parts of the double-precision function $J_{\nu}(z)$ are stored in array z.

DISCUSSION

The incomplete beta function B(p, q, x) is defined by the equation

$$B(p,q,x) = \int_0^x t^{p-1} (1-t)^{q-1} dt$$
 (288)

and the incomplete gamma function $\Gamma(p,x)$ is defined by the equation

$$\Gamma(p,x) = \int_0^x t^{p-1} e^{-t} dt$$
 (289)

A new subroutine BETAX computes directly the incomplete beta function and a new subroutine GAMMAX computes directly the incomplete gamma function for arbitrary real order and real argument. More efficient subroutines for the incomplete beta ratio of half integer order and the incomplete gamma ratio of arbitrary order have been prepared by A. R. DiDonato^{25,28}.

The potential of a rectangular plate is useful for the computation of flow around struts²⁷ and hulls²⁸.

The single precision Bessel functions were checked by comparison with

double-precision computations. The single precision $J_n(z)$ was compared directly with the double-precision $J_n(z)$. The single-precision $Y_n(z)$ was compared with double-precision values from the equation

$$Y_n(z) = \frac{1}{\pi} \left[\frac{\partial J_{\nu}(z)}{\partial \nu} - (-1)^n \frac{\partial J_{-\nu}(z)}{\partial \nu} \right]_{\nu=n}$$
 (290)

where the partial derivatives with respect to ν were estimated by finite differences between values with $\nu=n\pm c$. The single precision $I_n(z)$ was compared with double precision values from the equation

$$I_n(z) = (-i)^n J_n(iz) (291)$$

when y was negative and from the equation

$$I_n(z) = i^n J_n(-iz) \tag{292}$$

when y was positive. The single precision $K_n(z)$ was compared with double precision values from the equation

$$K_{n}(z) = \frac{1}{2} (-1)^{n} \left[\frac{\partial I_{-\nu}(z)}{\partial \nu} - \frac{\partial I_{\nu}(z)}{\partial \nu} \right]_{\nu=n}$$
 (293)

where the partial derivatives with respect to ν were estimated by finite differences between values with $\nu=n\pm\epsilon$. The values of the functions $I_{\nu}(z)$ were derived from the equation

$$I_{\nu}(z) = e^{-\nu \frac{\pi}{2} t} J_{\nu}(iz) \tag{294}$$

when y was negative, and from the equation

$$I_{\nu}(z) = e^{\nu \frac{\pi}{2}i} J_{\nu}(-iz) \tag{295}$$

when y was positive. The first order difference across a point is in error only in the third order, and the accuracy of the difference is one and a half precision when the difference in argument is at the half precision level.

On page 265 of *Theory of Bessel Functions* by Watson² there is a figure which gives the boundaries for various combinations of s_1 and s_2 in the ν z-plane. This figure agrees with the analysis herewith for real z but does not show the relation of boundaries at one third the angle of rotation of z which is characteristic of the nodal lines.

Subroutines for $J_{\nu}(z)$ and $I_{\nu}(z)$ have been programmed by Amos, Daniel, and Weston¹⁰. Their subroutines are valid for positive real argument and positive real order. They supplement the classical series with the Debye approximation, and they use the Olver approximation where the Debye approximation is ineffective. A subroutine for $Y_{\nu}(z)$ has been programmed by Cody, Motley, and Fullerton¹¹. Their subroutine is valid for positive real argument and positive real order. It uses a sequence of Taylor series expansions for lowest orders, and it uses ascending recurrence to reach higher orders. The names of the subroutines for all four Bessel functions are

The first three subroutines have been checked against double precision computations. Four subroutines in the present project are valid for complex argument but for integer order. They supplement the classical series with rational approximations at small orders and use recurrence to extend the range of orders. The names of these

subroutines are

BSSLJ

BSSLY

BSSLI

BSSLK

The new subroutines are more compact than the other subroutines. They are more efficient where they use rational approximations. Otherwise the new subroutines are as efficient at low orders as the other subroutines would be if they were converted to complex arithmetic. Conversion of arithmetic from real to complex may increase the time of computation by $1\frac{2}{3}$ on the CDC 6600 where there can be parallel processing. The accuracies of the new subroutines for low orders are within one digit of the accuracies of the other subroutines. The efficiencies and the accuracies of the new subroutines deteriorate with increase of order into the range of order where the Debye approximation is used.

CONCLUSION

The Debye approximation can be used for the computation of Bessel functions of complex order and complex argument everywhere except in a zone of rounding error where the value of the Bessel function is relatively small. In the zone of rounding error the convergent series with ascending recurrence gives better accuracy than the Debye approximation with descending recurrence.

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APPENDIX A

LEGENDRE FUNCTIONS

LEGENDRE FUNCTIONS

An analysis of Legendre functions of integral order is to be found in *Modern Analysis* by Whittaker and Watson¹. The differential equation for the Legendre functions is

$$(1-z^2)\frac{d^2w}{dz^2} - 2z\frac{dw}{dz} + n(n+1)w = 0$$
 (1)

The Legendre function of the first kind is given by the Schläfli integral,

$$P_n(z) = \frac{1}{2^{n+1}\pi i} \oint \frac{(t^2 - 1)^n}{(t - z)^{n+1}} dt$$
 (2)

where the contour of integration encircles z once counterclockwise. That this integral satisfies the differential equation is easily verified since substitution in the differential equation leads to the circuit integral,

$$(1-z^2)\frac{d^2P_n}{dz^2} - 2z\frac{dP_n}{dz} + n(n-1)P_n = \frac{n+1}{2^{n+1}\pi i} \oint \frac{d}{dt} \left\{ \frac{(t^2-1)^{n+1}}{(t-z)^{n+2}} \right\} dt$$
 (3)

That the integral coincides with the Legendre polynomial is verified when the integral is evaluated for $z=\pm 1$.

The Schläfli integral may be derived by $n\cdot$ fold differentiation of the Cauchy integral

$$(z^2 - 1)^n = \frac{1}{2\pi i} \oint \frac{(t^2 - 1)^n}{(t - z)} dt$$
 (4)

Thus the Legendre polynomials are given by the Rodrigues formula.

$$P_n(z) = \frac{1}{2^n n!} \frac{d^n}{dz^n} (z^2 - 1)^n \tag{5}$$

Expansion of the identity

$$\frac{1}{2^{n+2}\pi i} \oint \frac{d}{dt} \left\{ \frac{(t^2-1)^{n+1}}{(t-z)^{n+1}} \right\} dt = 0$$
 (6)

leads to the equation

$$P_{n+1}(z) = z P_n(z) = \frac{1}{2^{n+1}\pi i} \oint \frac{(t^2 - 1)^n}{(t - z)^n} dt$$
 (7)

Expansion of the identity

$$\frac{1}{2^{n+1}\pi i} \oint \frac{d}{dt} \left\{ t \frac{(t^2 - 1)^n}{(t - z)^n} \right\} dt = 0$$
 (8)

leads to the equation

$$nz P_n(z) = n P_{n-1}(z) = \frac{n+1}{2^{n+1}\pi i} \oint \frac{(t^2-1)^n}{(t-z)^n} dt$$
 (9)

Elimination leads to the recurrence equation

$$n P_{n-1}(z) = (2n+1)z P_n(z) + (n+1)P_{n+1}(z) = 0$$
 (10)

and differentiation leads to the recurrence equation

$$(2n+1)P_n(z) = P'_{n+1}(z) - P'_{n-1}(z)$$
(11)

Thus all of the Legendre functions and their derivatives may be synthesized from the two functions of lowest order.

Differentiation of the recurrence equations leaves one term of lower order in each. Repeated differentiation with elimination of the term of lower order leads to the recurrence equation

$$(n+m)\frac{d^{m}P_{n+1}}{dz^{m}}-(2n+1)z\frac{d^{m}P_{n}}{dz^{m}}+(n-m+1)\frac{d^{m}P_{n+1}}{dz^{m}}=0$$
 (12)

which connects the derivatives of functions of progressively increasing order. Repeated differentiation $\,$ of the differential equation leads to the recurrence equation

$$(n-m)(n-m+1)\frac{d^{m-1}P_n}{dz^{m-1}} - 2mz\frac{d^mP_n}{dz^m} + (1-z^2)\frac{d^{m+1}P_n}{dz^{m+1}} = 0$$
 (13)

which connects the progressively higher derivatives of functions of common order. The Legendre function of the second kind is given by the integral,

$$Q_n(z) = \frac{1}{2^{n+1}} \int_{-1}^{+1} \frac{(1-t^2)^n}{(z-t)^{n+1}} dt$$
 (14)

Substitution of the integral in the differential equation and in the recurrence equations shows that $Q_n(z)$ satisfies the same equations as $P_n(z)$ provided that $\Re e(n+1) > 0$.

APPENDIX B

MULTIPLE-PRECISION COMPUTATIONS

MULTIPLE-PRECISION COMPUTATIONS

Formula Algebraic Processor

FLAP, or Formula Algebraic Processor, is a computational system which has been developed by Morris¹⁸ for the manipulation of mathematical expressions. The FLAP system refers to LISP, or List Processor, which manipulates lists of numbers or symbols. As a checkout of the numerical feature of FLAP, high-precision values of Bernoulli numbers and Riemann zeta functions have been computed. Values were computed to 80 digits with an accuracy of 75 digits, and then the values have been truncated back to 64 digits. The values have been punched on cards and are printed in Appendix C.

Bernoulli Numbers

There are two principal versions of the Bernoulli numbers. The older version is derived from the definition

$$\frac{1}{2}z \cot \frac{1}{2}z = 1 - \sum_{n=1}^{\infty} B_n \frac{z^{2n}}{(2n)!}$$
 (1)

where B_n is the *n*th Bernoulli number in the older definition. The newer version is derived from the definition

$$\frac{z}{e^z - 1} = \sum_{n=0}^{\infty} B_n \frac{z^n}{n!}$$
 (2)

where B_n is the *n*th Bernoulli number in the newer definition. The Bernoulli number B_n in the older definition is equivalent to $(-1)^{n-1}B_{2n}$ in the newer definition. The change of definition adds one number to the set and makes some formulae more compact.

Values of B_n in the newer definition can be obtained by the division of z by the series expansion for $e^z - 1$. The first few values are given by the equations

$$B_0 = 1$$
, $B_1 = -\frac{1}{2}$, $B_2 = \frac{1}{6}$, $B_3 = 0$, $B_4 = -\frac{1}{30}$, $B_5 = 0$, $B_6 = \frac{1}{42}$ (3)

If z is replaced by -z in the definition equation to give terms which are subtracted from the terms of the definition equation, then cancellation of terms leads to the equation

$$z = -2 \sum_{n=0}^{\infty} B_{2n+1} \frac{z^{2n+1}}{(2n+1)!}$$
 (4)

Comparison of coefficients of powers of z shows that the Bernoulli numbers of odd order satisfy the equation

$$B_{2n+1} = 0 (n > 0) (5)$$

If z is replaced by -z in the definition equation to give terms which are added to the terms of the definition equation, then cancellation of terms leads to the equation

$$\frac{1}{2}z \coth \frac{1}{2}z = \sum_{n=0}^{\infty} B_{2n} \frac{z^{2n}}{(2n)!}$$
 (6)

Substitution of 2iz for z leads to the equation

$$\cot z = \sum_{n=0}^{\infty} \frac{(-1)^n 2^{2n} B_{2n}}{(2n)!} z^{2n-1}$$
 (7)

which gives the Maclaurin expansion for the cotangent. From the identity

$$2 \cot 2z = \cot z - \tan z \tag{8}$$

may be derived the equation

$$\tan z = -\sum_{n=1}^{\infty} \frac{(-1)^n 2^{2n} (2^{2n} - 1) B_{2n}}{(2n)!} z^{2n-1}$$
(9)

which gives the Maclaurin expansion for the tangent.

If z is real, then integration around a contour which is bounded by the real axis, a line at i parallel to the real axis, and the imaginary axis, but does not contain the points 0, i, leads to the equation

$$\int_0^\infty \frac{\sin zt}{e^{2\pi t} - 1} dt = \frac{1}{4} \coth \frac{1}{2}z - \frac{1}{2z}$$
 (2 real) (10)

Substitution for $\coth \frac{1}{2}z$ its series expansion in terms of Bernoulli numbers, substitution for $\sin zt$ its series expansion in powers of zt, and comparison of coefficients shows that the even-ordered Bernoulli numbers are given by the equation

$$B_{2n} = -(-1)^n 4n \int_0^\infty \frac{t^{2n-1}}{e^{2\pi t} - 1} dt$$
 (11)

A change of variable in the integrand expresses the Bernoulli numbers in terms of Riemann zeta functions of even order.

Values of Bernoulli numbers have been obtained from Tables of the Higher Mathematical Functions by Davis²³. They are listed in Table I at the same level of accuracy as the other numbers which have been obtained through FLAP. Values of Bernoulli numbers for use in the computer were computed by the method of Knuth and Buckholtz²². The derivative of the nth power of the tangent is given by the equation

$$\frac{d}{dz}\tan^{n}z = n\tan^{n-1}z(1+\tan^{2}z)$$
 (12)

Thus the derivative of a polynomial in powers of $\tan z$ remains a polynomial in powers of $\tan z$. The derivative of the power polynomial

$$\sum_{n=0}^{N} a_n \tan^n z \tag{13}$$

is obtained by the transformation

$$a_n \to (n-1)a_{n-1} + (n+1)a_{n+1}$$
 (14)

If a_1 is unity and all other coefficients a_n are zero initially, then iteration of the transformation gives all of the derivatives of $\tan z$, from which numerical values for the coefficients of the Maclaurin series can be computed. From the coefficients of the Maclaurin series are computed the Bernoulli numbers.

Bernoulli Polynomials

Bernoulli polynomials were derived from an unconventional generating function by Whittaker and Watson¹. Their polynomials were terminated with terms in z or z^2 , whereas the conventional polynomials are terminated with terms in 1 or z. The conventional definition is to be preferred because then the polynomials are terminated automatically when factorials of negative integers appear in the denominators of their terms.

Bernoulli polynomials are defined by the equation

$$t \frac{e^{zt}}{e^t - 1} = \sum_{n=0}^{\infty} B_n(z) \frac{t^n}{n!}$$
 (15)

where $B_n(z)$ is the *n*th Bernoulli polynomial. Term by term multiplication of the series expansion for $t/(e^t-1)$ by the series expansion for e^{zt} , and comparison of coefficients leads to the equation

$$B_n(z) = \sum_{k=0}^{n} \frac{n!}{(n-k)!k!} B_k z^{n-k}$$
 (16)

Thus the nth polynomial $B_n(z)$ is of the nth degree. Differentiation of the terms of this polynomial n-m times is expressed by the equation

$$B_n^{(n-m)}(z) = \sum_{k=0}^m \frac{n!}{(m-k)!k!} B_k z^{m-k}$$
 (17)

Special values for z = 0 are given by the equations

$$B_n(0) = B_n \tag{m : n) (18)$$

and

$$B_n^{(n-m)}(0) = \frac{n!}{m!} B_m \qquad (m-n)$$
 (19)

Thus the Bernoulli numbers are the constants in the Bernoulli polynomials

Subtraction of the terms in the generating equation from the same terms with z replaced by z+1 leads to the equation

$$t e^{zt} = \sum_{n=0}^{\infty} \left\{ B_n(z+1) - B_n(z) \right\} \frac{t^n}{n!}$$
 (20)

Series expansion of ezt and comparison of coefficients lead to the equation

$$B_n(z+1) - B_n(z) = nz^{n-1} \tag{21}$$

Differentiation of the terms of this equation n - m times is expressed by the equation

$$B_n^{(n-m)}(z+1) - B_n^{(n-m)}(z) = \frac{n!}{(m-1)!} z^{m-1}$$
 (22)

Special values for $z \approx 0$ are given by the equations

and

Thus the Bernoulli polynomials are the same at both ends of the range $0 \ge z \le 1$ if the order $n \ne 1$.

A comparison of coefficients of the powers of t in the identity

$$t\frac{e^{(1-z)t}}{e^t-1} = -t\frac{e^{-zt}}{e^{-t}-1}$$
 (25)

shows that the Bernoulli polynomials satisfy the equation

$$B_n(1-z) = (-1)^n B_n(z)$$
 (26)

Thus the even-ordered polynomials are symmetric and the odd-ordered polynomials are antisymmetric with respect to the midpoint of the range $0 \le z \le 1$.

A comparison of coefficients of the powers of t in the identity

$$t \frac{e^{\frac{1}{2}t}}{e^t - 1} = \frac{t}{e^{\frac{1}{2}t} - 1} - \frac{t}{e^t - 1} \tag{27}$$

shows that special values for $z = \frac{1}{2}$ are given by the equation

$$B_n(\frac{1}{2}) = (2^{1-n} + 1)B_n \tag{28}$$

Thus the Bernoulli polynomials have opposite signs at the midpoint and at the ends of the range $0 \le z \le 1$.

Differentiation of the Bernoulli polynomials is expressed by the equation

$$B_n'(z) = n B_{n-1}(z) \tag{29}$$

Integration of the Bernoulli polynomials is expressed by the equation

$$\int_{0}^{1} B_{n}(z) dz = \frac{1}{n+1} \left\{ B_{n+1}(1) - B_{n+1}(0) \right\}$$
 (30)

Thus the integral of a Bernoulli polynomial is zero in the range $0 \ge z \le 1$ if the order $n \ne 0$.

Further differentiation of the Bernoulli polynomials is expressed by the equation

$$B_n''(z) = n(n-1)B_{n-2}(z) \tag{31}$$

The polynomial $B_1(z)$ of first order is monotonic with a uniform sign throughout each side of the midpoint of the range $0 \le z \le 1$. The second derivative of the next higher odd-ordered polynomial has a uniform sign throughout either half of the range $0 \le z \le 1$, and the polynomial has roots only at $0, \frac{1}{2}, 1$. By induction it may be inferred that all higher odd-ordered polynomials have the same property. The first derivative of each even-ordered polynomial has a uniform sign throughout each side of the midpoint of the range $0 \le z \le 1$. Each even-ordered polynomial has only two roots in the range $0 \le z \le 1$. The absolute value of every even-ordered polynomial is a maximum at the ends of the range.

Euler-Maclaurin Expansion

An elegant derivation of the Euler-Maclaurin formula has been given by Whittaker and Watson¹. However, their unconventional definition of the Bernoulli polynomials warrants a review of their derivation. They started with a formula which they attributed to Darboux.

Let f(z) be analytic at all points on a straight line which joins α to z, and let $\varphi(t)$

be any polynomial of degree n in t. Then if $0 \le t \le 1$, differentiation is expressed by the equation

$$\frac{d}{dt} \sum_{m=1}^{n} (-1)^{m} (z-a)^{m} \varphi^{(n-m)}(t) f^{(m)}(a+(z-a)t)
= \sum_{m=1}^{n} (-1)^{m} (z-a)^{m} \varphi^{(n-m+1)}(t) f^{(m)}(a+(z-a)t)
+ \sum_{m=1}^{n} (-1)^{m} (z-a)^{m+1} \varphi^{(n-m)}(t) f^{(m+1)}(a+(z-a)t)$$
(32)

In the first summation on the right side of the equation the substitution of m+1 for m leads to the cancellation of all terms of the summations except the first term of the first summation and the last term of the second summation. Thus the equation can be reduced to

$$\frac{d}{dt} \sum_{m=1}^{n} (-1)^{m} (z-a)^{m} \varphi^{(n-m)}(t) f^{(m)}(a+(z-a)t)
= -(z-a) \varphi^{(n)}(t) f'(a+(z-a)t) + (-1)^{n} (z-a)^{n+1} \varphi(t) f^{(n+1)}(a+(z-a)t)$$
(33)

Inasmuch as $\varphi(t)$ is a polynomial of *n*th degree, the *n*th derivative $\varphi^{(n)}(t)$ is constant and equal to $\varphi^{(n)}(0)$ or $\varphi^{(n)}(1)$. Integration with respect to t from 0 to 1 gives the equation

$$\sum_{m=0}^{n} (-1)^{m} (z-a)^{m} \left[\varphi^{(n-m)}(1) f^{(m)}(z) - \varphi^{(n-m)}(0) f^{(m)}(a) \right]$$

$$= (-1)^{n} (z-a)^{n+1} \int_{0}^{1} \varphi(t) f^{(n+1)}(a+(z-a)t) dt$$
(34)

Let the polynomial $\varphi(t)$ be identified with the polynomial $B_n(t)$.

Substitution of the special values for the two Bernoulli numbers of lowest order in the Darboux identity, and substitutions of 2k for m and 2n for n lead to the Euler-Maclaurin expansion $^{13-15}$

$$f(z) - f(a) = \frac{1}{2}(z - a)\{f'(z) + f'(a)\}$$

$$- \sum_{k=1}^{n} \frac{(z - a)^{2k} B_{2k}}{(2k)!} \left\{ f^{(2k)}(z) - f^{(2k)}(a) \right\}$$

$$+ \frac{(z - a)^{2n+1}}{(2n)!} \int_{0}^{1} B_{2n}(t) f^{(2n+1)}(a + (z - a)t) dt$$
(35)

Integration by parts in this equation continues the summation through additional terms.

Addition of the *n*th term of the summation to the integral in the equation is equivalent to the replacement of $B_{2n}(t)$ in the integrand by $B_{2n}(t) - B_{2n}$. Let the difference $B_{2n}(t) - B_{2n}$ be replaced by its average value $-B_{2n}$. Then the expansion is

expressed by the equation

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$$f(z) - f(a) = \frac{1}{2}(z - a)\{f'(z) + f'(a)\}$$

$$- \sum_{k=1}^{n-1} \frac{(z - a)^{2k} B_{2k}}{(2k)!} \left\{ f^{(2k)}(z) - f^{(2k)}(a) \right\}$$

$$- \frac{(z - a)^{2n+1} B_{2n}}{(2n)!} f^{(2n+1)}(a + (z - a)\theta)$$
(36)

where θ is some number in the range $0 \le \theta \le 1$. The first term on the right side of this equation expresses the trapezoidal rule for $\int_{-t}^{t} f'(t) dt$, the summation provides a correction for the trapezoidal rule, and the last term provides an estimate of the error in the correction.

Riemann Zeta Function

The Riemann zeta function $\zeta(s)$ is defined in terms of its argument s by the equations

$$\zeta(s) = \sum_{k=1}^{\infty} \frac{1}{k^{s}} = \frac{1}{\Gamma(s)} \int_{0}^{\infty} \frac{x^{s-1}}{e^{x} - 1} dx$$
 (37)

Direct evaluation of the series to an acceptable level of accuracy is not feasible for a small value of s. In the special case where s is an even integer 2n, the Riemann zeta function is given by the equation

$$\zeta(2n) = -\frac{(-1)^n (2\pi)^{2n} B_{2n}}{2(2n)!} \tag{38}$$

Otherwise application of the Euler-Maclaurin expansion gives the equation

$$\zeta(s) = \sum_{k=1}^{K-1} \frac{1}{k^{s}} + \frac{1}{2K^{s}} + \frac{1}{(s-1)K^{s-1}} + \sum_{m=1}^{M-1} \frac{B_{2m}}{(2m)!} \frac{\Gamma(s)}{\Gamma(s+2m-2)} \frac{1}{K^{s+2m-1}} + \frac{B_{2M}}{(2M)!} \frac{\Gamma(s)}{\Gamma(s+2M-1)} \sum_{k=K}^{\infty} \frac{1}{(k+\theta)^{s+2M}}$$
(39)

Consideration of the magnitude of the remainder by Morris has indicated that if K=41 and $s \ge 2$, then $M \le 39$ for an error of less than 4×10^{-74} . High-precision values of the Riemann zeta function for integer values of the argument are listed in Table II. The most accurate values which previously have been computed only had fifty digits²¹

Gamma Function

The logarithm of the gamma function is defined by the equation

$$\log \Gamma(1+z) = -\gamma z + \sum_{n=1}^{\infty} \left\{ \frac{z}{n} + \log n - \log(n+z) \right\}$$
 (40)

The first derivative is given by the equation

$$\frac{d}{dz}\log\Gamma(1+z) = -\gamma + \sum_{n=1}^{\infty} \left\{ \frac{1}{n} - \frac{1}{n+z} \right\}$$
 (41)

The higher derivatives are given by the equation

$$\frac{d^{m}}{dz^{m}}\log\Gamma(1+z)=(-1)^{m}(m-1)!\sum_{n=1}^{\infty}\frac{1}{(n+z)^{m}}$$
(42)

Thus the Taylor series expansion of the logarithm of the gamma function is given by the equation

$$\log \Gamma(1+z) = -\gamma z + \sum_{m=2}^{\infty} \frac{(-1)^m \zeta(m)}{m} z^m$$
(43)

Addition of the Taylor series expansion for log(1+z) gives the equation

$$\log \Gamma(2+z) = (1-\gamma)z + \sum_{m=2}^{\infty} (-1)^m \frac{\{\zeta(m)-1\}}{m} z^m$$
 (44)

Let $\log \Gamma(2+z)$ be expressed by a series in accordance with the equation

$$\log \Gamma(2+z) = -\sum_{k=1}^{\infty} a_k z^k \tag{45}$$

and let $1/\Gamma(2+z)$ be expressed by a series in accordance with the equation

$$\frac{1}{\Gamma(2+z)} = \sum_{m=0}^{\infty} b_m z^m \tag{46}$$

Differentiation and substitution gives the equation

$$\sum_{n=0}^{\infty} (n+1)b_{n+1}z^n = \sum_{m=0}^{\infty} b_m z^m \sum_{k=0}^{\infty} (k+1)a_{k+1}z^k$$
 (47)

Comparison of coefficients gives the equation

$$(n+1)b_{n+1} = \sum_{k=0}^{n} (k+1)\alpha_{k+1}b_{n-k}$$
 (48)

from which the coefficients can be computed by recurrence. Let $1/\Gamma(1+z)$ be expressed by a series in accordance with the equation

$$\frac{1}{\Gamma(1+z)} = \sum_{m=0}^{\infty} c_m z^m \tag{49}$$

The coefficients are related by the equation

$$c_m = b_{m-1} + b_m \tag{50}$$

The first two coefficients are given by the equations

$$c_0 = 1 c_1 = \gamma (51)$$

A high-precision value of γ was obtained from the published literature ^{19,20}. High-precision values of the coefficients in the convergent series are given for the gamma function in Table III, and are given for the digamma function in Table V.

The logarithm of the gamma function is expressed by the equation

$$\log \Gamma(z) = (z - \frac{1}{2})\log z - z + \frac{1}{2}\log (2\pi) + \sum_{m=1}^{N} \frac{B_{2m}}{2m(2m-1)z^{2m-1}}$$
 (52)

High-precision values of the coefficients in the asymptotic series are given for the

gamma function in Table IV, and are given for the digamma function in Table VI.

Multiple-Precision Package

MP, or Multiple-Precision Package is a collection of subroutines which have been developed by Brent²⁴. A multiple-precision number is represented by an array of floating-point numbers. The first number in the array defines the sign of the number. The next number in the array gives the exponent of the number. The remaining numbers in the array express the fraction of the number. Each successive number in the fraction is the coefficient of a progressively more negative power of the base. The number of coefficients in the composition of the fraction is unlimited. The number of bits in the base may have any value not exceeding half the number of bits in the fraction of a floating-point number. Otherwise multiple-precision multiplication would be unduly cumbersome. Included in the package are routines for arithmetic and special functions.

APPENDIX C

MULTIPLE-PRECISION NUMBERS

TABLE I

Bernoulli Numbers

 B_n -7.0921568627450980392156862745098039215686274509803921568627450980 E 000 $5.4971177944862155388471177944862155388471177944862155388471177944 \\ E+O11177944862155388471177944 \\ E+O1117794486215538847117794 \\ E+O1117794488521571 \\ E+O11177948871 \\ E+O11177948871 \\ E+O11177948871 \\ E+O11177948871 \\ E+O111779448871 \\ E+O1117794871 \\ E+O111779471 \\ E+O117779471 \\ E+O111779471 \\ E+O1117779471 \\ E+O1117779471 \\ E+O1117779471 \\ E+O1117779471 \\ E+O1117779471 \\ E+O11177777 \\ E+O117777 \\ E+O117777 \\ E+O117777 \\ E+O117777 \\ E+O11777 \\ E+O1177$ 6.1921231884057971014492753623188405797101449275362318840579710144 E + 036.0158087390064236838430386817483591677140064236838430386817483591E+08- 1.5116315767092156862745098039215686274509803921568627450980392156 E+ 10 - 1.9296579341940068148632668144863266814486326681448632668144863266 E+ 16

TABLE I (Continued)

TABLE II Riemann Zeta Function

 $\zeta(n)$

n

TABLE II (Continued)

 $\zeta(n)$ $1.0000000000000035527136913371136732984695340593429921456555030626 \pm 000$ $1.000000000000000000016940658945097991654064927471248619403036417 \mp 0.06$ $1.00000000000000000000008470329472546998348246992609182167522283864 \pm 669$ $1.0000000000000000000004235164736272833347862270483357934408810971 \\ + another an artist of the contraction of the contractio$ 1.0000000000000000000000529395592033987032381391230291850558663756 F 000 1.000000000000000000000000041359030627651609260093824555081412852.57 Figure $1.0000000000000000000000000516987882845643132041013321663555128936 \pm oc$ 1.0000000000000000000000000001615587133892632521206011405705227272611663

TABLE III

Convergent Series for Gamma Function

TABLE III (Continued)

n

TABLE IV Asymptotic Series for Gamma Function

 $B_{\underline{2m}}$ m 2m(2m-1)8.417508411.91752691752691752691752691752691752691752691752691752691752691752691751.3402864044168391994478951000690131124913733609385783298826777087E+012.1320333960919373896975058982136838557465453319851702055948769801E+16 1.0217752965257000775652876280535855003940110323089046493301812450 E+18 5.3575472173300203610827709191969204484849040543658816499867814010 E+19 $9.2528471761204163072302423483476227795193312434691745036572622779\,E+26022779\,E+12022749\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+120227\,E+1202$ $6.0451834059958569677431482387545472860661443959671962074063016080\,E+30$ 5.4206704715700945451934778148261000136612021857923497267759562841 E+32 5.3036588551197005966548392430697586436992926354055490979566255361 E+36 1.0536966953357141803754804927641810189648373375011415525114155251E+452.0817356522089565462424808241263562311317343264149979189335880113 E+49 $8.5299728203005518816208400522162278887807044700382824140089545446\,E+55$ 1.5064172809340598576695117360379879076101930840250545639808412745 E + 582.7893494703831636871288381686312781712347568886054688103193038537 E+60 5.4093504352860415005763561871884152582336290276915242378260371885 E+62

TABLE V
Convergent Series for Digamma Function

TABLE V (Continued)

nc,

TABLE VI

Asymptotic Series for Digamma Function

 B_{2m} m 2m $3.0539543302701197438039543302701197438039543302701197438039543302 \pm 0.00$ $2.8146014492753623188405797101449275362318840579710144927536231884\,E + 0.2231884\,E + 0.223184\,E +$ 3.60751054639804639804639804639804639804639804639804639804639804639.7493682385057471264367816091954022988505747126436781609195402298E+054.82414483548501703715816703621581670362158167036215816703621581672.0040310656516252738108421663238938986447292095132626694088488108 E+16 $9.1677436031953307756992753623188405797101449275362318840579710144 \, E+1881618111 \, E+188161811 \, E+18816181 \, E+1881618181 \, E+18816181 \, E+1881618181 \, E+1881618181 \, E+1881618181 \, E+1881618181 \, E+1881618181 \, E+188161818181 \, E+1881618181 \, E+1881618181 \, E+1881618181 \, E+1881618181 \, E+1881618181 \, E+1881618181$ 2.5180471921451095697089023320225526107879049055519643754937872584 E+21 5.0890659468662289689766332915911925287356321839080459770114942528E+284.1147288792557978697665486067619336158192090395480225988700564971E+303.5666582095375556109684574608651828987790251936206457623697179487E+323.30660898765775767256802146704392100833333333333333333333333333333353.2715634236478716264211227015668703413608149509803921568627450980 E+36 3.861427983270525889309272020023265011977794166666666666666666666 E+40 4.5892974432454332168863989006092836062174201580239009816474605206 E+42 1.081363544997165469635403335113385960717774904774815833333333333335E+492.5019479041560462843656661498516623460905275166032394894009320246 E+53 $4.1067052335810212479752045004071650019779998716090053258928714859\,E+55$ $1.2804546887939508790190849756322897214686641214212963793837150833\, E+60012414212963793837150833\, E+60012414212963793837150837150833\, E+60012414212963793837150833\, E+60012414212963793837150833\, E+60012414212963793837150833\, E+600124142129637938371508371508371508371508371508371508371508371508371508371508371508371508371508371508371508007150807150807150807150$ 2.4267340392333524078020892067092120089742384930867578649777943527 E+62

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