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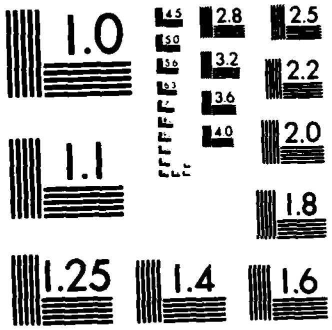

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SIMPLIFIED CONTINUED FRACTION CALCULATION OF SPHERICAL BESSEL FUNCTIONS

SEPTEMBER 1984

By

W. J. Lentz

Approved for public release; distribution unlimited.

US Army Electronics Research and Development Command

Atmospheric Sciences Laboratory

White Sands Missile Range, NM 88002

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A technique of generating spherical Bessel functions of real or complex argument is developed. A negative simple continued fraction is defined and error corrections developed for the calculation of the continued fraction. FORTRAN IV programs for spherical Bessel functions of real and complex argument are presented. The technique is simple, fast, and of higher accuracy than comparable techniques currently in use to evaluate spherical Bessel functions.

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CONTENTS

1. INTRODUCTION

A continued fraction technique[1,2] has been developed for the calculation of the ratios of spherical Bessel functions of complex argument used in Mie calculations.[3,4] When the spherical Bessel functions of complex argument themselves are required, the same technique may be applied with several simplifications. Spherical Bessel functions of complex argument have wide ranging applications in physics, electronics, and meteorology. The purpose of this report is to develop the simplified formulae for the calculation of spherical Bessel functions of complex argument and to present several algorithms that correctly calculate the functions. The technique is essentially based on a new method of evaluating continued fractions.

There are now four distinctly different methods that allow one to evaluate a continued fraction. Three of these methods are detailed in Gautschi,[5] and the fourth in Lentz.[1] The Lentz[6] continued fraction algorithm is of much more general application than just spherical Bessel functions. This algorithm essentially transforms a continued fraction into an infinite product, whereas the previous three methods convert to infinite series or recursions that have stability problems.

2. SIMPLE CONTINUED FRACTION

A simple continued fraction may be defined as:

$$F = a_1 + \frac{1}{a_2} + \frac{1}{a_3} + \dots + \frac{1}{a_n} + \dots \tag{1}$$

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[1] W. J. Lentz, 1973, A New Method of Computing Spherical Bessel Functions of Complex Argument with Tables, ECOM 5509, AD 767223, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

[2] W. J. Lentz, 1976, "Generating Bessel Functions in Mie Scattering Calculations Using Continued Fractions," Appl Opt, 15:668

[3] W. J. Wiscombe, 1980, "Improved Mie Scattering Algorithms," Appl Opt, 19:1505

[4] G. Grehan and G. Gouesbet, 1979, "Mie Theory Calculations: New Progress, with Emphasis on Particle Sizing," Appl Opt, 18:3489

[5] W. Gautschi, 1967, SIAM, Rev 9, No 1

[6] W. J. Lentz, 1982, A Simplification of Lentz's Algorithm, ASL-TR-0118, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

where none of the a_i may be zero. The a_i may be complex or negative, and the nth convergent of the continued fraction is defined as:

$$F_n = a_1 + \frac{1}{a_2} + \frac{1}{a_3} + \cdots \frac{1}{a_n} \quad (2)$$

This simple continued fraction might better be called a positive simple continued fraction because all the terms are added. One method of evaluating equation (2) is to start at a_n, take the reciprocal and add to a_{n-1} until a_1 is reached. The only trick is to know at which a_n to start for a given accuracy. Unfortunately, two terms in the iteration process may cancel, or nearly cancel, causing unpredictable errors in the final answer. Let us therefore review a new technique to evaluate continued fractions.[2]

Let us make a further change of notation to define a simple continued fraction more compactly.

$$F_n = [a_1, a_2, a_3, \ldots, a_n] \quad (3)$$

Lentz[2] has shown that this continued fraction may be transformed to an equivalent form, which begins at a_1 rather than some indeterminate a_n.

$$F_n = \frac{[a_1]\,[a_2, a_1]\,[a_3, a_2, a_1] \ldots [a_n, a_{n-1}, \ldots, a_1]}{[a_2]\quad [a_3, a_2] \ldots [a_n, a_{n-1}, \ldots, a_2]} \quad (4)$$

Although this formula may appear complicated, one generates successive numerators and denominators by taking the reciprocal and adding to the previous numerator or denominator. A numerical example and an algorithm for equation (4) may be found in reference 6.

---

[5] W. J. Lentz, 1976, "Generating Bessel Functions in Mie Scattering Calculations Using Continued Fractions," Appl Opt, 15:668

[6] W. J. Lentz, 1982, A Simplification of Lentz's Algorithm, ASL-TR-0118, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

Since the a_i might be negative, one will note that any given term $[a_i, a_{i-1}, \ldots, a_{1(\text{or } 2)}]$ might be inaccurate due to cancellation of common digits in the sum. In this case, an algorithm improvement has been devised.[2]

$$\text{Let} \quad [a_{m-1}, \ldots, a_1] = \alpha$$

$$\text{If} \quad [a_m, \ldots, a_1] = \beta = a_m + 1/\alpha \approx 0$$

$$\text{then} \quad [a_{m+1}, \ldots, a_1] = \gamma = a_{m+1} + 1/\beta \to \infty$$

$$\text{let} \quad [a_{m+2}, \ldots, a_1] = Z = a_{m+2} + 1/\gamma$$

$$\text{then} \quad \zeta = \beta\gamma = \beta \, \frac{a_{m+1}\beta + 1}{\beta} = a_{m+1}\beta + 1 \qquad (5)$$

ζ is the product of the next two terms. If β is identically zero, then ζ is one. Z the next term is then:

$$Z = \frac{a_{m+2}\gamma + 1}{\gamma} = \frac{a_{m+2}(a_{m+1}\beta + 1) + \beta}{a_{m+1}\beta + 1} \qquad (6)$$

$$Z = a_{m+2} + \beta/\zeta$$

Note that the above formulae apply to <u>both</u> the numerator and the denominator since the form is independent of whether a_1 or a_2 is used. In fact, accuracy can be increased by using the algorithm improvement any time a common number of digits cancel to reducing accuracy in the generation of β. When a given numerator such as β is equal to its corresponding denominator to the number of desired digits, the fraction may be said to have converged to the desired accuracy. Reasonable accuracy may also be obtained by only considering the case when β is identically zero, and the simplier algorithm will improve execution time significantly.

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[2] W. J. Lentz, 1976, "Generating Bessel Functions in Mie Scattering Calculations Using Continued Fractions," <u>Appl Opt</u>, 15:668

3. SIMPLIFIED FORMULAE

The continued fraction representation for the ratio of Bessel functions of consecutive order is given by:

$$\frac{J_{v-1}}{J_v} = F = [a_1, a_2, \ . \ . \ . \ , a_n, \ . \ . \ .] \tag{7}$$

where the $a_n = (-1)^{n+1} 2(v+n-1)/x$, v is the order, and x is the argument. A simplification is possible in this case because every other term is of opposite sign. The alternating sign can be eliminated by transforming the simple continued fraction to a simple negative continued fraction using equation (5) of 3.10.1 of Abramowitz.[7]

$$F_n = a_1 + \frac{c_2}{c_2 a_2 +} \frac{c_2 c_3}{c_3 a_3 +} \frac{c_3 c_4}{c_4 a_4 +} \cdots + \frac{c_{n-1} c_n}{c_n a_n} \tag{8}$$

If $c_{2m} = -1$ and $c_{2m+1} = 1$ and $b_{2m} = a_{2m}$ and $b_{2m+1} = a_{2m+1}$

then

$$G_n = b_1 - \frac{1}{b_2} - \frac{1}{b_3} - \frac{1}{b_4} - \cdots - \frac{1}{b_n} \tag{9}$$

which will be defined as a negative simple continued fraction. None of the b_i may be zero, but they may be complex or negative. In like manner, a new notation may be defined for the nth convergent G_n.

$$\begin{aligned} G_n &= [-]\ [b_1, b_2, \ldots, b_n] \\ &= \quad [b_1, -b_2, b_3, -b_4, b_5, -b_6, \ldots, b_n] \end{aligned} \tag{10}$$

---

[7]M. Abramowitz, F. W. J. Olver, and H. A. Antosiewicz, 1965, Handbook of Mathematical Functions, M. Abramowitz and I. A. Stegun, editors, Applied Mathematics Series 55, chapters 3, 9, and 10, US Government Printing Office, Washington, DC

where the first equation is a negative simple continued fraction and the second equation an equivalent positive simple continued fraction.

The need for this additional complexity will become apparent when the formulae for the spherical Bessel functions is derived.

The equivalent algorithm for negative continued fractions is:

$$G_n = [-] \frac{[b_1]\,[b_2, b_1]\ \ldots\ [b_n, \ldots, b_1]}{[b_2]\,[b_3, b_2]\ \ldots\ [b_n, \ldots, b_2]} \tag{11}$$

The algorithm improvement for negative continued fractions follows directly from the definition of the b_m.

$$\zeta = \beta\gamma = b_{m+1}\beta - 1 \tag{12}$$

$$Z = b_{m+2} - \beta/\zeta \tag{13}$$

The above formulae may apply to either the numerator or denominator or both completely independently.

4. SPHERICAL BESSEL FUNCTIONS

One straightforward way to calculate the consecutive orders of Bessel functions by the continued fraction technique is to multiply appropriate ratios by an initial value

$$1/j_n = 1/j_0 \, \frac{j_0}{j_1} \, \frac{j_1}{j_2} \, \frac{j_2}{j_3} \, \frac{\cdots}{\cdots} \, \frac{j_{n-1}}{j_n} \tag{14}$$

The initial value for spherical Bessel functions of complex argument is easily calculated from equation 10.1.11 of Abramowitz.[7]

$$j_0(x) = \sin(x)/x \tag{15}$$

In terms of a negative continued fraction $b_m = 2(v+m-1)/x$ where $v = n + 0.5$ is the order and m is the number of the term in the continued fraction.

Let $b_{n,m} = 2(n + m - 0.5)/x$

This definition is exactly equivalent to the previous b_m, and it allows one to keep track of both the order of the Bessel function ratio and the order of the continued fraction term. Using this notation, the product of n continued fraction ratios and an initial value becomes:

$$1/j_n = 1/j_0 \frac{[-]\ [b_{1,1}][b_{1,2},b_{1,1}] \ldots [b_{n,1}][b_{n,2},b_{n,1}] \ldots}{[b_{1,2}] \ldots \quad [b_{n,2}][b_{n,3},b_{n,2}] \ldots} \tag{16}$$

Some of the terms in the numerator and denominator are identical and cancel; for example, $[b_{1,2}] = [b_{2,1}]$. The terms that are generally identical are:

$$[b_{s,m+1}]_{num} = [b_{s-1,m}]_{den}$$

$$[b_{s,m+2},b_{s,m+1}]_{num} = [b_{s-1,m+1},b_{s-1,m}]_{den}$$

$$\ldots\ldots$$

A simple rule to use to understand the terms that are identical is to note that lower order denominators cancel the next higher order numerators. All of the denominators corresponding to the ratio of Bessel functions of a given order cancel all of the numerators of the next higher order ratio of Bessel functions. All that is left is the numerator of the ratio j_0/j_1 and the denominator of the ratio j_{n-1}/j_n. This cancellation is not approximate. Every term is exactly identical if the proper terms are considered. Let us consider a numerical example for clarification. Let $x = 1.0$ in $j_9(x)$.

---

[7]M. Abramowitz, F. W. J. Olver, and H. A. Antosiewicz, 1965, Handbook of Mathematical Functions, M. Abramowtiz and I. A. Stegun, editors, Applied Mathematics Series 55, chapters 3, 9, and 10, US Government Printing Office, Washington, DC

$$1/j_9 = (3)(4.666)(6.785714286)(8.852631589)(10.88703924)(12.90814766) \,*$$

$$(14.92252955)(16.93298723)(18.94094367)\frac{(20.94720432)(22.95226093)}{(21)\quad(22.95238095)} \,*$$

$$\frac{(24.95643131)(26.95993017)}{(24.95643154)(26.95993017)} * 1/\sin(1) = (1.4913765 \times 10^{-9})^{-1}$$

Note that there are nine terms before the denominator begins, and convergence is rapid once the continued fraction is begun.

It is important to realize that the error correction algorithm improvement applies to the first nine terms above as well as to the terms in the numerator and denominator of the complete continued fraction. The application of the algorithm improvement is completely independent of what is happening elsewhere; and in a properly constructed algorithm, no loss of accuracy will occur due to cancellation of digits in addition or subtraction.

5. FORTRAN PROGRAMS

The first FORTRAN IV program in the appendix is a simplified version of the spherical Bessel function formulae developed above. The only error check is for a term being identically zero in either the numerator or denominator. In that case, the error bypass is implemented through the algorithm improvement as detailed in reference 6. If a given term is zero, the product of that term and the next in the algorithm improvement is one. Therefore, it is sufficient to simply skip the product and reciprocal.

The second FORTRAN IV program is essentially the same program modified slightly for complex arguments. The test for convergence is also appropriately modified. Both of these programs have been checked against tables[1] of spherical Bessel functions and found to be more accurate than the tables. Remember that the final answer is scaled by powers of 10**50 so that overflow will not occur in the computer. The displayed answer must be adjusted to account for this if the values are used in computations.

---

[6] W. J. Lentz, 1982, A Simplification of Lentz's Algorithm, ASL-TR-0118, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

[7] W. J. Lentz, 1973, A New Method of Computing Spherical Bessel Functions of Complex Argument with Tables, ECOM 5509, AD 767223, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM

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2. Lentz, W. J., 1976, "Generating Bessel Functions in Mie Scattering Calculations Using Continued Fractions," Appl Opt, 15:668.

3. Wiscombe, W. J., 1980, "Improved Mie Scattering Algorithms," Appl Opt, 19:1505.

4. Grehan, G., and G. Gouesbet, "Mie Theory Calculations: New Progress, with Emphasis on Particle Sizing," Appl Opt, 18:3489.

5. Gautschi, W., 1967, SIAM, Rev 9, No 1.

6. Lentz, W. J., 1982, A Simplification of Lentz's Algorithm, ASL-TR-0118, US Army Atmospheric Sciences Laboratory, White Sands Missile Range, NM.

7. Abramowitz, M., F. W. J. Olver, and H. A. Antosiewicz, 1965, Handbook of Mathematical Functions, M. Abramowitz and I. A. Stegun, editors, Applied Mathematics Series 55, chapters 3, 9, and 10, US Government Printing Office, Washington, DC.

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APPENDIX

FORTRAN ALGORITHM LISTINGS

NOVA FORTRAN 5, Version 6.16 -- Monday, April 23, 1984 11:27:53 AM

FBESSEL.FR

```
            COMPILER DOUBLE PRECISION
      C     PROGRAM FBESSEL CALCULATES SPHERICAL BESSEL FUNCTIONS OF THE FIRST
      C     KIND BY LENTZ CONTINUED FRACTION WITH A CHECK FOR ZERO ONLY
      C     IN THE NUMERATOR AND DENOMINATOR CALCULATIONS
      C     SEE APPLIED OPTICS VOL 15, NO 3 MARCH 1976 P668.
      C***********************************************************************
            INTEGER ICOUNT,N
            REAL V,XINC,AN,JO,JN,X,NUM,DEN,PDT,SCALE
      C***********************************************************************
      1     TYPE "INPUT ORDER, ARGUMENT OF SPHERICAL BESSEL FUNCTION"
            ACCEPT N,X
            PDT=1.0
            V=FLOAT(N)+0.5
            NUM=0.0
            DEN=0.0
            SCALE=0.0
            AN=1.0/X
            XINC=2.0/X
            ICOUNT=0
      C     IF N IS ZERO, THE INITIAL VALUE SIN(X)/X IS USED
            IF(N.EQ.0) GOTO 20
      17    AN=AN+XINC
            NUM=AN-NUM
            IF(NUM.EQ.0.0) GOTO 18
            PDT=PDT*NUM
            NUM=1.0/NUM
            IF(ABS(PDT).LT.1.0D50) GOTO 18
            PDT=PDT*1.0D-50
            SCALE=SCALE-50.
      18    ICOUNT=ICOUNT+1
            IF(ICOUNT.LE.N) GOTO 19
            DEN=AN-DEN
            IF(DEN.EQ.0.0) GOTO 19
            PDT=PDT/DEN
            DEN=1.0/DEN
      19    IF(NUM.NE.DEN.OR.ICOUNT.LT.5) GOTO 17
      20    JO=SIN(X)/X
            JN=JO/PDT
            WRITE(10,100) JN,SCALE,X,V,ICOUNT
      100   FORMAT(1H ,"JN=",D20.10,"  POWER OF 10 SCALE=",F6.0,/,1H ,"X=",(E14.6),
           X "  V=",F6.1,"  COUNT=",I5)
            GOTO 1
            END
```

Identifier	References					
AN	8	17	22	23	32	
DEN	8	15	32	33	34	35	36
ICOUNT	7	19	30	31	36	39	
JN	8	38	39				
JO	8	37	38				
N	7	11	13	21	31		
NUM	8	14	23	24	25	26	36
PDT	8	12	25	27	28	34	38
SCALE	8	16	29	39			
V	8	13	39				
X	8	11	17	18	37	39	
XINC	8	18	22				
1	10	42					
100	41	39					
17	22	36					
18	24	27	30				
19	31	33	36				
20	21	37					

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FCBESSEL.FR

```
      COMPILER DOUBLE PRECISION
C     PROGRAM FCBESSEL CALCULATES BESSEL FUNCTIONS BY FIRST RATIO METHOD
C     AND SIMPLIFICATIONS WITH ONLY A CHECK FOR ZERO. NO ACCURACY IMPROVEMENT
C     IS IMPLEMENTED

C*********************************************************************************
      REAL COUNT,V,SCALE
      COMPLEX XINC,AN,JO,JN,X,NUM,DEN,PDT
C*********************************************************************************
1     TYPE "INPUT N,COMPLEX X"
      ACCEPT N,X
      PDT=1.0
      V=FLOAT(N)
      NUM=0.0
      DEN=0.0
      SCALE=0.0
      AN=1.0/X
      XINC=2.0/X
      COUNT=0
C     IF N IS ZERO, USE THE INITIAL VALUE SIN(X)/S
      IF(N.EQ.0) GOTO 20
17    AN=AN+XINC
      NUM=AN-NUM
      IF(NUM.EQ.0.0) GOTO 18
      PDT=PDT*NUM
      NUM=1.0/NUM
      IF(ABS(REAL(PDT)).LT.1.D50) GOTO 18
      PDT=PDT*1.D-50
      SCALE=SCALE-50
18    COUNT=COUNT+1.0
      IF(COUNT.LE.V) GOTO 19
      DEN=AN-DEN
      IF(DEN.EQ.0.0) GOTO 19
      PDT=PDT/DEN
      DEN=1.0/DEN
19    IF(COUNT.LT.5.0) GOTO 17
C     THIS CHECK FOR THE COMPLEX NUMERATOR EQUAL TO THE COMPLEX
C     DENOMINATOR MAY BE MACHINE DEPENDENT
      IF(REAL(NUM).NE.REAL(DEN).OR.AIMAG(NUM).NE.AIMAG(DEN)) GOTO 17
20    JO=CSIN(X)/X
      JN=JO/PDT
      WRITE(10,100) JN,SCALE,X,V,COUNT
100   FORMAT(1H ,"JN=",2(D20.10)," POWER OF 10 SCALE=",F6.0,/,1H ,"X=",
     X 2(E14.6)," N=",F6.0," COUNT=",F8.0)
      GOTO 1
      END
```

Identifier	References						
AN	8	17	22	23	32		
COUNT	7	19	30	31	36	42	
DEN	8	15	32	33	34	35	39
JN	8	41	42				
JO	8	40	41				
N	11	13	21				
NUM	8	14	23	24	25	26	39
PDT	8	12	25	27	28	34	41
SCALE	7	16	29	42			
V	7	13	31	42			
X	8	11	17	18	40	42	
XINC	8	18	22				
1	10	45					
100	44	42					
17	22	36	39				
18	24	27	30				
19	31	33	36				
20	21	40					

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