S21BDF – NAG Fortran Library Routine Document

Note. Before using this routine, please read the Users' Note for your implementation to check the interpretation of bold italicised terms and other implementation-dependent details.

1 Purpose

S21BDF returns a value of the symmetrised elliptic integral of the third kind, via the routine name.

2 Specification

```
real FUNCTION S21BDF(X, Y, Z, R, IFAIL)
INTEGER              IFAIL
real                 X, Y, Z, R
```

3 Description

This routine calculates an approximation to the integral

$$R_J(x,y,z,\rho) = \frac{3}{2}\int_0^\infty \frac{dt}{(t+\rho)\sqrt{(t+x)(t+y)(t+z)}}$$

where x, y, $z \geq 0$, $\rho \neq 0$ and at most one of x, y and z is zero.

If $\rho < 0$, the result computed is the Cauchy principal value of the integral.

The basic algorithm, which is due to Carlson [2] and [3], is to reduce the arguments recursively towards their mean by the rule:

$$\begin{aligned}
x_0 &= x, y_0 = y, z_0 = z, \rho_0 = \rho \\
\mu_n &= (x_n + y_n + z_n + 2\rho_n)/5 \\
X_n &= 1 - x_n/\mu_n \\
Y_n &= 1 - y_n/\mu_n \\
Z_n &= 1 - z_n/\mu_n \\
P_n &= 1 - \rho_n/\mu_n \\
\lambda_n &= \sqrt{x_n y_n} + \sqrt{y_n z_n} + \sqrt{z_n x_n} \\
x_{n+1} &= (x_n + \lambda_n)/4 \\
y_{n+1} &= (y_n + \lambda_n)/4 \\
z_{n+1} &= (z_n + \lambda_n)/4 \\
\rho_{n+1} &= (\rho_n + \lambda_n)/4 \\
\alpha_n &= \left[\rho_n(\sqrt{x_n} + \sqrt{y_n} + \sqrt{z_n}) + \sqrt{x_n y_n z_n}\right]^2 \\
\beta_n &= \rho_n(\rho_n + \lambda_n)^2
\end{aligned}$$

For n sufficiently large,

$$\epsilon_n = \max(|X_n|, |Y_n|, |Z_n|, |P_n|) \sim \frac{1}{4^n}$$

and the function may be approximated by a 5th order power series

$$\begin{aligned}
R_J(x,y,z,\rho) = {} & 3\sum_{m=0}^{n-1} 4^{-m} R_C(\alpha_m, \beta_m) \\
& + \frac{4^{-n}}{\sqrt{\mu_n^3}}\left[1 + \frac{3}{7}S_n^{(2)} + \frac{1}{3}S_n^{(3)} + \frac{3}{22}(S_n^{(2)})^2 + \frac{3}{11}S_n^{(4)} + \frac{3}{13}S_n^{(2)}S_n^{(3)} + \frac{3}{13}S_n^{(5)}\right]
\end{aligned}$$

where $S_n^{(m)} = (X_n^m + Y_n^m + Z_n^m + 2P_n^m)/2m$.

The truncation error in this expansion is bounded by $3\epsilon_n^6/\sqrt{(1-\epsilon_n)^3}$ and the recursion process is terminated when this quantity is negligible compared with the ***machine precision***. The routine may fail either because it has been called with arguments outside the domain of definition or with arguments so extreme that there is an unavoidable danger of setting underflow or overflow.

Note. $R_J(x,x,x,x) = x^{-\frac{3}{2}}$, so there exists a region of extreme arguments for which the function value is not representable.

4 References

[1] Abramowitz M and Stegun I A (1972) *Handbook of Mathematical Functions* Dover Publications (3rd Edition)

[2] Carlson B C (1978) Computing elliptic integrals by duplication *Preprint* Department of Physics, Iowa State University

[3] Carlson B C (1988) A table of elliptic integrals of the third kind *Math. Comput.* **51** 267–280

5 Parameters

1: X — ***real*** *Input*

2: Y — ***real*** *Input*

3: Z — ***real*** *Input*

4: R — ***real*** *Input*

On entry: the arguments x, y, z and ρ of the function.

Constraint: X, Y, Z $\geq$ 0.0, R $\neq$ 0.0 and at most one of X, Y and Z may be zero.

5: IFAIL — INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

If on entry IFAIL = 0 or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL = 1

On entry, at least one of X, Y and Z is negative, or at least two of them are zero; the function is undefined.

IFAIL = 2

On entry, R = 0.0; the function is undefined.

IFAIL = 3

On entry, either R is too close to zero, or any two of X, Y and Z are too close to zero; there is a danger of setting overflow.

IFAIL = 4

On entry, at least one of X, Y, Z and R is too large; there is a danger of setting underflow.

7 Accuracy

In principle the routine is capable of producing full ***machine precision***. However round-off errors in internal arithmetic will result in slight loss of accuracy. This loss should never be excessive as the algorithm does not involve any significant amplification of round-off error. It is reasonable to assume that the result is accurate to within a small multiple of the ***machine precision***.

8 Further Comments

Users should consult the Chapter Introduction which shows the relationship of this function to the classical definitions of the elliptic integrals.

If the argument R is equal to any of the other arguments, the function reduces to the integral R_D, computed by S21BCF.

9 Example

This example program simply generates a small set of non-extreme arguments which are used with the routine to produce the table of low accuracy results.

9.1 Program Text

Note. The listing of the example program presented below uses bold italicised terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     S21BDF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*     .. Local Scalars ..
      real             R, RJ, X, Y, Z
      INTEGER          IFAIL, IX, IY, IZ
*     .. External Functions ..
      real             S21BDF
      EXTERNAL         S21BDF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S21BDF Example Program Results'
      WRITE (NOUT,*)
      WRITE (NOUT,*) '    X      Y      Z      R        S21BDF  IFAIL'
      WRITE (NOUT,*)
      DO 60 IX = 1, 3
         X = IX*0.5e0
         DO 40 IY = IX, 3
            Y = IY*0.5e0
            DO 20 IZ = IY, 3
               Z = IZ*0.5e0
               R = 2.0e0
               IFAIL = 1
*
               RJ = S21BDF(X,Y,Z,R,IFAIL)
*
               WRITE (NOUT,99999) X, Y, Z, R, RJ, IFAIL
   20       CONTINUE
   40    CONTINUE
   60 CONTINUE
      STOP
*
99999 FORMAT (1X,4F7.2,F12.4,I5)
      END
```

9.2 Program Data

None.

9.3 Program Results

```
 S21BDF Example Program Results

     X       Y       Z       R         S21BDF  IFAIL

    0.50    0.50    0.50    2.00      1.1184    0
    0.50    0.50    1.00    2.00      0.9221    0
    0.50    0.50    1.50    2.00      0.8115    0
    0.50    1.00    1.00    2.00      0.7671    0
    0.50    1.00    1.50    2.00      0.6784    0
    0.50    1.50    1.50    2.00      0.6017    0
    1.00    1.00    1.00    2.00      0.6438    0
    1.00    1.00    1.50    2.00      0.5722    0
    1.00    1.50    1.50    2.00      0.5101    0
    1.50    1.50    1.50    2.00      0.4561    0
```