

NAG Library Routine Document

S21BDF

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

double precision FUNCTION S21BDF(X, Y, Z, R, IFAIL)

INTEGER

IFAIL

double precision

X, Y, Z, R

3 Description

S21BDF 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 (1979) and Carlson (1988), is to reduce the arguments recursively towards their mean by the rule:

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

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 fifth 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 $3\epsilon_n/\sqrt{(1-\epsilon_n)^3}$ 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

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

Carlson B C (1979) Computing elliptic integrals by duplication *Numerische Mathematik* **33** 1–16

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

5 Parameters

- | | | |
|----|-----------------------------|--------------|
| 1: | X – <i>double precision</i> | <i>Input</i> |
| 2: | Y – <i>double precision</i> | <i>Input</i> |
| 3: | Z – <i>double precision</i> | <i>Input</i> |
| 4: | R – <i>double precision</i> | <i>Input</i> |

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 | <i>Input/Output</i> |
|----|-----------------|---------------------|

On entry: IFAIL must be set to 0, –1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

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

For environments where it might be inappropriate to halt program execution when an error is detected, the value –1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, if you are not familiar with this parameter, the recommended value is 0. **When the value –1 or 1 is used it is essential to test the value of IFAIL on exit.**

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 or warnings 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

$R = 0.0$; 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. See also the Users' Note for your implementation.

IFAIL = 4

On entry, at least one of X, Y, Z and R is too large; there is a danger of setting underflow. See also the Users' Note for your implementation.

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

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

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

9 Example

This example 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

```
*      S21BDF Example Program Text
*      Mark 14 Revised. NAG Copyright 1989.
*      .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
*      .. Local Scalars ..
      DOUBLE PRECISION R, RJ, X, Y, Z
      INTEGER          IFAIL, IX, IY, IZ
*      .. External Functions ..
      DOUBLE PRECISION 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*0.5D0
        DO 40 IY = IX, 3
          Y = IY*0.5D0
          DO 20 IZ = IY, 3
            Z = IZ*0.5D0
            R = 2.0D0
            IFAIL = 1

*
            RJ = S21BDF(X,Y,Z,R,IFAIL)
*
            IF (IFAIL.GE.0) THEN
              WRITE (NOUT,99999) X, Y, Z, R, RJ, IFAIL
            ELSE
              WRITE (NOUT,99998) IFAIL
              GO TO 80
            END IF
          20 CONTINUE
        40 CONTINUE
      60 CONTINUE
*
```

```
      80 CONTINUE
*
99999 FORMAT (1X,4F7.2,F12.4,I5)
99998 FORMAT (1X,' ** S21BDF returned with IFAIL = ',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
