S20ADF – 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

S20ADF returns a value for the Fresnel Integral $C(x)$, via the routine name.

2 Specification

```
real FUNCTION S20ADF(X, IFAIL)
INTEGER            IFAIL
real               X
```

3 Description

This routine evaluates an approximation to the Fresnel Integral

$$C(x) = \int_0^x \cos\left(\frac{\pi}{2}t^2\right) dt.$$

Note. $C(x) = -C(-x)$, so the approximation need only consider $x \geq 0.0$.

The routine is based on three Chebyshev expansions:

For $0 < x \leq 3$,

$$C(x) = x{\sum_{r=0}}' a_r T_r(t) \text{ , with } t = 2\left(\frac{x}{3}\right)^4 - 1;$$

For $x > 3$,

$$C(x) = \frac{1}{2} + \frac{f(x)}{x}\sin\left(\frac{\pi}{2}x^2\right) - \frac{g(x)}{x^3}\cos\left(\frac{\pi}{2}x^2\right),$$

where $f(x) = {\sum_{r=0}}' b_r T_r(t)$,

and $g(x) = {\sum_{r=0}}' c_r T_r(t)$, with $t = 2\left(\frac{3}{x}\right)^4 - 1$.

For small x, $C(x) \simeq x$. This approximation is used when x is sufficiently small for the result to be correct to ***machine precision***.

For large x, $f(x) \simeq \frac{1}{\pi}$ and $g(x) \simeq \frac{1}{\pi^2}$. Therefore for moderately large x, when $\frac{1}{\pi^2 x^3}$ is negligible compared with $\frac{1}{2}$, the second term in the approximation for $x > 3$ may be dropped. For very large x, when $\frac{1}{\pi x}$ becomes negligible, $C(x) \simeq \frac{1}{2}$. However there will be considerable difficulties in calculating $\sin\left(\frac{\pi}{2}x^2\right)$ accurately before this final limiting value can be used. Since $\sin\left(\frac{\pi}{2}x^2\right)$ is periodic, its value is essentially determined by the fractional part of x^2. If $x^2 = N+\theta$, where N is an integer and $0 \leq \theta < 1$, then $\sin\left(\frac{\pi}{2}x^2\right)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain some significance in the calculation of $\sin\left(\frac{\pi}{2}x^2\right)$ either all the way to the very large x limit, or at least until the integer part of $\frac{x}{2}$ is equal to the maximum integer allowed on the machine.

4 References

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

5 Parameters

1: X — ***real*** *Input*

On entry: the argument x of the function.

2: 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

There are no failure exits from this routine. The parameter IFAIL has been included for consistency with other routines in this chapter.

7 Accuracy

Let δ and ϵ be the relative errors in the argument and result respectively.

If δ is somewhat larger than the ***machine precision*** (i.e if δ is due to data errors etc.), then ϵ and δ are approximately related by:

$$\epsilon \simeq \left| \frac{x \cos\left(\frac{\pi}{2} x^2\right)}{C(x)} \right| \delta.$$

Figure 1 shows the behaviour of the error amplification factor $\left| \frac{x \cos\left(\frac{\pi}{2} x^2\right)}{C(x)} \right|$.

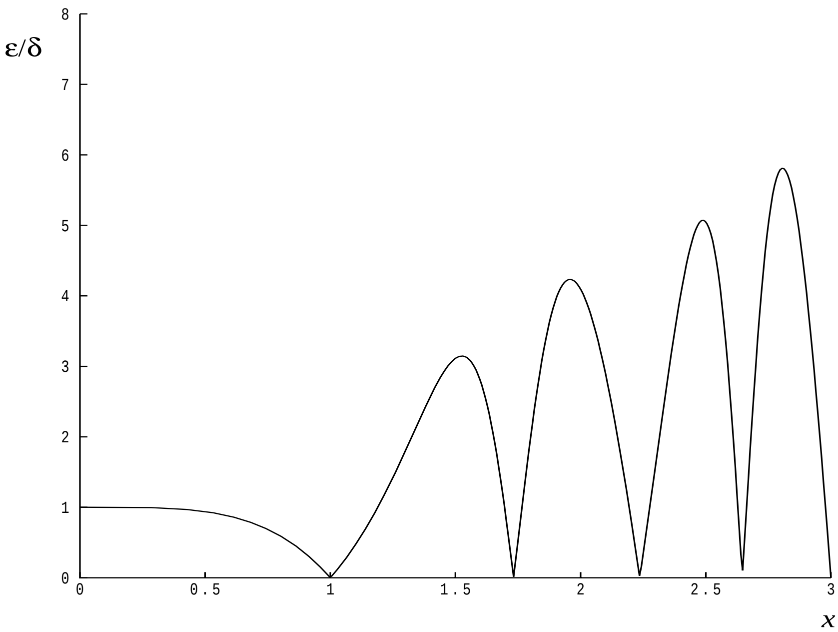

Figure 1

However, if δ is of the same order as the ***machine precision***, then rounding errors could make ϵ slightly larger than the above relation predicts.

For small x, $\epsilon \simeq \delta$ and there is no amplification of relative error.

For moderately large values of x,

$$|\epsilon| \simeq \left| 2x \cos\left(\frac{\pi}{2} x^2\right) \right| |\delta|$$

and the result will be subject to increasingly large amplification of errors. However the above relation breaks down for large values of x (i.e., when $\frac{1}{x^2}$ is of the order of the ***machine precision***); in this region the relative error in the result is essentially bounded by $\frac{2}{\pi x}$.

Hence the effects of error amplification are limited and at worst the relative error loss should not exceed half the possible number of significant figures.

8 Further Comments

None.

9 Example

The example program reads values of the argument x from a file, evaluates the function at each value of x and prints the 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.

```
*     S20ADF Example Program Text
*     Mark 14 Revised.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      real             X, Y
      INTEGER          IFAIL
*     .. External Functions ..
      real             S20ADF
      EXTERNAL         S20ADF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S20ADF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '     X           Y        IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) X
      IFAIL = 1
*
      Y = S20ADF(X,IFAIL)
*
      WRITE (NOUT,99999) X, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,1P,2e12.3,I7)
      END
```

9.2 Program Data

```
S20ADF Example Program Data
             0.0
             0.5
             1.0
             2.0
             4.0
             5.0
             6.0
             8.0
             10.0
             -1.0
             1000.0
```

9.3 Program Results

```
 S20ADF Example Program Results

      X           Y        IFAIL

   0.000E+00   0.000E+00      0
   5.000E-01   4.923E-01      0
   1.000E+00   7.799E-01      0
   2.000E+00   4.883E-01      0
   4.000E+00   4.984E-01      0
   5.000E+00   5.636E-01      0
   6.000E+00   4.995E-01      0
   8.000E+00   4.998E-01      0
   1.000E+01   4.999E-01      0
  -1.000E+00  -7.799E-01      0
   1.000E+03   5.000E-01      0
```