NAG Fortran Library Routine Document

S20ACF

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

S20ACF returns a value for the Fresnel Integral $S(x)$, via the routine name.

2   Specification

```
real FUNCTION S20ACF(X, IFAIL)
INTEGER            IFAIL
real               X
```

3   Description

This routine evaluates an approximation to the Fresnel Integral

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

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

The routine is based on three Chebyshev expansions:

For $0 < x \leq 3$,

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

For $x > 3$,

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

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

and $g(x) = \sideset{}{'}\sum_{r=0} c_r T_r(t)$,

with $t = 2\left(\frac{3}{x}\right)^4 - 1$.

For small x, $S(x) \simeq \frac{\pi}{6}x^3$. This approximation is used when x is sufficiently small for the result to be correct to **machine precision**. For very small x, this approximation would underflow; the result is then set exactly to zero.

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, $S(x) \simeq \frac{1}{2}$. However there will be considerable difficulties in calculating $\cos\left(\frac{\pi}{2}x^2\right)$ accurately before this final limiting value can be used. Since $\cos\left(\frac{\pi}{2}x^2\right)$ 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 $\cos\left(\frac{\pi}{2}x^2\right)$ depends on θ and on N modulo 4. By exploiting this fact, it is possible to retain significance in

the calculation of $\cos\left(\frac{\pi}{2}x^2\right)$ 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

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

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. Users who are unfamiliar with this parameter should refer to Chapter P01 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, for users 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

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:

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

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

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, $\epsilon \simeq 3\delta$ and hence there is only moderate amplification of relative error. Of course for very small x where the correct result would underflow and exact zero is returned, relative error-control is lost.

For moderately large values of x,

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

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.
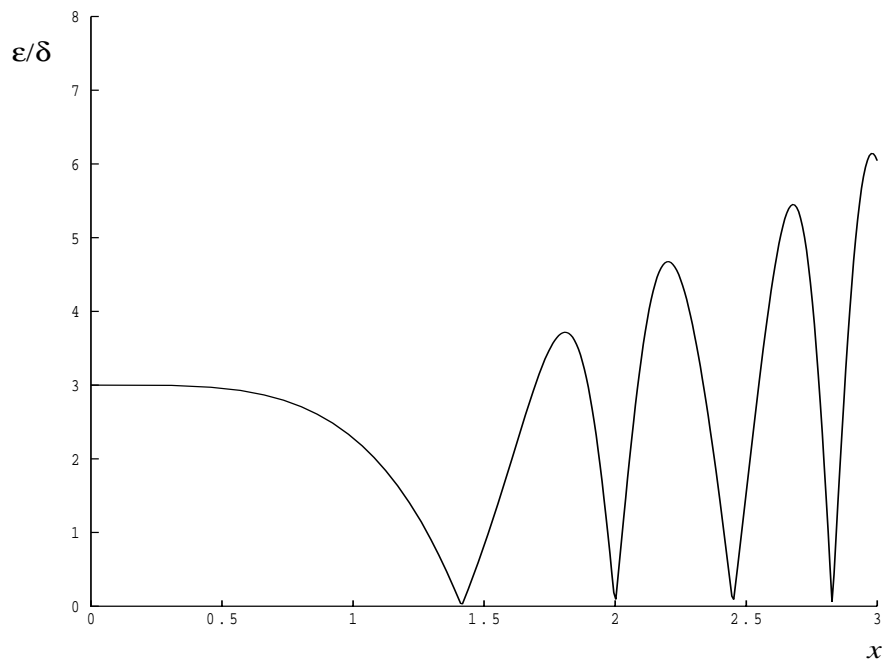

Figure 1

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.

```
*      S20ACF 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             S20ACF
       EXTERNAL         S20ACF
*      .. Executable Statements ..
       WRITE (NOUT,*) 'S20ACF 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 = S20ACF(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

```
S20ACF 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

```
 S20ACF Example Program Results

      X           Y          IFAIL

   0.000E+00   0.000E+00       0
   5.000E-01   6.473E-02       0
   1.000E+00   4.383E-01       0
   2.000E+00   3.434E-01       0
   4.000E+00   4.205E-01       0
   5.000E+00   4.992E-01       0
   6.000E+00   4.470E-01       0
   8.000E+00   4.602E-01       0
   1.000E+01   4.682E-01       0
  -1.000E+00  -4.383E-01       0
   1.000E+03   4.997E-01       0
```