

# NAG Library Routine Document

## S15AFF

**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

S15AFF returns a value for Dawson's Integral,  $F(x)$ , via the routine name.

### 2 Specification

*double precision* FUNCTION S15AFF(X, IFAIL)  
 INTEGER IFAIL  
*double precision* X

### 3 Description

S15AFF evaluates an approximation for Dawson's Integral

$$F(x) = e^{-x^2} \int_0^x e^{t^2} dt.$$

The routine is based on two Chebyshev expansions:

For  $0 < |x| \leq 4$ ,

$$F(x) = x \sum_{r=0}^l a_r T_r(t), \quad \text{where} \quad t = 2\left(\frac{x}{4}\right)^2 - 1.$$

For  $|x| > 4$ ,

$$F(x) = \frac{1}{x} \sum_{r=0}^l b_r T_r(t), \quad \text{where} \quad t = 2\left(\frac{4}{x}\right)^2 - 1.$$

For  $|x|$  near zero,  $F(x) \simeq x$ , and for  $|x|$  large,  $F(x) \simeq \frac{1}{2x}$ . These approximations are used for those values of  $x$  for which the result is correct to *machine precision*. For very large  $x$  on some machines,  $F(x)$  may underflow and then the result is set exactly to zero (see the Users' Note for your implementation for details).

### 4 References

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

### 5 Parameters

- 1: X – *double precision* *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. 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

There are no failure exits from this routine.

## 7 Accuracy

Let  $\delta$  and  $\epsilon$  be the relative errors in the argument and result respectively.

If  $\delta$  is considerably greater than the *machine precision* (i.e., if  $\delta$  is due to data errors etc.), then  $\epsilon$  and  $\delta$  are approximately related by:

$$\epsilon \simeq \left| \frac{x(1 - 2xF(x))}{F(x)} \right| \delta.$$

The following graph shows the behaviour of the error amplification factor  $\left| \frac{x(1 - 2xF(x))}{F(x)} \right|$ :

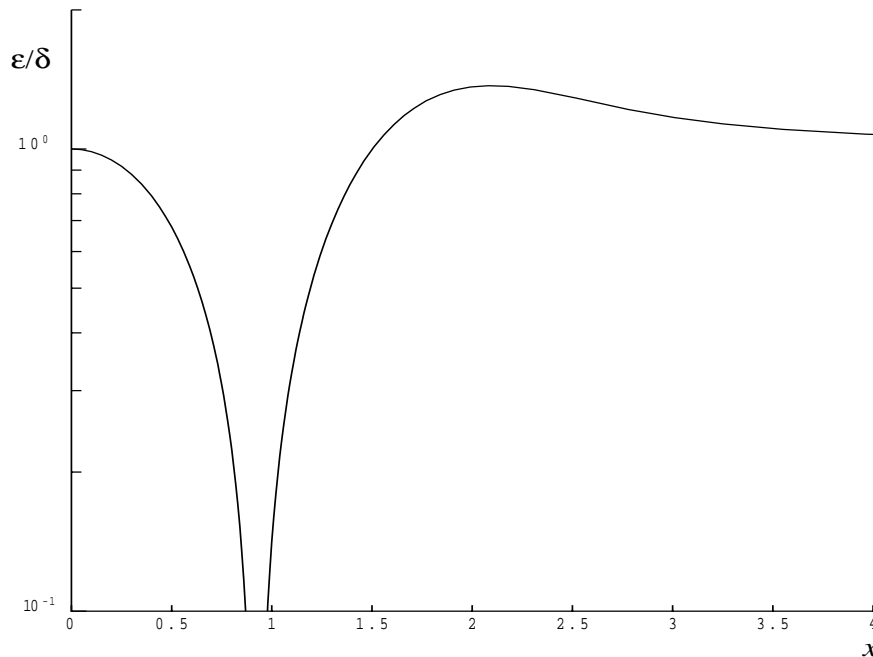


Figure 1

However if  $\delta$  is of the same order as *machine precision*, then rounding errors could make  $\epsilon$  somewhat larger than the above relation indicates. In fact  $\epsilon$  will be largely independent of  $x$  or  $\delta$ , but will be of the order of a few times the *machine precision*.

## 8 Further Comments

None.

## 9 Example

This example 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

```

*      S15AFF Example Program Text
*      Mark 14 Revised. NAG Copyright 1989.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER       (NIN=5,NOUT=6)
*      .. Local Scalars ..
      DOUBLE PRECISION X, Y
      INTEGER          IFAIL
*      .. External Functions ..
      DOUBLE PRECISION S15AFF
      EXTERNAL        S15AFF
*      .. Executable Statements ..
      WRITE (NOUT,*) 'S15AFF 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 = S15AFF(X,IFAIL)
*
      IF (IFAIL.GE.0) THEN
          WRITE (NOUT,99999) X, Y, IFAIL
          GO TO 20
      ELSE
          WRITE (NOUT,99998) IFAIL
      END IF
40     CONTINUE
*
99999  FORMAT (1X,1P,2E12.3,I7)
99998  FORMAT (1X,' ** S15AFF returned with IFAIL = ',I5)
      END

```

## 9.2 Program Data

```

S15AFF Example Program Data
      -2.0
      -0.5
      1.0
      1.5
      2.0
      5.0
      10.0

```

## 9.3 Program Results

S15AFF Example Program Results

X	Y	IFAIL
-2.000E+00	-3.013E-01	0
-5.000E-01	-4.244E-01	0
1.000E+00	5.381E-01	0
1.500E+00	4.282E-01	0
2.000E+00	3.013E-01	0
5.000E+00	1.021E-01	0
1.000E+01	5.025E-02	0

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