NAG Fortran Library Routine Document

S15DDF

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

S15DDF computes values of the function $w(z) = e^{-z^2} \operatorname{erfc}(-iz)$, for ***complex*** z.

2 Specification

```
complex FUNCTION S15DDF(Z, IFAIL)
INTEGER                  IFAIL
complex                  Z
```

3 Description

This routine computes values of the function $w(z) = e^{-z^2} \operatorname{erfc}(-iz)$, where $\operatorname{erfc} z$ is the complementary error function

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2}\, dt,$$

for ***complex*** z. The method used is that in Gautschi (1970) for z in the first quadrant of the complex plane, and is extended for z in other quadrants via the relations $w(-z) = 2e^{-z^2} - w(z)$ and $w(\bar{z}) = \overline{w(-z)}$. Following advice in Gautschi (1970), and van der Laan and Temme (1984), the code in Gautschi (1969) has been adapted to work in various precisions up to 18 decimal places. The real part of $w(z)$ is sometimes known as the Voigt function.

4 References

Gautschi W (1970) Efficient computation of the complex error function *SIAM J. Numer. Anal.* **7** 187–198

Gautschi W (1969) Algorithm 363: Complex error function *Comm. ACM* **12** 635

van der Laan C G and Temme N M (1984) Calculation of special functions: the gamma function, the exponential integrals and error-like functions *CWI Tract 10* Centre for Mathematics and Computer Science, Amsterdam

5 Parameters

1: Z – ***complex*** *Input*

On entry: the argument z 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

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 $= 1$

The real part of the result overflows, and is set to the largest safe number with the correct sign. The imaginary part of the result is meaningful.

IFAIL $= 2$

The imaginary part of the result overflows, and is set to the largest safe number with the correct sign. The real part of the result is meaningful.

IFAIL $= 3$

Both real and imaginary parts of the result overflow, and are set to the largest safe number with the correct signs.

IFAIL $= 4$

The result returned is accurate to less than half precision, due to the size of an intermediate result.

IFAIL $= 5$

The result returned has no precision, due to the size of an intermediate result, and is set to zero.

7 Accuracy

The accuracy of the returned result depends on the argument z. If z lies in the first or second quadrant of the complex plane (i.e., $\mathrm{Im}\, z$ is greater than or equal to zero), the result should be accurate almost to ***machine precision***, except that there is a limit of about 18 decimal places on the achievable accuracy because constants in the routine are given to this precision. With such arguments, IFAIL can only return as zero.

If however $\mathrm{Im}\, z$ is less than zero, accuracy may be lost in two ways; firstly, in the evaluation of e^{-z^2}, if $\mathrm{Im}(-z^2)$ is large, in which case a warning will be issued through IFAIL $= 4$ or 5; and secondly, near the zeros of the required function, where precision is lost due to cancellation, in which case no warning is given – the result has absolute accuracy rather than relative accuracy. Note also that in this half-plane, one or both parts of the result may overflow – this is signalled through IFAIL $= 1$, 2 or 3.

8 Further Comments

The time taken for a call of S15DDF depends on the argument z, the time increasing as $|z| \rightarrow 0.0$.

This routine may be used to compute values of $\mathrm{erfc}\, z$ and $\mathrm{erf}\, z$ for ***complex*** z by the relations $\mathrm{erfc}\, z = e^{-z^2} w(iz)$, $\mathrm{erf}\, z = 1 - \mathrm{erfc}\, z$. (For ***real*** arguments, S15ADF and S15AEF should be used.)

9 Example

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

```
*     S15DDF Example Program Text
*     Mark 14 Release.  NAG Copyright 1989.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          W, Z
      INTEGER          IFAIL
*     .. External Functions ..
      complex          S15DDF
      EXTERNAL         S15DDF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S15DDF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '               Z                                W'
   20 READ (NIN,*,END=40) Z
      IFAIL = 0
*
      W = S15DDF(Z,IFAIL)
*
      WRITE (NOUT,99999) Z, W
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,'(',F12.4,',',F12.4,')      (',F12.4,',',F12.4,')')
      END
```

9.2 Program Data

```
S15DDF Example Program Data
 ( 1.00E0,   0.00E0)       - Values for Z.
 (-3.01E0,   0.75E0)
 ( 2.75E0,  -1.52E0)
 (-1.33E0,  -0.54E0)
```

9.3 Program Results

```
 S15DDF Example Program Results

              Z                                W
 (      1.0000,      0.0000)      (      0.3679,      0.6072)
 (     -3.0100,      0.7500)      (      0.0522,     -0.1838)
 (      2.7500,     -1.5200)      (     -0.1015,      0.1654)
 (     -1.3300,     -0.5400)      (     -0.1839,     -0.7891)
```