NAG Toolbox for MATLAB

s15dd

1 Purpose

s15dd computes values of the function $w(z) = e^{-z^2}\operatorname{erfc}(-iz)$, for ***complex*16*** z.

2 Syntax

```
[result, ifail] = s15dd(z)
```

3 Description

s15dd 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*16*** 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 1969 Algorithm 363: Complex error function *Comm. ACM* **12** 635

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

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

5.1 Compulsory Input Parameters

1: **z – complex scalar**

The argument z of the function.

5.2 Optional Input Parameters

None.

5.3 Input Parameters Omitted from the MATLAB Interface

None.

5.4 Output Parameters

1: **result – complex scalar**

The result of the function.

2: **ifail – int32 scalar**

0 unless the function detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the function:

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 function are given to this precision. With such arguments, **ifail** can only return as **ifail** $= 0$.

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 $\mathrm{Im}\left(-z^2\right)$ 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 s15dd depends on the argument z, the time increasing as $|z| \rightarrow 0.0$.

s15dd may be used to compute values of $\mathrm{erfc}\, z$ and $\mathrm{erf}\, z$ for ***complex*16*** z by the relations $\mathrm{erfc}\, z = e^{-z^2} w(iz)$, $\mathrm{erf}\, z = 1 - \mathrm{erfc}\, z$. (For double arguments, s15ad and s15ae should be used.)

9 Example

```
z = complex(1, +0);
[result, ifail] = s15dd(z)
```

```
result =
   0.3679 + 0.6072i
ifail =
```

0