

PACKAGE SPECIFICATION

1 SUMMARY

To evaluate the function $e^{-z^2} \operatorname{erfc}(-iz)$ for complex *z*, viz.

$$W(z) = e^{-z^2} \left(1 + \frac{2i}{\sqrt{\pi}} \int_0^z e^{t^2} dt \right)$$

W(z) is evaluated for z = x + iy, x, y > 0 using the approximations

(a) if $|z| \le 1$ integrate first few terms of expansion of e^{t^2} .

(b) if $1 < |z| \le 4$ and y < 1.4 integrate the Taylor series expansion of e^{t^2} about points in the region at which the value of W(z) is known.

(c) if 1 < |z| and y > 1.4 numerically integrate

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z-t} dt$$

using the midpoint rule or Gauss-Hermite.

For outside the region x, y > 0 the relations

 $W(-z) = 2e^{-z^2} - W(z)$ and $W(\overline{z}) = \overline{W}(z)$ are used.

ATTRIBUTES — Version: 1.0.0. Types: FC01A; FC01AD. Original date: February 1964. Origin: A.Bailey*, Harwell.

2 HOW TO USE THE PACKAGE

The single precision version

CALL FC01A(X,Y,U,V)

The double precision version

CALL FC01AD(X,Y,U,V)

- X is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to x the real part of the argument z=x+iy. **Restriction:** x > 0.
- Y is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to y the imaginary part of the argument z=x+iy. **Restriction:** y>0.
- U is a REAL (DOUBLE PRECISION in the D version) variable which is set by the subroutine to the real part of the computed value of the function W(z).
- V is a REAL (DOUBLE PRECISION in the D version) variable which is set by the subroutine to the imaginary part of the computed value of the function W(z).

HSL ARCHIVE

3 GENERAL INFORMATION

Use of common: none.

Workspace: none.

Other subroutines: none.

Input/Output: none.

Restrictions:

x > 0,

y>0.

4 METHOD

W(z) is evaluated for z in the first quadrant, other values being calculated from

$$W(-z) = 2e^{z^2} - W(z)$$

and

$$W(\bar{z}) = \bar{W}(-z)$$

Within the first quadrant the approximations are computed as follows

- (a) If |z| < 1, then W(z) is calculated by integrating the first few terms of the expansion of e^{t^2} .
- (b) If 1 < |z| < 4 and y < 1.4 integration of a Taylor series expansion of e^{r^2} about one of a number of fixed points in the region, at which the value of W(z) is known.
- (c) If 1 < |z| < 4 and y > 1.4 the integral

$$W(z) = \frac{i}{\pi} \int_{-\infty}^{\infty} \frac{e^{-t^2}}{z - t} dt$$

is calculated using the midpoint rule.

(d) If |z| > 4 the above integral representation is calculated using a Gauss-Hermite quadrature formula.

At the boundaries of the various regions, the function is calculated by two methods and linear interpolation is used to give a continuous error curve.