FC16

PACKAGE SPECIFICATION HSL ARCHIVE

1 SUMMARY

To **compute values of the plasma dispersion function**

$$u(x,y) = \frac{1}{\pi} \int_{-\infty}^{\infty} \frac{y\, e^{-t^2}\, dt}{(x-t)^2 + y^2}$$

to an accuracy of 6 decimals for a series of n equally spaced values of $x = x_s,\ x_s+\delta,\ \ldots,\ x_s+(n-1)\delta$ at a fixed value of y.

ATTRIBUTES — **Version:** 1.0.0. **Remark:** using `FC16` is faster than making repeated calls to `FC01`. **Types:** `FC16A`, `FC16AD`. **Calls:** `FC07`. **Original date:** February 1983. **Origin:** A. R. Curtis, Harwell.

2 HOW TO USE THE PACKAGE

2.1 Argument list and calling sequence

The single precision version

```
CALL FC16A(Y,XS,DELTA,N,U)
```

The double precision version

```
CALL FC16AD(Y,XS,DELTA,N,U)
```

`Y` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the value of y. **Restriction:** $y > 0$. This argument is not altered by the subroutine.

`XS` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the value of x_s the smallest value of x for which $u(x,y)$ is required. This argument is not altered by the subroutine.

`DELTA` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the value of δ the interval between consecutive x values. **Restriction:** $\delta > 0$. This argument is not altered by the subroutine.

`N` is an `INTEGER` variable which must be set by the user to the value of n the total number of x values. **Restriction:** $n > 0$. This argument is not altered by the subroutine.

`U` is a `REAL` (`DOUBLE PRECISION` in the D version) array of dimension at least n in which the subroutine will return the values of $u(x,y)$ for $x = x_s,\ x_s+\delta,\ \ldots,\ x_s+(n-1)\delta$.

3 GENERAL INFORMATION

Use of common: none.

Workspace: None.

Other routines called directly: `FC07` is called.

Input/output: none.

Restrictions:

$y > 0$,

$n > 0$,

$\delta > 0$.

Accuracies:

6 decimal places.

4 METHOD

4.1 Method

The function $u(x, y)$ is the real part of the complex analytic function

$$w(z) = e^{-z^2} erfc(-iz), \qquad z = x+iy$$

(i) for $x^2 + y^2 \geq 36$ the asymptotic formula

$$w(z) = iz \left(\frac{0.5124242}{z^2 - 0.2752551} + \frac{0.05176536}{z^2 - 2.724745} \right)$$

(page 328*ref*1) is computed; it is correct to the required accuracy in this region, but if $y < 6$ values are also computed by method (ii) below in a small transition interval, and smooth interpolation used between the two values.

(ii) Within the above circle, the differential equations

$$\frac{du}{dx} = 2(vy - ux)$$
$$\frac{dv}{dx} = 2(\pi^{-1/2} - uy - vx)$$

are solved, to accuracy 10^{-6}, from initial values

$$u(0, y) = e^{y^2} erfc(y)$$
$$v(0, y) = 0$$

Values for negative x are obtained by using the fact that u is an even function of x.

4.2 Accuracy and timing

All computation is done in double precision internally; however, as the method is only capable of 6-decimal accuracy the main advantage of `FC16AD` is the double precision accumulation of x.

The c.p.u. time taken by the subroutine is given approximately by

$$t_{cpu} = t_0(y) + t_1 n_1 + t_2 n_2$$

where n_1 is the number of x values outside the circle $x^2 + y^2 = 36$ and n_2 is the number inside. On an IBM/3081, $t_1 = 10$ μsec, $t_2 = 7$ μsec, and $t_0(y)$ decreases from just under 5 *m*sec for very small y, through about 3 *m*sec at $y \approx 1.2$, 2 *m*sec at $y \approx 2.8$, to about 5 *m*sec just below $y = 6$; for $Y \geq 6$ (where $n_2 = 0$) t_0 is about 50 μsec.

References

1. M.Abramowitz and I.A.Stegun, 'Handbook of Mathematical Functions', Dover (New York) 1965.
2. A.R.Curtis, 'Calculation of the Mixed Doppler-Lorentz Line-shape Function', AERE report R.10837 (1983).