NAG Fortran Library Routine Document

S14AFF

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

S14AFF returns the value of the kth derivative of the psi function $\psi(z)$ for complex z and $k = 0, 1, \ldots, 4$, via the routine name.

2 Specification

```
complex FUNCTION S14AFF(Z, K, IFAIL)
INTEGER                 K, IFAIL
complex                 Z
```

3 Description

This routine evaluates an approximation to the kth derivative of the psi function $\psi(z)$ given by

$$\psi^{(k)}(z) = \frac{d^k}{dz^k}\psi(z) = \frac{d^k}{dz^k}\left(\frac{d}{dz}\log_{\mathrm{e}}\Gamma(z)\right),$$

where $z = x + iy$ is complex provided $y \neq 0$ and $k = 0, 1, \ldots, 4$. If $y = 0$, z is real and thus $\psi^{(k)}(z)$ is singular when $z = 0, -1, -2, \ldots$.

Note that $\psi^{(k)}(z)$ is also known as the *polygamma* function. Specifically, $\psi^{(0)}(z)$ is often referred to as the *digamma* function and $\psi^{(1)}(z)$ as the *trigamma* function in the literature. Further details can be found in Abramowitz and Stegun (1972).

S14AFF is based on a modification of the method proposed by Kölbig (1972).

To obtain the value of $\psi^{(k)}(z)$ when z is real, S14AEF can be used.

4 References

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

Kölbig K S (1972) Programs for computing the logarithm of the gamma function, and the digamma function, for complex arguments *Comp. Phys. Comm.* **4** 221–226

5 Parameters

1: Z – ***complex*** *Input*

On entry: the argument z of the function.

Constraint: Re(Z) must not be 'too close' (see Section 6) to a non-positive integer when Im(Z) = 0.0.

2: K – INTEGER *Input*

On entry: the function $\psi^{(k)}(z)$ to be evaluated.

Constraint: $0 \leq \mathrm{K} \leq 4$.

3: 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 $= 1$

On entry, K < 0,
or K > 4,
or Re(Z) is 'too close' to a non-positive integer when Im(Z) $= 0.0$. That is, ABS(Re(Z) $-$ NINT(Re(Z))) $<$ ***machine precision*** $\times$ NINT(ABS(Re(Z))).

IFAIL $= 2$

The evaluation has been abandoned due to the likelihood of overflow. The result is returned as zero.

7 Accuracy

Empirical tests have shown that the maximum relative error is a loss of approximately two decimal places of precision.

8 Further Comments

None.

9 Example

The example program evaluates the psi (trigamma) function $\psi^{(1)}(z)$ at $z = -1.5 + 2.5i$, 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.

```
*     S14AFF Example Program Text.
*     Mark 20 Release. NAG Copyright 2001.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*     .. Local Scalars ..
      complex          Y, Z
      INTEGER          IFAIL, K
*     .. External Functions ..
      complex          S14AFF
      EXTERNAL         S14AFF
*     .. Executable Statements ..
      WRITE (NOUT,*) 'S14AFF Example Program Results'
```

```
*     Skip heading in data file
      READ (NIN,*)
      WRITE (NOUT,*)
      WRITE (NOUT,*) '       Z           K         (D^K/DZ^K)psi(Z)',
     +  '          IFAIL'
      WRITE (NOUT,*)
   20 READ (NIN,*,END=40) Z, K
      IFAIL = 0
*
      Y = S14AFF(Z,K,IFAIL)
*
      WRITE (NOUT,99999) Z, K, Y, IFAIL
      GO TO 20
   40 STOP
*
99999 FORMAT (1X,'(',F5.1,',',F5.1,' )',I6,'   (',1P,E12.4,',',E12.4,
     +       ' )',I7)
      END
```

9.2 Program Data

```
S14AFF Example Program Data
 (-1.5, 2.5)   1  : Values of Z and K
```

9.3 Program Results

```
 S14AFF Example Program Results

        Z           K         (D^K/DZ^K)psi(Z)          IFAIL

 ( -1.5,  2.5 )     1   ( -1.9737E-01, -2.4271E-01 )      0
```