

NAG 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 k th derivative of the psi function $\psi(z)$ for complex z and $k = 0, 1, \dots, 4$, via the routine name.

2 Specification

```
complex*16 FUNCTION S14AFF(Z, K, IFAIL)
INTEGER                                K, IFAIL
complex*16                            Z
```

3 Description

S14AFF evaluates an approximation to the k th derivative of the psi function $\psi(z)$ given by

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

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

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*16*** *Input*
On entry: the argument z of the function.
Constraint: $\text{Re}(Z)$ must not be ‘too close’ (see Section 6) to a nonpositive integer when $\text{Im}(Z) = 0.0$.
- 2: K – INTEGER *Input*
On entry: the function $\psi^{(k)}(z)$ to be evaluated.
Constraint: $0 \leq K \leq 4$.

3: IFAIL – INTEGER

Input/Output

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction 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, if you are 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 $\text{Re}(Z)$ is 'too close' to a nonpositive integer when $\text{Im}(Z) = 0.0$. That is,
 $\text{abs}(\text{Re}(Z) - \text{nint}(\text{Re}(Z))) < \text{machine precision} \times \text{nint}(\text{abs}(\text{Re}(Z)))$.

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

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

9.1 Program Text

```
*      S14AFF Example Program Text
*      Mark 20 Release. NAG Copyright 2001.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
*      .. Local Scalars ..
      COMPLEX *16      Y, Z
      INTEGER          IFAIL, K
*      .. External Functions ..
      COMPLEX *16      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 = 1
*
      Y = S14AFF(Z,K,IFAIL)
*
      IF (IFAIL.GE.0) THEN
        WRITE (NOUT,99999) Z, K, Y, IFAIL
        GO TO 20
      ELSE
        WRITE (NOUT,99998) IFAIL
      END IF
40  CONTINUE
*
99999 FORMAT (1X,'( ',F5.1,', ',F5.1,', ' ),I6,' ( ',1P,E12.4,', ',E12.4,
+          ' )',I7)
99998 FORMAT (1X,' ** S14AFF returned with IFAIL = ',I5)
      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
