

# 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,  
 $\text{abs}(\text{Re}(Z) - \text{nint}(\text{Re}(Z))) < \textit{machine precision} \times \text{nint}(\text{abs}(\text{Re}(Z)))$ .

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 <sup>K</sup> /DZ <sup>K</sup> )psi(Z)	IFAIL
( -1.5, 2.5 )	1	( -1.9737E-01, -2.4271E-01 )	0

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