

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 function name.

2 Specification

```
FUNCTION S14AFF (Z, K, IFAIL)
COMPLEX (KIND=nag_wp) S14AFF
INTEGER          K, IFAIL
COMPLEX (KIND=nag_wp) 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 (KIND=nag_wp) *Input*
On entry: the argument z of the function.
Constraint: Z.re must not be 'too close' (see Section 6) to a non-positive integer when Z.im = 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.

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.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

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 non-positive 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

```

Program s14affe

!      S14AFF Example Program Text

!      Mark 24 Release. NAG Copyright 2012.

!      .. Use Statements ..
      Use nag_library, Only: nag_wp, s14aff
!      .. Implicit None Statement ..
      Implicit None
!      .. Parameters ..
      Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
      Complex (Kind=nag_wp)      :: y, z
      Integer                     :: ifail, ioerr, k

```

```

!      .. 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)'
      Write (nout,*)

data: Do
      Read (nin,*,Iostat=ioerr) z, k

      If (ioerr<0) Then
         Exit data
      End If

      ifail = -1
      y = s14aff(z,k,ifail)

      If (ifail<0) Then
         Exit data
      End If

      Write (nout,99999) z, k, y
End Do data

99999 Format (1X,'(,F5.1,',',F5.1,')',I6,' (',1P,E12.4,',',E12.4,')')
      End Program s14affe

```

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)

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

```
