

# NAG Library Function Document

## nag\_complex\_erfc (s15ddc)

### 1 Purpose

nag\_complex\_erfc (s15ddc) computes values of the function  $w(z) = e^{-z^2} \operatorname{erfc}(-iz)$ , for Complex  $z$ .

### 2 Specification

```
#include <nag.h>
#include <nags.h>

Complex nag_complex_erfc (Complex z, NagError *fail)
```

### 3 Description

nag\_complex\_erfc (s15ddc) computes values of the function  $w(z) = e^{-z^2} \operatorname{erfc}(-iz)$ , where  $\operatorname{erfc} z$  is the complementary error function

$$\operatorname{erfc} z = \frac{2}{\sqrt{\pi}} \int_z^\infty e^{-t^2} dt,$$

for Complex  $z$ . The method used is that in Gautschi (1970) for  $z$  in the first quadrant of the complex plane, and is extended for  $z$  in other quadrants via the relations  $w(-z) = 2e^{-z^2} - w(z)$  and  $w(\bar{z}) = \overline{w(-z)}$ . Following advice in Gautschi (1970) and van der Laan and Temme (1984), the code in Gautschi (1969) has been adapted to work in various precisions up to 18 decimal places. The real part of  $w(z)$  is sometimes known as the Voigt function.

### 4 References

Gautschi W (1969) Algorithm 363: Complex error function *Comm. ACM* **12** 635

Gautschi W (1970) Efficient computation of the complex error function *SIAM J. Numer. Anal.* **7** 187–198

van der Laan C G and Temme N M (1984) Calculation of special functions: the gamma function, the exponential integrals and error-like functions *CWI Tract 10* Centre for Mathematics and Computer Science, Amsterdam

### 5 Arguments

- 1: **z** – Complex *Input*  
On entry: the argument  $z$  of the function.
- 2: **fail** – NagError \* *Input/Output*  
The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

### NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

An unexpected error has been triggered by this function. Please contact NAG.

See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

### NE\_NO\_LICENCE

Your licence key may have expired or may not have been installed correctly.

See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

### NE\_RESULT\_HALF\_PRECISION

Result has less than half precision when entered with argument  $z = (\langle value \rangle, \langle value \rangle)$ .

### NE\_RESULT\_IMAGINARY\_OVERFLOW

Imaginary part of result overflows when entered with argument  $z = (\langle value \rangle, \langle value \rangle)$ .

### NE\_RESULT\_NO\_PRECISION

Result has no precision when entered with argument  $z = (\langle value \rangle, \langle value \rangle)$ .

### NE\_RESULT\_OVERFLOW

Both real and imaginary parts of result overflow when entered with argument  $z = (\langle value \rangle, \langle value \rangle)$ .

### NE\_RESULT\_REAL\_OVERFLOW

Real part of result overflows when entered with argument  $z = (\langle value \rangle, \langle value \rangle)$ .

## 7 Accuracy

The accuracy of the returned result depends on the argument  $z$ . If  $z$  lies in the first or second quadrant of the complex plane (i.e.,  $\text{Im}(z)$  is greater than or equal to zero), the result should be accurate almost to *machine precision*, except that there is a limit of about 18 decimal places on the achievable accuracy because constants in the function are given to this precision. With such arguments, **fail** can only return as **fail.code** = NE\_NOERROR.

If however  $\text{Im}(z)$  is less than zero, accuracy may be lost in two ways; firstly, in the evaluation of  $e^{-z^2}$ , if  $\text{Im}(-z^2)$  is large, in which case a warning will be issued through **fail.code** = NE\_RESULT\_HALF\_PRECISION or NE\_RESULT\_NO\_PRECISION; and secondly, near the zeros of the required function, where precision is lost due to cancellation, in which case no warning is given – the result has absolute accuracy rather than relative accuracy. Note also that in this half-plane, one or both parts of the result may overflow – this is signalled through **fail.code** = NE\_RESULT\_IMAGINARY\_OVERFLOW, NE\_RESULT\_OVERFLOW or NE\_RESULT\_REAL\_OVERFLOW.

## 8 Parallelism and Performance

nag\_complex\_erfc (s15ddc) is not threaded in any implementation.

## 9 Further Comments

The time taken for a call of `nag_complex_erfc` (s15ddc) depends on the argument  $z$ , the time increasing as  $|z| \rightarrow 0.0$ .

`nag_complex_erfc` (s15ddc) may be used to compute values of  $\operatorname{erfc} z$  and  $\operatorname{erf} z$  for Complex  $z$  by the relations  $\operatorname{erfc} z = e^{-z^2} w(iz)$ ,  $\operatorname{erf} z = 1 - \operatorname{erfc} z$ . (For double arguments, `nag_erfc` (s15adc) and `nag_erf` (s15aec) should be used.)

## 10 Example

This example reads values of the argument  $z$  from a file, evaluates the function at each value of  $z$  and prints the results.

### 10.1 Program Text

```
/* nag_complex_erfc (s15ddc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <nag.h>
#include <stdio.h>
#include <nag_stdlib.h>
#include <nags.h>

int main(void)
{
    Integer exit_status = 0;
    Complex w, z;
    NagError fail;

    INIT_FAIL(fail);

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[^\\n]");
#else
    scanf("%*[^\\n]");
#endif
    printf("nag_complex_erfc (s15ddc) Example Program Results\\n");
    printf("          z                      w\\n");
#ifdef _WIN32
    while (scanf_s(" (%lf,%lf)%*[^\\n] ", &z.re, &z.im) != EOF)
#else
    while (scanf(" (%lf,%lf)%*[^\\n] ", &z.re, &z.im) != EOF)
#endif
    {
        /* nag_complex_erfc (s15ddc).
         * Scaled complex complement of error function,
         * exp(-z^2)erfc(-iz)
         */
        w = nag_complex_erfc(z, &fail);
        if (fail.code != NE_NOERROR) {
            printf("Error from nag_complex_erfc (s15ddc).\\n%s\\n", fail.message);
            exit_status = 1;
            goto END;
        }
        printf("(%.4f,%.4f)    (%.4f,%.4f)\\n", z.re, z.im, w.re, w.im);
    }
}
```

END:

```
    return exit_status;  
}
```

## 10.2 Program Data

nag\_complex\_erfc (s15ddc) Example Program Data

```
( 1.00,  0.00)  
(-3.01,  0.75)  
( 2.75, -1.52)  
(-1.33, -0.54)      - Values for z.
```

## 10.3 Program Results

nag\_complex\_erfc (s15ddc) Example Program Results

$z$		$w$	
( 1.0000,	0.0000)	( 0.3679,	0.6072)
( -3.0100,	0.7500)	( 0.0522,	-0.1838)
( 2.7500,	-1.5200)	( -0.1015,	0.1654)
( -1.3300,	-0.5400)	( -0.1839,	-0.7891)

---