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 3.6 in the Essential Introduction).

6 Error Indicators and Warnings

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.

NE_RESULT_HALF_PRECISION

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

NE_RESULT_IMAGINARY_OVERFLOW

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

NE_RESULT_NO_PRECISION

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

NE_RESULT_OVERFLOW

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

NE_RESULT_REAL_OVERFLOW

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

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., $\mathrm{Im}(z)$ 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 $\mathrm{Im}(z)$ is less than zero, accuracy may be lost in two ways; firstly, in the evaluation of e^{-z^2}, if $\mathrm{Im}(-z^2)$ 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

Not applicable.

9 Further Comments

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

nag_complex_erfc (s15ddc) may be used to compute values of $\mathrm{erfc}\, z$ and $\mathrm{erf}\, z$ for Complex z by the relations $\mathrm{erfc}\, z = e^{-z^2} w(iz)$, $\mathrm{erf}\, z = 1 - \mathrm{erfc}\, z$. (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.
 *
 * Copyright 2002 Numerical Algorithms Group.
 *
 * Mark 7, 2002.
 */

#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 */
  scanf("%*[^\n]");
  printf("nag_complex_erfc (s15ddc) Example Program Results\n");
  printf("          z                     w\n");
  while (scanf(" (%lf,%lf)%*[^\n] ", &z.re, &z.im) != EOF)
    {
      /* 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("(%8.4f,%8.4f)   (%8.4f,%8.4f)\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)
```