# 2.16 Complex Error Function $w(z)$

## A. Purpose

Compute the Fadeeva function $w(z)$, defined by Equation 7.1.3 in [1]:

$$w(z) = e^{-z^2}\left[1 + \frac{2i}{\sqrt{\pi}}\int_0^z e^{t^2}dt\right]. \qquad (1)$$

The Fadeeva function is related to the error function by

$$w(z) = e^{-z^2}\,\mathrm{erfc}(-iz),$$

to Dawson's integral

$$F(z) = e^{-z^2}\int_0^z e^{t^2}dt, \text{ by } \quad \frac{2i}{\sqrt{\pi}}F(z) = w(z) - e^{-z^2},$$

to the Fresnel integrals

$$C(z) = \int_0^z \cos\left(\frac{\pi}{2}t^2\right)dt, \text{ and } \; S(z) = \int_0^z \sin\left(\frac{\pi}{2}t^2\right)dt,$$

by

$$C(z) + iS(z) = \frac{1+i}{2}\left[1 - e^{i\pi z^2/2}w\left(\frac{\sqrt{\pi}}{2}(1+i)z\right)\right],$$

and to the Voigt functions $V(x,y)$ and $L(x,y)$ (used in spectroscopy and astronomy — see [2]) by $V(x,y) = \Re w(z)$ and $L(x,y) = \Im w(z)$, where $z = x + iy$.

## B. Usage

### B.1 Program Prototype, Single Precision

**COMPLEX Z, W**

**INTEGER IFLAG**

**CALL CWOFZ (Z, W, IFLAG)**

### B.2 Argument Definitions

**Z** [in] Argument at which the function is to be evaluated.

**W** [out] Value of $w(z)$, where $z$ is given by the argument Z.

**IFLAG** [out] A flag indicating success or failure of the computation:

- 0 means $w(z)$ was successfully calculated,
- +1 means $w(z)$ was not successfully calculated because it would have no significant digits.
- −1 means $w(z)$ was not successfully calculated because it would overflow.

See Section E, Error Procedures and Restrictions, for a discussion of values of Z that result in nonzero values of IFLAG. If IFLAG is nonzero, the real and imaginary parts of W are set to the largest representable number.

### B.3 Modifications for Double Precision

Change the subprogram name to ZWOFZ. On computers that support a double precision complex data type, frequently spelled COMPLEX*16, and on which double precision complex is represented by an array of two double precision numbers, with the first being the real part, and the second being the imaginary part, change the type declarations of Z and W so that Z and W are declared to be of type double precision complex. On machines that do not support double precision complex, change the declarations of Z and W to

**DOUBLE PRECISION Z(2), W(2)**

In the latter case, put the real part of $z$ into Z(1), and the imaginary part of $z$ into Z(2), and find the real and imaginary parts of $w(z)$ in W(1) and W(2), respectively.

## C. Examples and Remarks

See DRCWOFZ and ODCWOFZ for an example of the usage of this subprogram.

## D. Functional Description

From Eq. (1) it is clear that $w(z)$ is analytic in the entire plane. In the upper half-plane, $0 \le |w(z)| < 1$, which may have been the original reason to consider $w(z)$ to be a generalization of erfc.

$w(z)$ satisfies the differential equation $w'(z) + 2zw(z) = 2i/\sqrt{\pi}$. Since $w(z)$ is analytic it satisfies the Cauchy-Riemann conditions. If we let $w(z) = u(z) + iv(z)$, and $z = x + iy$, where $u$, $v$, $x$ and $y$ are real, the Cauchy-Riemann conditions, together with the differential equation, give us $u_x = 2yv - 2xu$ and $u_y = 2xv + 2yu - 2\pi^{1/2}$. In some applications, particularly related to spectroscopy, one needs $V(x,y)$, $L(x,y)$, $V_x(x,y)$ and $V_y(x,y)$. We have already, above, identified $V(x,y)$ as $u(z)$ and $L(x,y)$ as $v(z)$. Thus, one can compute these four functions by computing $w(z)$ alone.

These subprograms are based on a subprogram by G. P. M. Poppe and C. M. J. Wijers described in [3] and [4]. The subprogram by Poppe and Wijers was modified to work in either single or double precision, and some tests of argument range were changed to be invoked only when necessary. Machine characteristics are discovered, and errors are processed, using MATH77 conventions. The

subprogram name was changed to conform to MATH77 naming conventions.

The algorithm uses three different methods. Inside the ellipse $(x/6.3)^2+(y/4.4)^2 \le .292^2$ the algorithm uses the series approximation given by Equation 7.1.6 in [1]. In the elliptic annulus $.292^2 < (x/6.3)^2 + (y/4.4)^2 \le 1.0$ the algorithm uses a Taylor series, with derivatives calculated by the Laplace continued fraction. Outside the latter ellipse, a Laplace continued fraction is used.

**Accuracy Tests**

The accuracy of the approximations was analyzed by Poppe and Wijers. They concluded that relative accuracy is maintained within 14 significant digits, except inside a circle of radius 0.126 around a zero of the function (all zeros of $w(z)$ are in the lower half-plane), where absolute accuracy is retained but relative accuracy is not. They also compared the accuracy of $w(z)$ to $\operatorname{erfc} z$ for several purely imaginary values of $z$. Their testing procedure is reported in [3].

We tested CWOFZ in four regions along the imaginary axis, where $w(z)$ is real, on an IBM PC/AT, by comparing to DERFCE. Each region was divided into 500 subregions, and a point was randomly selected in each subregion. The maximum errors are shown below, where ULP means "error in units of last position of the reference result," and $\rho \approx 1.192 \times 10^{-7}$ is the round-off level for IEEE single precision arithmetic.

| Range | ULP | Absolute | Relative |
|---|---|---|---|
| [0..0.75] | 2.42 | 1.21 $\rho$ | 2.29 $\rho$ |
| [0.75..1.2848] | 19.05 | 4.76 $\rho$ | 12.95 $\rho$ |
| [1.2848..4.4] | 6.05 | 1.23 $\rho$ | 3.49 $\rho$ |
| [4.4..100] | 2.19 | 0.12 $\rho$ | 1.43 $\rho$ |

In the range [0.75..1.2848] errors grow as $x$ increases. Errors are four times larger near 1.2848 than near 0.75.

We tested ZWOFZ in five regions along the imaginary axis, where $w(z)$ is real, on an IBM PC/AT, by comparing to an extended precision calculation of $\exp(x^2)\operatorname{erfc} x$. Each region was divided into 200 subregions, and a point was randomly selected in each subregion. The maximum errors are shown below, where $\rho \approx 2.22 \times 10^{-16}$ is the round-off level for IEEE double precision arithmetic.

| Range | ULP | Absolute | Relative |
|---|---|---|---|
| [0..0.75] | 1.47 | 0.73 $\rho$ | 1.35 $\rho$ |
| [0.75..1.2848] | 14.29 | 3.57 $\rho$ | 9.84 $\rho$ |
| [1.2848..3.4469] | 6.23 | 0.78 $\rho$ | 4.44 $\rho$ |
| [3.4469..4.4] | 14.20 | 1.78 $\rho$ | 13.42 $\rho$ |
| [4.4..100] | 3.02 | 0.19 $\rho$ | 1.52 $\rho$ |

In the range [0.75..1.2848] errors grow as $x$ increases. Errors are four times larger near 1.2848 than near 0.75.

We tested ZWOFZ in four regions along the real axis on an IBM PC/AT, by comparing the imaginary part of the result to an extended precision calculation of Dawson's integral, $F(x)$. Each region was divided into 200 subregions, and a point was randomly selected in each subregion. The maximum errors are as follows.

| Range | ULP | Absolute | Relative |
|---|---|---|---|
| [0..1.83960] | 2.21 | 0.93 $\rho$ | 1.73 $\rho$ |
| [1.8396..2.95] | 17.28 | 3.90 $\rho$ | 11.20 $\rho$ |
| [2.95..6.3] | 8.99 | 1.12 $\rho$ | 6.24 $\rho$ |
| [6.3..100] | 1.59 | 0.06 $\rho$ | 0.90 $\rho$ |

We tested ZWOFZ along the real axis on an IBM PC/AT, by comparing the real part of the result to an extended precision calculation of $\exp(-x^2)$, in the range [0..10]. The maximum error was 2.04 ULP; the maximum absolute error was 0.26 $\rho$; the maximum relative error was 0.45 $\rho$. The largest errors occurred near the change of method at $x = 1.8396$.

**References**


1. Milton Abramowitz and Irene A. Stegun, **Handbook of Mathematical Functions**, *Applied Mathematics Series 55*, National Bureau of Standards (1966).
2. S. S. Penner, **Quantitative Molecular Spectroscopy and Gas Emissivities**, Addison Wesley, Reading, Mass. (1959).
3. G. P. M. Poppe and C. M. J. Wijers, *More efficient computation of the complex error function*, **ACM Trans. on Math. Software 16**, 1 (March 1990) 38–46.
4. G. P. M. Poppe and C. M. J. Wijers, *Algorithm 680: Evaluation of the complex error function*, **ACM Trans. on Math. Software 16**, 1 (March 1990) 47.


## E. Error Procedures and Restrictions

$w(z)$ is computable throughout the upper half plane without restriction. To compute $w(z)$ in the lower half plane we use $w(-z) = 2\exp(-z^2) - w(z)$. Since $\exp(-z^2) = \exp(\Re z^2)[\cos(\Im z^2) + i\sin(\Im z^2)]$, we must have $x^2-y^2 < \ln\ \Omega$, where $\Omega$ is the largest representable floating point number. Argument reduction in computing sin and cos causes loss of precision, and so we restrict $2|xy| < \rho^{-1/2}$, where $\rho$ is the smallest positive number such that the floating point representation of $1.0 + \rho$ is different from 1.0. If $y < 0$ and $x^2 - y^2 \ge \ln\ \Omega$ the error processor (see Chapter 19.2) is invoked with LEVEL = 2, and IFLAG is set to $-1$. If $y < 0$ and $2|xy| \ge \rho^{-1/2}$ the error message processor is invoked with LEVEL = 2, and IFLAG is set to $+1$. The usual action of the error message processor when invoked with LEVEL = 2 is to halt execution of the program. This action may be altered by calling ERMSET (see Chapter 19.2).

## F. Supporting Information

| Entry | Required Files |
|---|---|
| **CWOFZ** | AMACH, CWOFZ, ERFIN, ERMOR, ERMSG, SERV1 |
| **ZWOFZ** | AMACH, DERV1, ERFIN, ERMOR, ERMSG, ZWOFZ |

Present version converted from ACM TOMS Algorithm 680, [4], by W. V. Snyder, 1991.

## DRCWOFZ

```
c      program DRCWOFZ
c>> 2009-10-27 DRCWOFZ Krogh/Snyder Added equivalence for Nag compiler.
c>> 1996-06-10 DRCWOFZ Krogh Moved formats up, M77CON changes for C.
c>> 1992-03-13 DRCWOFZ WV Snyder Created from DRCWOFZ
c>> 1991-11-20 DRCWOFZ WV Snyder Original Code
c Conversion should only be done from "Z" to "C" for processing to C.
c--C replaces "?": DR?WOFZ, ?WOFZ
c
c      Demonstration driver for CWOFZ.
c
       complex Z, W
       real ZR(2), WR(2)
       equivalence ( Z, ZR ), ( W, WR )
       integer IFLAG
       integer IX, IY
c
c      Evaluate w(z) at 25 points [0..4] x [0..4] in the complex plane.
c
10     format ('  x   y         Re w              Im w')
20     format (2i3, 2g17.8)
       print 10
       do 40 ix = 0, 4
          do 30 iy = 0, 4
             z = cmplx(real(ix), real(iy))
             call cwofz (zr, wr, iflag)
             print 20, ix, iy, w
30        continue
40     continue
       stop
       end
```

## ODCWOFZ

```
  x   y          Re w              Im w
  0   0     1.0000000          0.0000000
  0   1    0.42758343          0.0000000
  0   2    0.25539580          0.0000000
  0   3    0.17900115          0.0000000
  0   4    0.13699944          0.0000000
  1   0    0.36787945         0.60715777
  1   1    0.30474424         0.20821901
  1   2    0.21849267       0.92997834E-01
  1   3    0.16426113       0.50197128E-01
  1   4    0.12988818       0.30778861E-01
  2   0  0.18315639E-01         0.34002644
  2   1    0.14023955         0.22221340
  2   2    0.14795277         0.13117969
  2   3    0.13075750       0.81112668E-01
  2   4    0.11213948       0.53489000E-01
  3   0  0.12340980E-03         0.20115739
  3   1  0.65317795E-01         0.17391835
  3   2  0.92710741E-01         0.12831692
  3   3  0.96402526E-01       0.91236345E-01
  3   4  0.90933919E-01       0.65592334E-01
  4   0  0.11253518E-06         0.14595355
  4   1  0.36281474E-01         0.13583903
```

| | | | |
|---|---|---|---|
| 4 | 2 | 0.59686974E−01 | 0.11321013 |
| 4 | 3 | 0.69790952E−01 | 0.89340016E−01 |
| 4 | 4 | 0.71570434E−01 | 0.69374524E−01 |