Author(s) : G.A. Erskine
Submitter : K.S. Kölbig
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Adaptive Complex Integration Along a Line Segment

Function subprograms `CGAUSS` and `WGAUSS` compute, to an attempted specified accuracy, the value of the complex integral

$$I = \int_A^B f(z)dz.$$

The path of integration is the directed line segment AB in the complex z-plane. The function $f(z)$ must be single-valued on this segment.

The double-precision version `WGAUSS` is available only on computers which support a `COMPLEX*16` Fortran data type.

Structure:

`FUNCTION` subprograms
User Entry Names: `CGAUSS`, `WGAUSS`
Files Referenced: `Unit 6`
External References: `MTLMTR` (N002), `ABEND` (Z035), user-supplied `FUNCTION` subprogram

Usage:

In any arithmetic expression,

`CGAUSS(F,A,B,EPS)`   or   `WGAUSS(F,A,B,EPS)`

has the approximate value of the integral I.

`F` Name of a user-supplied `FUNCTION` subprogram, declared `EXTERNAL` in the calling program. This subroutine must set `F(Z)` $= f($`Z`$)$.

`A,B` End-points of integration interval.

`EPS` Accuracy parameter (see **Accuracy**).

`CGAUSS` is of type `COMPLEX`, `WGAUSS` is of type `COMPLEX*16`, and the arguments `F`, `A`, `B`, and `Z` (in `F`) have the same type as the function name. `EPS` is of type `REAL` for `CGAUSS` and of type `DOUBLE PRECISION` for `WGAUSS`.

Method:

For any line segment $[a, b]$ we define $g_8(a, b)$ and $g_{16}(a, b)$ to be the 8-point and 16-point Gaussian quadrature approximations to

$$\int_a^b f(z)dz$$

and define

$$r(a, b) = \frac{|g_{16}(a, b) - g_8(a, b)|}{1 + |g_{16}(a, b)|}.$$

Then, with G = `CGAUSS` or `WGAUSS`,

$$G = \sum_{i=1}^{k} g_{16}(z_{i-1}, z_i),$$

where, starting with $z_0 = A$ and finishing with $z_k = B$, the subdivision points z_i $(i = 1, 2, \ldots)$ are given by

$$z_i = z_{i-1} + \lambda(B - z_{i-1}),$$

with λ equal to the first member of the sequence $1, 1/2, 1/4, \ldots$ for which $r(z_{i-1}, z_i) <$ `EPS`. If, at any stage in the process of subdivision, the ratio

$$q = \left| \frac{z_i - z_{i-1}}{B - A} \right|$$

is so small that $1 + 0.005q$ is indistinguishable from 1 to machine accuracy, an error exit occurs with the function value set equal to zero.

Accuracy:

Unless there is severe cancellation of positive and negative values of $f(z)$ over the interval $[A, B]$, the argument `EPS` may be considered as specifying a bound on the *relative* error of I in the case $|I| > 1$, and a bound on the *absolute* error in the case $|I| < 1$. More precisely, if k is the number of sub-intervals contributing to the approximation (see **Method**), and if

$$I_{abs} = \int_A^B |f(z)| dz,$$

then the relation

$$\frac{|G - I|}{I_{abs} + k} < \texttt{EPS}$$

will nearly always be true, provided the routine terminates without printing an error message. For functions f having no singularities in the closed interval $[A, B]$ the accuracy will usually be much higher than this.

Error handling:

Error `D113.1`: The requested accuracy (see **Method**) cannot be obtained. The function value is set equal to zero, and a message is written on `Unit 6`, unless subroutine `MTLSET` (N002) has been called.

Notes:

Values of the function $f(z)$ at the end-points of the line segment A and B are not required. The subprogram may therefore be used when these values are undefined.

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