

PACKAGE SPECIFICATION

QD01

HSL ARCHIVE

1 SUMMARY

To evaluate integrals of the form

$$\int_{a}^{b} f(t) \sin xt \, dt$$

and

$$\int_{a}^{b} f(t) \cos xt \, dt$$

to a specified absolute accuracy.

Filon's method is used where a **quadrature formula** is derived by approximating to f(x) by a piecewise quadratic interpolant. The user must provide a subroutine to evaluate the function f(x).

The subroutine is of greater efficiency than Simpson's rule only if |u| > 1; the greater the value of u the more marked is the increase in efficiency.

ATTRIBUTES — Version: 1.0.0. Remark: The method is to be preferred to Simpson's Rule when $|x(b-a)| \ge 10$. Types: QD01A; QD01AD. Calls: F (a user subroutine). Original date: 1968. Origin: W.E.Hart, Harwell.

2 HOW TO USE THE PACKAGE

2.1 Argument list

The single precision version

CALL QD01A(EPS, ISUBMX, U, A, B, JCS, SINT, CINT)

The double precision version

CALL QD01AD(EPS, ISUBMX, U, A, B, JCS, SINT, CINT)

- EPS is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to the absolute accuracy required in the integral values.
- ISUBMX is an INTEGER variable which must be set by the user to the maximum number of iterations the subroutine is allowed to perform (10 is suggested); this argument is a safety valve which causes a return to the calling program if convergence is not reached.
- U is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to the value of the constant *u*, see section 1.
- A is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to *a* the lower limit of the range of integration.
- B is a REAL (DOUBLE PRECISION in the D version) variable which must be set by the user to *b* the upper limit of the range of integration.
- JCS is an INTEGER variable which must be set by the user to select which integrals are required. The possible values are:



- 3 both integrals are computed.
- SINT is a REAL (DOUBLE PRECISION in the D version) variable which is set by the subroutine to the value of the sine integral.
- CINT is a REAL (DOUBLE PRECISION in the D version) variable which is set by the subroutine to the value of the cosine integral.

2.2 The function subroutine

The user must provide a Fortran FUNCTION subroutine to evaluate the function f(x) for any x in the range $a \le x \le b$. It must have the form:

The single precision version

REAL FUNCTION F(X) F= function value RETURN END

The double precision version

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DOUBLE PRECISION FUNCTION F(X)
DOUBLE PRECISION X
F= function value
RETURN
END
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Note that both single and double precision subroutines have the same name.

3 GENERAL INFORMATION

Workspace: none.

Use of common: none.

Other routines called directly: user-supplied function subroutine, see §2.2.

Input/output: none.

4 METHOD

The method used is Filon's method: a quadrature formula is derived by approximating to f(x) by a piecewise quadratic interpolant.