1 SUMMARY

To **evaluate the integral**

$$\int_a^b f(x)\,dx$$

using one of five Newton-Coates m strip formulae: Trapesoidal rule (m=1), Simpson's rule (m=2), the $\frac{3}{8}$-th rule (m=3) and the four-strip formula (m=4) and the five-strip formula (m=5).

The user chooses the integration step h and supplies the tabulated integrand values: f_i, f_{i+1}, f_{i+2},..., f_{i+nm}, at equal intervals h in $a \le x \le b$; where n is the number of times the quadrature must be applied to cover the range and m is the number values required by each application of the quadrature.

Double length accumulation of intermediate results is carried out to minimize rounding errors.

ATTRIBUTES — **Version:** 1.0.0. **Remark:** One of the adaptive quadrature subroutines, `QA02`, `QA04` or `QA05` may give better results than `QA01`. **Types:** `QA01A; QA01AD.` **Original date:** August 1967. **Origin:** M.J.Hopper, Harwell.

2 HOW TO USE THE PACKAGE

2.1 Argument list and calling sequence

The single precision version

```
Q=QA01A(F,I,M,N,H)
```

The double precision version

```
DOUBLE PRECISION QA01AD,Q
Q=QA01AD(F,I,M,N,H)
```

Note: `QA01A` and `QA01AD` are `FUNCTION` subroutines and `QA01AD` must be declared `DOUBLE PRECISION` in the calling program.

`F` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length at least i+mn in which the user must put the tabulated values of $f(x)$. The value of $f(a)$ should be stored in `F(i)` and the rest following so that `F(i+j)` = $f(a+jh)$ j=0,1,2,...,mn. The argument is not altered by the subroutine.

`I` is an `INTEGER` variable which must be set by the user to i the subscript of the element of `F` containing the value of $f(a)$. Normally i=1. This argument is not altered by the subroutine.

`M` is an `INTEGER` variable which must be set by the user to m to choose the quadrature formula (Note that the quadrature uses m+1 function values). The values of m accepted by `QA01` are:

1 Trapesoidal rule,

2 Simpson's rule,

3 The three-eighths rule,

4 The four-strip formula,

5 The five-strip formula.

`N` is an `INTEGER` which must be set by the user to n the number of times the quadrature is to be applied to cover the range from a to b=a+mnh.

`H` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to h the tabulation interval. If the value of the integral is required to a prescribed accuracy it is the user's responsibility to choose an h which is sufficiently small. See section 4 for comments on choosing h and note that $h=(b-a)/mn$.

3 GENERAL INFORMATION

Use of common: None.

Workspace: None.

Other routines called directly: None.

Input/output: None.

4 METHOD

The first five Newton-Coates quadrature formulae with error terms are:

Trapesoidal: $Q=\frac{h}{2}(f_0+f_1),\quad E_1=-\frac{h^3}{12}f^{(2)}(\xi),$

Simpson's: $Q=\frac{h}{3}(f_0+4f_1+f_2),\quad E_2=-\frac{h^5}{90}f^{(4)}(\xi),$

$\frac{3}{8}$-ths rule: $Q=\frac{3h}{8}(f_0+3f_1+3f_2+f_3),\quad E_3=-\frac{3h^5}{80}f^{(4)}(\xi),$

Four-strip: $Q=\frac{2h}{45}(7f_0+32f_1+12f_2+32f_3+7f_4),\quad E_4=-\frac{8h^7}{945}f^{(6)}(\xi),$

Five-strip: $Q=\frac{5h}{288}(19f_0+75f_1+50f_2+50f_3+75f_4+19F_5),\quad E_5=-\frac{275h^7}{12096}f^{(6)}(\xi),$

where for illustration purposes the integration is made over the points $x_0, x_1, ..., x_m$ and where $f^{(k)}(\xi)$ is the value of the k-th derivative at some point ξ, in $x_0\le\xi\le x_m$.

The step size required to achieve a given accuracy ε can be determined by finding an h such that $|E_m|<\varepsilon$. This is not always possible unless a reasonable estimate of the derivative value is available. An alternative procedure is to carry out a sequence of integrations, halving h at each stage and observing the convergence of the sequence of values so obtained. A further possibility is to use finite differences to approximate the derivative values. However, this is likely to prove just as costly as repeating the integration. Note: the error term for the whole range a to b is $n\,E_m$ where in this case $a\le\xi\le b$.

5 EXAMPLE OF USE

Suppose we require to evaluate the integral

$$Q=\int_0^1 \sin x\,dx$$

with an absolute accuracy of 10^{-12} and we chose to use Simpson's rule, i.e. m=2.

First decide the value of h that will achieve the accuracy. Let n be the number of times the quadrature must be applied to cover the range 0 to 1 and take the error estimate

$$E=n|E_2|=\frac{nh^5}{90}|f^{(4)}(\xi)|\quad 0\le\xi\le1$$

Now h is required such that $E < \varepsilon = 10^{-12}$. Using the fact that $|f^{(4)}(x)| = |\sin(x)| \le 1$ for all x and that $h = \frac{1}{2n}$ we have that

$$\frac{1}{90 \times 2^5 \times n^4} < \varepsilon$$

so that

$$n = \left[\left(\frac{1}{90 \times 2^5 \times \varepsilon} \right)^{\frac{1}{4}} \right] + 1$$

will do. The value of h is given by $h = 1/2n$.

The following code might then be used:

```
      DOUBLE PRECISION F(200),X,H,Q,QA01AD
C       SET THE ACCURACY REQUIRED
      EPS=1E-12
C       NUMBER OF TIMES QUADRATURE IS TO BE APPLIED
      N=INT(1./(2880.*EPS)**.25}+1
C       TABULATION INTERVAL
      H=.5D0/DFLOAT(N)
C       SELECT SIMPSON'S RULE
      M=2
      N1=M*N+1
C       SET ARRAY OF INTEGRAND VALUES
      DO 10 J=1,N1
      F(J)=DSIN(H*DFLOAT(J-1))
   10 CONTINUE
C       SET POSITION OF FIRST INTEGRAND VALUE (IN F(1))
      I=1
C       EVALUATE THE INTEGRAL
      Q=QA01AD(F,I,M,N,H)
        - -
        - -
```