1 SUMMARY

To **tabulate an integral function** of the form

$$g(x) = g(a) + \int_a^x f(t)\,dt$$

at points $x=a, a+h,...,a+mh$ to a **specified accuracy.**

The subroutine uses a variable step Simpson's rule using at each step an integration step, based on 4th differences, which is chosen small enough to achieve the required accuracy.

The user must specify a minimum integration step-size and provide a subroutine to evaluate the integrand $f(x)$.

ATTRIBUTES — Version: 1.0.0. **Types:** `QA03A`; `QA03AD`. **Calls:** `CALCIN` (a user subroutine). **Original date:** March 1963. **Origin:** M.J.D.Powell, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The argument list

The single precision version

```
CALL QA03A(G,H,A,B,ACC,DXMIN)
```

The double precision version

```
CALL QA03AD(G,H,A,B,ACC,DXMIN)
```

`G` is a `REAL` (`DOUBLE PRECISION` in the D version) array into which the subroutine will put the values of $g(x)$ at the tabulation points. The user must set `G(1)` to the value of $g(a)$ before calling the subroutine. The array must be at least of length $m+1$, see section 1 for a definition of m.

`H` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to h the interval of tabulation. **Restriction:** $h \leq \frac{1}{2}(b-a)$.

`A` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to a the first tabulation point.

`B` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to b the end of the range of tabulation.

`ACC` is a `REAL` variable which must be set by the user to the absolute accuracy required in the tabulated values of $g(x)$.

`DXMIN` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the minimum step length to be used in the evaluation of the integral by Simpson's Rule. **Restriction:** `DXMIN` $< \frac{1}{4}h$.

This parameter may be used to limit the amount of time spent trying unsuccessfully to integrate an ill-defined $f(t)$. If trouble is not expected set `DXMIN` very small relative to h and `ACC`. Note: for each step of the integration the step size δx must approximately satisfy

$$\texttt{ACC} > \frac{\delta x^5}{90}|f^{(4)}(\xi)| \qquad a \leq \xi \leq b$$

where $f^{(4)}(t)$ is the fourth derivative of $f(t)$. If the subroutine is unable to achieve the accuracy with a step length $\geq$ `DXMIN` a message is printed to that effect. In this event the array `G` will contain the values of $g(x)$ up to the

point of failure and the rest of the array will be set to zero.

2.2 The subroutine to evaluate f(t)

The user must provide a subroutine called CALCIN to calculate a value of $f(t)$ for any t in the range a to $a+mh$ where m equals the largest integer less than or equal to $(b-a)/h+\frac{1}{2}$. The subroutine must be of the form

```
SUBROUTINE CALCIN(T,F)
```

T is a REAL (DOUBLE PRECISION in the D version) variable which will contain on entry the value of t for the required $f(t)$.

F is a REAL (DOUBLE PRECISION in the D version) variable which CALCIN must set to the value of $f(t)$.

3 GENERAL INFORMATION

Use of common: None.

Workspace: None.

Other routines called directly: requires a user written subroutine called CALCIN.

Input/output: error message, see DXMIN.

4 METHOD

The integration is worked out by Simpson's Rule, the step length being chosen by the subroutine so that the specified accuracy is achieved in all tabulated values of $g(x)$. This step length is adjusted automatically by the subroutine for different parts of the range so that unnecessary values of $f(t)$ are not called for.