1 SUMMARY

To **evaluate the integral** $\int_a^b f(x)\,dx$ to a **specified absolute 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. **Remark:** Unless only limited accuracy is required, or storage is limited, either `QA04` or `QA05` may be better, especially on *difficult integrands.* **Types:** `QA02A`; `QA02AD`. **Calls:** `FD05`, `CALCIN` (a user subroutine). **Original date:** March 1963. **Origin:** M.J.D.Powell and A.R.Curtis, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The argument list

The single precision version

```
SUBROUTINE QA02A(ANSWER,A,B,ERR,HMIN)
```

The double precision version

```
SUBROUTINE QA02AD(ANSWER,A,B,ERR,HMIN)
```

`ANSWER` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which is set by the subroutine to the value of the integral, except when an error return occurs in which case it is set to zero (see section 4).

`A` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to a the lower limit of integration. It is not altered by the subroutine.

`B` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to b the upper limit of integration. It is not altered by the subroutine.

`ERR` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the absolute error to be allowed in the computed value of the integral. It is not altered by the subroutine.

`HMIN` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the smallest step-length to be used by the subroutine in calculating the integral. This parameter ensures that the subroutine will return after not more than $(b–a)/h$ values of $f(x)$ have been calculated. The argument is not altered by the subroutine. Note: `HMIN` must be such that `HMIN` $< (b–a)/16$.

2.2 The user supplied subroutine

The user is required to write a subroutine called `CALCIN` to provide values of $f(x)$ in the range $a \le x \le b$. Note that both single and double precision versions are called `CALCIN`.

```
SUBROUTINE CALCIN(X,F)
```

`X` is a `REAL` (`DOUBLE PRECISION` in the D version) variable in which `QA02` will pass the x value corresponding to the required $f(x)$ value.

`F` is a `REAL` (`DOUBLE PRECISION` in the D version) variable which the subroutine `CALCIN` must return the function value $f(x)$.

2.3 Use of common

The subroutine makes reference to a common block.

The single precision version

```
COMMON/QA02B/ VAL,EST,LP
```

The double precision version

```
COMMON/QA02BD/ VAL,EST,LP
```

VAL is a REAL (DOUBLE PRECISION in the D version) variable which contains on return the best estimate found of the integral (it is exactly equal to ANSWER if no diagnostic is given).

EST is a REAL (DOUBLE PRECISION in the D version) variable which contains on return an estimate of the error on VAL. While this estimate is often pessimistic, it can be over-optimistic on singular or other *difficult* integrands.

LP is an INTEGER variable which is used as the Fortran unit number for diagnostic output (normally 6 but may be changed).

This common statement need not be included in the calling program unless it is desired to refer to one of its variables.

2.4 Output from the subroutine

No printing from QA02 occurs unless it is unable to evaluate the integral to the accuracy requested, i.e. it requires a step-length less than HMIN. In this case an appropriate diagnostic is printed and ANSWER is set to 0. However the subroutine continues with a relaxed error criterion, which it restores to the original value later if possible. It always returns the best answer it can obtain, and an error estimate on it, via the common block QA02BD (see §2.3), thus enabling an answer to be obtained although ANSWER has been set to zero.

4 METHOD

The method is Simpson’s rule with the step length chosen to achieve the required accuracy. The step length varies over the range of integration according to error estimates based on 4-th differences as follows:

If the modulus of a 4-th difference is found to exceed 180.*ERR/(B-A) the step length is halved, and if one is found to be less than 9.*ERR/(B-A) an attempt is made to double the step length.