1 SUMMARY

Given a **cubic spline** $s(x)$ defined by knots ξ_i, function values $s_i = s(\xi_i)$ and derivative values $g_i = \frac{d}{dx}s(\xi_i)$, i=1,2,...,n, n≥2 and given **integration limits** a **and** b**, and parameters** ϕ and $\bar{x}$ the subroutine evaluates

$$Q(\phi, \bar{x}) = \int_a^b e^{-|\phi|(x-\bar{x})^2} s(x)\, dx$$

The subroutine is not restricted to cubic splines and may be used with any piece-wise cubic function that has a continuous first derivative and which can be specified by its values and first derivative values at the joins.

The subroutine can be applied to the problem of **folding a Gaussian into a function.**

ATTRIBUTES — **Version:** 1.0.0. **Types:** `QG04A`, `QG04AD`. **Calls:** `FC07`, `FC08`, `QG02`. **Original date:** May 1975. **Origin:** S.Marlow, Harwell.

2 HOW TO USE THE PACKAGE

2.1 The argument list and calling sequence

The single precision version

```
Q=QG04A(A,B,N,XI,S,G,PHI,XBAR)
```

The double precision version

```
DOUBLE PRECISION QG04AD
   -        -
Q=QG04AD(A,B,N,XI,S,G,PHI,XBAR)
```

The arguments

`A,B` are `REAL` (`DOUBLE PRECISION` in the D version) variables which must be set by the user to the lower and upper limits of the integration respectively. If either a or b is outside the range of the knots the integral is calculated on the assumption that $s(x)$=0 for $x < \xi_1$ and $x > \xi_n$. If $a > b$ the sign of the integral is appropriately modified.

`N` is an `INTEGER` variable which must be set by the user to n the number of knot points. **Restriction:** $n \geq 2$.

`XI` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length at least n which must be set by the user to the knot values ξ_i, i=1,2,..,n. These must be ordered and distinct so that $\xi_1 < \xi_2 < ... < \xi_n$.

`S` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length at least n which must be set by the user to the spline values s_i=$s(\xi_i)$, i=1,2,..,n.

`G` is a `REAL` (`DOUBLE PRECISION` in the D version) array of length at least n which must be set by the user to the first derivative values g_i, i=1,2,...,n at the knots.

`PHI` is `REAL` (`DOUBLE PRECISION` in the D version) variable which must be set by the user to the value of ϕ. Only the modulus of ϕ is used by the subroutine.

`XBAR` is a `REAL` (`DOUBLE PRECISION` in the D version) variable and must be set by the user to the value of $\bar{x}$.

Function value

QG04A and QG04AD are Fortran FUNCTION subroutines and will be set to the value of the integral on return.

2.2 The COMMON area and diagnostic messages

Associated with the subroutine is a named common area which the user may reference. To do this the calling program will require a COMMON statement of the form.

The single precision version

```
COMMON/QG04B/ LP,IERR
```

The double precision version

```
COMMON/QG04BD/ LP,IERR
```

LP is an INTEGER variable (initial value = 6 for line printer) and specifies the Fortan output stream number to be used for diagnostic printing. It may be reset by the user to any valid stream number. If LP is zero or negative printing is suppressed.

IERR is an INTEGER variable and is always set by the subroutine to one of the following values.

IERR $=0$ successful entry to subroutine.

IERR $=-1$ value of N was less than 2.

IERR >0 then $\xi_i > \xi_{i+1}$, where $i=$ IERR, that is the knots did not satisfy the original conditions.

3 GENERAL INFORMATION

Use of common: a common area called QG04B/BD is used.

Workspace: none.

Other routines called directly: calls FC07, FC08, QG02A/AD.

Input/output: diagnostic messages are printed in the event of errors.

Restrictions: $n \ge 2$, $\xi_1 < \xi_2 < ... < \xi_n$.

4 METHOD

The subroutine first ensures that the limits a and b are sensible. The integral Q can then be expressed as

$$Q = \int_a^{x_j} f_{j-1}(x)\,dx + + \sum_{i=j}^{k} \int_{x_i}^{x_{i+1}} f_i(x)\,dx + \int_{x_{k+1}}^{b} f_{k+1}(x)\,dx$$

or

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

if both a and b are inside the same interval, where the $f_i(x)$, i=j−1,...,k+1 are of the form $s_i(x)e^{-|\phi|(x-\bar{x})^2}$ and $s_i(x)$ are simple cubics in x. Each of the integrals is reduced by integration by parts to an analytic function and a multiple of the integral $\int e^{-x^2}\,dx$ between suitable limits. This integral is evaluated by using the Error function or the complementary Error function, the choice being made to minimise loss of accuracy.