NAG Fortran Library Routine Document

E01BHF

Note: before using this routine, please read the Users' Note for your implementation to check the interpretation of **bold italicised** terms and other implementation-dependent details.

1   Purpose

E01BHF evaluates the definite integral of a piecewise cubic Hermite interpolant over the interval $[a, b]$.

2   Specification

```
SUBROUTINE E01BHF(N, X, F, D, A, B, PINT, IFAIL)
INTEGER          N, IFAIL
real             X(N), F(N), D(N), A, B, PINT
```

3   Description

This routine evaluates the definite integral of a piecewise cubic Hermite interpolant, as computed by E01BEF, over the interval $[a, b]$.

If either a or b lies outside the interval from X(1) to X(N) computation of the integral involves extrapolation and a warning is returned.

The routine is derived from routine PCHIA in Fritsch (1982).

4   References

Fritsch F N (1982) PCHIP final specifications *Report UCID-30194* Lawrence Livermore National Laboratory

5   Parameters

1:    N – INTEGER   *Input*
2:    X(N) – **real** array   *Input*
3:    F(N) – **real** array   *Input*
4:    D(N) – **real** array   *Input*

On entry: N, X, F and D must be unchanged from the previous call of E01BEF.

5:    A – **real**   *Input*
6:    B – **real**   *Input*

On entry: the interval $[a, b]$ over which integration is to be performed.

7:    PINT – **real**   *Output*

On exit: the value of the definite integral of the interpolant over the interval $[a, b]$.

8:    IFAIL – INTEGER   *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL = 0 unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the

value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6   Error Indicators and Warnings

If on entry IFAIL $= 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL $= 1$

> On entry, N < 2.

IFAIL $= 2$

> The values of X(r), for $r = 1, 2, \ldots, $N, are not in strictly increasing order.

IFAIL $= 3$

> On entry, at least one of A or B lies outside the interval [X(1),X(N)], and extrapolation was performed to compute the integral. The value returned is therefore unreliable.

7   Accuracy

The computational error in the value returned for PINT should be negligible in most practical situations.

8   Further Comments

The time taken by the routine is approximately proportional to the number of data points included within the interval $[a, b]$.

9   Example

This example program reads in values of N, X, F and D. It then reads in pairs of values for A and B, and evaluates the definite integral of the interpolant over the interval [A,B] until end-of-file is reached.

9.1   Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*      E01BHF Example Program Text
*      Mark 14 Revised.  NAG Copyright 1989.
*      .. Parameters ..
       INTEGER          NIN, NOUT
       PARAMETER        (NIN=5,NOUT=6)
       INTEGER          NMAX
       PARAMETER        (NMAX=50)
*      .. Local Scalars ..
       real             A, B, PINT
       INTEGER          IFAIL, N, R
*      .. Local Arrays ..
       real             D(NMAX), F(NMAX), X(NMAX)
*      .. External Subroutines ..
       EXTERNAL         E01BHF
*      .. Executable Statements ..
       WRITE (NOUT,*) 'E01BHF Example Program Results'
*      Skip heading in data file
       READ (NIN,*)
       READ (NIN,*) N
       IF (N.GT.0 .AND. N.LE.NMAX) THEN
          DO 20 R = 1, N
```

```
              READ (NIN,*) X(R), F(R), D(R)
   20      CONTINUE
           WRITE (NOUT,*)
           WRITE (NOUT,*) '                                    Integral'
           WRITE (NOUT,*) '         A           B      over (A,B)'
*          Read A, B pairs until end of file and compute
*          definite integrals
   40      READ (NIN,*,END=60) A, B
           IFAIL = 0
*
           CALL E01BHF(N,X,F,D,A,B,PINT,IFAIL)
*
           WRITE (NOUT,99999) A, B, PINT
           GO TO 40
        END IF
   60 STOP
*
99999 FORMAT (1X,3F13.4)
      END
```

9.2 Program Data

```
E01BHF Example Program Data
 9                                  N, the number of data points
   7.990  0.00000E+0  0.00000E+0  X(R), F(R), D(R)
   8.090  0.27643E-4  5.52510E-4
   8.190  0.43749E-1  0.33587E+0
   8.700  0.16918E+0  0.34944E+0
   9.200  0.46943E+0  0.59696E+0
   10.00  0.94374E+0  6.03260E-2
   12.00  0.99864E+0  8.98335E-4
   15.00  0.99992E+0  2.93954E-5
   20.00  0.99999E+0  0.00000E+0
   7.99        20.0                 A, B pairs until end of file
   10.0        12.0
   12.0        10.0
   15.0        15.0
```

9.3 Program Results

```
 E01BHF Example Program Results

                          Integral
         A          B     over (A,B)
      7.9900    20.0000      10.7648
     10.0000    12.0000       1.9622
     12.0000    10.0000      -1.9622
     15.0000    15.0000       0.0000
```