

NAG 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 (KIND=nag_wp) X(N), F(N), D(N), A, B, PINT
```

3 Description

E01BHF 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 Arguments

- | | | |
|----|---------------------------------|--------------|
| 1: | N – INTEGER | <i>Input</i> |
| 2: | X(N) – REAL (KIND=nag_wp) array | <i>Input</i> |
| 3: | F(N) – REAL (KIND=nag_wp) array | <i>Input</i> |
| 4: | D(N) – REAL (KIND=nag_wp) array | <i>Input</i> |

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

- | | | |
|----|------------------------|--------------|
| 5: | A – REAL (KIND=nag_wp) | <i>Input</i> |
| 6: | B – REAL (KIND=nag_wp) | <i>Input</i> |

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

- | | | |
|----|---------------------------|---------------|
| 7: | PINT – REAL (KIND=nag_wp) | <i>Output</i> |
|----|---------------------------|---------------|

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

- | | | |
|----|-----------------|---------------------|
| 8: | IFAIL – INTEGER | <i>Input/Output</i> |
|----|-----------------|---------------------|

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this argument you should refer to Section 3.4 in How to Use the NAG Library and its Documentation for details.

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, if you are not familiar with this argument, the

recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

On exit: IFAIL = 0 unless the routine detects an error or a warning has been flagged (see Section 6).

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 $r = 1, 2, \dots, N$, 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.

IFAIL = -99

An unexpected error has been triggered by this routine. Please contact NAG.

See Section 3.9 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -399

Your licence key may have expired or may not have been installed correctly.

See Section 3.8 in How to Use the NAG Library and its Documentation for further information.

IFAIL = -999

Dynamic memory allocation failed.

See Section 3.7 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

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

8 Parallelism and Performance

E01BHF is not threaded in any implementation.

9 Further Comments

The time taken by E01BHF is approximately proportional to the number of data points included within the interval $[a, b]$.

10 Example

This example 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.

10.1 Program Text

```

Program e01bhfe

!      E01BHF Example Program Text

!      Mark 26 Release. NAG Copyright 2016.

!      .. Use Statements ..
      Use nag_library, Only: e01bhf, nag_wp
!      .. Implicit None Statement ..
      Implicit None
!      .. Parameters ..
      Integer, Parameter          :: nin = 5, nout = 6
!      .. Local Scalars ..
      Real (Kind=nag_wp)          :: a, b, pint
      Integer                     :: ifail, ioerr, n, r
!      .. Local Arrays ..
      Real (Kind=nag_wp), Allocatable :: d(:), f(:), x(:)
!      .. Executable Statements ..
      Write (nout,*) 'E01BHF Example Program Results'

!      Skip heading in data file
      Read (nin,*)

      Read (nin,*) n
      Allocate (d(n),f(n),x(n))

      Do r = 1, n
         Read (nin,*) x(r), f(r), d(r)
      End Do

      Write (nout,*)
      Write (nout,*) '
      Write (nout,*) '
                        A                B          Integral'
                        over (A,B)'

data: Do
      Read (nin,*,Iostat=ioerr) a, b

      If (ioerr<0) Then
         Exit data
      End If

      ifail = 0
      Call e01bhf(n,x,f,d,a,b,pint,ifail)

      Write (nout,99999) a, b, pint
End Do data

99999 Format (1X,3F13.4)
End Program e01bhfe

```

10.2 Program Data

```

E01BHF Example Program Data
9
7.990  0.00000E+0  0.00000E+0
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
10.0    12.0
12.0    10.0
15.0    15.0

```

N, the number of data points
X(R), F(R), D(R)

A, B pairs until end of file

10.3 Program Results

E01BHF Example Program Results

A	B	Integral 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
