### F04AHF - NAG Fortran Library Routine Document

**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

F04AHF calculates the accurate solution of a set of real linear equations with multiple right-hand sides, AX = B, with iterative refinement, where A has been factorized by F03AFF.

## 2 Specification

```
SUBROUTINE FO4AHF(N, IR, A, IA, AA, IAA, P, B, IB, EPS, X, IX, BB, 1 IBB, K, IFAIL)

INTEGER N, IR, IA, IAA, IB, IX, IBB, K, IFAIL

real A(IA,N), AA(IAA,N), P(N), B(IB,IR), EPS, 1 X(IX,IR), BB(IBB,IR)
```

# 3 Description

To solve a set of real linear equations AX = B, the routine must be preceded by a call to F03AFF which computes an LU factorization of A with partial pivoting, PA = LU, where P is a permutation matrix, L is lower triangular and U is unit upper triangular. An approximation to X is found by forward and backward substitution. The residual matrix R = B - AX is then calculated using **additional precision**, and a correction D to X is found by solving LUD = PR. X is replaced by X + D, and this iterative refinement of the solution is repeated until full machine accuracy has been obtained.

### 4 References

[1] Wilkinson J H and Reinsch C (1971) Handbook for Automatic Computation II, Linear Algebra Springer-Verlag

### 5 Parameters

1: N — INTEGER Input

On entry: n, the order of the matrix A.

2: IR — INTEGER

On entry: r, the number of right-hand sides.

3: A(IA,N) — real array

On entry: the n by n matrix A.

4: IA — INTEGER Input

On entry: the first dimension of the array A as declared in the (sub)program from which F04AHF is called.

Constraint: IA  $\geq$  N.

5: AA(IAA,N) — real array Input

On entry: details of the LU factorization, as returned by F03AFF.

6: IAA — INTEGER Input

On entry: the first dimension of the array AA as declared in the (sub)program from which F04AHF is called.

Constraint: IAA  $\geq$  N.

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7: P(N) — real array

On entry: details of the row interchanges as returned by F03AFF.

8: B(IB,IR) - real array

On entry: the n by r right-hand side matrix B.

9: IB — INTEGER Input

On entry: the first dimension of the array B as declared in the (sub)program from which F04AHF is called.

Constraint:  $IB \geq N$ .

10: EPS - real Input

On entry: EPS must be set to the value of the machine precision.

11: X(IX,IR) — real array

On exit: the n by r solution matrix X.

12: IX — INTEGER

On entry: the first dimension of the array X as declared in the (sub)program from which F04AHF is called.

Constraint:  $IX \geq N$ .

13: BB(IBB,IR) - real array

Output

On exit: the n by r final residual matrix R = B - AX.

14: IBB — INTEGER Input

On entry: the first dimension of the array BB as declared in the (sub)program from which F04AHF is called.

Constraint: IBB > N.

15: K — INTEGER Output

 $On\ exit:$  the number of iterations needed in the refinement process.

16: IFAIL — INTEGER Input/Output

On entry: IFAIL must be set to 0, -1 or 1. For users not familiar with this parameter (described in Chapter P01) the recommended value is 0.

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

# 6 Error Indicators and Warnings

Errors detected by the routine:

IFAIL = 1

The matrix A is too ill-conditioned to produce a correctly rounded solution.

# 7 Accuracy

The computed solutions should be correct to full machine accuracy. For a detailed error analysis see Wilkinson and Reinsch [1] page 106.

#### 8 Further Comments

The time taken by the routine is approximately proportional to  $n^2r$ .

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## 9 Example

To solve the set of linear equations AX = B where

$$A = \begin{pmatrix} 33 & 16 & 72 \\ -24 & -10 & -57 \\ -8 & -4 & -17 \end{pmatrix} \text{ and } B = \begin{pmatrix} -359 \\ 281 \\ 85 \end{pmatrix}.$$

#### 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.

```
FO4AHF Example Program Text
   Mark 14 Revised. NAG Copyright 1989.
   .. Parameters ..
   INTEGER
                     NMAX, IR, IAA, IA, IB, IX, IBB
   PARAMETER
                     (NMAX=8, IR=1, IAA=NMAX, IA=NMAX, IB=NMAX, IX=NMAX,
                     IBB=NMAX)
   INTEGER
                     NIN, NOUT
   PARAMETER
                     (NIN=5,NOUT=6)
   .. Local Scalars ..
   real
                    D1, EPS
   INTEGER
                     I, ID, IFAIL, J, K, N
   .. Local Arrays ..
                     A(IA,NMAX), AA(IAA,NMAX), B(IB,IR), BB(IBB,IR),
                    P(NMAX), X(IX,IR)
   .. External Functions ..
   real
                    XO2AJF
   EXTERNAL
                    XO2AJF
   .. External Subroutines ..
   EXTERNAL
                     FO3AFF, FO4AHF
   .. Executable Statements ...
   WRITE (NOUT,*) 'F04AHF Example Program Results'
   Skip heading in data file
   READ (NIN,*)
   READ (NIN,*) N
   WRITE (NOUT,*)
   IF (N.GT.O .AND. N.LE.NMAX) THEN
      READ (NIN,*) ((AA(I,J),J=1,N),I=1,N)
      DO 40 I = 1, N
         DO 20 J = 1, N
            A(J,I) = AA(J,I)
         CONTINUE
20
40
      CONTINUE
      EPS = XO2AJF()
      IFAIL = 1
      Crout decomposition
      CALL FO3AFF(N, EPS, AA, IAA, D1, ID, P, IFAIL)
      IF (IFAIL.NE.O) THEN
         WRITE (NOUT, 99998) 'Error in FO3AFF. IFAIL =', IFAIL
         READ (NIN,*) ((B(I,J),J=1,IR),I=1,N)
         IFAIL = 1
         Accurate solution of linear equations
         CALL FO4AHF(N, IR, A, IA, AA, IAA, P, B, IB, EPS, X, IX, BB, IBB, K, IFAIL)
```

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```
*
            IF (IFAIL.NE.O) THEN
               WRITE (NOUT,99998) 'Error in FO4AHF. IFAIL =', IFAIL
            ELSE
               WRITE (NOUT,*) ' Solution'
               DO 60 I = 1, N
                  WRITE (NOUT,99999) (X(I,J),J=1,IR)
   60
               CONTINUE
            END IF
         END IF
      ELSE
         WRITE (NOUT,99998) 'N is out of range: N = ', N
      END IF
      STOP
99999 FORMAT (1X,8F9.4)
99998 FORMAT (1X,A,I5)
      END
```

## 9.2 Program Data

## 9.3 Program Results

FO4AHF Example Program Results

Solution 1.0000 -2.0000 -5.0000

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