Package MC31 was designed for use by package MA32 which has itself been superseded; the use of this routine is not recommended.

## 1 SUMMARY

This subroutine performs the arithmetic operations corresponding to two steps of Gaussian elimination.
ATTRIBUTES - Version: 1.0.0. Types: MC31A; MC31AD. Remark: This is a double pivot version of MC32. Calls: None. Language: A Cray-2 assembler version is available and is more than twice as fast as the equivalent vectorized version Fortran code. Original date: August 1986. Origin: I.S. Duff, Harwell and A. K. Dave, CRAY Research (UK) Ltd.

## 2 HOW TO USE THE PACKAGE

Each call to MC31 is equivalent to the execution of the Fortran code :

```
    DO 20 J=1,LFRONT
        DO 10 I=1,KFRONT
        FA(I,J) = FA(I,J) + PVKOL (I,1)*QQ(1,J) + PVKOL (I, 2)*QQ (2,J)
    CONTINUE
20 CONTINUE
```


### 2.1 Argument list

The single precision version
CALL MC31A (FA, NFRONT, KFRONT, LFRONT, PVKOL, QQ)

## The double precision version

CALL MC31AD (FA, NFRONT, KFRONT, LFRONT, PVKOL, QQ)
FA is a REAL (DOUBLE PRECISION in the D version) array of two dimensions, with leading dimension NFRONT. The user must set the leading KFRONT by LFRONT subarray to the values of the matrix entries prior to the Gaussian elimination steps to be executed by the call to MC31A/AD. On exit, FA contains the values of the matrix entries after the Gaussian elimination step. Only the leading KFRONT by LFRONT subarray is modified by MC31A/AD.

NFRONT is an INTEGER variable which must be set on entry to the leading dimension of arrays FA and PVKOL. It is not altered by MC31A/AD.
KFRONT is an INTEGER variable which must be set on entry to the number of entries in the pivot column (excluding the pivot). It is not altered by MC31A/AD.

LFRONT is an INTEGER variable which must be set on entry to the number of entries in the pivot row (excluding the pivot). It is not altered by MC31A/AD.
PVKOL is a REAL (DOUBLE PRECISION in the D version) array of two dimensions, with leading dimension NFRONT. The user must set the first NFRONT by 2 elements of this to the negative of the subdiagonal entries in the two pivot columns. PVKOL is not altered by MC31A/AD.

QQ is a REAL (DOUBLE PRECISION in the D version) array of two dimensions, with leading dimension 2 and a second dimension of at least LFRONT. The user must set these to the superdiagonal entries in the pivot rows divided by the pivots. $Q Q$ is not altered by MC31A/AD .

### 2.3 Common

None.

### 2.4 Errors and diagnostic messages

None.

## 3 GENERAL INFORMATION

Workspace: There are no work arrays used by MC31A/AD.
Use of common: The subroutine does not use any common areas or auxiliary subroutines.
Other routines called directly: None
Input/output: None
Portability: There is a CRAY-2 Assembler Language version available.
Restrictions: None.

## 4 METHOD

For the CRAY version, CRAY Assembler Language (CAL) is used to ensure that the vector PVKOL is kept in the vector registers throughout the sequence of inner loops. Thus there is only one memory fetch/store for each arithmetic operation and a maximum asymptotic rate of nearly 280 Megaflops is possible.

For systems of moderate size, $n<50$, a Gaussian elimination program based around this subroutine will typically run 1.5 times faster than the equivalent program based around the single pivot subroutine $M C 32 \mathrm{~A} / \mathrm{AD}$, and for large systems it will typically run 1.75 times faster.

## 5 EXAMPLE OF USE

The following example shows the use of the subroutine MC31A to factorise a full matrix using Gaussian elimination without pivoting.

```
PROGRAM MC31T
PARAMETER( NMAX = 20 , NMAXP1 = NMAX + 1 )
REAL A (NMAX, NMAXP1), PVKOL (NMAX, 2), QQ (2,NMAX), RHS1,
+ ZERO, EPSOLN, A11, A12, A21, A22, TMAX, ERRMAX
INTEGER I, J, K, N, NMK, NMKP1, POSITN
EXTERNAL FA01AS
REAL FA01AS
DATA ZERO/0.0E0/, EPSOLN/1.0E-09/
WRITE (6,99999)
N = NMAX
C GENERATE RANDOM MATRIX WITH
C RIGHT HAND SIDE AS COLUMN N+1.
DO 20 I=1,N
    RHS1 = ZERO
    DO 10 J=1,N
        A(I,J) = FA01AS (-1)
```

```
        RHS1 = RHS1 + A(I,J)*FLOAT (J)
        CONTINUE
        A(I,N+1) = RHS1
    CONTINUE
    EACH PASS THROUGH THIS LOOP PERFORMS TWO
    STEPS OF GAUSSIAN ELIMINATION.
    DO 70 K=1,N,2
        NMK = N - K - 1
    HOLD TWO BY TWO BLOCK.
    A11 = A(K,K)
    A12 = A(K,K+1)/A11
C STORE UPPER TRIANGLE READY FOR BACKSOLUTION.
    A (K,K+1) = A12
    JUMP IF AT LAST ONE BY ONE PIVOT.
    IF (NMK.GE.O) THEN
            SAVE REST OF TWO BY TWO BLOCK.
            A21 = -A (K+1,K)
            A22 = A (K+1,K+1) + A21*A12
            CREATE QQ
            DO 50 I=1,NMK+1
                QQ(1,I) = A(K,K+I+1)/A11
                QQ(2,I) = (A (K+1,K+I+1) +A21*QQ(1,I)) /A22
                STORE UPPER TRIANGLE READY FOR BACKSOLUTION.
                A(K,K+I+1) = QQ(1,I)
                A(K+1,K+I+1)=QQ(2,I)
            CONTINUE
            CREATE PVKOL
            DO 30 I=1,NMK
                PVKOL (I,1) = -A (K+I+1,K)
                PVKOL(I, 2) = -(A(K+I+1,K+1) + PVKOL (I,1)*A12)
            CONTINUE
            IF (NMK .NE. O) THEN
                    PERFORM GAUSSIAN ELIMINATION
                    CALL MC31A(A (K+2,K+2), NMAX, NMK, NMK+1, PVKOL, QQ)
            ENDIF
        ENDIF
    CONTINUE
    PERFORM BACK SUBSTITUTION
    DO }90\mathrm{ I=N-1,1,-1
        DO 80 J=I+1,N
            A(I,N+1) = A(I,N+1) - A(I,J)*A(J,N+1)
        CONTINUE
    CONTINUE
    CONTINUE
    PRINT MAXIMUM ERROR AND THE ASSOCIATED COMPONENT
    ERRMAX = ZERO
    POSITN = 0
    DO 110 I=1,N
        TMAX = AMAX1( ABS (A (I,N+1) -FLOAT (I)), ERRMAX)
        IF (TMAX .NE. ERRMAX) THEN
            POSITN = I
            ERRMAX = TMAX
        ENDIF
    110 CONTINUE
    WRITE(6,99998) ERRMAX , POSITN , A(POSITN,N+1)
99999 FORMAT (' OUTPUT FROM TEST OF MC31A ')
```

```
99998 FORMAT (' MAXIMUM ERROR = ',E12.5,' ATTAINED AT COMPONENT ',I2/
    + ' VALUE OF COMPONENT = ',E12.5 )
        STOP
        END
```

This produces the following output
OUTPUT FROM TEST OF MC31A
MAXIMUM ERROR $=0.65995 E-10$ ATTAINED AT COMPONENT 1
VALUE OF COMPONENT $=0.10000 \mathrm{E}+01$

