

## F02WQFP

### NAG Parallel Library Routine Document

**Note:** Before using this routine, please read the Users' Note for your implementation to check for implementation-dependent details. You are advised to enclose any calls to NAG Parallel Library routines between calls to Z01AAFP and Z01ABFP.

## 1 Description

F02WQFP computes the Singular Value Decomposition (SVD) of a real matrix whose columns are distributed on a logical 2-d processor grid.

The SVD of an  $m$  by  $n$  real rectangular matrix  $A$  (where  $m \geq n$ ) may be defined in the form

$$A = \begin{bmatrix} U | \tilde{U} \end{bmatrix} \begin{bmatrix} \Sigma \\ 0 \end{bmatrix} V^T = U \Sigma V^T$$

where  $U$  is an  $m \times n$  matrix of left singular vectors,  $\tilde{U}$  is an  $m \times (m - n)$  matrix,  $V$  is an  $n \times n$  orthogonal matrix of right singular vectors, and  $\Sigma$  is an  $n \times n$  diagonal matrix of singular values. The singular values  $\sigma_1, \sigma_2, \dots, \sigma_n$  are non-negative and in non-increasing order of magnitude. The matrix  $\begin{bmatrix} U | \tilde{U} \end{bmatrix}$  is orthogonal.

For the case,  $m < n$  the SVD may be defined in the form

$$A = U \begin{bmatrix} \Sigma | 0 \end{bmatrix} \begin{bmatrix} V | \tilde{V} \end{bmatrix}^T = U \Sigma V^T$$

where  $U$  is an  $m \times m$  orthogonal matrix,  $V$  is an  $n \times m$  matrix of right singular vectors,  $\tilde{V}$  is an  $n \times (n - m)$  matrix, and  $\Sigma$  is an  $m \times m$  diagonal matrix of singular values. The matrix  $\begin{bmatrix} V | \tilde{V} \end{bmatrix}$  is orthogonal.

In general, matrices  $\tilde{V}$  and  $\tilde{U}$  are not unique. For convenience in the description of the routine, the definition of singular values is extended when  $m < n$  by defining  $\sigma_{m+1} = \dots = \sigma_n = 0$ . In that case, the columns of  $\tilde{V}$  may be considered as right singular vectors corresponding to zero singular values.

F02WQFP computes only the left singular vectors  $U$  which correspond to non-zero singular values. Optionally all right singular vectors  $V$  (including  $\tilde{V}$  if  $m < n$ ) are computed.

## 2 Specification

```

SUBROUTINE F02WQFP(ICNTXT, M, N, A, LDA, VWANT, NX, NR, IFAIL)
DOUBLE PRECISION  A(0:LDA-1,0:*)
INTEGER           ICNTXT, M, N, LDA, NX, NR, IFAIL
LOGICAL          VWANT

```

## 3 Data Distribution

### 3.1 Definitions

The following definitions are used in describing the data distribution within this document:

- $m_p$  – the number of rows in the logical processor grid.
- $n_p$  – the number of columns in the logical processor grid.
- $p$  –  $m_p \times n_p$ , the total number of processors in the logical processor grid.
- $p_d$  – the number of logical processors which hold columns of the matrix  $A$ .
- $N_b$  – the maximum number of columns of the matrix  $A$  held locally on a logical processor.
- $N_x$  – the actual number of columns of the matrix  $A$  held locally on a logical processor, where  $0 \leq N_x \leq N_b$ .
- $n_r$  – the number of non-zero singular values computed by a logical processor, where  $0 \leq n_r \leq N_x$ .
- $[x]$  – the ceiling function of  $x$  which gives the smallest integer which is not less than  $x$ .

## 3.2 Global and Local Arguments

The input arguments `M`, `N`, `VWANT` and `IFAIL` are global and so must have the same value on entry to the routine on each processor. The output argument `IFAIL` is global and so will have the same value on exit from the routine on each processor. The remaining arguments are local.

## 3.3 Distribution Strategy

Columns of the matrix  $A$  are allocated to logical processors on the 2-d grid row by row (i.e., in row major ordering of the grid) starting from the  $\{0,0\}$  logical processor. Each logical processor that contains columns of the matrix contains  $N_b = \lceil n/p \rceil$  columns, except the last processor that actually contains data, for which the number of columns held may be less than  $N_b$ . This processor will contain  $\text{mod}(n, N_b)$  columns if  $\text{mod}(n, N_b) \neq 0$ , and will contain  $N_b$  columns otherwise. Some logical processors may not contain any columns of the matrix if  $n$  is not large relative to  $p$ , but if  $n > (p-1)^2$  then all processors will certainly contain columns of the matrix.

The number of logical processors that contain columns of the matrix is given by  $p_d = \lceil n/N_b \rceil$ .

The following example illustrates a case where the last processor with data is not the last processor of the grid. Furthermore the number of columns on the last processor with data is not equal to the number of columns on other processors.

If  $m_p = 2$ ,  $n_p = 4$  then  $p = m_p \times n_p = 8$ . If  $n = 41$  then  $N_b = \lceil n/p \rceil = \lceil 5.125 \rceil = 6$ ,  $\text{mod}(n, N_b) = 5 \neq 0$  and  $p_d = \lceil n/N_b \rceil = \lceil 6.833 \rceil = 7$ .

processor $\{0,0\}$ $N_x = 6$ columns (1:6)	processor $\{0,1\}$ $N_x = 6$ columns (7:12)	processor $\{0,2\}$ $N_x = 6$ columns (13:18)	processor $\{0,3\}$ $N_x = 6$ columns (19:24)
processor $\{1,0\}$ $N_x = 6$ columns (25:30)	processor $\{1,1\}$ $N_x = 6$ columns (31:36)	processor $\{1,2\}$ $N_x = 5$ columns (37:41)	processor $\{1,3\}$ $N_x = 0$

If the data is distributed incorrectly, the routine may fail to produce correct results or will exit with an error flag. Routines to assist with distribution of data can be found in Chapters F01 and X04.

## 4 Arguments

- 1: ICNTXT — INTEGER *Local Input*  
*On entry:* the BLACS context used by the communication mechanism, usually returned by a call to Z01AAFP.
- 2: M — INTEGER *Global Input*  
*On entry:*  $m$ , the number of rows of  $A$ .  
*Constraint:*  $M \geq 0$ .
- 3: N — INTEGER *Global Input*  
*On entry:*  $n$ , the number of columns of  $A$ .  
*Constraint:*  $N \geq 0$ .
- 4: A(0:LDA-1,0:\*) — DOUBLE PRECISION array *Local Input/Local Output*  
**Note:** the size of the second dimension of the array  $A$  must be at least  $N_x + 1$  where  $N_x$  is the number of columns of  $A$  held locally by the logical processor. The array  $A$  is not referenced if  $N_x = 0$ .  
*On entry:*  $A(1 : m, 1 : N_x)$  must contain columns of the matrix  $A$ , as defined by the distribution strategy (see Section 3.3).  
*On exit:*  $A(0, 1 : N_x)$  contains  $N_x$  singular values of the matrix  $A$  stored on this logical processor. They are ordered locally and globally (in the row major ordering of the processors) in non-increasing order of magnitude.

$A(1 : m, 1 : n_r)$  contains the left singular vectors corresponding to non-zero singular values. A left singular vector is not computed if the corresponding singular value and the corresponding elements of  $A$  are set to zero.

If  $VWANT = .TRUE.$ , then  $A(m+1 : m+n, 1 : N_x)$  contains the right singular vectors corresponding to the singular values held on this logical processor.

The remainder of the array is used as workspace and contains no useful information.

- 5:** LDA — INTEGER *Local Input*  
*On entry:* the size of the first dimension of the array  $A$  as declared in the (sub)program from which F02WQFP is called.  
*Constraint:*  $LDA \geq M + N + 2$  if  $VWANT = .TRUE.$ ; otherwise  $LDA \geq M + 2$ .
- 6:** VWANT — LOGICAL *Global Input*  
*On entry:* VWANT must be set to  $.TRUE.$  if right singular vectors are also required.
- 7:** NX — INTEGER *Local Output*  
*On exit:*  $N_x$ , the actual number of columns of the matrix  $A$  held on the logical processor.
- 8:** NR — INTEGER *Local Output*  
*On exit:*  $n_r$ , the number of non-zero singular values held on the logical processor.
- 9:** IFAIL — INTEGER *Global Input/Global Output*  
*On entry:* IFAIL must be set to 0,  $-1$  or 1. For users not familiar with this parameter (described in the Essential Introduction) the recommended values are:  
     IFAIL = 0, if multigridding is **not** employed;  
     IFAIL =  $-1$ , if multigridding is employed.  
*On exit:* IFAIL = 0 unless the routine detects an error (see Section 5).

## 5 Errors and Warnings

If on entry IFAIL = 0 or  $-1$ , explanatory error messages are output from the root processor (or processor  $\{0,0\}$  when the root processor is not available) on the current error message unit (as defined by X04AAF).

Errors detected by the routine:

IFAIL =  $-2000$

The routine has been called with an invalid value of ICNTXT on one or more processors.

IFAIL =  $-1000$

The logical processor grid and library mechanism (Library Grid) have not been correctly defined, see Z01AAFP.

IFAIL =  $-i$

On entry, the  $i$ th argument had an invalid value. This error occurred either because a global argument did not have the same value on all logical processors, or because its value on one or more processors was incorrect. An explanatory message distinguishes between these two cases.

IFAIL = 1

The Jacobi algorithm has not converged.

## 6 Further Comments

### 6.1 Algorithmic Detail

The algorithm is based on a one-sided Jacobi method, see Hestenes [2].

## 6.2 Parallelism Detail

The algorithm uses a linear array of logical processors. This linear array is mapped to the 2-d array based on the row major ordering beginning from the  $\{0,0\}$  logical processor on the 2-d array. Most of the communication is between neighbours on the linear array of processors.

## 6.3 Accuracy

The computed factors  $U$ ,  $\Sigma$  and  $V$  satisfy the relation

$$U\Sigma V^T = A + E,$$

where

$$\|E\| \leq c\epsilon\|A\|,$$

$\epsilon$  being the *machine precision*,  $c$  is a modest function of  $m$  and  $n$  and  $\|\cdot\|$  denotes the 2-norm.

## 7 References

- [1] Dongarra J J and Whaley R C (1995) A users' guide to the BLACS v1.0. *LAPACK Working Note 94 (Technical Report CS-95-281)* Department of Computer Science, University of Tennessee, 107 Ayres Hall, Knoxville, TN 37996-1301, USA.  
URL: <http://www.netlib.org/lapack/lawns/lawn94.ps>
- [2] Hestenes M R (1958) Inversion of matrices by biorthogonalization and related results *J. SIAM* **6** 51–90

## 8 Example

To find the singular value decomposition of the 4 by 7 matrix  $A$  given by

$$A = \left( \begin{array}{cc|cc|cc|c} 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 & 1.0 \\ 0.0 & 0.0 & 0.0 & 1.0 & 1.0 & 1.0 & 1.0 \end{array} \right)$$

and to print results on the root processor. The routine F01ZRFP is used to generate the matrix  $A$  on a 2 by 2 logical processor grid. The number of columns of the matrix  $A$  on each logical processor,  $N_x$ , is equal to 2 on logical processors  $\{0,0\}$ ,  $\{0,1\}$ , and  $\{1,0\}$ . On the final logical processor  $\{1,1\}$ ,  $N_x = 1$ .

The routine X04BFFP is used to bring results to the root processor and print the results. The results are the non-zero singular values, and the corresponding left and right singular vectors.

### 8.1 Example Text

```
*      F02WQFP Example Program Text
*      NAG Parallel Library Release 2. NAG Copyright 1996.
*      .. Parameters ..
      INTEGER          NOUT
      PARAMETER        (NOUT=6)
      INTEGER          M, N, MM, NM
      PARAMETER        (M=4,N=7,MM=20,NM=20)
      INTEGER          MG, NG
      PARAMETER        (MG=2,NG=2)
      INTEGER          LDA, TDA
      PARAMETER        (LDA=MM+NM+2,TDA=(NM/(MG*NG)+2))
      CHARACTER*25     FORMT
      PARAMETER        (FORMT='F12.4')
      LOGICAL          VWANT
      PARAMETER        (VWANT=.TRUE.)
```

```

*      .. Local Scalars ..
INTEGER          ICNTXT, ICOFF, IFAIL, MP, NP, NR, NX
LOGICAL          ROOT
CHARACTER        CNUMOP, TITOP
*      .. Local Arrays ..
DOUBLE PRECISION A(0:LDA-1,0:TDA-1), W(LDA,TDA)
*      .. External Functions ..
INTEGER          OFFSET
LOGICAL          Z01ACFP
EXTERNAL         OFFSET, Z01ACFP
*      .. External Subroutines ..
EXTERNAL         F01ZRFP, F02WQFP, GMATA, X04BFFP, Z01AAFP,
+               Z01ABFP
*      .. Executable Statements ..
ROOT = Z01ACFP()

*
IF (ROOT) THEN
  WRITE (NOUT,*) 'F02WQFP Example Program Results'
  WRITE (NOUT,*)
END IF

*
Define the 2D processor grid
*
MP = MG
NP = NG
IFAIL = 0

*
CALL Z01AAFP(ICNTXT,MP,NP,IFAIL)

*
Generate the matrix A
*
IFAIL = 0

*
CALL F01ZRFP(ICNTXT,GMATA,M,N,A(1,1),LDA,NX,IFAIL)

*
Compute the SVD
*
IFAIL = 0

*
CALL F02WQFP(ICNTXT,M,N,A,LDA,VWANT,NX,NR,IFAIL)

*
Print singular values
*
IF (ROOT) THEN
  WRITE (NOUT,*) 'Singular values'
  WRITE (NOUT,*)
  TITOP = 'N'
  CNUMOP = 'G'
END IF
ICOFF = 0
IFAIL = 0

*
CALL X04BFFP(ICNTXT,NOUT,1,NR,A(0,1),LDA,FORMT,TITOP,CNUMOP,ICOFF,
+           W,LDA,IFAIL)

*
Print left singular vectors
*
IF (ROOT) THEN

```

```

        WRITE (NOUT,*) 'Left singular vectors'
        WRITE (NOUT,*)
    END IF
    IFAIL = 0
*
    CALL X04BFFP(ICNTXT,NOUT,M,NR,A(1,1),LDA,FORMAT,TITOP,CNUMOP,ICOFF,
+              W,LDA,IFAIL)
*
*   Print right singular vectors (full set)
*
    IF (ROOT) THEN
        WRITE (NOUT,*) 'Right singular vectors (full set)'
        WRITE (NOUT,*)
    END IF
    IFAIL = 0
*
    CALL X04BFFP(ICNTXT,NOUT,N,NX,A(M+1,1),LDA,FORMAT,TITOP,CNUMOP,
+              ICOFF,W,LDA,IFAIL)
*
*   Print right singular vectors (which define the null space)
*
    IF (ROOT) THEN
        WRITE (NOUT,*) 'Right singular vectors (null space only)'
        WRITE (NOUT,*)
        CNUMOP = 'L'
    END IF
*
*   (Integer function OFFSET gives the additive offset required to
*   transform the local column number to the global column number.)
*
    ICOFF = OFFSET(ICNTXT,N)
    IFAIL = 0
*
    CALL X04BFFP(ICNTXT,NOUT,N,NX-NR,A(M+1,NR+1),LDA,FORMAT,TITOP,
+              CNUMOP,ICOFF,W,LDA,IFAIL)
*
    IFAIL = 0
*
*   Undefine the grid
*
    CALL Z01ABFP(ICNTXT,'N',IFAIL)
*
    STOP
    END
*
    SUBROUTINE GMATA(M,J1,J2,AL,LDAL)
*
*   GMATA generates the block A( 1: M, J1: J2 ) of the matrix A such
*   that
*
*       a(i,j) = 0.0 if i >= j
*       a(i,j) = 1.0 else
*
*   in the array AL.
*
*   .. Scalar Arguments ..
    INTEGER          J1, J2, LDAL, M
*   .. Array Arguments ..

```

```

      DOUBLE PRECISION AL(LDAL,*)
*      .. Local Scalars ..
      INTEGER          I, J, L
*      .. Executable Statements ..
      L = 1
      DO 40 J = J1, J2
        DO 20 I = 1, M
          IF (J.GE.I) THEN
            AL(I,L) = 1.0
          ELSE
            AL(I,L) = 0.0
          END IF
        20 CONTINUE
        L = L + 1
      40 CONTINUE
*
*      End of GMATA.
*
      RETURN
      END
*
      INTEGER FUNCTION OFFSET(ICNTXT,N)
*
*      Integer function OFFSET gives the (additive) offset required to
*      transform the local column number to the global column number if
*      the distribution corresponds to the data structure
*      in F01ZRFP, F02FQFP or F02WQFP.
*
*      .. Scalar Arguments ..
      INTEGER          ICNTXT, N
*      .. Local Scalars ..
      INTEGER          ME, MP, MYCOL, MYROW, NB, NP, P
*      .. External Subroutines ..
      EXTERNAL        BLACS_GRIDINFO
*      .. Intrinsic Functions ..
      INTRINSIC      MOD
*      .. Executable Statements ..
      CALL BLACS_GRIDINFO(ICNTXT,MP,NP,MYROW,MYCOL)
      P = MP*NP
      IF (P.GT.N) THEN
        NB = 1
      ELSE
        NB = N/P
        IF (MOD(N,P).NE.0) THEN
          NB = NB + 1
        END IF
      END IF
      ME = MP*MYROW + MYCOL
      OFFSET = ME*NB
*
*      End of OFFSET.
*
      RETURN
      END

```

## 8.2 Example Data

None.

### 8.3 Example Results

#### F02WQFP Example Program Results

##### Singular values

1	2
4.4485	1.1983
3	4
0.6953	0.5396

##### Left singular vectors

1	2
0.5653	-0.6145
0.5368	-0.1866
0.4811	0.3713
0.4011	0.6706
3	4
0.4832	0.2631
-0.5164	-0.6406
-0.4478	0.6559
0.5471	-0.3002

##### Right singular vectors (full set)

1	2
0.1271	-0.5128
0.2477	-0.6685
0.3559	-0.3587
0.4460	0.2009
0.4460	0.2009
0.4460	0.2009
0.4460	0.2009
3	4
0.6950	0.4877
-0.0477	-0.6996
-0.6917	0.5159
0.0951	-0.0405
0.0951	-0.0405
0.0951	-0.0405
0.0951	-0.0405
5	6
0.0000	0.0000
0.0000	0.0000
0.0000	0.0000
0.8573	-0.1227
-0.3436	-0.3632
-0.3436	-0.3632
-0.1700	0.8492
7	
0.0000	
0.0000	

0.0000  
0.0000  
-0.7071  
0.7071  
0.0000

Right singular vectors (null space only)

5	6
0.0000	0.0000
0.0000	0.0000
0.0000	0.0000
0.8573	-0.1227
-0.3436	-0.3632
-0.3436	-0.3632
-0.1700	0.8492

7
0.0000
0.0000
0.0000
0.0000
-0.7071
0.7071
0.0000

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