

NAG Fortran Library Routine Document

F07CPF (ZGTSVX)

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

F07CPF (ZGTSVX) uses the LU factorization to compute the solution to a complex system of linear equations

$$AX = B, \quad A^T X = B \quad \text{or} \quad A^H X = B,$$

where A is a tridiagonal matrix of order N and X and B are n by r matrices. Error bounds on the solution and a condition estimate are also provided.

2 Specification

```

SUBROUTINE F07CPF (FACT, TRANS, N, NRHS, DL, D, DU, DLF, DF, DUF, DU2,
1 IPIV, B, LDB, X, LDX, RCOND, FERR, BERR, WORK, RWORK,
2 INFO)
    INTEGER          N, NRHS, IPIV(*), LDB, LDX, INFO
    double precision RCOND, FERR(*), BERR(*), RWORK(*)
    complex*16       DL(*), D(*), DU(*), DLF(*), DF(*), DUF(*), DU2(*),
1 B(LDB,*), X(LDX,*), WORK(*)
    CHARACTER*1      FACT, TRANS

```

The routine may be called by its LAPACK name ***zgtsvx***.

3 Description

The following steps are performed:

1. If FACT = 'N', the LU decomposition is used to factor the matrix A as $A = LU$, where L is a product of permutation and unit lower bidiagonal matrices and U is upper triangular with nonzeros in only the main diagonal and first two super-diagonals.
2. If some $u_{ii} = 0$, so that U is exactly singular, then the routine returns with INFO = i . Otherwise, the factored form of A is used to estimate the condition number of the matrix A . If the reciprocal of the condition number is less than ***machine precision***, INFO = $N + 1$ is returned as a warning, but the routine still goes on to solve for X and compute error bounds as described below.
3. The system of equations is solved for X using the factored form of A .
4. Iterative refinement is applied to improve the computed solution matrix and to calculate error bounds and backward error estimates for it.

4 References

Anderson E, Bai Z, Bischof C, Blackford S, Demmel J, Dongarra J J, Du Croz J J, Greenbaum A, Hammarling S, McKenney A and Sorensen D (1999) *LAPACK Users' Guide* (3rd Edition) SIAM, Philadelphia URL: <http://www.netlib.org/lapack/lug>

Golub G H and Van Loan C F (1996) *Matrix Computations* (3rd Edition) Johns Hopkins University Press, Baltimore

Higham N J (2002) *Accuracy and Stability of Numerical Algorithms* (2nd Edition) SIAM, Philadelphia

5 Parameters

- 1: FACT – CHARACTER*1 *Input*
On entry: specifies whether or not the factored form of A has been supplied on entry:
 if FACT = 'F', DLF, DF, DUF, DU2 and IPIV contain the factored form of A ; DL, D, DU, DLF, DF, DUF, DU2 and IPIV will not be modified;
 if FACT = 'N', the matrix will be copied to DLF, DF and DUF and factored.
Constraint: FACT = 'F' or 'N'.

- 2: TRANS – CHARACTER*1 *Input*
On entry: specifies the form of the system of equations:
 if TRANS = 'N', $AX = B$ (No transpose);
 if TRANS = 'T', $A^T X = B$ (Transpose);
 if TRANS = 'C', $A^H X = B$ (Conjugate transpose).
Constraint: TRANS = 'N', 'T' or 'C'.

- 3: N – INTEGER *Input*
On entry: n , the order of the matrix A .
Constraint: $N \geq 0$.

- 4: NRHS – INTEGER *Input*
On entry: r , the number of right-hand sides, i.e., the number of columns of the matrix B .
Constraint: NRHS ≥ 0 .

- 5: DL(*) – **complex*16** array *Input*
Note: the dimension of the array DL must be at least $\max(1, N - 1)$.
On entry: the $(n - 1)$ sub-diagonal elements of A .

- 6: D(*) – **complex*16** array *Input*
Note: the dimension of the array D must be at least $\max(1, N)$.
On entry: the n diagonal elements of A .

- 7: DU(*) – **complex*16** array *Input*
Note: the dimension of the array DU must be at least $\max(1, N - 1)$.
On entry: the $(n - 1)$ super-diagonal elements of A .

- 8: DLF(*) – **complex*16** array *Input/Output*
Note: the dimension of the array DLF must be at least $\max(1, N - 1)$.
On entry: if FACT = 'F', DLF contains the $(n - 1)$ multipliers that define the matrix L from the LU factorization of A .
On exit: if FACT = 'N', DLF contains the $(n - 1)$ multipliers that define the matrix L from the LU factorization of A .

- 9: DF(*) – **complex*16** array *Input/Output*
Note: the dimension of the array DF must be at least $\max(1, N)$.
On entry: if FACT = 'F', DF contains the n diagonal elements of the upper triangular matrix U from the LU factorization of A .

On exit: if FACT = 'N', DF contains the n diagonal elements of the upper triangular matrix U from the LU factorization of A .

- 10: DUF(*) – **complex*16** array *Input/Output*

Note: the dimension of the array DUF must be at least $\max(1, N - 1)$.

On entry: if FACT = 'F', DUF contains the $(n - 1)$ elements of the first super-diagonal of U .

On exit: if FACT = 'N', DUF contains the $(n - 1)$ elements of the first super-diagonal of U .

- 11: DU2(*) – **complex*16** array *Input/Output*

Note: the dimension of the array DU2 must be at least $\max(1, N - 2)$.

On entry: if FACT = 'F', DU2 contains the $(n - 2)$ elements of the second super-diagonal of U .

On exit: if FACT = 'N', DU2 contains the $(n - 2)$ elements of the second super-diagonal of U .

- 12: IPIV(*) – INTEGER array *Input/Output*

Note: the dimension of the array IPIV must be at least $\max(1, N)$.

On entry: if FACT = 'F', IPIV contains the pivot indices from the LU factorization of A .

On exit: if FACT = 'N', IPIV contains the pivot indices from the LU factorization of A ; row i of the matrix was interchanged with row $IPIV(i)$. $IPIV(i)$ will always be either i or $i + 1$; $IPIV(i) = i$ indicates a row interchange was not required.

- 13: B(LDB,*) – **complex*16** array *Input*

Note: the second dimension of the array B must be at least $\max(1, NRHS)$.

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

- 14: LDB – INTEGER *Input*

On entry: the first dimension of the array B as declared in the (sub)program from which F07CPF (ZGTSVX) is called.

Constraint: $LDB \geq \max(1, N)$.

- 15: X(LDX,*) – **complex*16** array *Output*

Note: the second dimension of the array X must be at least $\max(1, NRHS)$.

On exit: if INFO = 0 or INFO = $N + 1$, the n by r solution matrix X .

- 16: LDX – INTEGER *Input*

On entry: the first dimension of the array X as declared in the (sub)program from which F07CPF (ZGTSVX) is called.

Constraint: $LDX \geq \max(1, N)$.

- 17: RCOND – **double precision** *Output*

On exit: the estimate of the reciprocal condition number of the matrix A . If RCOND is less than the **machine precision** (in particular, if RCOND = 0), the matrix is singular to working precision. This condition is indicated by a return code of INFO > 0.

- 18: FERR(*) – **double precision** array *Output*

Note: the dimension of the array FERR must be at least $\max(1, NRHS)$.

On exit: if INFO = 0 or INFO = $N + 1$, an estimate of the forward error bound for each computed solution vector, such that $\|\hat{x}_j - x_j\|_\infty / \|x_j\|_\infty \leq FERR(j)$ where \hat{x}_j is the j th column of the computed solution returned in the array X and x_j is the corresponding column of the exact solution

X. The estimate is as reliable as the estimate for RCOND, and is almost always a slight overestimate of the true error.

19: BERR(*) – **double precision** array *Output*

Note: the dimension of the array BERR must be at least $\max(1, \text{NRHS})$.

On exit: if $\text{INFO} = 0$ or $\text{INFO} = N + 1$, an estimate of the componentwise relative backward error of each computed solution vector \hat{x}_j (i.e., the smallest relative change in any element of A or B that makes \hat{x}_j an exact solution).

20: WORK(*) – **complex*16** array *Workspace*

Note: the dimension of the array WORK must be at least $\max(1, 2 \times N)$.

21: RWORK(*) – **double precision** array *Workspace*

Note: the dimension of the array RWORK must be at least $\max(1, N)$.

22: INFO – INTEGER *Output*

On exit: $\text{INFO} = 0$ unless the routine detects an error (see Section 6).

6 Error Indicators and Warnings

Errors or warnings detected by the routine:

$\text{INFO} < 0$

If $\text{INFO} = -i$, the i th argument had an illegal value. An explanatory message is output, and execution of the program is terminated.

$\text{INFO} > 0$ and $\text{INFO} \leq N$

If $\text{INFO} = i$, u_{ii} is exactly zero. The factorization has not been completed unless $i = N$, but the factor U is exactly singular, so the solution and error bounds could not be computed. $\text{RCOND} = 0$ is returned.

$\text{INFO} = N + 1$

U is nonsingular, but RCOND is less than **machine precision**, so that the matrix A is numerically singular. A solution to the equations $AX = B$, and corresponding error bounds, have nevertheless been computed because there are some situations where the computed solution can be more accurate than the value of RCOND would suggest.

7 Accuracy

For each right-hand side vector b , the computed solution \hat{x} is the exact solution of a perturbed system of equations $(A + E)\hat{x} = b$, where

$$|E| \leq c(n)\epsilon|L||U|,$$

$c(n)$ is a modest linear function of n , and ϵ is the **machine precision**. See Section 9.3 of Higham (2002) for further details.

If x is the true solution, then the computed solution \hat{x} satisfies a forward error bound of the form

$$\frac{\|x - \hat{x}\|_{\infty}}{\|\hat{x}\|_{\infty}} \leq w_c \text{cond}(A, \hat{x}, b)$$

where $\text{cond}(A, \hat{x}, b) = \frac{\|A^{-1}\|_{\infty} (\|A\|\|\hat{x}\| + \|b\|)}{\|\hat{x}\|_{\infty}} \leq \text{cond}(A) = \|A^{-1}\|_{\infty} \|A\|_{\infty} \leq \kappa_{\infty}(A)$. If \hat{x} is the j th column of X , then w_c is returned in $\text{BERR}(j)$ and a bound on $\|x - \hat{x}\|_{\infty} / \|\hat{x}\|_{\infty}$ is returned in $\text{FERR}(j)$. See Section 4.4 of Anderson *et al.* (1999) for further details.

8 Further Comments

The total number of floating point operations required to solve the equations $AX = B$ is proportional to nr .

The condition number estimation typically requires between four and five solves and never more than eleven solves, following the factorization. The solution is then refined, and the errors estimated, using iterative refinement.

In practice the condition number estimator is very reliable, but it can underestimate the true condition number; see Section 15.3 of Higham (2002) for further details.

The real analogue of this routine is F07CBF (DGTSVX).

9 Example

To solve the equations

$$AX = B,$$

where A is the tridiagonal matrix

$$A = \begin{pmatrix} -1.3 + 1.3i & 2.0 - 1.0i & 0 & 0 & 0 \\ 1.0 - 2.0i & -1.3 + 1.3i & 2.0 + 1.0i & 0 & 0 \\ 0 & 1.0 + 1.0i & -1.3 + 3.3i & -1.0 + 1.0i & 0 \\ 0 & 0 & 2.0 - 3.0i & -0.3 + 4.3i & 1.0 - 1.0i \\ 0 & 0 & 0 & 1.0 + 1.0i & -3.3 + 1.3i \end{pmatrix}$$

and

$$B = \begin{pmatrix} 2.4 - 5.0i & 2.7 + 6.9i \\ 3.4 + 18.2i & -6.9 - 5.3i \\ -14.7 + 9.7i & -6.0 - 0.6i \\ 31.9 - 7.7i & -3.9 + 9.3i \\ -1.0 + 1.6i & -3.0 + 12.2i \end{pmatrix}.$$

Estimates for the backward errors, forward errors and condition number are also output.

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.

```
*      F07CPF Example Program Text
*      Mark 21 Release. NAG Copyright 2004.
*      .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          NMAX, NRHSMX
      PARAMETER        (NMAX=50,NRHSMX=4)
      INTEGER          LDB, LDX
      PARAMETER        (LDB=NMAX,LDX=NMAX)
*      .. Local Scalars ..
      DOUBLE PRECISION RCOND
      INTEGER          I, IFAIL, INFO, J, N, NRHS
*      .. Local Arrays ..
      COMPLEX *16      B(LDB,NRHSMX), D(NMAX), DF(NMAX), DL(NMAX-1),
+                     DLF(NMAX-1), DU(NMAX-1), DU2(NMAX-2),
+                     DUF(NMAX-1), WORK(2*NMAX), X(LDX,NRHSMX)
      DOUBLE PRECISION BERR(NRHSMX), FERR(NRHSMX), RWORK(NMAX)
      INTEGER          IPIV(NMAX)
      CHARACTER        CLABS(1), RLABS(1)
*      .. External Subroutines ..
      EXTERNAL         X04DBF, ZGTSVX
*      .. Executable Statements ..
      WRITE (NOUT,*) 'F07CPF Example Program Results'
      WRITE (NOUT,*)
```

```

*      Skip heading in data file
      READ (NIN,*)
      READ (NIN,*) N, NRHS
      IF (N.LE.NMAX .AND. NRHS.LE.NRHSMX) THEN
*
*      Read the tridiagonal matrix A from data file
*
      READ (NIN,*) (DU(I),I=1,N-1)
      READ (NIN,*) (D(I),I=1,N)
      READ (NIN,*) (DL(I),I=1,N-1)
*
*      Read the right hand matrix B
*
      READ (NIN,*) ((B(I,J),J=1,NRHS),I=1,N)
*
*      Solve the equations AX = B
*
      CALL ZGTSVX('No factors','No transpose',N,NRHS,DL,D,DU,DLF,DF,
+              DUF,DU2,IPIV,B,LDB,X,LDX,RCOND,FERR,BERR,WORK,
+              RWORK,INFO)
*
      IF ((INFO.EQ.0) .OR. (INFO.EQ.N+1)) THEN
*
*      Print solution, error bounds and condition number
*
      IFAIL = 0
      CALL X04DBF('General',' ',N,NRHS,X,LDX,'Bracketed','F7.4',
+              'Solution(s)','Integer',RLABS,'Integer',CLABS,
+              80,0,IFAIL)
*
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Backward errors (machine-dependent)'
      WRITE (NOUT,99999) (BERR(J),J=1,NRHS)
      WRITE (NOUT,*)
      WRITE (NOUT,*)
+      'Estimated forward error bounds (machine-dependent)'
      WRITE (NOUT,99999) (FERR(J),J=1,NRHS)
      WRITE (NOUT,*)
      WRITE (NOUT,*) 'Estimate of reciprocal condition number'
      WRITE (NOUT,99999) RCOND
*
      IF (INFO.EQ.N+1) THEN
        WRITE (NOUT,*)
        WRITE (NOUT,*)
+        'The matrix A is singular to working precision'
      END IF
      ELSE
      WRITE (NOUT,99998) 'The (', INFO, ', ', INFO, ')',
+      ' element of the factor U is zero'
      END IF
      ELSE
      WRITE (NOUT,*) 'NMAX and/or NRHSMX too small'
      END IF
      STOP
*
99999 FORMAT ((3X,1P,7E11.1))
99998 FORMAT (1X,A,I3,A,I3,A,A)
      END

```

9.2 Program Data

F07CPF Example Program Data

```

      5      2                                     :Values of N and NRHS
      ( 2.0, -1.0) ( 2.0, 1.0) ( -1.0, 1.0) ( 1.0, -1.0) :End of DU
      ( -1.3, 1.3) ( -1.3, 1.3) ( -1.3, 3.3) ( -0.3, 4.3)
      ( -3.3, 1.3)                                     :End of D
      ( 1.0, -2.0) ( 1.0, 1.0) ( 2.0, -3.0) ( 1.0, 1.0) :End of DL
      ( 2.4, -5.0) ( 2.7, 6.9)
      ( 3.4, 18.2) ( -6.9, -5.3)
      (-14.7, 9.7) ( -6.0, -0.6)
      ( 31.9, -7.7) ( -3.9, 9.3)
      ( -1.0, 1.6) ( -3.0, 12.2)                       :End of B

```

9.3 Program Results

F07CPF Example Program Results

Solution(s)

```

                                     1      2
1  ( 1.0000, 1.0000) ( 2.0000,-1.0000)
2  ( 3.0000,-1.0000) ( 1.0000, 2.0000)
3  ( 4.0000, 5.0000) (-1.0000, 1.0000)
4  (-1.0000,-2.0000) ( 2.0000, 1.0000)
5  ( 1.0000,-1.0000) ( 2.0000,-2.0000)

```

Backward errors (machine-dependent)

```

6.2E-17      5.0E-17

```

Estimated forward error bounds (machine-dependent)

```

5.2E-14      7.2E-14

```

Estimate of reciprocal condition number

```

5.4E-03

```
