NAG Library Routine Document

F08UTF (ZPBSTF)

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

F08UTF (ZPBSTF) computes a split Cholesky factorization of a complex Hermitian positive definite band matrix.

2 Specification

```
SUBROUTINE F08UTF (UPLO, N, KB, BB, LDBB, INFO)

INTEGER                N, KB, LDBB, INFO
COMPLEX (KIND=nag_wp) BB(LDBB,*)
CHARACTER(1)           UPLO
```

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

3 Description

F08UTF (ZPBSTF) computes a split Cholesky factorization of a complex Hermitian positive definite band matrix B. It is designed to be used in conjunction with F08USF (ZHBGST).

The factorization has the form $B = S^{\mathrm{H}}S$, where S is a band matrix of the same bandwidth as B and the following structure: S is upper triangular in the first $(n+k)/2$ rows, and transposed — hence, lower triangular — in the remaining rows. For example, if $n = 9$ and $k = 2$, then

$$S = \begin{pmatrix} s_{11} & s_{12} & s_{13} & & & & & & \\ & s_{22} & s_{23} & s_{24} & & & & & \\ & & s_{33} & s_{34} & s_{35} & & & & \\ & & & s_{44} & s_{45} & & & & \\ & & & & s_{55} & & & & \\ & & & s_{64} & s_{65} & s_{66} & & & \\ & & & & s_{75} & s_{76} & s_{77} & & \\ & & & & & s_{86} & s_{87} & s_{88} & \\ & & & & & & s_{97} & s_{98} & s_{99} \end{pmatrix}.$$

4 References

None.

5 Arguments

1: UPLO – CHARACTER(1) *Input*

On entry: indicates whether the upper or lower triangular part of B is stored.

UPLO = 'U'
The upper triangular part of B is stored.

UPLO = 'L'
The lower triangular part of B is stored.

Constraint: UPLO = 'U' or 'L'.

2: N – INTEGER *Input*

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

Constraint: $\mathrm{N} \geq 0$.

3: KB – INTEGER *Input*

On entry: if $\mathrm{UPLO} = \text{'U'}$, the number of superdiagonals, k_b, of the matrix B.

If $\mathrm{UPLO} = \text{'L'}$, the number of subdiagonals, k_b, of the matrix B.

Constraint: $\mathrm{KB} \geq 0$.

4: BB(LDBB, $*$) – COMPLEX (KIND=nag_wp) array *Input/Output*

Note: the second dimension of the array BB must be at least $\max(1, \mathrm{N})$.

On entry: the n by n Hermitian positive definite band matrix B.

The matrix is stored in rows 1 to $k_b + 1$, more precisely,

if $\mathrm{UPLO} = \text{'U'}$, the elements of the upper triangle of B within the band must be stored with element B_{ij} in $\mathrm{BB}(k_b + 1 + i - j, j)$ for $\max(1, j - k_b) \leq i \leq j$;

if $\mathrm{UPLO} = \text{'L'}$, the elements of the lower triangle of B within the band must be stored with element B_{ij} in $\mathrm{BB}(1 + i - j, j)$ for $j \leq i \leq \min(n, j + k_b)$.

On exit: B is overwritten by the elements of its split Cholesky factor S.

5: LDBB – INTEGER *Input*

On entry: the first dimension of the array BB as declared in the (sub)program from which F08UTF (ZPBSTF) is called.

Constraint: $\mathrm{LDBB} \geq \mathrm{KB} + 1$.

6: INFO – INTEGER *Output*

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

6 Error Indicators and Warnings

$\mathrm{INFO} < 0$

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

$\mathrm{INFO} > 0$

If $\mathrm{INFO} = i$, the factorization could not be completed, because the updated element $b(i,i)$ would be the square root of a negative number. Hence B is not positive definite. This may indicate an error in forming the matrix B.

7 Accuracy

The computed factor S is the exact factor of a perturbed matrix $(B + E)$, where

$$|E| \leq c(k+1)\epsilon|S^{\mathrm{H}}||S|,$$

$c(k+1)$ is a modest linear function of $k+1$, and ϵ is the ***machine precision***. It follows that $|e_{ij}| \leq c(k+1)\epsilon\sqrt{(b_{ii}b_{jj})}$.

8 Parallelism and Performance

F08UTF (ZPBSTF) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the X06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this routine. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The total number of floating-point operations is approximately $4n(k+1)^2$, assuming $n \gg k$.

A call to F08UTF (ZPBSTF) may be followed by a call to F08USF (ZHBGST) to solve the generalized eigenproblem $Az = \lambda Bz$, where A and B are banded and B is positive definite.

The real analogue of this routine is F08UFF (DPBSTF).

10 Example

See Section 10 in F08USF (ZHBGST).