

# NAG Library Function Document

## nag\_zptrfs (f07jvc)

### 1 Purpose

nag\_zptrfs (f07jvc) computes error bounds and refines the solution to a complex system of linear equations  $AX = B$ , where  $A$  is an  $n$  by  $n$  Hermitian positive definite tridiagonal matrix and  $X$  and  $B$  are  $n$  by  $r$  matrices, using the modified Cholesky factorization returned by nag\_zpttrf (f07jrc) and an initial solution returned by nag\_zpttrs (f07jsc). Iterative refinement is used to reduce the backward error as much as possible.

### 2 Specification

```
#include <nag.h>
#include <nagf07.h>

void nag_zptrfs (Nag_OrderType order, Nag_UploType uplo, Integer n,
                Integer nrhs, const double d[], const Complex e[], const double df[],
                const Complex ef[], const Complex b[], Integer pdb, Complex x[],
                Integer pdx, double ferr[], double berr[], NagError *fail)
```

### 3 Description

nag\_zptrfs (f07jvc) should normally be preceded by calls to nag\_zpttrf (f07jrc) and nag\_zpttrs (f07jsc). nag\_zpttrf (f07jrc) computes a modified Cholesky factorization of the matrix  $A$  as

$$A = LDL^H,$$

where  $L$  is a unit lower bidiagonal matrix and  $D$  is a diagonal matrix, with positive diagonal elements. nag\_zpttrs (f07jsc) then utilizes the factorization to compute a solution,  $\hat{X}$ , to the required equations. Letting  $\hat{x}$  denote a column of  $\hat{X}$ , nag\_zptrfs (f07jvc) computes a *component-wise backward error*,  $\beta$ , the smallest relative perturbation in each element of  $A$  and  $b$  such that  $\hat{x}$  is the exact solution of a perturbed system

$$(A + E)\hat{x} = b + f, \quad \text{with} \quad |e_{ij}| \leq \beta |a_{ij}|, \quad \text{and} \quad |f_j| \leq \beta |b_j|.$$

The function also estimates a bound for the *component-wise forward error* in the computed solution defined by  $\max |x_i - \hat{x}_i| / \max |\hat{x}_i|$ , where  $x$  is the corresponding column of the exact solution,  $X$ .

Note that the modified Cholesky factorization of  $A$  can also be expressed as

$$A = U^H D U,$$

where  $U$  is unit upper bidiagonal.

### 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 <http://www.netlib.org/lapack/lug>

### 5 Arguments

- 1: **order** – Nag\_OrderType *Input*  
*On entry:* the **order** argument specifies the two-dimensional storage scheme being used, i.e., row-major ordering or column-major ordering. C language defined storage is specified by

**order** = Nag\_RowMajor. See Section 2.3.1.3 in How to Use the NAG Library and its Documentation for a more detailed explanation of the use of this argument.

*Constraint:* **order** = Nag\_RowMajor or Nag\_ColMajor.

- 2:   **uplo** – Nag\_UploType *Input*  
*On entry:* specifies the form of the factorization as follows:  
**uplo** = Nag\_Upper  
 $A = U^H D U$ .  
**uplo** = Nag\_Lower  
 $A = L D L^H$ .  
*Constraint:* **uplo** = Nag\_Upper or Nag\_Lower.
  
- 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**  $\geq 0$ .
  
- 5:   **d**[ $dim$ ] – const double *Input*  
**Note:** the dimension,  $dim$ , of the array **d** must be at least  $\max(1, n)$ .  
*On entry:* must contain the  $n$  diagonal elements of the matrix of  $A$ .
  
- 6:   **e**[ $dim$ ] – const Complex *Input*  
**Note:** the dimension,  $dim$ , of the array **e** must be at least  $\max(1, n - 1)$ .  
*On entry:* if **uplo** = Nag\_Upper, **e** must contain the  $(n - 1)$  superdiagonal elements of the matrix  $A$ .  
If **uplo** = Nag\_Lower, **e** must contain the  $(n - 1)$  subdiagonal elements of the matrix  $A$ .
  
- 7:   **df**[ $dim$ ] – const double *Input*  
**Note:** the dimension,  $dim$ , of the array **df** must be at least  $\max(1, n)$ .  
*On entry:* must contain the  $n$  diagonal elements of the diagonal matrix  $D$  from the  $LDL^T$  factorization of  $A$ .
  
- 8:   **ef**[ $dim$ ] – const Complex *Input*  
**Note:** the dimension,  $dim$ , of the array **ef** must be at least  $\max(1, n - 1)$ .  
*On entry:* if **uplo** = Nag\_Upper, **ef** must contain the  $(n - 1)$  superdiagonal elements of the unit upper bidiagonal matrix  $U$  from the  $U^H D U$  factorization of  $A$ .  
If **uplo** = Nag\_Lower, **ef** must contain the  $(n - 1)$  subdiagonal elements of the unit lower bidiagonal matrix  $L$  from the  $LDL^H$  factorization of  $A$ .
  
- 9:   **b**[ $dim$ ] – const Complex *Input*  
**Note:** the dimension,  $dim$ , of the array **b** must be at least  
 $\max(1, p_{db} \times nrhs)$  when **order** = Nag\_ColMajor;  
 $\max(1, n \times p_{db})$  when **order** = Nag\_RowMajor.

The  $(i, j)$ th element of the matrix  $B$  is stored in

$$\begin{aligned} &\mathbf{b}[(j-1) \times \mathbf{pdb} + i - 1] \text{ when } \mathbf{order} = \text{Nag\_ColMajor}; \\ &\mathbf{b}[(i-1) \times \mathbf{pdb} + j - 1] \text{ when } \mathbf{order} = \text{Nag\_RowMajor}. \end{aligned}$$

*On entry:* the  $n$  by  $r$  matrix of right-hand sides  $B$ .

- 10: **pdb** – Integer *Input*

*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **b**.

*Constraints:*

$$\begin{aligned} &\text{if } \mathbf{order} = \text{Nag\_ColMajor}, \mathbf{pdb} \geq \max(1, \mathbf{n}); \\ &\text{if } \mathbf{order} = \text{Nag\_RowMajor}, \mathbf{pdb} \geq \max(1, \mathbf{nrhs}). \end{aligned}$$

- 11: **x[dim]** – Complex *Input/Output*

**Note:** the dimension,  $dim$ , of the array **x** must be at least

$$\begin{aligned} &\max(1, \mathbf{pdx} \times \mathbf{nrhs}) \text{ when } \mathbf{order} = \text{Nag\_ColMajor}; \\ &\max(1, \mathbf{n} \times \mathbf{pdx}) \text{ when } \mathbf{order} = \text{Nag\_RowMajor}. \end{aligned}$$

The  $(i, j)$ th element of the matrix  $X$  is stored in

$$\begin{aligned} &\mathbf{x}[(j-1) \times \mathbf{pdx} + i - 1] \text{ when } \mathbf{order} = \text{Nag\_ColMajor}; \\ &\mathbf{x}[(i-1) \times \mathbf{pdx} + j - 1] \text{ when } \mathbf{order} = \text{Nag\_RowMajor}. \end{aligned}$$

*On entry:* the  $n$  by  $r$  initial solution matrix  $X$ .

*On exit:* the  $n$  by  $r$  refined solution matrix  $X$ .

- 12: **pdx** – Integer *Input*

*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **x**.

*Constraints:*

$$\begin{aligned} &\text{if } \mathbf{order} = \text{Nag\_ColMajor}, \mathbf{pdx} \geq \max(1, \mathbf{n}); \\ &\text{if } \mathbf{order} = \text{Nag\_RowMajor}, \mathbf{pdx} \geq \max(1, \mathbf{nrhs}). \end{aligned}$$

- 13: **ferr[nrhs]** – double *Output*

*On exit:* estimate of the forward error bound for each computed solution vector, such that  $\|\hat{x}_j - x_j\|_\infty / \|\hat{x}_j\|_\infty \leq \mathbf{ferr}[j-1]$ , 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 almost always a slight overestimate of the true error.

- 14: **berr[nrhs]** – double *Output*

*On exit:* estimate of the component-wise 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).

- 15: **fail** – NagError \* *Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

### NE\_BAD\_PARAM

On entry, argument  $\langle value \rangle$  had an illegal value.

### NE\_INT

On entry,  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $\mathbf{n} \geq 0$ .

On entry,  $\mathbf{nrhs} = \langle value \rangle$ .

Constraint:  $\mathbf{nrhs} \geq 0$ .

On entry,  $\mathbf{pdb} = \langle value \rangle$ .

Constraint:  $\mathbf{pdb} > 0$ .

On entry,  $\mathbf{pdx} = \langle value \rangle$ .

Constraint:  $\mathbf{pdx} > 0$ .

### NE\_INT\_2

On entry,  $\mathbf{pdb} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $\mathbf{pdb} \geq \max(1, \mathbf{n})$ .

On entry,  $\mathbf{pdb} = \langle value \rangle$  and  $\mathbf{nrhs} = \langle value \rangle$ .

Constraint:  $\mathbf{pdb} \geq \max(1, \mathbf{nrhs})$ .

On entry,  $\mathbf{pdx} = \langle value \rangle$  and  $\mathbf{n} = \langle value \rangle$ .

Constraint:  $\mathbf{pdx} \geq \max(1, \mathbf{n})$ .

On entry,  $\mathbf{pdx} = \langle value \rangle$  and  $\mathbf{nrhs} = \langle value \rangle$ .

Constraint:  $\mathbf{pdx} \geq \max(1, \mathbf{nrhs})$ .

### NE\_INTERNAL\_ERROR

An internal error has occurred in this function. Check the function call and any array sizes. If the call is correct then please contact NAG for assistance.

An unexpected error has been triggered by this function. Please contact NAG.

See Section 2.7.6 in How to Use the NAG Library and its Documentation for further information.

### NE\_NO\_LICENCE

Your licence key may have expired or may not have been installed correctly.

See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

## 7 Accuracy

The computed solution for a single right-hand side,  $\hat{x}$ , satisfies an equation of the form

$$(A + E)\hat{x} = b,$$

where

$$\|E\|_{\infty} = O(\epsilon)\|A\|_{\infty}$$

and  $\epsilon$  is the *machine precision*. An approximate error bound for the computed solution is given by

$$\frac{\|\hat{x} - x\|_\infty}{\|x\|_\infty} \leq \kappa(A) \frac{\|E\|_\infty}{\|A\|_\infty},$$

where  $\kappa(A) = \|A^{-1}\|_\infty \|A\|_\infty$ , the condition number of  $A$  with respect to the solution of the linear equations. See Section 4.4 of Anderson *et al.* (1999) for further details.

Function nag\_zptcon (f07juc) can be used to compute the condition number of  $A$ .

## 8 Parallelism and Performance

nag\_zptrfs (f07jvc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag\_zptrfs (f07jvc) 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 function. 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 required to solve the equations  $AX = B$  is proportional to  $nr$ . At most five steps of iterative refinement are performed, but usually only one or two steps are required.

The real analogue of this function is nag\_dptrfs (f07jhc).

## 10 Example

This example solves the equations

$$AX = B,$$

where  $A$  is the Hermitian positive definite tridiagonal matrix

$$A = \begin{pmatrix} 16.0 & 16.0 - 16.0i & 0 & 0 \\ 16.0 + 16.0i & 41.0 & 18.0 + 9.0i & 0 \\ 0 & 18.0 - 9.0i & 46.0 & 1.0 + 4.0i \\ 0 & 0 & 1.0 - 4.0i & 21.0 \end{pmatrix}$$

and

$$B = \begin{pmatrix} 64.0 + 16.0i & -16.0 - 32.0i \\ 93.0 + 62.0i & 61.0 - 66.0i \\ 78.0 - 80.0i & 71.0 - 74.0i \\ 14.0 - 27.0i & 35.0 + 15.0i \end{pmatrix}.$$

Estimates for the backward errors and forward errors are also output.

### 10.1 Program Text

```
/* nag_zptrfs (f07jvc) Example Program.
*
* NAGPRODCODE Version.
*
* Copyright 2016 Numerical Algorithms Group.
*
* Mark 26, 2016.
*/

#include <stdio.h>
```

```

#include <nag.h>
#include <nagx04.h>
#include <nag_stdlib.h>
#include <nagf07.h>
#include <nagf16.h>

int main(void)
{
    /* Scalars */
    Integer exit_status = 0, i, j, n, nrhs, pdb, pdx;
    Nag_OrderType order;

    /* Arrays */
    Complex *b = 0, *e = 0, *ef = 0, *x = 0;
    double *berr = 0, *d = 0, *df = 0, *ferr = 0;

    /* Nag Types */
    NagError fail;

#ifdef NAG_COLUMN_MAJOR
#define B(I, J) b[(J - 1) * pdb + I - 1]
    order = Nag_ColMajor;
#else
#define B(I, J) b[(I - 1) * pdb + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);

    printf("nag_zptrfs (f07jvc) Example Program Results\n\n");
    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n]");
#else
    scanf("%*[\n]");
#endif

#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%" NAG_IFMT "%*[\n]", &n, &nrhs);
#else
    scanf("%" NAG_IFMT "%" NAG_IFMT "%*[\n]", &n, &nrhs);
#endif
    if (n < 0 || nrhs < 0) {
        printf("Invalid n or nrhs\n");
        exit_status = 1;
        goto END;
    }
    if (!(b = NAG_ALLOC(n * nrhs, Complex)) ||
        !(e = NAG_ALLOC(n - 1, Complex)) ||
        !(ef = NAG_ALLOC(n - 1, Complex)) ||
        !(x = NAG_ALLOC(n * nrhs, Complex)) ||
        !(berr = NAG_ALLOC(nrhs, double)) ||
        !(d = NAG_ALLOC(n, double)) ||
        !(df = NAG_ALLOC(n, double)) || !(ferr = NAG_ALLOC(nrhs, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
#ifdef NAG_COLUMN_MAJOR
    pdb = n;
    pdx = n;
#else
    pdb = nrhs;
    pdx = nrhs;
#endif

    /* Read the lower bidiagonal part of the tridiagonal matrix A from */
    /* data file */
#ifdef _WIN32

```

```

    for (i = 0; i < n; ++i)
        scanf_s("%lf", &d[i]);
#else
    for (i = 0; i < n; ++i)
        scanf("%lf", &d[i]);
#endif
#ifdef _WIN32
    scanf_s("%*[^\\n]");
#else
    scanf("%*[^\\n]");
#endif
#ifdef _WIN32
    for (i = 0; i < n - 1; ++i)
        scanf_s(" ( %lf , %lf )", &e[i].re, &e[i].im);
#else
    for (i = 0; i < n - 1; ++i)
        scanf(" ( %lf , %lf )", &e[i].re, &e[i].im);
#endif
#ifdef _WIN32
    scanf_s("%*[^\\n]");
#else
    scanf("%*[^\\n]");
#endif

    /* Read the right hand matrix B */
    for (i = 1; i <= n; ++i)
        for (j = 1; j <= nrhs; ++j)
#ifdef _WIN32
            scanf_s(" ( %lf , %lf )", &B(i, j).re, &B(i, j).im);
#else
            scanf(" ( %lf , %lf )", &B(i, j).re, &B(i, j).im);
#endif
#ifdef _WIN32
    scanf_s("%*[^\\n]");
#else
    scanf("%*[^\\n]");
#endif

    /* Copy A into DF and EF, and copy B into X */
    for (i = 0; i < n; ++i)
        df[i] = d[i];
    for (i = 0; i < n - 1; ++i) {
        ef[i].re = e[i].re;
        ef[i].im = e[i].im;
    }

    /* Copy B into X using nag_zge_copy (f16tfc). */
    nag_zge_copy(order, Nag_NoTrans, n, nrhs, b, pdb, x, pdx, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_zge_copy (f16tfc).\\n%s\\n", fail.message);
        exit_status = 1;
        goto END;
    }

    /* Factorize the copy of the tridiagonal matrix A
     * using nag_zpttrf (f07jrc).
     */
    nag_zpttrf(n, df, ef, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_zpttrf (f07jrc).\\n%s\\n", fail.message);
        exit_status = 1;
        goto END;
    }

    /* Solve the equations AX = B using nag_zpttrs (f07jsc). */
    nag_zpttrs(order, Nag_Lower, n, nrhs, df, ef, x, pdx, &fail);
    if (fail.code != NE_NOERROR) {
        printf("Error from nag_zpttrs (f07jsc).\\n%s\\n", fail.message);
        exit_status = 1;
        goto END;
    }
}

```

```

/* Improve the solution and compute error estimates
 * using nag_zptrfs (f07jvc).
 */
nag_zptrfs(order, Nag_Lower, n, nrhs, d, e, df, ef, b, pdb, x, pdx,
           ferr, berr, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_zptrfs (f07jvc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Print the solution using nag_gen_complx_mat_print_comp (x04dbc). */
fflush(stdout);
nag_gen_complx_mat_print_comp(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n,
                              nrhs, x, pdx, Nag_BracketForm, "%7.4f",
                              "Solution(s)", Nag_IntegerLabels, 0,
                              Nag_IntegerLabels, 0, 80, 0, 0, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_complx_mat_print_comp (x04dbc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
}

/* Print the the forward and backward error estimates */
printf("\nBackward errors (machine-dependent)\n");
for (j = 0; j < nrhs; ++j)
    printf("%11.1e%s", berr[j], j % 7 == 6 ? "\n" : " ");

printf("\n\nEstimated forward error bounds (machine-dependent)\n");
for (j = 0; j < nrhs; ++j)
    printf("%11.1e%s", ferr[j], j % 7 == 6 ? "\n" : " ");

END:
    NAG_FREE(b);
    NAG_FREE(e);
    NAG_FREE(ef);
    NAG_FREE(x);
    NAG_FREE(berr);
    NAG_FREE(d);
    NAG_FREE(df);
    NAG_FREE(ferr);

    return exit_status;
}

#undef B

```

## 10.2 Program Data

```

nag_zptrfs (f07jvc) Example Program Data
      4          2          : n, nrhs
      16.0       41.0       46.0       21.0 : diagonal d
( 16.0, 16.0) ( 18.0, -9.0) ( 1.0, -4.0) : sub-diagonal e
( 64.0, 16.0) (-16.0,-32.0)
( 93.0, 62.0) ( 61.0,-66.0)
( 78.0,-80.0) ( 71.0,-74.0)
( 14.0,-27.0) ( 35.0, 15.0)          : matrix B

```

## 10.3 Program Results

nag\_zptrfs (f07jvc) Example Program Results

```

Solution(s)
      1          2
1 ( 2.0000, 1.0000) (-3.0000,-2.0000)
2 ( 1.0000, 1.0000) ( 1.0000, 1.0000)
3 ( 1.0000,-2.0000) ( 1.0000,-2.0000)
4 ( 1.0000,-1.0000) ( 2.0000, 1.0000)

```



Backward errors (machine-dependent)  
0.0e+00      0.0e+00

Estimated forward error bounds (machine-dependent)  
9.0e-12      6.1e-12

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