

# NAG Library Function Document

## nag\_dpbrfs (f07hhc)

### 1 Purpose

nag\_dpbrfs (f07hhc) returns error bounds for the solution of a real symmetric positive definite band system of linear equations with multiple right-hand sides,  $AX = B$ . It improves the solution by iterative refinement, in order to reduce the backward error as much as possible.

### 2 Specification

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

void nag_dpbrfs (Nag_OrderType order, Nag_UploType uplo, Integer n,
                Integer kd, Integer nrhs, const double ab[], Integer pdab,
                const double afb[], Integer pdafb, const double b[], Integer pdb,
                double x[], Integer pdx, double ferr[], double berr[], NagError *fail)
```

### 3 Description

nag\_dpbrfs (f07hhc) returns the backward errors and estimated bounds on the forward errors for the solution of a real symmetric positive definite band system of linear equations with multiple right-hand sides  $AX = B$ . The function handles each right-hand side vector (stored as a column of the matrix  $B$ ) independently, so we describe the function of nag\_dpbrfs (f07hhc) in terms of a single right-hand side  $b$  and solution  $x$ .

Given a computed solution  $x$ , the function computes the *component-wise backward error*  $\beta$ . This is the size of the smallest relative perturbation in each element of  $A$  and  $b$  such that  $x$  is the exact solution of a perturbed system

$$|\delta a_{ij}| \leq \beta |a_{ij}| \quad \text{and} \quad |\delta b_i| \leq \beta |b_i|.$$

Then the function estimates a bound for the *component-wise forward error* in the computed solution, defined by:

$$\max_i |x_i - \hat{x}_i| / \max_i |x_i|$$

where  $\hat{x}$  is the true solution.

For details of the method, see the f07 Chapter Introduction.

### 4 References

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

### 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 3.2.1.3 in the Essential Introduction 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 whether the upper or lower triangular part of  $A$  is stored and how  $A$  is to be factorized.  
**uplo** = Nag\_Upper  
 The upper triangular part of  $A$  is stored and  $A$  is factorized as  $U^T U$ , where  $U$  is upper triangular.  
**uplo** = Nag\_Lower  
 The lower triangular part of  $A$  is stored and  $A$  is factorized as  $LL^T$ , where  $L$  is lower triangular.  
*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: **kd** – Integer *Input*  
*On entry:*  $k_d$ , the number of superdiagonals or subdiagonals of the matrix  $A$ .  
*Constraint:* **kd**  $\geq 0$ .
- 5: **nrhs** – Integer *Input*  
*On entry:*  $r$ , the number of right-hand sides.  
*Constraint:* **nrhs**  $\geq 0$ .
- 6: **ab**[*dim*] – const double *Input*  
**Note:** the dimension, *dim*, of the array **ab** must be at least  $\max(1, \mathbf{pdab} \times \mathbf{n})$ .  
*On entry:* the  $n$  by  $n$  original symmetric positive definite band matrix  $A$  as supplied to nag\_dpbtfr (f07hdc).
- 7: **pdab** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) of the matrix in the array **ab**.  
*Constraint:* **pdab**  $\geq \mathbf{kd} + 1$ .
- 8: **afb**[*dim*] – const double *Input*  
**Note:** the dimension, *dim*, of the array **afb** must be at least  $\max(1, \mathbf{pdafb} \times \mathbf{n})$ .  
*On entry:* the Cholesky factor of  $A$ , as returned by nag\_dpbtfr (f07hdc).
- 9: **pdafb** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) of the matrix in the array **afb**.  
*Constraint:* **pdafb**  $\geq \mathbf{kd} + 1$ .
- 10: **b**[*dim*] – const double *Input*  
**Note:** the dimension, *dim*, of the array **b** must be at least  
 $\max(1, \mathbf{pdb} \times \mathbf{nrhs})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{n} \times \mathbf{pdb})$  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  $r$  right-hand side matrix  $B$ .

11: **pdb** – Integer *Input*

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

*Constraints:*

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

12: **x[*dim*]** – double *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  $r$  solution matrix  $X$ , as returned by nag\_dpbttrs (f07hec).

*On exit:* the improved solution matrix  $X$ .

13: **pdx** – Integer *Input*

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

*Constraints:*

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

14: **ferr[*nrhs*]** – double *Output*

*On exit:* **ferr**[ $j-1$ ] contains an estimated error bound for the  $j$ th solution vector, that is, the  $j$ th column of  $X$ , for  $j = 1, 2, \dots, r$ .

15: **berr[*nrhs*]** – double *Output*

*On exit:* **berr**[ $j-1$ ] contains the component-wise backward error bound  $\beta$  for the  $j$ th solution vector, that is, the  $j$ th column of  $X$ , for  $j = 1, 2, \dots, r$ .

16: **fail** – NagError \* *Input/Output*

The NAG error argument (see Section 3.6 in the Essential Introduction).

## 6 Error Indicators and Warnings

### NE\_ALLOC\_FAIL

Dynamic memory allocation failed.

See Section 3.2.1.2 in the Essential Introduction for further information.

### NE\_BAD\_PARAM

*On entry,* argument  $\langle \text{value} \rangle$  had an illegal value.

**NE\_INT**

On entry, **kd** =  $\langle value \rangle$ .  
 Constraint: **kd**  $\geq 0$ .

On entry, **n** =  $\langle value \rangle$ .  
 Constraint: **n**  $\geq 0$ .

On entry, **nrhs** =  $\langle value \rangle$ .  
 Constraint: **nrhs**  $\geq 0$ .

On entry, **pdab** =  $\langle value \rangle$ .  
 Constraint: **pdab**  $> 0$ .

On entry, **pdafb** =  $\langle value \rangle$ .  
 Constraint: **pdafb**  $> 0$ .

On entry, **pdb** =  $\langle value \rangle$ .  
 Constraint: **pdb**  $> 0$ .

On entry, **pdx** =  $\langle value \rangle$ .  
 Constraint: **pdx**  $> 0$ .

**NE\_INT\_2**

On entry, **pdab** =  $\langle value \rangle$  and **kd** =  $\langle value \rangle$ .  
 Constraint: **pdab**  $\geq$  **kd** + 1.

On entry, **pdafb** =  $\langle value \rangle$  and **kd** =  $\langle value \rangle$ .  
 Constraint: **pdafb**  $\geq$  **kd** + 1.

On entry, **pdb** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .  
 Constraint: **pdb**  $\geq$  max(1, **n**).

On entry, **pdb** =  $\langle value \rangle$  and **nrhs** =  $\langle value \rangle$ .  
 Constraint: **pdb**  $\geq$  max(1, **nrhs**).

On entry, **pdx** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .  
 Constraint: **pdx**  $\geq$  max(1, **n**).

On entry, **pdx** =  $\langle value \rangle$  and **nrhs** =  $\langle value \rangle$ .  
 Constraint: **pdx**  $\geq$  max(1, **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 3.6.6 in the Essential Introduction for further information.

**NE\_NO\_LICENCE**

Your licence key may have expired or may not have been installed correctly.  
 See Section 3.6.5 in the Essential Introduction for further information.

**7 Accuracy**

The bounds returned in **ferr** are not rigorous, because they are estimated, not computed exactly; but in practice they almost always overestimate the actual error.

**8 Parallelism and Performance**

nag\_dpbrfs (f07hhc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag\_dpbrfs (f07hhc) 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

For each right-hand side, computation of the backward error involves a minimum of  $8nk$  floating-point operations. Each step of iterative refinement involves an additional  $12nk$  operations. This assumes  $n \gg k$ . At most five steps of iterative refinement are performed, but usually only one or two steps are required.

Estimating the forward error involves solving a number of systems of linear equations of the form  $Ax = b$ ; the number is usually 4 or 5 and never more than 11. Each solution involves approximately  $4nk$  operations.

The complex analogue of this function is nag\_zpbrfs (f07hvc).

## 10 Example

This example solves the system of equations  $AX = B$  using iterative refinement and to compute the forward and backward error bounds, where

$$A = \begin{pmatrix} 5.49 & 2.68 & 0.00 & 0.00 \\ 2.68 & 5.63 & -2.39 & 0.00 \\ 0.00 & -2.39 & 2.60 & -2.22 \\ 0.00 & 0.00 & -2.22 & 5.17 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 22.09 & 5.10 \\ 9.31 & 30.81 \\ -5.24 & -25.82 \\ 11.83 & 22.90 \end{pmatrix}.$$

Here  $A$  is symmetric and positive definite, and is treated as a band matrix, which must first be factorized by nag\_dpbtrf (f07hdc).

### 10.1 Program Text

```

/* nag_dpbrfs (f07hhc) Example Program.
 *
 * Copyright 2014 Numerical Algorithms Group.
 *
 * Mark 7, 2001.
 */

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

int main(void)
{
    /* Scalars */
    Integer      i, j, k, kd, n, nrhs, pdab, pdafb, pdb, pdx;
    Integer      ferr_len, berr_len;
    Integer      exit_status = 0;
    Nag_UploType uplo;
    NagError     fail;
    Nag_OrderType order;
    /* Arrays */
    char         nag_enum_arg[40];
    double       *ab = 0, *afb = 0, *b = 0, *berr = 0, *ferr = 0, *x = 0;

#ifdef NAG_COLUMN_MAJOR
#define AB_UPPER(I, J)  ab[(J-1)*pdab + k + I - J - 1]
#define AB_LOWER(I, J) ab[(J-1)*pdab + I - J]
#define AFB_UPPER(I, J) afb[(J-1)*pdafb + k + I - J - 1]

```

```

#define AFB_LOWER(I, J)  afb[(J-1)*pdafb + I - J]
#define B(I, J)         b[(J-1)*pdb + I - 1]
#define X(I, J)         x[(J-1)*pdx + I - 1]
    order = Nag_ColMajor;
#else
#define AB_UPPER(I, J)  ab[(I-1)*pdab + J - I]
#define AB_LOWER(I, J) ab[(I-1)*pdab + k + J - I - 1]
#define AFB_UPPER(I, J) afb[(I-1)*pdafb + J - I]
#define AFB_LOWER(I, J) afb[(I-1)*pdafb + k + J - I - 1]
#define B(I, J)         b[(I-1)*pdb + J - 1]
#define X(I, J)         x[(I-1)*pdx + J - 1]
    order = Nag_RowMajor;
#endif

    INIT_FAIL(fail);

    printf("nag_dpbrfs (f07hhc) 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%"NAG_IFMT"%*[\n] ", &n, &kd, &nrhs);
#else
    scanf("%"NAG_IFMT%"NAG_IFMT%"NAG_IFMT"%*[\n] ", &n, &kd, &nrhs);
#endif
    pdab = kd + 1;
    pdafb = kd + 1;
#ifdef NAG_COLUMN_MAJOR
    pdb = n;
    pdx = n;
#else
    pdb = nrhs;
    pdx = nrhs;
#endif

    ferr_len = nrhs;
    berr_len = nrhs;

    /* Allocate memory */
    if (!(berr = NAG_ALLOC(berr_len, double)) ||
        !(ferr = NAG_ALLOC(ferr_len, double)) ||
        !(ab = NAG_ALLOC((kd+1) * n, double)) ||
        !(afb = NAG_ALLOC((kd+1) * n, double)) ||
        !(b = NAG_ALLOC(n * nrhs, double)) ||
        !(x = NAG_ALLOC(n * nrhs, double)))
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }

    /* Read A from data file */
#ifdef _WIN32
    scanf_s(" %39s%*[\n] ", nag_enum_arg, _countof(nag_enum_arg));
#else
    scanf(" %39s%*[\n] ", nag_enum_arg);
#endif
    /* nag_enum_name_to_value (x04nac).
     * Converts NAG enum member name to value
     */
    uplo = (Nag_UploType) nag_enum_name_to_value(nag_enum_arg);

    k = kd + 1;
    if (uplo == Nag_Upper)
    {
        for (i = 1; i <= n; ++i)

```

```

        {
            for (j = i; j <= MIN(i+kd, n); ++j)
#ifdef _WIN32
                scanf_s("%lf", &AB_UPPER(i, j));
#else
                scanf("%lf", &AB_UPPER(i, j));
#endif
        }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif
    }
    else
    {
        for (i = 1; i <= n; ++i)
        {
            for (j = MAX(1, i-kd); j <= i; ++j)
#ifdef _WIN32
                scanf_s("%lf", &AB_LOWER(i, j));
#else
                scanf("%lf", &AB_LOWER(i, j));
#endif
        }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif
    }
    /* Read B from data file */
    for (i = 1; i <= n; ++i)
    {
        for (j = 1; j <= nrhs; ++j)
#ifdef _WIN32
            scanf_s("%lf", &B(i, j));
#else
            scanf("%lf", &B(i, j));
#endif
    }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endif
    /* Copy A to AF and B to X */
    if (uplo == Nag_Upper)
    {
        for (i = 1; i <= n; ++i)
        {
            for (j = i; j <= MIN(i+kd, n); ++j)
                AFB_UPPER(i, j) = AB_UPPER(i, j);
        }
    }
    else
    {
        for (i = 1; i <= n; ++i)
        {
            for (j = MAX(1, i-kd); j <= i; ++j)
                AFB_LOWER(i, j) = AB_LOWER(i, j);
        }
    }
    for (i = 1; i <= n; ++i)
    {
        for (j = 1; j <= nrhs; ++j)
            X(i, j) = B(i, j);
    }
    /* Factorize A in the array AFP */
    /* nag_dpbtrf (f07hdc).
    * Cholesky factorization of real symmetric

```

```

    * positive-definite band matrix
    */
nag_dpbtrf(order, uplo, n, kd, afb, pdafb, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_dpbtrf (f07hdc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Compute solution in the array X */
/* nag_dpbtrs (f07hec).
 * Solution of real symmetric positive-definite band system
 * of linear equations, multiple right-hand sides, matrix
 * already factorized by nag_dpbtrf (f07hdc)
 */
nag_dpbtrs(order, uplo, n, kd, nrhs, afb, pdafb, x, pdx, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_dpbtrs (f07hec).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Improve solution, and compute backward errors and */
/* estimated bounds on the forward errors */
/* nag_dpbrfs (f07hhc).
 * Refined solution with error bounds of real symmetric
 * positive-definite band system of linear equations,
 * multiple right-hand sides
 */
nag_dpbrfs(order, uplo, n, kd, nrhs, ab, pdab, afb, pdafb,
            b, pdb, x, pdx, ferr, berr, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_dpbrfs (f07hhc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Print details of solution */

/* nag_gen_real_mat_print (x04cac).
 * Print real general matrix (easy-to-use)
 */
fflush(stdout);
nag_gen_real_mat_print(order, Nag_GeneralMatrix, Nag_NonUnitDiag, n, nrhs, x,
                       pdx, "Solution(s)", 0, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_gen_real_mat_print (x04cac).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
}
printf("\nBackward errors (machine-dependent)\n");
for (j = 1; j <= nrhs; ++j)
    printf("%11.1e%s", berr[j-1], j%7 == 0?"\n":" ");
printf("\nEstimated forward error bounds (machine-dependent)\n");
for (j = 1; j <= nrhs; ++j)
    printf("%11.1e%s", ferr[j-1], j%7 == 0?"\n":" ");
printf("\n");
END:
NAG_FREE(berr);
NAG_FREE(ferr);
NAG_FREE(ab);
NAG_FREE(afb);
NAG_FREE(b);
NAG_FREE(x);
return exit_status;
}

```



## 10.2 Program Data

```
nag_dpbrfs (f07hhc) Example Program Data
  4  1  2          :Values of n, kd and nrhs
  Nag_Lower       :Value of uplo
  5.49
  2.68    5.63
          -2.39    2.60
          -2.22    5.17    :End of matrix A
  22.09    5.10
  9.31    30.81
  -5.24  -25.82
  11.83    22.90          :End of matrix B
```

## 10.3 Program Results

```
nag_dpbrfs (f07hhc) Example Program Results
```

```
Solution(s)
```

	1	2
1	5.0000	-2.0000
2	-2.0000	6.0000
3	-3.0000	-1.0000
4	1.0000	4.0000

```
Backward errors (machine-dependent)
```

```
1.1e-16    1.1e-16
```

```
Estimated forward error bounds (machine-dependent)
```

```
2.1e-14    3.0e-14
```

---