

# NAG Library Function Document

## nag\_dporfs (f07fhc)

### 1 Purpose

nag\_dporfs (f07fhc) returns error bounds for the solution of a real symmetric positive definite 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_dporfs (Nag_OrderType order, Nag_UploType uplo, Integer n,
                 Integer nrhs, const double a[], Integer pda, const double af[],
                 Integer pdaf, const double b[], Integer pdb, double x[], Integer pdx,
                 double ferr[], double berr[], NagError *fail)
```

### 3 Description

nag\_dporfs (f07fhc) returns the backward errors and estimated bounds on the forward errors for the solution of a real symmetric positive definite 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\_dporfs (f07fhc) 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

$$(A + \delta A)x = b + \delta b$$

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

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 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 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: **nrhs** – Integer *Input*  
*On entry:*  $r$ , the number of right-hand sides.  
*Constraint:* **nrhs**  $\geq 0$ .
- 5: **a**[*dim*] – const double *Input*  
**Note:** the dimension, *dim*, of the array **a** must be at least  $\max(1, \mathbf{pda} \times \mathbf{n})$ .  
*On entry:* the  $n$  by  $n$  original symmetric positive definite matrix  $A$  as supplied to nag\_dpotrf (f07fdc).
- 6: **pda** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) of the matrix in the array **a**.  
*Constraint:* **pda**  $\geq \max(1, \mathbf{n})$ .
- 7: **af**[*dim*] – const double *Input*  
**Note:** the dimension, *dim*, of the array **af** must be at least  $\max(1, \mathbf{pdaf} \times \mathbf{n})$ .  
*On entry:* the Cholesky factor of  $A$ , as returned by nag\_dpotrf (f07fdc).
- 8: **pdaf** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) of the matrix in the array **af**.  
*Constraint:* **pdaf**  $\geq \max(1, \mathbf{n})$ .
- 9: **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  
 $\mathbf{b}[(j-1) \times \mathbf{pdb} + i - 1]$  when **order** = Nag\_ColMajor;  
 $\mathbf{b}[(i-1) \times \mathbf{pdb} + j - 1]$  when **order** = Nag\_RowMajor.  
*On entry:* the  $n$  by  $r$  right-hand side matrix  $B$ .

- 10: **pdb** – Integer *Input*  
*On entry:* the stride separating row or column elements (depending on the value of **order**) in the array **b**.  
*Constraints:*  
 if **order** = Nag\_ColMajor, **pdb**  $\geq \max(1, \mathbf{n})$ ;  
 if **order** = Nag\_RowMajor, **pdb**  $\geq \max(1, \mathbf{nrhs})$ .
- 11: **x**[*dim*] – double *Input/Output*  
**Note:** the dimension, *dim*, of the array **x** must be at least  
 $\max(1, \mathbf{pdx} \times \mathbf{nrhs})$  when **order** = Nag\_ColMajor;  
 $\max(1, \mathbf{n} \times \mathbf{pdx})$  when **order** = Nag\_RowMajor.  
 The (*i*, *j*)th element of the matrix *X* is stored in  
 $\mathbf{x}[(j-1) \times \mathbf{pdx} + i - 1]$  when **order** = Nag\_ColMajor;  
 $\mathbf{x}[(i-1) \times \mathbf{pdx} + j - 1]$  when **order** = Nag\_RowMajor.  
*On entry:* the *n* by *r* solution matrix *X*, as returned by nag\_dpotrs (f07fec).  
*On exit:* the improved 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:*  
 if **order** = Nag\_ColMajor, **pdx**  $\geq \max(1, \mathbf{n})$ ;  
 if **order** = Nag\_RowMajor, **pdx**  $\geq \max(1, \mathbf{nrhs})$ .
- 13: **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, ..., *r*.
- 14: **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, ..., *r*.
- 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 *value* had an illegal value.

**NE\_INT**

On entry, **n** =  $\langle value \rangle$ .

Constraint: **n**  $\geq 0$ .

On entry, **nrhs** =  $\langle value \rangle$ .

Constraint: **nrhs**  $\geq 0$ .

On entry, **pda** =  $\langle value \rangle$ .

Constraint: **pda**  $> 0$ .

On entry, **pda**f =  $\langle value \rangle$ .

Constraint: **pda**f  $> 0$ .

On entry, **pdb** =  $\langle value \rangle$ .

Constraint: **pdb**  $> 0$ .

On entry, **pdx** =  $\langle value \rangle$ .

Constraint: **pdx**  $> 0$ .

**NE\_INT\_2**

On entry, **pda** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

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

On entry, **pda**f =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

Constraint: **pda**f  $\geq \max(1, \mathbf{n})$ .

On entry, **pdb** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

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

On entry, **pdb** =  $\langle value \rangle$  and **nrhs** =  $\langle value \rangle$ .

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

On entry, **pdx** =  $\langle value \rangle$  and **n** =  $\langle value \rangle$ .

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

On entry, **pdx** =  $\langle value \rangle$  and **nrhs** =  $\langle value \rangle$ .

Constraint: **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 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\_dporfs (f07fhc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag\_dporfs (f07fhc) 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  $4n^2$  floating-point operations. Each step of iterative refinement involves an additional  $6n^2$  operations. 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  $2n^2$  operations.

The complex analogue of this function is `nag_zporfs` (f07fvc).

## 10 Example

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

$$A = \begin{pmatrix} 4.16 & -3.12 & 0.56 & -0.10 \\ -3.12 & 5.03 & -0.83 & 1.18 \\ 0.56 & -0.83 & 0.76 & 0.34 \\ -0.10 & 1.18 & 0.34 & 1.18 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 8.70 & 8.30 \\ -13.35 & 2.13 \\ 1.89 & 1.61 \\ -4.14 & 5.00 \end{pmatrix}.$$

Here  $A$  is symmetric positive definite and must first be factorized by `nag_dpotrf` (f07fdc).

### 10.1 Program Text

```
/* nag_dporfs (f07fhc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

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

int main(void)
{
    /* Scalars */
    Integer berr_len, ferr_len, i, j, n, nrhs, pda, pdaf, pdb, pdx;
    Integer exit_status = 0;
    Nag_UploType uplo;
    NagError fail;
    Nag_OrderType order;

    /* Arrays */
    char nag_enum_arg[40];
    double *a = 0, *af = 0, *b = 0, *berr = 0, *ferr = 0, *x = 0;

#ifdef NAG_COLUMN_MAJOR
#define A(I, J)  a[(J-1)*pda + I - 1]
#define AF(I, J) af[(J-1)*pdaf + I - 1]
#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 A(I, J)  a[(I-1)*pda + J - 1]
#endif
```

```

#define AF(I, J) af[(I-1)*pdaf + J - 1]
#define B(I, J)  b[(I-1)*pdb + J - 1]
#define X(I, J)  x[(I-1)*pdx + J - 1]
    order = Nag_RowMajor;
#endifif

    INIT_FAIL(fail);

    printf("nag_dporfs (f07fhc) Example Program Results\n\n");

    /* Skip heading in data file */
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endifif
#ifdef _WIN32
    scanf_s("%" NAG_IFMT "%" NAG_IFMT "%*[\n] ", &n, &nrhs);
#else
    scanf("%" NAG_IFMT "%" NAG_IFMT "%*[\n] ", &n, &nrhs);
#endifif
#ifdef NAG_COLUMN_MAJOR
    pda = n;
    pdaf = n;
    pdb = n;
    pdx = n;
#else
    pda = n;
    pdaf = n;
    pdb = nrhs;
    pdx = nrhs;
#endifif
    ferr_len = nrhs;
    berr_len = nrhs;

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

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

    if (uplo == Nag_Upper) {
        for (i = 1; i <= n; ++i) {
            for (j = i; j <= n; ++j)
#ifdef _WIN32
                scanf_s("%lf", &A(i, j));
#else
                scanf("%lf", &A(i, j));
#endifif
        }
    }
#ifdef _WIN32
    scanf_s("%*[\n] ");
#else
    scanf("%*[\n] ");
#endifif

```

```

        scanf("%*[^\\n] ");
#endif
    }
    else {
        for (i = 1; i <= n; ++i) {
            for (j = 1; j <= i; ++j)
#ifdef _WIN32
                scanf_s("%lf", &A(i, j));
#else
                scanf("%lf", &A(i, j));
#endif
        }
#ifdef _WIN32
        scanf_s("%*[^\\n] ");
#else
        scanf("%*[^\\n] ");
#endif
    }

    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 <= n; ++j)
            AF(i, j) = A(i, j);
    }
}
else {
    for (i = 1; i <= n; ++i) {
        for (j = 1; j <= i; ++j)
            AF(i, j) = A(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 AF */
/* nag_dpotrf (f07fdc).
 * Cholesky factorization of real symmetric
 * positive-definite matrix
 */
nag_dpotrf(order, uplo, n, af, pdaf, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dpotrf (f07fdc).\\n%s\\n", fail.message);
    exit_status = 1;
    goto END;
}
/* Compute solution in the array X */
/* nag_dpotrs (f07fec).
 * Solution of real symmetric positive-definite system of
 * linear equations, multiple right-hand sides, matrix
 * already factorized by nag_dpotrf (f07fdc)
 */
nag_dpotrs(order, uplo, n, nrhs, af, pdaf, x, pdx, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dpotrs (f07fec).\\n%s\\n", fail.message);
    exit_status = 1;
    goto END;
}

```

```

}
/* Improve solution, and compute backward errors and */
/* estimated bounds on the forward errors */
/* nag_dporfs (f07fhc).
 * Refined solution with error bounds of real symmetric
 * positive-definite system of linear equations, multiple
 * right-hand sides
 */
nag_dporfs(order, uplo, n, nrhs, a, pda, af, pdaf, b, pdb, x, pdx,
           ferr, berr, &fail);
if (fail.code != NE_NOERROR) {
    printf("Error from nag_dporfs (f07fhc).\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

/* Print 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 || j == nrhs ? "\n" : " ");
END:
NAG_FREE(a);
NAG_FREE(af);
NAG_FREE(b);
NAG_FREE(berr);
NAG_FREE(ferr);
NAG_FREE(x);
return exit_status;
}

```

## 10.2 Program Data

nag\_dporfs (f07fhc) Example Program Data

4	2					:Values of n and nrhs
		Nag_Lower				:Value of uplo
4.16						
-3.12	5.03					
0.56	-0.83	0.76				
-0.10	1.18	0.34	1.18			:End of matrix A
8.70	8.30					
-13.35	2.13					
1.89	1.61					
-4.14	5.00					:End of matrix B

## 10.3 Program Results

nag\_dporfs (f07fhc) Example Program Results

Solution(s)		
	1	2
1	1.0000	4.0000
2	-1.0000	3.0000
3	2.0000	2.0000
4	-3.0000	1.0000



Backward errors (machine-dependent)  
6.7e-17 7.9e-17  
Estimated forward error bounds (machine-dependent)  
2.3e-14 2.3e-14

---