NAG Library Function Document

nag_zpbrfs (f07hvc)

1 Purpose

nag_zpbrfs (f07hvc) returns error bounds for the solution of a complex Hermitian 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_zpbrfs (Nag_OrderType order, Nag_UploType uplo, Integer n,
     Integer kd, Integer nrhs, const Complex ab[], Integer pdab,
     const Complex afb[], Integer pdafb, const Complex b[], Integer pdb,
     Complex x[], Integer pdx, double ferr[], double berr[], NagError *fail)
```

3 Description

nag_zpbrfs (f07hvc) returns the backward errors and estimated bounds on the forward errors for the solution of a complex Hermitian 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_zpbrfs (f07hvc) 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* β. 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

$$\begin{gathered}(A + \delta A)x = b + \delta b \\ \left|\delta a_{ij}\right| \leq \beta\left|a_{ij}\right| \quad \text{and} \quad \left|\delta b_i\right| \leq \beta\left|b_i\right|.\end{gathered}$$

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

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

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 $U^{\mathrm{H}}U$, where U is upper triangular.

uplo = Nag_Lower
The lower triangular part of A is stored and A is factorized as LL^{H}, 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: $\mathbf{n} \geq 0$.

4: **kd** – Integer *Input*

On entry: k_d, the number of superdiagonals or subdiagonals of the matrix A.

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

5: **nrhs** – Integer *Input*

On entry: r, the number of right-hand sides.

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

6: **ab**[dim] – const Complex *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 Hermitian positive definite band matrix A as supplied to nag_zpbtrf (f07hrc).

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: $\mathbf{pdab} \geq \mathbf{kd} + 1$.

8: **afb**[dim] – const Complex *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_zpbtrf (f07hrc).

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: $\mathbf{pdafb} \geq \mathbf{kd} + 1$.

10: **b**[dim] – const Complex *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.

11: **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, $\mathbf{pdb} \geq \max(1, \mathbf{n})$;
if **order** = Nag_RowMajor, $\mathbf{pdb} \geq \max(1, \mathbf{nrhs})$.

12: $\mathbf{x}[dim]$ – Complex *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_zpbtrs (f07hsc).

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:

if **order** = Nag_ColMajor, $\mathbf{pdx} \geq \max(1, \mathbf{n})$;
if **order** = Nag_RowMajor, $\mathbf{pdx} \geq \max(1, \mathbf{nrhs})$.

14: $\mathbf{ferr}[\mathbf{nrhs}]$ – double *Output*

On exit: $\mathbf{ferr}[j-1]$ contains an estimated error bound for the jth solution vector, that is, the jth column of X, for $j = 1, 2, \ldots, r$.

15: $\mathbf{berr}[\mathbf{nrhs}]$ – double *Output*

On exit: $\mathbf{berr}[j-1]$ contains the component-wise backward error bound β for the jth solution vector, that is, the jth column of X, for $j = 1, 2, \ldots, r$.

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 $\langle value \rangle$ had an illegal value.

NE_INT

On entry, $\mathbf{kd} = \langle value \rangle$.
Constraint: $\mathbf{kd} \geq 0$.

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, $\mathbf{pdab} = \langle value \rangle$.
Constraint: $\mathbf{pdab} > 0$.

On entry, $\mathbf{pdafb} = \langle value \rangle$.
Constraint: $\mathbf{pdafb} > 0$.

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, $\mathbf{pdab} = \langle value \rangle$ and $\mathbf{kd} = \langle value \rangle$.
Constraint: $\mathbf{pdab} \geq \mathbf{kd} + 1$.

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

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 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_zpbrfs (f07hvc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_zpbrfs (f07hvc) 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 $32nk$ real floating-point operations. Each step of iterative refinement involves an additional $48nk$ real 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 5 and never more than 11. Each solution involves approximately $16nk$ real operations.

The real analogue of this function is nag_dpbrfs (f07hhc).

10 Example

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

$$A = \begin{pmatrix} 9.39 + 0.00i & 1.08 - 1.73i & 0.00 + 0.00i & 0.00 + 0.00i \\ 1.08 + 1.73i & 1.69 + 0.00i & -0.04 + 0.29i & 0.00 + 0.00i \\ 0.00 + 0.00i & -0.04 - 0.29i & 2.65 + 0.00i & -0.33 + 2.24i \\ 0.00 + 0.00i & 0.00 + 0.00i & -0.33 - 2.24i & 2.17 + 0.00i \end{pmatrix}$$

and

$$B = \begin{pmatrix} -12.42 + 68.42i & 54.30 - 56.56i \\ -9.93 + 0.88i & 18.32 + 4.76i \\ -27.30 - 0.01i & -4.40 + 9.97i \\ 5.31 + 23.63i & 9.43 + 1.41i \end{pmatrix}.$$

Here A is Hermitian positive definite, and is treated as a band matrix, which must first be factorized by nag_zpbtrf (f07hrc).

10.1 Program Text

```
/* nag_zpbrfs (f07hvc) 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];
  Complex       *ab = 0, *afb = 0, *b = 0, *x = 0;
  double        *berr = 0, *ferr = 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_zpbrfs (f07hvc) 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, Complex)) ||
      !(afb = NAG_ALLOC((kd+1) * n, Complex)) ||
      !(b = NAG_ALLOC(n * nrhs, Complex)) ||
      !(x = NAG_ALLOC(n * nrhs, Complex)))
    {
      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 , %lf )", &AB_UPPER(i, j).re,
                     &AB_UPPER(i, j).im);
#else
              scanf(" ( %lf , %lf )", &AB_UPPER(i, j).re,
                     &AB_UPPER(i, j).im);
#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 , %lf )", &AB_LOWER(i, j).re,
                     &AB_LOWER(i, j).im);
#else
              scanf(" ( %lf , %lf )", &AB_LOWER(i, j).re,
                     &AB_LOWER(i, j).im);
#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 , %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 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).re = AB_UPPER(i, j).re;
            AFB_UPPER(i, j).im = AB_UPPER(i, j).im;
          }
      }
    }
  else
    {
      for (i = 1; i <= n; ++i)
        {
          for (j = MAX(1, i-kd); j <= i; ++j)
            {
              AFB_LOWER(i, j).re = AB_LOWER(i, j).re;
              AFB_LOWER(i, j).im = AB_LOWER(i, j).im;
            }
        }
    }
  for (i = 1; i <= n; ++i)
    {
      for (j = 1; j <= nrhs; ++j)
        {
          X(i, j).re = B(i, j).re;
          X(i, j).im = B(i, j).im;
        }
    }
  /* Factorize A in the array AFP */
  /* nag_zpbtrf (f07hrc).
   * Cholesky factorization of complex Hermitian
   * positive-definite band matrix
   */
  nag_zpbtrf(order, uplo, n, kd, afb, pdafb, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_zpbtrf (f07hrc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Compute solution in the array X */
  /* nag_zpbtrs (f07hsc).
   * Solution of complex Hermitian positive-definite band
   * system of linear equations, multiple right-hand sides,
   * matrix already factorized by nag_zpbtrf (f07hrc)
   */
  nag_zpbtrs(order, uplo, n, kd, nrhs, afb, pdafb, x, pdx, &fail);
  if (fail.code != NE_NOERROR)
    {
      printf("Error from nag_zpbtrs (f07hsc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Improve solution, and compute backward errors and */
  /* estimated bounds on the forward errors */
  /* nag_zpbrfs (f07hvc).
   * Refined solution with error bounds of complex Hermitian
   * positive-definite band system of linear equations,
   * multiple right-hand sides
   */
  nag_zpbrfs(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_zpbrfs (f07hvc).\n%s\n", fail.message);
      exit_status = 1;
      goto END;
    }
  /* Print details of solution */

  /* nag_gen_complx_mat_print_comp (x04dbc).
   * Print complex general matrix (comprehensive)
   */
  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;
    }
  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_zpbrfs (f07hvc) Example Program Data
  4  1  2                                                 :Values of n, kd and nrhs
  Nag_Lower                                               :Value of uplo
 ( 9.39, 0.00)
 ( 1.08, 1.73) ( 1.69, 0.00)
               (-0.04,-0.29) ( 2.65, 0.00)
                             (-0.33,-2.24) ( 2.17, 0.00)  :End of matrix A
 (-12.42,68.42) (54.30,-56.56)
 ( -9.93, 0.88) (18.32,  4.76)
 (-27.30,-0.01) (-4.40,  9.97)
 (  5.31,23.63) ( 9.43,  1.41)                            :End of matrix B
```

10.3 Program Results

```
nag_zpbrfs (f07hvc) Example Program Results

 Solution(s)
                    1                  2
 1  (-1.0000, 8.0000)  ( 5.0000,-6.0000)
 2  ( 2.0000,-3.0000)  ( 2.0000, 3.0000)
 3  (-4.0000,-5.0000)  (-8.0000, 4.0000)
 4  ( 7.0000, 6.0000)  (-1.0000,-7.0000)

Backward errors (machine-dependent)
    8.2e-17     5.4e-17
Estimated forward error bounds (machine-dependent)
    3.6e-14     3.0e-14
```