NAG Fortran Library Routine Document

C06PSF

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

C06PSF computes the discrete Fourier transforms of m sequences, stored as columns of an array, each containing n complex data values.

2 Specification

```
SUBROUTINE C06PSF(DIRECT, N, M, X, WORK, IFAIL)
INTEGER           N, M, IFAIL
complex           X(N*M), WORK(N*M+N+15)
CHARACTER*1       DIRECT
```

3 Description

Given m sequences of n complex data values z_j^p, for $j = 0, 1, \ldots, n-1$ and $p = 1, 2, \ldots, m$, this routine simultaneously calculates the (**forward** or **backward**) discrete Fourier transforms of all the sequences defined by

$$\hat{z}_k^p = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} z_j^p \times \exp\left(\pm i \frac{2\pi jk}{n}\right), \quad k = 0, 1, \ldots, n-1; \quad p = 1, 2, \ldots, m.$$

(Note the scale factor $\frac{1}{\sqrt{n}}$ in this definition.) The minus sign is taken in the argument of the exponential within the summation when the forward transform is required, and the plus sign is taken when the backward transform is required. A call of the routine with DIRECT = 'F' followed by a call with DIRECT = 'B' will restore the original data.

The routine uses a variant of the fast Fourier transform (FFT) algorithm (Brigham (1974)) known as the Stockham self-sorting algorithm, which is described in Temperton (1983b). Special code is provided for the factors 2, 3, 4 and 5.

4 References

Brigham E O (1974) *The Fast Fourier Transform* Prentice-Hall

Temperton C (1983b) Self-sorting mixed-radix fast Fourier transforms *J. Comput. Phys.* **52** 1–23

5 Parameters

1: DIRECT – CHARACTER*1 *Input*

On entry: if the **F**orward transform as defined in Section 3 is to be computed, then DIRECT must be set equal to 'F'. If the **B**ackward transform is to be computed then DIRECT must be set equal to 'B'.

Constraint: DIRECT = 'F' or 'B'.

2: N – INTEGER *Input*

3: M – INTEGER *Input*

4: X(N∗M) – ***complex*** array *Input/Output*

On entry: the complex data must be stored in X as if in a two-dimensional array of dimension $(0 : \mathrm{N}-1, 1 : \mathrm{M})$; each of the m sequences is stored in a **column** of the array. In other words, if the elements of the pth sequence to be transformed are denoted by z_j^p, for $j = 0, 1, \ldots, n-1$ and X is declared as $\mathrm{X}(0 : \mathrm{N}-1, 1 : \mathrm{M})$, then $\mathrm{X}(j, p)$ must contain z_j^p.

On exit: X is overwritten by the complex transforms.

5: WORK(N∗M+N+15) – ***complex*** array *Workspace*

6: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. Users who are unfamiliar with this parameter should refer to Chapter P01 for details.

On exit: IFAIL $= 0$ unless the routine detects an error (see Section 6).

For environments where it might be inappropriate to halt program execution when an error is detected, the value -1 or 1 is recommended. If the output of error messages is undesirable, then the value 1 is recommended. Otherwise, for users not familiar with this parameter the recommended value is 0. **When the value -1 or 1 is used it is essential to test the value of IFAIL on exit.**

6 Error Indicators and Warnings

If on entry IFAIL $= 0$ or -1, explanatory error messages are output on the current error message unit (as defined by X04AAF).

Errors or warnings detected by the routine:

IFAIL $= 1$

IFAIL $= 2$

IFAIL $= 3$

IFAIL $= 4$

IFAIL $= 5$

7 Accuracy

Some indication of accuracy can be obtained by performing a subsequent inverse transform and comparing the results with the original sequence (in exact arithmetic they would be identical).

8 Further Comments

The time taken by the routine is approximately proportional to $nm \times \log n$, but also depends on the factors of n. The routine is fastest if the only prime factors of n are 2, 3 and 5, and is particularly slow if n is a large prime, or has large prime factors.

9 Example

This program reads in sequences of complex data values and prints their discrete Fourier transforms (as computed by C06PSF with DIRECT set to 'F'). Inverse transforms are then calculated using C06PSF with DIRECT set to 'B' and printed out, showing that the original sequences are restored.

9.1 Program Text

Note: the listing of the example program presented below uses ***bold italicised*** terms to denote precision-dependent details. Please read the Users' Note for your implementation to check the interpretation of these terms. As explained in the Essential Introduction to this manual, the results produced may not be identical for all implementations.

```
*     C06PSF Example Program Text.
*     Mark 19 Release. NAG Copyright 1999.
*     .. Parameters ..
      INTEGER          NIN, NOUT
      PARAMETER        (NIN=5,NOUT=6)
      INTEGER          MMAX, NMAX
      PARAMETER        (MMAX=5,NMAX=20)
*     .. Local Scalars ..
      INTEGER          I, IFAIL, J, M, N
*     .. Local Arrays ..
      complex          WORK(NMAX+MMAX*NMAX+15), X(MMAX*NMAX)
*     .. External Subroutines ..
      EXTERNAL         C06PSF
*     .. Intrinsic Functions ..
      INTRINSIC        real, imag
*     .. Executable Statements ..
      WRITE (NOUT,*) 'C06PSF Example Program Results'
*     Skip heading in data file
      READ (NIN,*)
   20 CONTINUE
      READ (NIN,*,END=120) M, N
      IF (M.LE.MMAX .AND. N.LE.NMAX) THEN
         DO 40 J = 1, M*N, N
            READ (NIN,*) (X(J+I),I=0,N-1)
   40    CONTINUE
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Original data values'
         DO 60 J = 1, M*N, N
            WRITE (NOUT,*)
            WRITE (NOUT,99999) 'Real ', (real(X(J+I)),I=0,N-1)
            WRITE (NOUT,99999) 'Imag ', (imag(X(J+I)),I=0,N-1)
   60    CONTINUE
         IFAIL = 0
*
         CALL C06PSF('F',N,M,X,WORK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Discrete Fourier transforms'
         DO 80 J = 1, M*N, N
            WRITE (NOUT,*)
            WRITE (NOUT,99999) 'Real ', (real(X(J+I)),I=0,N-1)
            WRITE (NOUT,99999) 'Imag ', (imag(X(J+I)),I=0,N-1)
   80    CONTINUE
*
         CALL C06PSF('B',N,M,X,WORK,IFAIL)
*
         WRITE (NOUT,*)
         WRITE (NOUT,*) 'Original data as restored by inverse transform'
         DO 100 J = 1, M*N, N
            WRITE (NOUT,*)
            WRITE (NOUT,99999) 'Real ', (real(X(J+I)),I=0,N-1)
            WRITE (NOUT,99999) 'Imag ', (imag(X(J+I)),I=0,N-1)
  100    CONTINUE
         GO TO 20
      ELSE
         WRITE (NOUT,*) 'Invalid value of M or N'
      END IF
  120 CONTINUE
```

```
      STOP
*
99999 FORMAT (1X,A,6F10.4)
      END
```

9.2 Program Data

```
C06PSF Example Program Data
     3     6
     (0.3854,0.5417)
     (0.6772,0.2983)
     (0.1138,0.1181)
     (0.6751,0.7255)
     (0.6362,0.8638)
     (0.1424,0.8723)
     (0.9172,0.9089)
     (0.0644,0.3118)
     (0.6037,0.3465)
     (0.6430,0.6198)
     (0.0428,0.2668)
     (0.4815,0.1614)
     (0.1156,0.6214)
     (0.0685,0.8681)
     (0.2060,0.7060)
     (0.8630,0.8652)
     (0.6967,0.9190)
     (0.2792,0.3355)
```

9.3 Program Results

```
 C06PSF Example Program Results

 Original data values

 Real     0.3854    0.6772    0.1138    0.6751    0.6362    0.1424
 Imag     0.5417    0.2983    0.1181    0.7255    0.8638    0.8723

 Real     0.9172    0.0644    0.6037    0.6430    0.0428    0.4815
 Imag     0.9089    0.3118    0.3465    0.6198    0.2668    0.1614

 Real     0.1156    0.0685    0.2060    0.8630    0.6967    0.2792
 Imag     0.6214    0.8681    0.7060    0.8652    0.9190    0.3355

 Discrete Fourier transforms

 Real     1.0737   -0.5706    0.1733   -0.1467    0.0518    0.3625
 Imag     1.3961   -0.0409   -0.2958   -0.1521    0.4517   -0.0321

 Real     1.1237    0.1728    0.4185    0.1530    0.3686    0.0101
 Imag     1.0677    0.0386    0.7481    0.1752    0.0565    0.1403

 Real     0.9100   -0.3054    0.4079   -0.0785   -0.1193   -0.5314
 Imag     1.7617    0.0624   -0.0695    0.0725    0.1285   -0.4335

 Original data as restored by inverse transform

 Real     0.3854    0.6772    0.1138    0.6751    0.6362    0.1424
 Imag     0.5417    0.2983    0.1181    0.7255    0.8638    0.8723

 Real     0.9172    0.0644    0.6037    0.6430    0.0428    0.4815
 Imag     0.9089    0.3118    0.3465    0.6198    0.2668    0.1614

 Real     0.1156    0.0685    0.2060    0.8630    0.6967    0.2792
 Imag     0.6214    0.8681    0.7060    0.8652    0.9190    0.3355
```