NAG Library Routine Document

C06PZF

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

C06PZF computes the three-dimensional inverse discrete Fourier transform of a trivariate Hermitian sequence of complex data values.

2 Specification

```
SUBROUTINE C06PZF (N1, N2, N3, Y, X, IFAIL)

INTEGER                N1, N2, N3, IFAIL
REAL (KIND=nag_wp)     X(N1*N2*N3)
COMPLEX (KIND=nag_wp)  Y((N1/2+1)*N2*N3)
```

3 Description

C06PZF computes the three-dimensional inverse discrete Fourier transform of a trivariate Hermitian sequence of complex data values $z_{j_1 j_2 j_3}$, for $j_1 = 0, 1, \dots, n_1 - 1$, $j_2 = 0, 1, \dots, n_2 - 1$ and $j_3 = 0, 1, \dots, n_3 - 1$.

The discrete Fourier transform is here defined by

$$\hat{x}_{k_1 k_2 k_3} = \frac{1}{\sqrt{n_1 n_2 n_3}} \sum_{j_1=0}^{n_1-1} \sum_{j_2=0}^{n_2-1} \sum_{j_3=0}^{n_3-1} z_{j_1 j_2 j_3} \times \exp\left(2\pi i \left(\frac{j_1 k_1}{n_1} + \frac{j_2 k_2}{n_2} + \frac{j_3 k_3}{n_3}\right)\right),$$

where $k_1 = 0, 1, \dots, n_1 - 1$, $k_2 = 0, 1, \dots, n_2 - 1$ and $k_3 = 0, 1, \dots, n_3 - 1$. (Note the scale factor of $\frac{1}{\sqrt{n_1 n_2 n_3}}$ in this definition.)

Because the input data satisfies conjugate symmetry (i.e., $z_{k_1 k_2 k_3}$ is the complex conjugate of $z_{(n_1 - k_1) k_2 k_3}$), the transformed values $\hat{x}_{k_1 k_2 k_3}$ are real.

A call of C06PYF followed by a call of C06PZF will restore the original data.

This routine calls C06PQF and C06PRF to perform multiple one-dimensional discrete Fourier transforms by the fast Fourier transform (FFT) algorithm in Brigham (1974) and Temperton (1983).

4 References

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

Temperton C (1983) Fast mixed-radix real Fourier transforms *J. Comput. Phys.* **52** 340–350

5 Parameters

1: N1 – INTEGER *Input*

On entry: n_1, the first dimension of the transform.

Constraint: N1 ≥ 1.

2: N2 – INTEGER *Input*

On entry: n_2, the second dimension of the transform.

Constraint: N2 ≥ 1.

3: N3 – INTEGER *Input*

On entry: n_3, the third dimension of the transform.

Constraint: N3 ≥ 1.

4: Y$((\mathrm{N1}/2 + 1) \times \mathrm{N2} \times \mathrm{N3})$ – COMPLEX (KIND=nag_wp) array *Input*

On entry: the Hermitian sequence of complex input dataset z, where $z_{j_1 j_2 j_3}$ is stored in $\mathrm{Y}(j_3 \times (n_1/2 + 1)n_2 + j_2 \times (n_1/2 + 1) + j_1 + 1)$, for $j_1 = 0, 1, \ldots, n_1/2$, $j_2 = 0, 1, \ldots, n_2 - 1$ and $j_3 = 0, 1, \ldots, n_3 - 1$. That is, if Y is regarded as a three-dimensional array of dimension $(0 : \mathrm{N1}/2, 0 : \mathrm{N2} - 1, 0 : \mathrm{N3} - 1)$, then $\mathrm{Y}(j_1, j_2, j_3)$ must contain $z_{j_1 j_2 j_3}$.

5: X$(\mathrm{N1} \times \mathrm{N2} \times \mathrm{N3})$ – REAL (KIND=nag_wp) array *Output*

On exit: the real output dataset $\hat{x}$, where $\hat{x}_{k_1 k_2 k_3}$ is stored in $\mathrm{X}(k_3 \times n_1 n_2 + k_2 \times n_1 + k_1 + 1)$, for $k_1 = 0, 1, \ldots, n_1 - 1$, $k_2 = 0, 1, \ldots, n_2 - 1$ and $k_3 = 0, 1, \ldots, n_3 - 1$. That is, if X is regarded as a three-dimensional array of dimension $(0 : \mathrm{N1} - 1, 0 : \mathrm{N2} - 1, 0 : \mathrm{N3} - 1)$, then $\mathrm{X}(k_1, k_2, k_3)$ contains $\hat{x}_{k_1 k_2 k_3}$.

6: IFAIL – INTEGER *Input/Output*

On entry: IFAIL must be set to 0, -1 or 1. If you are unfamiliar with this parameter you should refer to Section 3.3 in the Essential Introduction for details.

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, if you are 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.**

On exit: IFAIL $= 0$ unless the routine detects an error or a warning has been flagged (see Section 6).

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 $= 1$

On entry, N1 $= \langle value \rangle$.
Constraint: N1 ≥ 1.

IFAIL $= 2$

On entry, N2 $= \langle value \rangle$.
Constraint: N2 ≥ 1.

IFAIL $= 3$

On entry, N3 $= \langle value \rangle$.
Constraint: N3 ≥ 1.

IFAIL = 4

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.

IFAIL = −999

Dynamic memory allocation failed.

7 Accuracy

Some indication of accuracy can be obtained by performing a forward transform using C06PYF and a backward transform using C06PZF, and comparing the results with the original sequence (in exact arithmetic they would be identical).

8 Further Comments

The time taken by C06PZF is approximately proportional to $n_1 n_2 n_3 \log(n_1 n_2 n_3)$, but also depends on the factors of n_1, n_2 and n_3. C06PZF is fastest if the only prime factors of n_1, n_2 and n_3 are 2, 3 and 5, and is particularly slow if one of the dimensions is a large prime, or has large prime factors.

Workspace is internally allocated by C06PZF. The total size of these arrays is approximately proportional to $n_1 n_2 n_3$.

9 Example

See Section 9 in C06PYF.