

UNITED STATES DEPARTMENT OF THE INTERIOR
GEOLOGICAL SURVEY

FORTRAN '77 PROGRAMS FOR COMPUTING DATA FITTING FUNCTIONS
BASED ON A PRINCIPLE OF MINIMUM INTEGRATED SQUARED CURVATURE

by

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This report consists of listings of FORTRAN '77 computer programs that implement a new algorithm for fitting a continuous, analytical function to a set of data points. The analytical function is defined in a one- or two-dimensional domain that contains the known data points. The fit satisfies the following criteria: (1) it passes through the known data points, and (2) the square of its curvature, integrated over the entire domain of the fit, is minimized.

The major programs, FOURGRID and FOURFIT, are intended to be self-documenting. These programs and the subroutines that they call have been extensively tested using data sets with up to 50 data points, with satisfactory results. The author is presently preparing a report on the mathematical algorithm that these programs implement.

```
SUBROUTINE FOURGRID(X,Y,F,N,DX,DY,XO,YO,MODE,WORK,NWRK,  
  LX,LY)
```

```
c  
c  
c 1.0 PURPOSE  
c
```

```
c Grids tabulated data in 2 dimensions using FOURFIT.  
c
```

```
c  
c 2.0 ARGUMENTS  
c
```

- ```
c 1. X - (input) real*4 array of x coordinates of known
c points, dimensioned (N).
c
c 2. Y - (input) real*4 array of y coordinates of known
c points, dimensioned (N).
c
c 3. F - (input) real*4 array of function values at the
c known points, dimensioned (N).
c
c 4. N - (input) integer number of known points.
c
c 5. DX - (input) grid interval in the x direction.
c
c 6. DY - (input) grid interval in the y direction.
c
c 7. XO - (input/output) x coordinate of lower left
c corner of grid (input or output parameter,
c depending on value of MODE).
c
c 8. YO - (input/output) y coordinate of lower left
c corner of grid (input or output parameter,
c depending on value of MODE).
c
c 9. MODE - (input)
c
c - if MODE.eq.1, then XO and YO are considered as
c input specifications of the minimum x and y
c values of the output grid.
c
c - if MODE.eq.2, then XO and YO are constructed by
c FOURGRID so that the grid is centered around
c the tabulated input data. XO and YO, which
c still represent the minimum x and y coordinates
c of the grid, are returned to the calling
c program.
c
c - if MODE has any other value, an error message
c is written and the program is STOPped.
c
c 10. WORK - (output) work and result array that must
c contain enough storage for all the work arrays used
```

c by FOURFIT. Real\*4 array dimensioned (NWRK). The  
c resulting grid is returned in WORK as a real\*4  
c array dimensioned (0:LX,0:LY).  
c

- c 11. NWRK - (input) size of WORK, integer input  
c parameter. Minimum NWRK is  $\max(N*(LX+1)*(LY+1)+$   
c  $2*N**2+5*N, 8*LX*LY)$ . LX and LY are computed by  
c FOURGRID as described below.  
c
- c 12. LX - (output) x size of the output grid.  
c
- c 13. LY - (output) y size of the output grid. LX and LY  
c are powers of 2 (because of the use of a radix-2  
c FFT), which are adjusted to the minimum size that  
c will span the input data range using either the  
c input values of X0 and Y0 or the values computed by  
c FOURGRID, depending on the value of MODE.  
c

### c 3.0 AUTHOR

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c

### c 4.0 TESTING SUMMARY

c FOURGRID was written in December, 1981, and tested on a  
c Digital Equipment Corporation VAX 11/780 computer, using  
c DEC's VAX FORTRAN compiler. The program is intended to  
c conform to FORTRAN '77 standards, and contains no known  
c non-FORTRAN '77 constructs.  
c

### c 5.0 CALLS SUBROUTINES:

- c - FOURFIT  
c  
c - FFT2D  
c  
c - TOCOMPLEX  
c  
c - TOREAL  
c

```
c
c 6.0 USAGE NOTES
c
```

```
c If all values of X or Y are the same, and if FFT2D is coded
c so that it will work with NX or NY = 1, then this program
c can be used to fit one-dimensional data.
c
```

```
c -----
c
c declarations:
c REAL*4 X(N),Y(N),F(N),WORK(NWRK)
c DATA PI/3.14159265/
```

```
c determine grid parameters.
c start by scanning for max and min values.
```

```
c XMIN=X(1)
c YMIN=Y(1)
c XMAX=XMIN
c YMAX=YMIN
c DO I=2,N
c XMAX=MAX(XMAX,X(I))
c YMAX=MAX(YMAX,Y(I))
c XMIN=MIN(XMIN,X(I))
c YMIN=MIN(YMIN,Y(I))
```

```
c END DO
```

```
c if MODE is 1, then use X0 and Y0 as minima.
```

```
c IF (MODE.EQ.1) THEN
c IF (XMIN.LT.X0) THEN
c WRITE(*,'(1X,A)') 'Minimum value in input X array is'//
c ' smaller than specified X0, MODE=1, in FOURGRID.'
c STOP
c ELSE
c XMIN=X0
c END IF
c IF (YMIN.LT.Y0) THEN
c WRITE(*,'(1X,A)') 'Minimum value in input Y array is'//
c ' smaller than specified Y0, MODE=1, in FOURGRID.'
c STOP
c ELSE
c YMIN=Y0
c END IF
```

```
c check for invalid value for MODE.
```

```
c ELSE
c IF (MODE.NE.2) THEN
c WRITE(*,'(1X,A)') 'Illegal value of MODE passed'//
c ' to FOURGRID.'
c STOP
c END IF
c END IF
```

```
c
```

```

c determine grid size.
 XSPAN=XMAX-XMIN
 YSPAN=YMAX-YMIN
 LX=1
 DO WHILE(LX*DX.LT.XSPAN)
 LX=2*LX
 END DO
 LY=1
 DO WHILE(LY*DY.LT.YSPAN)
 LY=2*LY
 END DO

c
c if MODE is 2, center the grid around the data.
 IF (MODE.EQ.2) THEN
 XO=(XMIN+XMAX)/2.-DX*(LX/2)
 YO=(YMIN+YMAX)/2.-DY*(LY/2)
 END IF

c
c check size of work array.
 MINSIZE=MAX(N*(LX+1)*(LY+1)+2*N**2+5*N,8*LX*LY)
 IF (NWRK.LT.MINSIZE) THEN
 WRITE(*,'(1X,A)') 'Error in FOURGRID:',
. 'Size of work array is not sufficient.',
. 'Grid parameters:'
 WRITE(*,'(4X,A,I6)') 'LX =',lx,'LY =',ly,
. 'Minimum NWRK =',minsize
 STOP
 END IF

c
c pointers for work array.
 I1=N*(LX+1)*(LY+1)+1
 I2=I1+N**2
 I3=I2+N**2
 I4=I3+N
 I5=I4+N
 I6=I5+N
 I7=I6+N

c
c rescale X and Y to principal interval for FOURFIT.
 DO I=1,N
 WORK(I6+I-1)=(X(I)-X0)/DX
 WORK(I7+I-1)=(Y(I)-Y0)/DY
 END DO

c
c get the Fourier cosine coefficients of the fit.
 CALL FOURFIT(WORK(I6),WORK(I7),F,N,
. FLOAT(LX),FLOAT(LY),WORK,LX,LY,WORK(I1),
. WORK(I2),WORK(I3),WORK(I4),WORK(I5))

c
c arrange them for Fourier transformation using FFT.
 CALL TOCOMPLEX(WORK,WORK,LX,LY,2*LX,2*LY)

c
c do the FFT.
 CALL FFT2D(WORK,2*LX,2*LY,-1.)

```

```
c squeeze out the imaginary part.
c CALL TOREAL(WORK,WORK,LX,LY)
c
c done
c END
```

```
SUBROUTINE FOURFIT(X,Y,F,N,SPANX,SPANY,D,NX,NY,M,MWORK,
V,W,LAMBDA)
```

## 1.0 PURPOSE

Computes the 2-D cosine transform of a fit to a function, using the principle of minimum integrated squared curvature. At the present time, the mathematical algorithm is undocumented, but it can be described briefly as follows: (1) we describe a function (the fit) in terms of a Fourier cosine series in D dimensions (the present programs work for D=1 or 2); (2) we use calculus of variations to minimize the square of the second derivative (or the square of del-squared) integrated over the domain of the fit, while the fit is simultaneously constrained to pass through the known data points.

## 2.0 ARGUMENTS

1. X - (input) array of X coordinates of known points, real\*4 array dimensioned (N). The calling program should ensure that all X values fall in the range 0. .le. X(i) .le. SPANX.
2. Y - (input) array of Y coordinates of known points, real\*4 array dimensioned (N). The calling program should ensure that all Y values fall in the range 0. .le. Y(i) .le. SPANY.
3. F - (input) array of values at known points, real\*4 array dimensioned (N).
4. N - (input) number of known points.
5. SPANX - (input) half the period of the function in the x dimension. Since the function must be even as well as periodic, it need be specified only over half a period in each dimension.
6. SPANY - (input) half the period of the function in the y dimension.
7. D - (output) work and result array, real\*4 dimensioned (0:NX,0:NY,N). The Fourier cosine coefficients are returned in the first panel of D [i.e. in D(0:NX,0:NY,1)].
8. NX - (input) the number of x-dimension frequencies included in the series. The highest frequency in the X dimension is  $NX \cdot \pi / \text{SPANX}$ .







```

 WTX=2.
 END IF
 YNORM=Y(I)/SPANX
 IF(ABS(YNORM-NINT(YNORM)).LT.1.E-5) THEN
 WTY=1.
 ELSE
 WTY=2.
 END IF
 W(I)=WTX*WTY
 END DO

```

c  
c  
c  
c

Compute the Fourier cosine transform of each sample function. Since each function is a delta function, the transform is done by a simple DFT rather than by an FFT.

```

 DKX=PI/SPANX
 DKY=PI/SPANX
 DO I=1,N
 CALL DCT(X(I),Y(I),DKX,DKY,D(0,0,I),NX,NY,W(I))
 END DO

```

c  
c  
c  
c  
c  
c  
c

In the frequency domain, compute the function that when operated on by the square of the Laplacian operator ( $\text{del}^{**4}$ ), yields each sampling function (i.e. a delta function at the location of the corresponding known point, plus delta functions at any symmetry points). This process must ignore the zero-frequency component, since that is destroyed by the Laplacian operator.

```

 DO I=1,N
 D(0,0,I)=(0.,0.)
 DO KX=0,NX
 WX=(KX*DKX)**2
 DO KY=MAX(0,1-KX),NY
 WY=(KY*DKY)**2
 WT=(WX+WY)**2
 D(KX,KY,I)=D(KX,KY,I)/WT
 END DO
 END DO
 END DO

```

c  
c  
c  
c  
c  
c  
c

Compute summed inverse transforms at the known sample points. The results are not equally weighted due to the presence of 0, 1, or 3 image points resulting from the required even symmetry in 2 dimensions. Since the result is required only at one point, this computation is most efficiently done by discrete cosine transform rather than by FFT.

```

 DO I=1,N
 DO J=1,I
 TEMPM=DICT(X(I),Y(I),DKX,DKY,D(0,0,J),NX,NY)*W(I)
 M(I,J)=TEMPM
 M(J,I)=TEMPM
 END DO
 END DO

```

c  
c

solve  $Mx=w$ .

```
CALL MATSOL(M,MWORK,V,W,N)
c
c determine <g>.
GDC=DOT(F,V,W,N)/SUM(V,W,N)
c
c solve My=f.
DO I=1,N
 LAMBDA(I)=W(I)*F(I)
END DO
CALL MATSOL(M,MWORK,LAMBDA,LAMBDA,N)
c
c determine Lagrange multipliers.
DO I=1,N
 LAMBDA(I)=GDC*V(I)-LAMBDA(I)
END DO
c
c Determine the positive-frequency part of the transform of
c the fit function, putting it into the first panel of D.
DO KX=0,NX
 DO KY=0,NY
 D(KX,KY,1)=-D(KX,KY,1)*LAMBDA(1)
 END DO
END DO
DO J=2,N
 DO KX=0,NX
 DO KY=0,NY
 D(KX,KY,1)=D(KX,KY,1)-D(KX,KY,J)*LAMBDA(J)
 END DO
 END DO
END DO
D(0,0,1)=GDC
c
c done
END
```

## SUBROUTINE FFT2D(F,M,N,S)

## 1.0 PURPOSE

Performs a 2-dimensional, radix-2 Fast Fourier Transform (FFT) in memory. This program is efficient only if the 2-D array can be stored in the user's physical memory space. If the array extends into virtual memory space on disk, then extensive paging will be incurred while doing the transform in the second dimension, which is the part performed by calls to FFT2.

## 2.0 ARGUMENTS

1. F - (input/output) complex\*8 array of input values that is Fourier transformed in place into the output values. Dimensioned (M,N).
2. M - (input) integer subscript range of first dimension of F. Must be an integral power of 2, or FFT will issue an error message and STOP.
3. N - (input) integer subscript range of second dimension of F. Must be an integral power of 2, or FFT2 will issue an error message and STOP.
4. S - (input) real\*4 sign of transform. Must equal +1. or -1., or FFT will issue an error messages and STOP.

## 3.0 AUTHOR

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## 4.0 TESTING SUMMARY

FFT2D is a simple driver to call FFT and FFT2. FFT does the transforms in the first dimension (whose points are contiguous). FFT2 does the transforms in the second dimension (whose points are non-contiguous). The program

was written in 1976 and run on a Honeywell Multics system, then recompiled and tested in December, 1982, on a Digital Equipment Corporation VAX 11/780. The program conforms to FORTRAN '77 standards and contains no known non-standard constructs.

## 5.0 CALLS SUBROUTINES:

- FFT
- FFT2

## 6.0 USAGE

### 6.1 Definition Of Result

The result  $F$  in terms of the input  $f$  (which occupies the same storage) is:

$$F(k,l) = \prod_{m=0}^{M-1} \prod_{n=0}^{N-1} f(m,n) e^{4iS(\pi)^2 klmn/MN}$$

for  $k = 0, 1, \dots, M-1$  and  $l = 0, 1, \dots, N-1$ .

where  $i$  is the square root of  $-1$ .

### 6.2 Transform Weighting

6.2.1 Unweighted Results - If FFT2D is called with  $S = +1.$ , then called again with  $S = -1.$ , and no weighting is applied to the array, then the result will be the original array multiplied by  $M*N$ .

6.2.2 Further Information - See FFT for information on appropriate weights to apply to make a scaled transform pair.

### 6.3 Subscript Range

c This program only uses the subscript ranges prescribed by M  
 c and N. The calling program can use a declaration of the  
 c form

c COMPLEX F(m1:m2,n1:n2)

c and the only restrictions are:

c m2-m1+1=M

c n2-n1+1=N

c which is to say, M and N are the number of elements in each  
 c dimension.

#### c 6.4 Efficiency

c This program is intended to work in physical memory. If F  
 c is larger than the user's share of physical memory, then  
 c extensive paging will occur during the calls to FFT2.

c -----  
 c COMPLEX\*8 F(0:M-1,0:N-1)

c perform transforms in 1st dimension.

c DO I=0,N-1

c CALL FFT(F(0,I),M,S)

c END DO

c perform transforms in 2nd dimension.

c DO J=0,M-1

c CALL FFT2(F(J,0),M,N,S)

c END DO

c done

c END

## SUBROUTINE FFT(F,N,S)

## 1.0 PURPOSE

Computes the radix-2 Fast Fourier Transform, using an in-place algorithm. Output F in terms of input f is:

$$F(k) = \prod_{j=0}^{N-1} f(j) e^{iSjk^2(\pi)/N}$$

where F and f are tabulated transform values that occupy the same storage. i is the square root of -1. S is the sign of the transform, +/-1. N is restricted to be an integral power of 2.

## 2.0 ARGUMENTS

1. F - (input/output) complex input array, N complex elements. The transform is done in place, so the result is returned to the calling program in F.
2. N - (input) the (integer) number of elements in F. The subscripts actually used in this routine are 0 to N-1. N is restricted to take on values of integral powers of 2. If N is not so specified, then an error message is issued and the program is STOPped.
3. S - (input) forward/reverse transform sign indicator. Must have a value of +1. or -1.. If S is specified with any other value, then an error message is issued and the program is STOPped.

## 3.0 AUTHOR

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#### 4.0 TESTING SUMMARY

This is a variation of a routine that has been used for many years; the author obtained its ancestor from Ralph Wiggins at MIT. This version has been coded to use some nice features of FORTRAN '77, such as subscripts that start at zero and logically controlled DO loops.

#### 5.0 CALLS SUBROUTINES:

None.

#### 6.0 USAGE NOTES

##### 6.1 Domain Spacings

If the distance between samples in the input domain is  $D$ , then the distance between samples in the output domain is  $D'$ , given by

$$D' = \frac{2*\pi}{D*N}$$

##### 6.2 Weights

6.2.1 This incarnation of FFT has no weighting applied for forward/reverse transformation, so the user can define "forward" with whichever sign he prefers.

6.2.2 To use FFT to estimate a Fourier integral, the user should multiply the input or the output by the input domain spacing. To make a transform pair, Fourier theory requires either the "forward" or the "reverse" integral to be multiplied by  $1/(2*\pi)$ , or both integrals to be multiplied by  $1/\text{sqrt}(2*\pi)$ .

6.2.3 If FFT is called once with  $S = +1.$ , then again with  $S = -1.$ , or vice-versa, the result will be the original array multiplied by  $N$ . This result is apparent from the foregoing discussion, which says the round-trip transform pair should be multiplied by  $(DD')/(2*\pi)$ , which is equal to  $1/N$ , from the formula in paragraph 6.1 .

```

c
c
c -----
c
COMPLEX F(0:N),W,WP,X,Y
INTEGER GROUPSTART,GROUPSIZE,HALFSIZE
c
c check validity of arguments
IF (ABS(S) .NE. 1.) THEN
 WRITE(*,*)' Illegal argument S passed to FFT.'
 STOP
END IF
NT=1
DO WHILE (NT .LT. N)
 NT=2*NT
END DO
IF (NT .GT. N) THEN
 WRITE(*,*)' FFT requires N to be a power of 2.'
 STOP
END IF
c
c Arguments are OK.
c
c Do subscript bit reversal.
c
c IREV is bit-reversed counter - set initial value:
IREV=N/2
c
c zero and N-1 are their own bit reverses; do the rest
DO I=1,N-2
c
c do the reversal only once (since forward and reverse
c counters each take on any given value one time):
IF (IREV .GT. I) THEN
 X=F(IREV)
 F(IREV)=F(I)
 F(I)=X
END IF
c
c step the bit-reverse counter, starting at most significant
c bit:
J=N/2
DO WHILE (IREV .GE. J)
 IREV=IREV-J
 J=J/2
END DO
 IREV=IREV+J
c
c end of bit reversal.
END DO
c
c set up for transform.
c
c W is the twiddle factor base, given by

```

```
c W = exp (i*2*pi/GROUPSIZE)
W=(-1.,0.)
c
c groupsize is the length of the subtransform:
GROUPSIZE=2
c
c loop through the group sizes.
DO WHILE (GROUPSIZE .LE. N)
c
c set half-groupsize.
HALFSIZE=GROUPSIZE/2
c
c loop for each group.
DO GROUPSTART=0,N-1,GROUPSIZE
c
c set the power of W, WP, which is the "twiddle factor".
WP=(1.,0.)
c
c loop through the halfgroup.
DO I=GROUPSTART,GROUPSTART+HALFSIZE-1
c
c apply the twiddle factor to the second halfgroup,
then add and subtract to get the next level output.
J=I+HALFSIZE
X=F(I)
Y=F(J)*WP
F(I)=X+Y
F(J)=X-Y
c
c next twiddle factor:
WP=WP*W
c
c end of loop through halfgroup.
END DO
c
c end of loop through all groups.
END DO
c
c W (twiddle factor base) for next size transform:
W=SQRT(W)
IF (AIMAG(W)*S .LT. 0.) W=-W
c
c next group size.
GROUPSIZE=2*GROUPSIZE
c
c end of loop through all group sizes.
END DO
c
c done.
END
```

## SUBROUTINE FFT2(F,M,N,S)

## 1.0 PURPOSE

Computes the radix-2 Fast Fourier Transform, using an in-place algorithm. This program is a duplicate of FFT except that it is coded to access every Mth element of the input array F rather than consecutive elements. Output F in terms of input f is:

$$F(k) = \prod_{j=0}^{N-1} f(j) e^{iSjk^2(\pi)/N}$$

where F and f are tabulated transform values that occupy the same storage. i is the square root of -1. S is the sign of the transform, +/-1. N is restricted to be an integral power of 2.

## 2.0 ARGUMENTS

1. F - (input/output) complex input array, M\*N complex elements. The transform is done in place, so the result is returned to the calling program in F.
2. M - (input) the (integer) skipping factor for accessing the array F. If M = 1, then FFT2 does exactly the same operation as FFT, accessing consecutive elements of F. If M = 2, every second element of F is accessed, etc..
3. N - (input) the (integer) number of elements in F. The subscripts actually used in this routine are 0 to N-1. N is restricted to take on values of integral powers of 2. If N is not so specified, then an error message is issued and the program is STOPped.
4. S - (input) forward/reverse transform sign indicator. Must have a value of +1. or -1.. If S is specified with any other value, then an error message is issued and the program is STOPped.

## 3.0 AUTHOR



6.2.3 If FFT2 is called once with  $S = +1.$ , then again with  $S = -1.$ , or vice-versa, the result will be the original array multiplied by  $N$ . This result is apparent from the foregoing discussion, which says the round-trip transform pair should be multiplied by  $(DD')/(2\pi)$ , which is equal to  $1/N$ , from the formula in paragraph 6.1 .

-----

declarations:

```
COMPLEX F(M,0:N-1),W,WP,X,Y
INTEGER GROUPSTART,GROUPSIZE,HALFSIZE
```

check validity of arguments

```
IF (ABS(S) .NE. 1.) THEN
```

```
 WRITE(*,*)' Illegal argument S passed to FFT2.'
```

```
 STOP
```

```
END IF
```

```
NT=1
```

```
DO WHILE (NT .LT. N)
```

```
 NT=2*NT
```

```
END DO
```

```
IF (NT .GT. N) THEN
```

```
 WRITE(*,*)' FFT2 requires N to be a power of 2.'
```

```
 STOP
```

```
END IF
```

Arguments are OK.

Do subscript bit reversal.

irev is bit-reversed counter - set initial value:

```
IREV=N/2
```

zero and n-1 are their own bit reverses; do the rest

```
DO I=1,N-2
```

do the reversal only once (since forward and reverse counters each take on any given value one time):

```
IF (IREV .GT. I) THEN
```

```
 X=F(1,IREV)
```

```
 F(1,IREV)=F(1,I)
```

```
 F(1,I)=X
```

```
END IF
```

step the bit-reverse counter, starting at most significant bit:

```
J=N/2
```

```
DO WHILE (IREV .GE. J)
```

```
 IREV=IREV-J
```

```
 J=J/2
```

```

 END DO
 IREV=IREV+J
c
c end of bit reversal.
 END DO
c
c
c set up for transform.
c
c w is the twiddle factor base, given by
c w = exp (i*2*pi/groupsize)
c W=(-1.,0.)
c
c groupsize is the length of the subtransform:
 GROUPSIZE=2
c
c loop through the group sizes.
 DO WHILE (GROUPSIZE .LE. N)
c
c set half-group size.
 HALFSIZE=GROUPSIZE/2
c
c loop for each group.
 DO GROUPSTART=0,N-1,GROUPSIZE
c
c set the power of w, wp, which is the "twiddle factor".
 WP=(1.,0.)
c
c loop through the half group.
 DO I=GROUPSTART,GROUPSTART+HALFSIZE-1
c
c apply the twiddle factor to the second half group,
c then add and subtract to get the next level output.
 J=I+HALFSIZE
 X=F(1,I)
 Y=F(1,J)*WP
 F(1,I)=X+Y
 F(1,J)=X-Y
c
c next twiddle factor:
 WP=WP*W
c
c end of loop through half group.
 END DO
c
c end of loop through all groups.
 END DO
c
c w (twiddle factor base) for next size transform:
 W=SQRT(W)
 IF (AIMAG(W)*S .LT. 0.) W=-W
c
c next group size.
 GROUPSIZE=2*GROUPSIZE
c

```

```
c end of loop through all groupsizes.
 END DO
c
c done.
 END
```



SUBROUTINE DCT(X,Y,DKX,DKY,D,NX,NY,WIM)

1.0 PURPOSE

Computes a Discrete Cosine Transform as described below:

If we have a two-dimensional sequence of delta functions that satisfy the conditions

1. Even symmetry about zero in both x and y.
2. Periodicity of  $2\pi/DKX$  and  $2\pi/DKY$ , respectively, in the x and y dimensions.

then that sequence can be represented as an infinite 2-dimensional Fourier cosine series. DCT computes the first NX columns and NY rows (i.e., a rectangle in the low-frequency part) of the 2-dimensional cosine series.

2.0 ARGUMENTS

1. X - (input) x coordinate of one of the series of delta functions.
2. Y - (input) y coordinate of one of the series of delta functions.
3. DKX - (input) frequency interval of cosine series in x dimension.
4. DKY - (input) frequency interval of cosine series in y dimension.
5. D - output array to hold 2-D cosine series. Real\*4 array dimensioned (0:NX,0:NY).
6. NX - (input) integer number of frequency components to determine in x direction. Maximum x frequency in output 2-D series is  $NX*DKX$ .
7. NY - (input) integer number of frequency components to determine in y direction. Maximum y frequency in output 2-D series is  $NY*DKY$ .
8. WIM - (input) real\*4 weight due to images of the point at (x,y). WIM is a multiplicative factor applied to the output. WIM will ordinarily have a value of 4 (for the delta function plus its three images), but is reduced by a factor of 2 for each symmetry-line that (X,Y) occupies. For example,

(0,0) lies on a symmetry line in the x dimension (reducing WIM to 2) and on a symmetry line in the y dimension (further reducing WIM to 1).

### 3.0 AUTHOR

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### 4.0 TESTING SUMMARY

DCT was written in December, 1981, and tested on a Digital Equipment Corporation VAX 11/780 computer, using DEC's VAX FORTRAN compiler. The program is intended to conform to FORTRAN '77 standards, and contains no known non-FORTRAN '77 constructs.

### 5.0 CALLS SUBROUTINES:

None.

### 6.0 USAGE

#### 6.1 Notes

This program is more efficient than the FFT for computing cosines at regular intervals. Note that DCT does not compute a complete transform, since the input function is restricted to be a single delta function plus its images. The true transform of the delta functions is not band-limited, so the use of DCT must be followed by some band-limiting procedure. When DCT is called by FOURFIT (for which it was originally coded), a factor of  $1/(kx^{**2} + ky^{**2})^{**2}$ , which is a strong band-limiting factor, is applied.

#### 6.2 Computed Output

The Fourier cosine series computed by DCT is

$$D(i,j) = \frac{WIM*DKX*DKY}{(pi**2)*w(i)*w(j)} \cos(X*DKX*i) \cos(Y*DKY*j)$$

$$i = (0,1,\dots,NX); \quad j = (0,1,\dots,NY).$$

where  $w(k)=2$  for  $k=0$  and  $w(k)=1$  otherwise.

### 6.3 Inverse Series

The output series is a partial representation of the input delta-function and its symmetric images, if there are any. The full representation is given by:

$$d(x,y) = \prod_{i=0}^{+\infty} \prod_{j=0}^{+\infty} D(i,j) \cos(x*DKX*i) \cos(y*DKY*j)$$

-----

declarations:

```
REAL*4 D(0:NX,0:NY)
COMPLEX*8 COSX,COSY,COSGENX,COSGENY
DATA PI/3.14159265/
```

weight factors

```
WT=WIM*DKX*DKY/PI**2
```

complex exponentials for cosine generation

```
COSGENX=EXP(CMPLX(0.,DKX*X))
```

```
COSGENY=EXP(CMPLX(0.,DKY*Y))
```

do the transform.

```
D(0,0)=WT/4.
```

```
COSX=WT/2.
```

```
DO KX=1,NX
```

```
 COSX=COSX*COSGENX
```

```
 D(KX,0)=REAL(COSX)
```

```
END DO
```

```
COSY=(1.,0.)
```

```
DO KY=1,NY
```

```
 COSY=COSY*COSGENY
```

```
 D(0,KY)=WT/2.*REAL(COSY)
```

```
 COSX=WT
```

```
 DO KX=1,NX
```

```
 COSX=COSX*COSGENX
```

```
 D(KX,KY)=REAL(COSX)*REAL(COSY)
```

```
 END DO
```

```
END DO
```

c  
c      done  
         END

REAL\*4 FUNCTION DICT(X,Y,DKX,DKY,D,NX,NY)

1.0 PURPOSE

DICT (Discrete Inverse Cosine Transform) is a real\*4 function that evaluates a 2-dimensional Fourier cosine series at one output point. Since the output is required at one point rather than over the entire transform domain, DICT is more efficient than a 2-dimensional FFT.

2.0 ARGUMENTS

1. X - (input) real\*4 x coordinate of point of evaluation.
2. Y - (input) real\*4 y coordinate of point of evaluation.
3. DKX - (input) real\*4 frequency interval in the x dimension.
4. DKY - (input) real\*4 frequency interval in the y dimension.
5. D - (input) coefficients of the 2-D cosine series, real\*4 array dimensioned (0:NX,0:NY).
6. NX - (input) integer number of non-zero-frequency terms to compute in the x dimension. Maximum frequency in the x dimension is NX\*DKX.
7. NY - (input) integer number of non-zero-frequency terms to compute in the y dimension. Maximum frequency in the y dimension is NY\*DKY.

3.0 AUTHOR

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4.0 TESTING SUMMARY

DICT was written in December, 1981, and tested on a Digital Equipment Corporation VAX 11/780 computer, using DEC's VAX FORTRAN compiler. The program is intended to conform to FORTRAN '77 standards and contains no known non-fortran constructs.

#### 5.0 CALLS SUBROUTINES:

None

#### 6.0 USAGE NOTES

The function value computed for DICT is given by:

$$\text{DICT} = \prod_{i=0}^{NX} \prod_{j=0}^{NY} D(i,j) \cos(X*DKX*i) \cos(Y*DKY*j)$$

-----

declarations:

```
REAL*4 D(0:NX,0:NY)
COMPLEX*8 COSX,COSY,COSGENX,COSGENY
```

complex exponentials for cosine generation

```
COSGENX=EXP(CMPLX(0.,X*DKX))
COSGENY=EXP(CMPLX(0.,Y*DKY))
```

addemup

```
SUM=0.
COSX=(1.,0.)
DO KX=0,NX
 COSY=(1.,0.)
 DO KY=0,NY
 SUM=SUM+REAL(COSX)*REAL(COSY)*D(KX,KY)
 COSY=COSY*COSGENY
 END DO
 COSX=COSX*COSGENX
END DO
```

done.

```
DICT=SUM
END
```

## SUBROUTINE MATSOL(A,AT,B,C,N)

## 1.0 PURPOSE

Solves the matrix equation  $Ab=c$ , where A is a real NxN matrix, c is a given vector, and b is an unknown vector. Solution is by Gaussian elimination with pivoting.

## 2.0 ARGUMENTS

1. A - (input) real\*4 array dimensioned (N,N). Matrix for solution, remains unchanged by operation of subroutine MATSOL.
2. AT - (work) real\*4 array dimensioned (N,N). Work array used to hold A and its modifications that occur during Gaussian elimination.
3. B - (output) real\*4 vector dimensioned (N). Result of solution of the matrix equation.
4. C - (input) real\*4 vector dimensioned (N). Right-side vector in matrix equation.
5. N - (input) integer size of matrix-vector problem.

## 3.0 AUTHOR

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## 4.0 TESTING SUMMARY

MATSOL was written in December, 1981. It was compiled on a Digital Equipment Corporation VAX 11/780 computer, using DEC's VAX FORTRAN '77 compiler. MATSOL contains no known non-FORTRAN '77 constructs.

MATSOL has been tested with adequate results with N as great as 50.

```
c
c
c 5.0 CALLS SUBROUTINES:
c
c
```

```
c None.
c
c
```

```
c
c 6.0 USAGE NOTES
c
```

```
c Gaussian elimination is used, with pivoting around the
c largest element in the elimination column. Output
c accuracy's dependence on N has not been established. All
c operations are done in single precision. No provision is
c made for detection of singular matrices; a divide-by-zero
c exception occurs if A is singular.
c
c
```

```
c
c REAL*4 A(N,N),AT(N,N),B(N),C(N)
```

```
c copy A into AT, C into B.
```

```
c DO I=1,N
c B(I)=C(I)
c DO J=1,N
c AT(I,J)=A(I,J)
c END DO
c END DO
```

```
c scan through elimination pivot points.
c DO IPIVOT=1,N-1
```

```
c search for largest number in pivot column.
```

```
c CMAX=ABS(AT(IPIVOT,IPIVOT))
c IMAX=IPIVOT
```

```
c DO I=IPIVOT+1,N
c CTEMP=ABS(AT(I,IPIVOT))
c IF(CTEMP.GT.CMAX) THEN
c CMAX=CTEMP
c IMAX=I
c END IF
c END DO
```

```
c swap it into pivot position.
```

```
c IF(IMAX.NE.IPIVOT) THEN
c DO J=IPIVOT,N
c T=AT(IPIVOT,J)
c AT(IPIVOT,J)=AT(IMAX,J)
c AT(IMAX,J)=T
c END DO
c T=B(IPIVOT)
c B(IPIVOT)=B(IMAX)
c B(IMAX)=T
c END IF
```



```
c
c do the elimination.
c PVAL=AT(IPIVOT,IPIVOT)
c BVAL=B(IPIVOT)
c
c scan down the rows.
c DO IROW=IPIVOT+1,N
c RATIO=AT(IROW,IPIVOT)/PVAL
c
c scan across row.
c DO J=IPIVOT+1,N
c
c eliminate.
c AT(IROW,J)=AT(IROW,J)-AT(IPIVOT,J)*RATIO
c
c END DO
c
c and adjust B in the same way.
c B(IROW)=B(IROW)-BVAL*RATIO
c
c END DO
c
c END DO
c
c back substitution.
c B(N)=B(N)/AT(N,N)
c
c scan up the rows.
c DO IPIVOT=N-1,1,-1
c
c add up the known parts.
c SUM=B(IPIVOT)
c DO J=IPIVOT+1,N
c SUM=SUM-AT(IPIVOT,J)*B(J)
c END DO
c
c determine the unknown.
c B(IPIVOT)=SUM/AT(IPIVOT,IPIVOT)
c
c END DO
c
c END
```

## SUBROUTINE TOCOMPLEX(DR,DC,LX,LY,MX,MY)

## 1.0 PURPOSE

Takes the real, 2-dimensional array DR and puts it into the bottom corner of the complex, 2-dimensional array DC, converting the real numbers into complex numbers with zero imaginary part.

## 2.0 ARGUMENTS

1. DR - (input) array of real numbers that are to be made complex and placed in the corresponding locations of the complex array DC (which must have the same or larger dimension). Dimensioned (0:LX, 0:LY).
2. DC - (output) complex array, dimensioned (0:MX-1, 0:MY-1).
3. LX - (input) integer dimension for DR.
4. LY - (input) integer dimension for DR.
5. MX - (input) integer dimension for DC. Must be greater than LX.
6. MY - (input) integer dimension for DC. Must be greater than LY.

## 3.0 AUTHOR

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## 4.0 TESTING SUMMARY

TOCOMPLEX was compiled and tested in December, 1981, on a Digital Equipment Corporation VAX 11/780 computer, using DEC's VAX FORTRAN '77 compiler. It contains no known non-FORTRAN '77 constructs.



## SUBROUTINE TOREAL(DC,DR,LX,LY)

## 1.0 PURPOSE

Performs the following operations on the complex output of an FFT:

- Keeps only the real part of the 2-dimensional FFT output, and only the part with even symmetry in the x dimension. This corresponds to terms of the form:

$$\frac{1}{2} \text{Real} \left[ e^{i(k_x x + k_y y)} + e^{i(-k_x x + k_y y)} \right]$$

This reduces to terms of the form:

$$\cos(k_x x) \cos(k_y y)$$

- Moves the result into the low-subscript corner of the array DR.

By keeping the specified terms, the operation of a 2-dimensional FFT followed by a call to TOREAL is equivalent to a 2-dimensional cosine transform.

## 2.0 ARGUMENTS

- DC - (input) array of complex numbers that are to be made real by discarding the imaginary part and keeping the part that is even in x, and placing the results in the corresponding locations of the real array DR. Dimensioned (0:2\*LX-1,0:2\*LY-1). DC is assumed to be arranged in the usual fashion for FFT arrays, with positive frequencies in the range (0:LX,0:LY) and negative frequencies in the range (LX+1:2\*LX-1,LY+1:2\*LY-1).
- DR - (output) complex array, dimensioned (0:LX,0:LY). Normally DR occupies the same storage as DC, since compression-in-place is possible.
- LX - (input) integer dimension for DC and DR.
- LY - (input) integer dimension for DC and DR.



END

REAL\*4 FUNCTION DOT(F,G,W,N)

### 1.0 PURPOSE

Computes the dot product of F and G, weighted by W. The function value is:

$$\text{DOT} = \sum_{i=1}^N F_i G_i W_i$$

### 2.0 ARGUMENTS

1. F - (input) real\*4 vector dimensioned (N). First factor of dot product.
2. G - (input) real\*4 vector dimensioned (N). Second factor of dot product.
3. W - (input) real\*4 vector dimensioned (N). Weighting factor of dot product.
4. N - (input) integer length of vectors in dot product.

### 3.0 AUTHOR

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### 4.0 TESTING SUMMARY

DOT was compiled and tested on a Digital Equipment Corporation VAX 11/780 computer, using DEC's VAX FORTRAN '77 compiler. It contains no known non-FORTRAN '77 constructs.

```
c
c 5.0 CALLS SUBROUTINES:
c
```

```
c None.
c
```

```
c 6.0 USAGE NOTES
c
```

```
c The weighting factor is included as a facility for FOURFIT,
c which applies weights to dot products according to the
c number of images possessed by a data point in a symmetric
c fitting domain. See FOURFIT documentation.
c
```

```
c -----
c
c declarations:
```

```
c REAL*4 F(N),G(N),W(N)
```

```
c clear the sum.
```

```
c SUM=0.
```

```
c addemup.
```

```
c DO I=1,N
```

```
c SUM=SUM+F(I)*G(I)*W(I)
```

```
c END DO
```

```
c transfer the answer to the function value.
```

```
c DOT=SUM
```

```
c done.
```

```
c END
```



## FUNCTION SUM(F,W,N)

## 1.0 PURPOSE

Computes the sum of F, weighted by W. The function value is:

$$\text{SUM} = \sum_{i=1}^N F_i W_i .$$

Obviously, this result can also be considered as the dot product of F and W.

## 2.0 ARGUMENTS

1. F - (input) real\*4 vector dimensioned (N). Vector to be summed.
2. W - (input) real\*4 vector dimensioned (N). Weights to be applied to summation vector.
3. N - (input) integer length of summation and weighting vectors.

## 3.0 AUTHOR

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## 4.0 TESTING SUMMARY

DOT was compiled and tested on a Digital Equipment Corporation VAX 11/780 computer, using DEC's VAX FORTRAN '77 compiler. It contains no known non-FORTRAN '77 constructs.

c 5.0 CALLS SUBROUTINES:

c  
c None.

c  
c  
c

c 6.0 USAGE NOTES

c  
c This routine is called by FOURFIT to compute summed elements  
c of vectors, with weights applied to compensate for the  
c number of images possessed by each known data point. See  
c FOURFIT documentation.

c  
c  
c

-----  
c declarations:

REAL\*4 F(N),W(N)

c  
c clear the sum.  
c SUM=0.

c  
c

addemup.

DO I=1,N

    SUM=SUM+F(I)\*W(I)

END DO

c  
c

done.

END