MRC CAMBRIDGE IMAGE PROCESSING SYSTEM

(Last update: 10-Jun-97)

CONTENTS

1. Overview and general philosophy

The system of image processing programs developed by past and present members of the Laboratory is used in various forms worldwide for determining the structure of macromolecular assemblies. The approach has been to study specimens with some form of symmetry, such as crystals or helical and icosahedral particles. Programs suitable for many kinds of 2-D and 3-D analysis have been written. The philosophy has been to write largely stand-alone FORTRAN programs for carrying out the various steps of processing. At the present time (November 2000), there are about 70 stand-alone programs, varying in length from a few lines to many thousands of lines of code. The unifying principle has been to use a standard format (MAPFORMAT) for images and Fourier transforms and postscript format for graphics files. These are also used in the crystallographic CCP4 system. In the later stages of some of the procedures, for example in high resolution electron crystallography, amplitudes and phases are put into a third standard format, that of LCF (labelled column format), which allows direct access to the X-ray crystallographic software in CCP4.

Libraries of standard subroutines are available for reading, writing and manipulating files. A user program written to accept files in these three formats and producing output in the same three formats thus fits directly into the system, with no need for any modifications to existing structures. The libraries can be invoked at the linking step on a DEC/Alpha or Silicon graphics under UNIX. We have produced FORTRAN user codes that will run under either system without modification.

MAPFORMAT involves each image or transform having an initial header block 1024 bytes long, which specifies the type and size of the file, the maximum, minimum and mean densities and information about origins. Most importantly it also contains a label field which provides a history of processing operations that have been applied to the image; the convention is that each program adds a label containing a one line description of the operation and time of running. More information about IMAGE format files and the subroutines (IMSUBS2000) for manipulating them is given in section 5. Briefly, the IMSUBS2000 routines are written in FORTRAN and themselves call lower level routines for the actual reading and writing; these lower level routines are written in FORTRAN and in C. Programs producing graphical output use PLOT2K routines and the resulting postscript format files can be sent to a laserprinter, or viewed on a terminal, using programs such as ghostscript or xview which may be installation dependent. Thus apart from getting digitized data into the system and hard copy out, the system of programs can be used as a coherent whole, independent of the particularities of the installation.

2. How to get started.

Installation is described in /image2000/README. First build all the libraries and executables using a .bld file specific to your system. Binaries will then be written to /image2000/bin and all have the extension .exe

2.1 Using existing libraries

For developing a new program, the following libraries might need to be invoked:

ifftlib	Fourier transform routines
imlib2k	Routines for handling image format
genlib	Lower level routines invoked by imlib
plot2klib	Graphics routines
misclib	Miscellaneous routines from mtzlib, lcflib, miscsubs

2.2 UNIX implementation

The standalone programs, while (mostly) written in standard FORTRAN, call various subroutines which hopefully carry all the machine specific subroutines. For UNIX implementation, the following source libraries will be needed, as discussed above (section 2.1):

```
ifftsub.for
imsubs2000.for
imsubs2.for
ccplib
diskio
library.c
unix
lcflib
mtzlib
miscsubs.for
plot2k.c
```

2.3 Example program showing use of image routines

Shown below is a simple example of a program to rotate an image by 90 degrees. Here only imlib2k and genlib would be needed.

```
C*ROTIM90.FOR************************************************************
C     Example program to rotate image 90 degrees
C     Input on logical stream IN, output on logical stream OUT
C
      DIMENSION ARRAY(1000000),TITLE(20),NXYZ(3),MXYZ(3),ALINE(1000),
     1 NXYZ1(3),MXYZ1(3),LABELS(20,10)
      CHARACTER DAT*24
      EQUIVALENCE (NX,NXYZ(1)),(NY,NXYZ(2)),(NZ,NXYZ(3))
C
      WRITE(6,1000)
1000  FORMAT('1',//'   ROTIM90 : Rotate image 90 degrees'//)
C     Open image stream 1 for input
      CALL IMOPEN(1,'IN','RO')
C     Read header block
      CALL IRDHDR(1,NXYZ,MXYZ,MODE,DMIN,DMAX,DMEAN)
C     Open image stream 2 for output
      CALL IMOPEN(2,'OUT','NEW')
C
C     Get date and time to include in new header label
      CALL FDATE(DAT)
      ENCODE(80,1100,TITLE) DAT
1100  FORMAT('  ROTIM90 : rotate image 90 degrees',A20)
C     Set new image dimensions, swapping x and y
      NXYZ1(1)=NXYZ(2)
      NXYZ1(2)=NXYZ(1)
      NXYZ1(3)=NXYZ(3)
      MXYZ1(1)=MXYZ(2)
      MXYZ1(2)=MXYZ(1)
      MXYZ1(3)=MXYZ(3)
C
C     Get labels from old image
      CALL IRTLAB(1,LABELS,NL)
C     Create new header, new dimensions, old MODE and LABELS
      CALL ICRHDR(2,NXYZ1,MXYZ1,MODE,LABELS,NL)
C     Write new header block adding label for this program step
      CALL IWRHDR(2,TITLE,1,DMIN,DMAX,DMEAN)
C
C     Loop over images in file - may be more than 1
      DO 300 IZ=1,NZ
C       Read an image, going to 99 if hit end of file
        CALL IRDSEC(1,ARRAY,*99)
C       Rotate 90 deg
        DO 200 JY=1,NX
          DO 210 JX=1,NY
            IND=(NY-JX)*NX+JY
210       ALINE(JX)=ARRAY(IND)
C         Write out new image a line at a time
          CALL IWRLIN(2,ALINE)
200     CONTINUE
300   CONTINUE
C
C     Close both image streams
      CALL IMCLOSE(1)
      CALL IMCLOSE(2)
      STOP
C     Here if end of file detected on reading
99    WRITE(6,1200)
1200  FORMAT(///'  End of file on stream 1')
      STOP
      END
```

3. Documentation and Index of existing stand-alone programs

P = Procedure i.e. Type the name and program will prompt you.
C = Command file which should be edited and entered as batch job.
I = Interactive program.

INDEX :

General programs for processing micrographs :

1.	HEADER	P	Prints out information in header records.
2.	LABEL	P	Image handling, does a few nice things.
3.	FFTRANS	C	Fast Fourier transform.
4.	TRNOUT	C	Output amplitudes & phases to line printer.
5.	TRMASK	C	Masks transform for filtering
6.	INTERPO	P	General 2D re-interpolation program
7.	BOXIM	C	Standard boxing program for selection of an area.
8.	BOXIMAGE	C	Similar to above, leaves boxed area in original position.
9.	IMEDIT	P	General editing program for image headers
10.	REMORIG	C	Remove origin peak in transform to correct background.
11.	TAPEREDGEK	C	Tapers the edge of an image to remove spikes.
12.	TWOFILE	C	Linear combination, or multiply/divide data in two files.
13.	TIF2MRC	C	Converts TIFF format files to MRC image format.
14.	MRC2TIF	C	Converts MRC image format to TIFF format.

2-dimensional processing programs :

1.	EMTILT	P	Calculate tilt angles from lattice parameters	(RH)
2.	MASKTRANA	C	Masks transform for filtering, like TRMASK	(RH)
3.	AUTOCORRL	C	Autocorrelation calc + expansion - use with QUADSERCH	(JMB)
4.	QUADSERCHK	C	Correlation peak search on lattice, with profile fit	(JMB)
5.	CCUNBENDK	C	Unbend image using list of peaks from QUADSERCH	(JMB/RH)
6.	MMBOXA	C	Sophisticated version of NNBOX, producing Amps, phases	(RH)
7.	TTBOXK	C	Corrects for tilted transfer function, gives Amps, phases	(RH)
8.	TTMASK	C	Combined MASKTRAN and TTBOX, masking + TTF corr on tilted	(RH)
9.	TTREFINE	C	Refines defocus, astig, tilt params on tilted images	(RH)
10.	CTFSEARCH	C	Refine or search for correct defocus, astigmatism	(RH)
11.	CTFAPPLYK	C	Applies CTF to data from MMBOX, with graphical output	(RH)
12.	CTFCALCK	C	Computes CTF curves for chosen values of Cs, KV, Defocus	(RH)
13.	CTFFIND2	C	Determines defocus and astigmatism. (RH)	
14.	CTFFINDA	C	Finds and applies CTF correction. (RH)	
15.	ORIGTILTK	C	Combine data from different images using crystal symmetry	(RH)
16.	LATLINEK	C	David Agard's least squares latline fit of Amps, phases	(DA)
17.	ALLSPACEA	C	Determines space group, origin, beamtilt on single image	(RH)
18.	AVRGAMPHS	C	Overall averaging of amplitude and phase projection data	(RH)
19.	MAKETRAN		Create reference transform from MTZ file - given defocus	(RH)
20.	SCALIMAMP3D		Scales image amplitudes to selected reference data	(RH)

Electron diffraction patterns :
---

1. BACKAUTOK C Calculates radial background and finds centre of pattern
2. AUTOINDEXK C Finds two simplest lattice vectors automatically
3. PICKAUTOK C Integrates and background corrects el.diff. spots
4. MERGEDIFF C Merges e.d. data and does a host of corrections
5. AVRGFDELF C Averages multiple measurements of delta-F from MERGEDIFF
6. SYNCFITP3 C Fits lattice line curves to output from MERGEDIFF
7. AVRGINTENS Overall averaging of electron diffraction ints. in projection

3-dimensional helical programs :
---

1. HLXSEARCH C Determine tilt and origin. (RAC)
2. HLXDUMP C Dumps layer line data from transform (RAC)
3. HLXFIT C Orientations & origins of different particles (RAC)
4. HLXAVG C Averages data from different particles (RAC)
5. HLXFOUR C Fourier program (RAC)
6. HLXPROJ C 2D filtered image from layer line data (RAC)
7. HLXDYAD C Imposes twofold normal to axis (JMS)
8. HLXSEPDAT C Feeder for HLXSEPR (RAC)
9. HLXSEPR C Separates overlapping Bessel functions (RAC)
10. HLXLLOUT C Graphs standard layer line data (RAC)
11. HLXSIMUL C Simulates image of helix (RAC)
12. HLXFITT C Orientations & origins of different particles (UNWIN)

Rotational averaging and filtering :
---

1. RFILTIM C Rotational filtering
2. ROTAV Rotational averaging of 2D images or 3D maps about z axis.
3. IMROTRAN Rotates/translates 2D image - search to maximise correlation.

General display programs :
---

1. LASERTONE General program for output of tone files. (TSH)
2. LASERTEXT General program for output of text files. (TSH)
3. HISTOK Makes histogram of densities in an image. (DAA/RH15)
4. Ximdisp General X-Windows based display program. (JMS)
5. THREED Displays 2D array as simulated 3D contoured surface.
6. SURF Calculates surface
7. LIGHT Displays 3D maps as shaded surfaces. (GV/RAC)

3.2 General programs for processing micrographs

1. HEADER: Version 1.00 11-Jun-87 RH

This is probably the simplest program of all. It simply reads the header information and prints it out. Information in EXTRA locations is also displayed.

2. LABEL: Version 1.28 29-MAR-00 RH

Runs online with prompts. This program is a general purpose program which carries out a variety of useful manipulations. The menu is given below.

Available modes of operation are:

```
    -2: Change INTEGER*2/INTEGER*1 output format
    -1: Change REAL/INTEGER*2 output format
     0: Change Labels
     1: Select region
     2: Linear OD stretch  ( y = mx + b )
     3: Logrithmic  OD stretch ( y = aLOGx + b )
     4: Average adjacent pixels
     5: Output amplitudes or Intensities'
     6: Output Phases (degrees)
     7: Output REAL part of Complex value
     8: Output IMAGINARY part of Complex value
   50: create stack of small boxes centred on coords read from list
    99: More options, mainly for display purposes
         1: VARIOUS 90 DEG TURNS AND MIRRORS
         2: GEOMETRIC STRETCH ( y = m**X )
         3: CUT OFF OVER - AND UNDERFLOWS
         4: GET RID OF OUTLIERS BY INTERPOLATION
```

3. FFTRANS: Version 2.03 22-APR-96 RH

This program will do 2 dimensional FFTs in either direction. The real-space origin is at (1,1) and the origin of reciprocal space is at (1,NY/2+1). The fourier transform of an image NX, NY is NX/2+1,NY complex values. Very large images (up to 8000 * 8000) are transformed using the disc based routine BIGFFT. The switch point is now determined by the available working set size. Small images are processed in core. On the Alliant, everything is in core. 3-dimensional images are treated as image stacks, each section being transformed independently; only single sections of large images may be used.

Input stream IN input image or fourier transform
Output stream OUT output fourier transform or image
No input parameters are required

4. TRNOUT: Version 1.19 29-Mar-00 RAC/JMS

Program to shift quadrant of FFT to produce suitable amplitude & phase output for the line printer i.e. the transform is continuous across the meridian. The output is log base 2 (amplitude) on a scale 0 to 9 and phase is in 10 degree intervals coded A - Z 0 - 9

At present can only put out central 129 columns about F(0,0).

Data input stream 5:
FMAX, IXMAX, IYMAX, XSHFT, YSHFT, IOUT (*)

FMAX sets the level above which all amps are set to 9
IXMAX sets halfwidth to be output in transform steps
IYMAX sets the number of Y lines output. Maximum 256.
XSHFT, YSHFT X & Y shift for phase origin in grid units
IOUT output flag
= 0 writes all output to unit 6
= 1 writes transform output directly to line printer
= 2 writes transform output directly to laserprinter
= 3 amps only to laserprinter
= 4 phases only to laserprinter

Transform input on stream 1 (IN)

Output amplitudes for TONE on stream 2 (OUT).

5. TRMASK: Version 2.0 11-Nov-00 RAC

Program for masking a fourier transform

Data input stream 3:

ISHAPE, IPIXEL (*)
if ISHAPE = 1,2 : IH(I), IK(I), XC(I), YC(I), RAD(I) (*)
if ISHAPE = 3: IH(I), IK(I), XC(I), YC(I), DELX(I), DELY (I) (*)

ISHAPE if = 1 hard edge circular holes
if = 2 soft edge circular holes gaussian weighted to EXP(-2) at edge
if = 3 hard edge rectangular holes
IPIXEL pixel size used in TONE display of transform (in 1/100 inch)
if IPIXEL=0, XC etc taken to be transform steps
IH, IK indices of spot
XC, YC hole centre in mm on TONE output measured from F(0,0) X positive across page to right, Y positive up page, from pixel centre to pixel centre.
RAD radius for circular holes in mm.
DELX half edge lengths for rectangular holes in mm.
DELY " " "

Transform input on stream 1 (IN)
Output masked transform on stream 2 (OUT)

6. INTERPO: Version 1.1 15-Nov-00 RH/RAC

This is a general 2-D interpolation program that allows the user to perform Rotations, Translations, Size alterations and Re-sampling on a skewed or distorted coordinate system.
All interpolation is done by the bi-quadratic method.
The rotation from OLD axis to NEW axis is positive for an anti-clockwise rotation.

7. BOXIM: Version 4.04 04-Apr-00 JMS/RH

(Largely obsolete, use Ximdisp unless special reasons for using BOXIM e.g. Large map)

BOXIM cuts out a specified area from a standard format image file. It is usual first to TONE the file from which a circular or polygonal area can be marked off. A mean density is calculated from the edge points of the box. For a circular area the edge coordinates are calculated line by line to determine whether or not a point lies inside or outside the area. For a polygonal area a line is constructed from each point vertically upwards; if it crosses an even number of box sides it lies outside. If not it lies inside and has the mean density subtracted from it thus 'floating' the new image. (For points close to a box side the slope of the line from the point to vertex 1 of the box side is calculated and compared with the slope of the box side). Finally the new image is moved to the bottom left hand corner of the new box and the rest of the array is padded with zeroes.

INPUT DATA:

FILIN input image file name

FILOUT output image file name

NXPAD,NYPAD,IPIXEL,NOVERT

NXPAD,NYPAD dimensions of output file in X & Y

IPIXEL pixel size of input (output from TONE)

NOVERT number of vertices, 0 for circular box

OX,OY phase origin position

if NOVERT = 0 then

CX,CY,RAD x,y coordinates of centre of circle & radius

else

IPX,IPY x,y coordinates of vertices NOVERT of these

8. BOXIMAGE: Version 3.41 29-Mar-00 JMS/RH

Simple boxing program to create circular or polygonal box with no change in image size. This makes it quite suitable for the FFT cross-correlation method.
Input original image on stream 1 (IN)
Output boxed image on stream 2 (OUT)
derived from BOXIM (27-AUG-82)

```
    1.    NOVERT              -number of vertices, 0 for circular box (*)
    2.    OX,OY          -phase origin position                   (*)
    3a.   CX,CY,RAD1,2,3,4  -centre coords and radii if circle      (*)
                            :note four radii are for a tapered toroidal
                            :mask. A simple circle would have RAD1,2=0
                            :and rad3,4 equal to the required radius.
 or 3b.   PX(I),PY(I)    -coords of vertices if polygon           (*)
                            :note origin is (0,0) at lower left corner.
```

NOTE : Specify points in image wrt origin (0,0) in bottom left corner.
Therefore the middle of a 1024x1024 image is (512,512).

IMPORTANT NOTE : This program does not float the image, but replaces densities outside box by the average along the inside perimeter.

9. IMEDIT: Version 5.0 01-Dec-00 JMS

Interactice program to allow editing of the header, but preserves the input file. Asks for input and output files, then :

```
change NXYZ size parameters......... 1
  change MXYZ sampling parameters..... 2
  change cell parameters.............. 3
  change origin on X,Y,Z.............. 4
  change fast, med, slow axes ........ 5
  change title........................ 6
  change symmetry operators........... 7
  recalculate min, max, mean.......... 8
  print selected area of file......... 9
  turn map.............................10
  invert densities ................... 11
  pad/float image .................... 12
```

10. REMORIG: Version 1.02 23-Jul-94 RH

Remove origin peak in transform in order to correct slowly
varying background in image. Uses inverted cosine bell
with elliptical shape specified by:

    IXZERO   X zero for filter in X steps
    IYZERO   Y zero for filter in Y steps

Input transform on stream 1 (IN)
Output weighted transform on stream 2 (OUT)
Data :

    IXZERO,IYZERO

11. TAPEREDGEK: Version 2.0 20-Aug-00 RH

Simple program to taper edges of a rectangular image so that there are
no sharp discontinuities which make the Fourier tranform contain spikes.
Input original image on stream 1 (IN)
Output featheredged image on stream 2 (OUT)

          --------------------INPUT-------------------
    CARD 1:IAVER,ISMOOTH,ITAPER
    CARD 2:JAVER,JSMOOTH,JTAPER
                IAVER,JAVER:depths of strips parallel to x & y over which
                      averaging takes place.
          ISMOOTH,JSMOOTH:for each pixel running average calculated
                      over area defined by (-ISMOOTH to ISMOOTH) x (IAVER).
                      (Similarly for JSMOOTH)
                ITAPER,JTAPER:depth over which tapering takes place.

12. TWOFILE: Version 2.05 15-Nov-00 RAC

Program to perform simple additions or multiplications on 2 images of
same dimensions and type (i.e. both must be real or both complex).

   Data   ICOMB
          WT1 , WT2   (Only needed if ICOMB=0)
          IORIGIN,ORIGXA,ORIGYA,ORIGXB,ORIGYB (Only needed for complex)

     ICOMB=-1 Divide two image densities pointwise real or complex.
     ICOMB=0 Linear combination (Addition) with weights WT1, WT2
     ICOMB=1 Multiply two image densities pointwise, real or complex.
     ICOMB=2 Multiply first image point by complex conjugate of second
               image point (only useful in complex image(Transform)).

     WT1,WT2 Weights for addition,   Result = (A*WT1 + B*WT2)

     IORIGIN   If 0, do not apply any extra origin shift (to complex images)
              If 1, apply origin shift ORIGXA,ORIGYA to image A(Stream IN1)
              If 2, apply origin shift ORIGXB,ORIGYB to image B(Stream IN2)
              If 3, apply origin shifts to images A and B

First image on stream 1 (IN1)
Second image on stream 2 (IN2)
Added or Multiplied image output on stream 3 (OUT)

13. TIF2MRC: Version 5.15 21-May-99 JMS

Program to convert tiff format files to MRC IMAGE. Prompts for input and output file names.

14. MRC2TIF: Version 1.5 18-Feb-97 JMS

Program to convert MRC IMAGE format files to tiff. Prompts for input and output file names.

3.3 2-Dimensional crystal processing programs :

3.3.1 Image analysis

1. EMTILT: Version 1.0 03-May-81 Peter Shaw

CALCULATE TILT ANGLES FROM TILTED AND UNTILTED RECIPROCAL CELL DEIMENSIONS.
CONVENTION FOR MEASURING TILT AXIS TO ASTAR IS THAT THE ANGLE IS
FROM TILTAXIS TO ASTAR IN THE DIRECTION GIVEN BY ASTAR TO BSTAR
BEING POSITIVE.

```
         ***** TILT ANGLE PROGRAM - PETER SHAW 3.5.81
                 UNTILTED ASTAR,BSTAR,GAMMASTAR ....?
                 TILTED ASTAR,BSTAR,GAMMASTAR .....?
    READ(5,*) A,B,GAMMA
    READ(5,*) AT,BT,GAMMAT
```

2. MASKTRANA: Version 2.04 03-Sep-95 RH

Program for masking a Fourier transform
Input transform in standard format on stream 1 (IN)
Output masked transform in standard format on stream 2 (OUT)
Control file contains parameters for generation of list of holes in
mask on stream 5, normal input stream (MASK)

Mask file in free format

- first record ISHAPE, IAMPLIMIT, ISPOTFILE
  ISHAPE=1 Hard edge circular holes
  2 Soft edge circular holes (Gaussian weighted to EXP(-2) at edge)
  3 Hard edge rectangular holes
  IAMPLIMIT if T then spots allowed through mask are limited in their maximum amplitude (they are reduced to 2x average)
  if F then no amplitude reduction is applied
  ISPOTFILE if F then input from stream 5 as in old program MASKTRAN
  if T then input from file SPOTS

- second record RAD (ISHAPE = 1 or 2) radius (circular holes)
  DELX,DELY (ISHAPE = 3) half edge lengths(rectangular holes)

- third record AX,AY,BX,BY,IHMIN,IHMAX,IKMIN,IKMAX,RMAX,ITYPE
  AX etc, lattice parameters from refined NNBOX output in grid units
  IHMIN etc, set min/max limits on H,K for lattice generator
  RMAX Cutoff radius in transform for lattice generator in grid units
  ITYPE if = 0, then generate all spots
  if = 1, then include only spots of given index (see below)

Followed by record for each required spot to be allowed through mask
IH,IK

Derived from TRMASK(Version 1.04)22-SEP-82 (RAC)

3. AUTOCORRL: Version 2.01 03-Jan-92 RH

This program was adapted from FFTRANS to include
1. Forward transform from image size NX,NY
2. Squaring of transform and placing in larger area
3. Back transform to produce autocorrelation size NX3,NY3

The real-space origin is at (1,1) and
the origin of reciprocal space is at (1,NY/2+1).
The FT of an image NX,NY is NX/2+1,NY complex value.

All transforms are done using Lynn ten Eyck's subroutines.
These allow arbitrary-sized images having a LARGEST PRIME
factor of 19!!.

Only input parameter determines change in size between input
and output image boxes.

Logical I/O assignments are:

IN	input image
OUT	output autocorrelation

4. QUADSERCHK: Version 4.0 23-08-00 RH

CROSS-CORRELATION SEARCHING PROGRAM SEARCHES A CROSS-CORRELATION
MAP CALCULATED SEPARATELY BY THE FFT METHOD BUT GIVES OUTPUT
CONSISTING OF A LIST OF CROSS-CORRELATION PEAKS AND POSITIONS.

NOW PREDICTS DIFFERENCE BETWEEN LATTICE POSITION AND SEARCH POSITION
FROM LOCAL AREA NEAR POINT, OF DIMENSIONS +/- NRANGE IN A AND B.
ON FIRST PASS ONLY THE AREA ALREADY PASSED IN THE SEARCH PROCEDURE
CONTAINS USEABLE INFORMATION;
IN OPTIONAL SECOND PASS THE AREA AHEAD
OF THE CURRENT POINT CONTAINS USEABLE INFORMATION STORED FROM PASS 1.

THIS PROGRAM PRODUCES :-

1. The file 'PROFDATA'; it contains the data for use in CCUNBENDA.
   First the information previously transferrd in file 'PIXPARMS';
   Then the list of best correlation peak positions and the
   heights of their correlation peaks.
2. A plot of the lattice positions searched in which; 1) error
   vectors are shown X10; 2) peak heights are shown as grey levels.
3. The file 'ERRORS'; this contains a list of the differences
   between actual positions of peaks and lattice positions. It
   can be used in a second pass through this program if some
   patches gave bad correlation peaks first time through and look
   as if they could be improved with hindsight

-------CORRELATION PEAKS ARE SEARCHED FOR AROUND THEIR
-------EXPECTED POSITION BASED ON INPUT LATTICE PARAMETERS

```
FILE STRUCTURE IS
  INPUT:
  CARDS ON UNIT 5 :
    1       IPASS,NRANGE            ! controls search learning algorithm.
    2       FILENAME                ! name of cross-correlation file
    3       ISIZEX,ISIZEY           ! SIZE OF TRANSFORM
    4       ASTR1,ASTR2,BSTR1,BSTR2,LREAL
                                    ! Lattice vectors, real(T) or recip(F)
    5       MINA,MAXA,MINB,MAXB     ! NUMBER UNIT CELLS TO SEARCH
    6       KDC,KDR                 ! RADIUS OF CORR SEARCH
    7       IC,IR                   ! POSN OF SEARCH START (0,0 IS ORIGIN)
    8       IPRNT                   ! YES/NO FOR DETAILED PRINTOUT
    9       RADLIMP,RADLIMQ,RADANGP ! ELLIPTICAL CUTOFF.

      IPASS -0 no error input or output, simple search only.
            -1 writes error file with peak positions for use in later pass.
            -2 reads error file for use in better initial peak predict.
      NRANGE- range of previous peaks used in prediction of next peak posn.
      ISIZEX- size of transform in x-pixels (eg. 3000,3000)
      ISIZEY-                  and y-pixels
      ASTR1 - reciprocal space lattice vectors.
      ASTR2 -       ""
      BSTR1 -       ""
      BSTR2 -       ""
      LREAL - use real space params if T, recip space if F
      MINA  - number of unit cells to search for in each direction from
      MAXA  - search origin IC,IR  e.g.(-120,120,-120,120)
      MINB  -   ""
      MAXB  -   ""
      KDC   - search over +/- this number of pixels on each side of the
      KDR   - predicted centre of each correlation peak.
      IC    - position of search origin for the first correlation peak
      IR    - relative to corner of image at 0,0 -  e.g.(1500,1500)
      IPRNT - more (Y) or less (N) printout
      RADLIMP- radius for profile fit in profile units in one direction
      RADLIMQ- same in orthogonal direction -- (20x smaller than pixels)
      RADANGP- angle relative to x-axis of RADLIMP (elliptical)

  INPUT FILES :
     ERRORS      - (Created if IPASS=1); Read if IPASS=2; Contains
                  - list of XERROR,YERROR,PEAK found when IPASS=1
                  - not written or read if IPASS=0
      PROFILE     - Profile used for matching against correlation peaks.
                  - This has been previously obtained from procedure
                  - AUTOCORRL
  OUTPUT FILES:
      PROFDATA    - File contains;
                  - Parameters to be transferred between programs,
                  - including data read in here, maximum value of
                  - peak height, raw list of correlation peak positions
                  - and heights produced by this program and to be used
                  - by CCUNBENDK
     ERRORS      - Produced when IPASS=1; File contains list of
                 XERROR(IA,IB),YERROR(IA,IB),PEAK(IA,IB)
```

5. CCUNBENDK: Version 6.0 23-Aug-00 RH

THE PROGRAM UNBENDS THE CRYSTAL USING OUTPUT
FROM THE CROSS-CORRELATION PEAK SEARCH PROGRAM, CCORSERCH OR
ITS LATER VARIANTS PROFSERCH AND QUADSERCH(0, 1, and 2)

CONTROL DATA :-
CARD 1 : FILE NAME OF INPUT IMAGE FILE.(ONLY HEADER READ IF IOUT=0).
CARD 2 : ITYPE,IOUT,IMAXCOR,ISTEP,LTAPER,RTAPER,LTABOUT
CARD 3 : IKNOTX,IKNOTY,EPS,FACTOR,TLTAXIS
CARD 4 : PLOT TITLE FOR DISTORTION CORRECTION DISPLAY.
and if IOUT = 1,
CARD 5 : FULL FILE NAME FOR OUTPUT OF CORRECTED IMAGE.
CARD 6 : TITLE TO BE ADDED TO CORRECTED IMAGE TITLE RECORD.

INPUT FILES:
CCORDATA - FILE OF PARAMETERS CONTAINING DETAILS OF THE CCORSERCH RUN AND
- RAW LIST OF CORRELATION PEAK POSITION AND HEIGHTS PRODUCED BY CCORSERCH.
PIX(NAME) - ORIGINAL DENSITOMETER RAW IMAGE FILE.

OUTPUT FILES:
PIXOUT(NAME1) - THE UNBENT IMAGE FILE, FULLY CORRECTED FOR THE SMOOTHED DISTORTION CORRECTIONS.
TABLEOUT - The unbending table as used inside the program - may be useful for creation of fixed distortion table, for example, to correct fibre optic distortion in in another program, e.g. pickprofa.for

OPTIONS ARE:
INTERPOLATION OF IMAGE DISTORTION TO PRODUCE
ITYPE = 0 ----- USES CORRELATION PEAKS EXACTLY WITHOUT SMOOTHING.
= 1 ----- SAME USING BICUBIC SPLINE FITTING (NAGLIB).

IOUT = 0 ----- NO OUTPUT, DIAGNOSTICS ONLY.
= 1 ----- CORRECTED IMAGE OUTPUT USING THE SMOOTHED PARAMETERS AS ABOVE.
ISTEP --------- SIZE OF GRID ON WHICH THE INTERPOLATED VECTORS ARE CALCULATED.
IMAXCOR ------- SIZE OF THE MAXIMUM ALLOWED CORRECTION, TO ENABLE THE SIZE OF EACH STRIP READ INTO CORE TO BE CALCULATED - (ISTEP + 2*IMAXCOR).
CORRECTIONS LARGER THAN IMAXCOR ARE REDUCED.
A FURTHER LIMIT THAT IMAXCOR IS NOT GREATER THAN ISTEP WAS INTRODUCED IN Nov-88 TO KEEP THE PROGRAM SIMPLE. BIGGER VALUES WILL NEED A MAJOR REWRITE.
LTAPER -------- T or F (logical*1) for application of a taperedge
RTAPER -------- Radius to be used from centre of ISTEP boxes.
LTABOUT ------- T or F (logical*1) for output of unbending table
IKNOTX -------- NUMBER OF KNOTS TO BE DISTRIBUTED ACROSS IMAGE IN BICUBIC SPLINE MODE OF SMOOTHING -- IKNOTX DESCRIBES DISTORTIONS PARALLEL TO THE TILTAXIS.
IKNOTY -------- NUMBER OF KNOTS -- IKNOTY DESCRIBES DISTORTIONS PERPENDICULAR TO THE TILTAXIS -- THIS WILL NEED TO BE SEVERAL TIMES HIGHER IF THE IMAGE IS OF A HIGHLY TILTED SPECIMEN.
EPS ----------- THRESHOLD FOR DETERMINATION OF RANK OF BICUBIC SPLINE FITTING MATRIX. TRY 0.00001 --- OTHERWISE SEE WRITE-UP FOR NAGLIB E02DAF SUBROUTINE.
THRESH -------- THRESHOLD OF CROSS-CORRELATION PEAK HEIGHT,

CALCULATED AS;
DENMAX (READ FROM CCORDATA) * FACTOR (READ FROM UNIT 5),
, BELOW WHICH THE PEAK IS NOT USED.
TLTAXIS ------- DIRECTION OF TILTAXIS RELATIVE TO NORMAL X-Y AXES OF
IMAGE.

6. MMBOX: Version 2.05 29-Mar-00 RH

More sophisticated version of NNBOX, prints out amplitudes & phases in N * N boxes from a Fourier transform

DATA:

```
    FILIN

    ISER,TITLE (I10,15A4)

    GU     (A)

    GENGRID(A)

    GENPTS (A)

    IPIXEL, IOUT,NUMSPOT, NOH, NOK, NHOR, NVERT  (*)

    FILOUT only if IOUT.NE.0

    XORIG, YORIG  (*)

    RINNER, ROUTER, IRAD, ACELL, BCELL, WIDTH, ABANG  (*)

if GENGRID :

    AX, AY, BX, BY (*)

if .not. GENGRID :

    IH(I), IK(I), X(I), Y(I)  (*)
```

ISER	serial number for run to be printed & output on IOUT.
TITLE	title to be printed & output on unit IOUT.
GU	if YES work in grid units, otherwise in mm.
GENGRID	if YES generate grid from lattice points (1,0) & (0,1)
GENPTS	if YES individual spots requested & generated from grid
IPIXEL	pixel size only used if .not.GU
IOUT	output unit number for serial number and title, then IH,IK,A,P,IQ terminated with IH=100.
NUMSPOT	number of spots to be printed, if 0 defaults to 20.
NOH, NOK	number of orders of spots in H & K direcions
NHOR, NVERT	box size in mm or grid units in horizontal & vertical directions, i.e. X & Y resp. (up to 20 grid units in each direction).
XORIG, YORIG	X & Y phase origin shifts to be added to those added to those read in on the transform
RINNER, ROUTER	inner & outer radius in mm, grid units or Angstroms, within which spots (centre of box) must fall.
IRAD	if IRAD = 0 radii are specified in mm or grid units. IRAD = 1 radii are in Angstroms using a, b, gamma
ACELL BCELL WIDTH ABANG	cell dimensions, thickness (Angstroms)and cell angle gamma. (used to calculate radii when IRAD = 1)
AX,AY,BX,BY	coordinates in mm or grid units of 1,0 & 0,1 spots respectively
IH, IK	indices of individual spot

X, Y coordinates of individual spot.

7. TTBOXK: Version 4.00 28-Aug-2000 RH

Prints out amplitudes & phases in N * N boxes from a Fourier transform, fully corrected for contrast transfer function in tilted image.
DATA :

1. FILIN -- full name of input file (.FFT)

2. ISER,TITLE (I10,17A4)

3. GENGRID (A)

4. GENPTS (A)

4a. LISTPTS (A)
4b. PLOTPTS (A)

5. ISIZEX,ISIZEY,DSTEP,XMAG,CS,KVOLT (*)

6. DFMID1,DFMID2,ANGAST,TLTAXIS,TLTANGL (*)

7. IOUT,NUMSPOT, NOH, NOK, NHOR, NVERT (*)

8. FILOUT only if IOUT.NE.0 -- full name of output file, formatted data.

9 RESMIN, RESMAX, XORIG, YORIG, SEGMNT (*)

10. if GENGRID or GENPTS : AX, AY, BX, BY (*)

11. if GENPTS : IH(I), IK(I) (*)
if .not.GENGRID and .not.GENPTS : IH(I), IK(I), X(I), Y(I) (*)

ISER serial number for run to be printed & output on IOUT.
TITLE title to be printed & output on unit IOUT.
GENGRID if YES generate grid from lattice points (1,0) & (0,1).
GENPTS if YES individual spots requested & generated from grid
if NO all spots within RESMIN to RESMAX generated.
LISTPTS if YES list spots whose amps and phases will be output.
PLOTPTS if YES plot spots with IQ<8 using symbol size propnl to 8-IQ
ISIZEX,Y size of image in x and y, checked against file-header.
DSTEP densitometer stepsize in microns.
XMAG magnification of micrograph.
CS spherical aberration coefficient in mm.
KVOLT microscope voltage in KV, used to calculate wavelength.
DFMID1 defocus in one direction (underfocus +ve)
DFMID2 defocus at 90-degs to above
ANGAST direction for DFMID1 in degrees relative to x,y in transform.
TLTAXIS direction of tiltaxis in degrees relative to x,y in transform,
should be between -90 and +90 degrees.
TLTANGL magnitude of tiltangle.
(+ve for less underfocus at start of scan(y=0)).
if tiltaxis is precisely parallel to y, then TLTANGL
should be positive for less underfocus at x=0.

```
   IOUT         output unit number for serial number and title, followed by
             IH,IK,A,P,IQ terminated with IH=100.
   NUMSPOT      number of spots to be printed.
   NOH, NOK     number of orders of spots in H & K directions to be generated.
   NHOR, NVERT  box size in grid units in horizontal & vertical directions,
                i.e. X & Y resp. ( up to 20 grid units in each
                direction).
   RESMIN, RESMAX inner & outer resolution limits in Angstroms within which
                 spots(centre of box) must fall.
   XORIG, YORIG X & Y phase origin shifts to be added to those
                added to those read in on the transform.
   SEGMNT       segment of reciprocal space within which spots
                must fall to be include in this run. +/- 90
                includes all spots, +45 is half data near tiltaxis
                -45 is half perpendicular to tilt axis.
   AX,AY,BX,BY  coordinates in grid units of 1,0 & 0,1 spots
                respectively.
   IH, IK       indices of individual spots required.
   X, Y         coordinates of individual spots required.


8. TTMASK:       Version    2.00  3-Jan-1992   RH
-------------------------------------------------------

Program for masking a Fourier transform, with simultaneous correction for *
   tilted contrast transfer function.                                      *
                                                                  *
   Output is written on top of input, so keep a copy if you think it will *
   need to be done more than once using different parameters.              *
                                                          *
   Input and output masked transform is on stream 1 (INOUT)                *
                                                                           *
   Data cards for control data file in free format                         *
                                                                           *
1.  ISIZEX,ISIZEY,DSTEP,XMAG,CS,KVOLT              (*)                  *
                                                                           *
2.  DFMID1,DFMID2,ANGAST,TLTAXIS,TLTANGL   (*)                          *
                                                                           *
3.   ISHAPE=1 Hard edge circular holes      (*)                           *
        2 Soft edge circular holes (Gaussian weighted to EXP(-2) at edge) *
                                                                           *
4.    RADMIN,RADMAX (ISHAPE = 1 or 2) radius (circular holes)   (*)       *
      MIN VALUE ON TILT AXIS; MAX VALUE AT 1200 rlu FROM TILT AXIS      *
       ISHAPE = 1 (Hard edged), = 2 (Gaussian fall off to exp(-2) at edge)*
                                                                           *
5.  AX,AY,BX,BY,IHMIN,IHMAX,IKMIN,IKMAX,RMAX,ITYPE,NUMSPOT  (*)           *
     AX    etc,lattice parameters from refined NNBOX output in grid units *
     IHMIN etc, set min/max limits on H,K for lattice generator           *
     RMAX  Cutoff radius in transform for lattice generator in grid units *
     ITYPE if = 0, then generate all spots                                *
           if = 1, then include only spots of given index (see below)     *
                                                                          *
6. Followed by record for each required spot to be allowed through mask   *
       IH,IK      (*)                                                     *
                                                                          *

   ISIZEX,Y       size of image in x and y, checked against file-header.
   DSTEP    densitometer stepsize in microns.
   XMAG     magnification of micrograph.
   CS               spherical aberration coefficient in mm.
   KVOLT    microscope voltage in KV, used to calculate wavelength.
   DFMID1   defocus in one direction (underfocus +ve)
   DFMID2   defocus at 90-degs to above
```

ANGAST direction for DFMID1 in degrees relative to x,y in transform.
TLTAXIS direction of tiltaxis in degrees relative to x,y in transform,
should be between -90 and +90 degrees.
TLTANGL magnitude of tiltangle.
(+ve for less underfocus at start of scan(y=0)).
if tiltaxis is precisely parallel to y, then TLTANGL
should be positive for less underfocus at x=0.

9. TTREFINE: Version 2.04 29-Mar-00 RH

Refines defocus, astigmatism, tiltaxis and tiltangle in images
of thin tilted crystals.
VERY IMPORTANT NOTE : The quality of image data required for success
in this type of least squares refinement is high, particularly
if more than one parameter is to be refined. BE VERY CAREFUL.

DATACARDS :

1. IMODE,NCYC,FSHIFT,LIST,MTZ,MAXIM,LISTS,ISHIFT,IREF (*)

2. FILIN -- full name of input file (.FFT)

3. ISIZEX,ISIZEY,DSTEP,XMAG,CS,KVOLT (*)

4. NUMSPOT, NOH, NOK, NHOR, NVERT (*)

5. RESMIN, RESMAX (*)

6. AX, AY, BX, BY (*)

7. ISPGRP,ORIGH,ORIGK,REVHK,ROT180,SGNXCH (*)

8. DFMID1,DFMID2,ANGAST,TLTAXIS,TLTANGL (*) These are parameters which
can be refined.

9. LABIN FC=F SIGFC=SIGF PHCAL=PHS FOM=FOM ## Program uses SIGFC as t+
the presence of F and F+
test for presence of ph+
data is input on stream+

IMODE	if = 1 Defocus refined = 2 Defocus and astigmatism refined. = 3 Tiltaxis refined. = 4 Tiltangle refined. = 5 All five parameters refined.
NCYC	Maximum number of cycles of refinement.
FSHIFT	Fractional shifts to be applied at each cycle.
LIST	if T, list spots whose amps and phases will be used, and list their resulting details.
MTZ	if T, reads in ref amplitudes from MTZ(or non-MTZ) file. if F, uses dummy amplitudes, in which case the various R-factors and residuals do not mean a lot.
MAXIM	IF T, the program simply maximises the corrected diffraction spot intensities. if F, the program minimises the rms R-factor against LCF amps.
LISTS	IF T, write output to data set 10 for use in statistics program
ISHIFT	IF T, adds 1/3(ax + bx); 1/3(ay +by) to lattice points for use in control calculations. If F does nothing.
IREF	if = 0 Set IREF=0. Read formatted data h,k,a,p; not LCF file = 1 Use LCF file ---- only needed if LCf.eq.T

```
     ISIZEX   size of image, used to check against image file-header.
     ISIZEY
     DSTEP    densitometer stepsize in microns.
     XMAG     magnification of micrograph.
     CS               spherical aberration coefficient in mm.
     KVOLT    microscope voltage in KV, used to calculate wavelength.
     NUMSPOT      number of spots to be printed out at each cycle.
     NOH, NOK     number of orders of spots in H & K directions to be generated.
     NHOR, NVERT  box size in grid units in horizontal & vertical directions,
                  i.e. X & Y resp. ( up to 20 grid units in each
                  direction).
     RESMIN, RESMAX inner & outer resolution limits in Angstroms within which
                   spots(centre of box) must fall.
     AX,AY,BX,BY  coordinates in grid units of 1,0 & 0,1 spots
                        respectively.
     DFMID1   defocus in one direction (underfocus +ve)
     DFMID2   defocus at 90-degs to above
     ANGAST   direction for DFMID1 in degrees relative to x,y in transform.
     TLTAXIS        direction of tiltaxis in degrees relative to x,y in
transform,
                    should be between -90 and +90 degrees.
     TLTANGL        magnitude of tiltangle.
                   (+ve for less underfocus at start of scan(y=0))
                      (or if TLTAXIS is parallel to y, at x=0)
     ISPGRP   two-dimensional space group number (1 - 17)
     ORIGH,ORIGK  phase origin shifts for (1,0) and (0,1) reflection to bring
              phases to the precise crystallographic origin (from ORIGMERG).
     REVHK    reverses H and K before comparing to reference data.
     ROT180   rotates by 180 degs about c-axis. (needed in p3)
     SGNXCH   rotates by 180 degs about a-axis. (needed in p121)
```

The function which this program minimises (when LCF=.TRUE. and MAXIM=.FALSE.) is :-

L = Sum of [1/sigma**2]*[Aobs-Aed*<ctf**2>]**2

where Aed is the scaled (sf+tf) electron diffraction data.
and Aobs is the result of convolution of the F.T. of the image with the F.T. of the function of ctf with position.
See Henderson et al, Utramic.(1986).

10. CTFSEARCH: Version 2.02 19-Mar-95 RH

Refine or search for correct defocus, astigmatisn on data derived from CTFREFINE originally, name changed 4.2.95 from untilted images.

Rectangular images possible; ISIZEX given in data; Y components of lattice parameters must be scaled by ISIZEX/ISIZEY before input.

PROGRAM TO REFINE C.T.F. OF AN IMAGE OF A TWO-DIMENSIONAL CRYSTAL BY ALTERING THE DEFOCUS AND ASTIGMATISM.

INPUT :-

PARAMETERS DESCRIBING IMAGE (AS IN CTFPLOT,CTFAPPLY,ORIGTILT)

CARD 0 : LIST LISTW QMAX ---
IF LIST=.TRUE. (T) GIVES EXTENSIVE OUTPUT OF NUMBERS
IF LISTW=.TRUE. GIVES INFORMATION FOR 'WILSON' PLOT
AS FOR LIST=.TRUE. BUT FOR Q <= QMAX

CARD 1 : AX AY BX BY ISIZEX DSTEP XMAG

CARD 2 : DFMID1 DFMID2 ANGAST CS KV

CARD 3 : TITLE FOR PLOT OF FINAL BEST FIT.

CARD 4 : ORIGH ORIGK TAXA TANGL REVHK ROT180 SGNXCH

CARD 5 : RESMIN RESMAX RESOLUTION LIMITS TO BE USED IN ANGSTROMS.

PARAMETERS DESCRIBING REFERENCE DATA

CARD 6 : ISPGRP,IREF,NCYC,IPHASE,DFSTEP,DFRANGE
(IREF=-1 if no reference data available)
(IREF=0 FOR PROJECTION DATA)
(IREF=1 FOR 3D LCF FILE DATA)
(IREF=2 FOR 3D MTZ FILE DATA)
NCYC IS MAX NUMBER OF CYCLES OF CTF REFINEMENT.
(IPHASE=0 uses only intensities for ctf-refine)
(IPHASE=1 uses amps and phases for complex refinement)
(IPHASE=2 uses phases alone for minimum residual)
DFSTEP,DFRANGE - stepsize and range for IPHASE=2 refinement

CARD 7 : FC=F SIGFC=SIGF PHCAL=PHS FOM=FOM ## (IF IREF=1 LCF CONTROL)

CARD 7 : LABIN AMP=F SIG=SIGF PHASE=PHS FOM=FOM ## (IF IREF=2 MTZ CONTROL)
PROGRAM USES SIGFC AS TEST FOR PRESENCE OF F
AND FOM AS TEST FOR PRESENCE OF MEASURED PHASE.

AX,AY - LATTICE PARAMETERS (FROM NNBOX) OF (1,0) AND (0,1)
BX,BY - IN GRID UNITS.
ISIZEX - SIZE OF DENSITOMETERED ARRAY IN X DIRECTION (E.G. 2048)
DSTEP - DENSITOMETER STEPSIZE IN MICRONS
XMAG - PRECISE MAGNIFICATION NORMALLY WORKED OUT FROM LATTICE PARAMETERS AND KNOWN CELL DIMENSIONS.
DFMID1 - DEFOCUS LEVEL (UNDERFOCUS +VE). IF DFMID2=DFMID1, IMAGE
DFMID2 - IS NON-ASTIGMATIC. OTHERWISE AMOUNT OF DEFOCUS IN TWO ORTHOGONAL DIRECTIONS, DFMID! BEING DEFOCUS IN DIRECTION ANGAST (DEGS) RELATIVE TO X AND Y OF THE FOURIER TRANSFORM
CS - SPHERICAL ABERRATION IN MM.
KV - E.M. ACCELERATING VOLTAGE

```
DATASTREAMS
 'INIMAGE'   - INPUT OF IMAGE DATA             H K AMP PHS IQ RMSBK
 'INREF'     - INPUT OF REFERENCE PROJECTION DATA    H K FOBS(I) PHASE
               ( IF FOBS BUT NO PHASE, SET PHASE = -999.0 )
 'HKLIN'     - INPUT OF REFERENCE 3D LCF OR MTZ DATA
 'WILSONCTF' - Output of data for Wilson plot using CURVY
 'SUMMARY'     - OUTPUT OF RESULTS, for updating of image_info

PARAMETERS TO BE CALCULATED
      (A)...PHASE AGREEMENT OVERALL, IF REFERENCE PHASE DATA EXISTS.
      (B)...CORRELATION COEFF BETWEEN IMAGE AND REFERENCE AMPLITUDES.

THE FUNCTION MINIMISED WILL BE :-
       L =  Sum of [(1/SIGMA**2) * (FIM**2-FREF**2*CTF**2)**2]    (IPHASE=0)
       L =  Sum of [(1/SIGMA**2) * (FIM*COS(DP)-FREF*CTF*)**2]    (IPHASE=1)
       L =  Sum of [DP]    (IPHASE=2)
             where DP is the phase difference between obs and ref data,
             and SIGMA is the error on FIM**2 and FIM respectively.
THIS IS THE SAME AS MAXIMISING      (1/SIGMA**2) * FIM**2 * FREF**2 * CTF**2

          where SIGMA = standard deviation of FIM**2


11. CTFAPPLYK : Version 2.00    13-08-00      RH
-----------------------------------------------

CTFAPPLY : derived from CTFPLOT giving automatic application of C.T.F. to
           phases input from MMBOX and output ready for ORIGTILT.
PROGRAM PLOTS SPOTS FROM MMBOX IN RECIPROCAL SPACE AND C.T.F. PLOT OF IMAGE.

INPUT PARAMETERS
    CARD 1    AX AY BX BY ISIZE DSTEP XMAG
    CARD 2    DFMID1 DFMID2 ANGAST CS KV
    CARD 3    ISER TITLE

       AX,AY   - LATTICE PARAMETERS (FROM NNBOX) OF (1,0) AND (0,1)
       BX,BY   -                                    IN GRID UNITS.
       ISIZE   - SIZE OF DENSITOMETERED ARRAY (E.G. 2048)
       DSTEP   - DENSITOMETER STEPSIZE IN MICRONS
       XMAG    - PRECISE MAGNIFICATION NORMALLY WORKED OUT FROM LATTICE
                  PARAMETERS AND KNOWN CELL DIMENSIONS.
       DFMID1  - DEFOCUS LEVEL (UNDERFOCUS +VE). IF DFMID2=DFMID1, IMAGE
       DFMID2  -  IS NON-ASTIGMATIC. OTHERWISE AMOUNT OF DEFOCUS IN TWO
                  ORTHOGONAL DIRECTIONS, DFMID1 BEING DEFOCUS IN DIRECTION
                  ANGAST (DEGS) RELATIVE TO X AND Y OF THE FOURIER TRANSFORM
       CS      - SPHERICAL ABERRATION IN MM.
       KV      - E.M. ACCELERATING VOLTAGE
       ISER    - SERIAL NUMBER AT HEAD OF OUTPUT FILE.
       TITLE   - TITLE FOR OUTPUT FILE.

 INPUT  DATASTREAM  'IN'
 OUTPUT DATASTREAM  'OUT'
```

12. CTFCALCK : Version 1.10 13-08-00 RH

PROGRAM TO COMPUTE CTF CURVES FOR CHOSEN VALUES OF
CS; KV; DEFOCUS RANGE;

Control cards

1.	KV,CS	voltage, spherical aberration
2.	DSSTEP,DSMAX	reciprocal Angstrom step and maximum
3.	DFSTART,DFEND,DFSTEP	defocus start, finish and interval Note that the number of plot pages will be (DFEND-DFSTART)/DFSTEP.

13. CTFFIND2 : Version 1.00 01-12-00 RH

CTFFIND2 - determines defocus and astigmatism for images of arbitrary size (MRC format). Astigmatic angle is measured form x axis (same convetiones as in the MRC 2D image processing programs).

CARD 1: Input file name for image
CARD 2: Output file name to check result
CARD 3: CS[mm], HT[kV], AmpCnst, XMAG, DStep[um]
CARD 4: Box, ResMin[A], ResMax[A], dFMin[A], dFMax[A], FStep

The output image file to check the result of the fitting shows the filtered average power spectrum of the input image in one half, and the fitted CTF (squared) in the other half. The two halfs should agree very well for a sucessfull fit.

CS: Spherical aberration coefficient of the objective in mm
HT: Electron beam voltage in kV
AmpCnst: Amount of amplitude contrast (fraction). For ice images 0.07, for negative stain about 0.15.
XMAG: Magnification of original image
DStep: Pixel size on scanner in microns
Box: Tile size. The program devides the image into square tiles and calculates the average power spectrum. Tiles with a significatly higher or lower variance are excluded; these are parts of the image which are unlikely to contain useful information (beam edge, film number etc). IMPORTANT: Box must have a value of power of 2.
ResMin: Low resolution end of data to be fitted.
ResMaX: High resolution end of data to be fitted.
dFMin: Starting defocus value for grid search in Angstrom. Positive values represent an underfocus. The program performs a systematic grid search of defocus values and astigmatism before fitting a CTF to machine precision.
dFMax: End defocus value for grid search in Angstrom.
FStep: Step width for grid search in Angstrom.

example command file (UNIX):

```
#!/bin/csh -x
#
#   ctffind2
#
```

```
time /public/image/bin/ctffind2.exe << eof
image.mrc
power.mrc
2.6,200.0,0.07,60000.0,28.0
128,100.0,15.0,30000.0,90000.0,5000.0
eof
#
```

14. CTFFINDA : Version 2.00 28-05-99 RH

This program will attempt to determine the defocus (not yet astigmatism) of any general image whether or not it contains crystalline areas. The program will also apply a CTF correction either by multiplication or division (accompanied by a Wiener filter). Both amplitude and phase contrast with astigmatism can be applied.

The input and output are Fourier transforms

Card input - four cards only

1. IFIND,IAPPLY,IMULT,CTFMINMOD,WAMP - function control (e.g. F T T 0.2 0.07)
2. DFMID1 DFMID2 ANGAST - defocus estimate
3. DSTEP XMAG CS KV - image parameters
4. RESMIN RESMAX - resolution limits to explore

Logical I/O assignments are:

IN	input image transform
OUT	output of ctf-corrected

*

IFIND	- CARRY OUT CTF DETERMINATION AND REFINEMENT, USING STARTING VALUES IF GIVEN - tries from half to double the given defocus using the given astigmatism as a guide to the possible range and therefore rapidity of angular variation
IAPPLY	- APPLY CTF, USING INPUT OR REFINED PARAMETERS
IMULT	- IF 'T' multiply by CTF, if 'F' divide by CTF
CTFMINMOD	- Minimum modulus of CTF to be used in denominator if IMULT='F'. This is similar to the normal Wiener filter
WAMP	- Amplitude Contrast: e.g. 0.07(120kV), 0.04(200kV), etc
ISIZE	- SIZE OF DENSITOMETERED ARRAY (E.G. 2000, 6000)
DFMID1	- DEFOCUS LEVEL (UNDERFOCUS +VE). IF DFMID2=DFMID1, IMAGE
DFMID2	- IS NON-ASTIGMATIC. OTHERWISE AMOUNT OF DEFOCUS IN TWO ORTHOGONAL DIRECTIONS, DFMID1 BEING DEFOCUS IN DIRECTION
ANGAST	(DEG) RELATIVE TO X AND Y OF THE FOURIER TRANSFORM
DSTEP	- DENSITOMETER STEPSIZE IN MICRONS
XMAG	- PRECISE MAGNIFICATION
CS	- SPHERICAL ABERRATION IN MM
KV	- E.M. ACCELERATING VOLTAGE
RESMIN	- RESOLUTION LIMITS TO BE USED IN ANGSTROMS
RESMAX	- " "

15. ORIGTILTK : Version 5.00 01-12-00 RH

THREE-DIMENSIONAL ORIGIN, BEAMTILT AND CRYSTAL TILT REFINEMENT.

NOW DOES REFINEMENT OF BEAM AND CRYSTAL TILTANGLES AND TILTAXES.
derived from ORIGMERG 13.4.84, (RH)
NOTE: TILT REFINEMENT (CRYSTAL AND BEAM) HAS BEEN TESTED ONLY IN
P3 30.12.84
P22121 8.8.88
P4212 4.4.94

THREE-DIMENSIONAL IMAGE COMBINING PROGRAM FOR ALL SEVENTEEN
TWO-SIDED PLANE GROUPS

THIS VERSION --
PRODUCES PLOTTER O/P ON FILE PLOT.PLT(SUBROUTINE GRAPH)
PRODUCES A MERGED LIST OF H,K,ZSTAR,AMPL,PHASE,FILMNO,
DESCRIPTIVE CODE(+/-IQ) ON UNIT 3.
THE MERGED LIST CAN THEN BE READ IN AND USED FOR
CYCLICAL ORIGIN REFINEMENT.
REFINES CRYSTAL TILTAXIS AN TILTANGLE.
REFINES BEAMTILT (MANIFESTED AS A RESOLUTION-DEPENDENT
SHIFT OF THE PHASE ORIGIN).

CARD INPUT ON UNIT 5

1 ISPGRP,NPROG,NTILT,NBEAM,ILIST,ALNG,BLNG,WIDTH,ANG,IPLOT,MINRFL (*)

2 IRUN,LHMIN,LHMAX,IQMAX,IBOXPHS,NREFOUT,NSHFTIN (*)

3 card 3 input depends on the value of NPROG chosen

IF NPROG.EQ.0
THE FIRST SET OF REFLECTIONS MUST BE FOR AN UNTILTED
IMAGE AND ONLY THE UNIQUE REFLECTIONS SHOULD BE PROVIDED
THIS OPTION IS MEANT FOR MERGING RAW DATA -- AS IN ORIGINAL
ORIGMERG - This set of data can have zero observations
provided that SCALE = 1.0 (or any non-zero value) on card 9
IF NPROG.EQ.1
THE FIRST SET OF DATA READ IN WILL BE FROM O/P OF A PREVIOUS
RUN OF ORIGMERG (UNIT 3 O/P). SUBSEQUENT FILMS WILL BE COMPARED
ONLY WITH THIS FIRST SET AND NO MERGED OUTPUT WILL BE POSSIBLE.
THIS OPTION IS MEANT FOR CYCLICAL ORIGIN REFINEMENT OF AN ALREADY
MERGED SET OF DATA.

3 IFILM,TITLE (I10,10A4)

3A Filename -- e.g. SS1:[RH15]P4151.APH (A)

Then the file contains data of following kind.
ISER (*)
IH,IK,A,P (*)
IH=900 (or EOF) --- THIS ENDS THE SET OF REFLECTIONS

```
IF  NPROG.EQ.2 (.LCF) -- (NO INPUT OF ABOVE CARDS 3,4,5, or 6)
 or NPROG.EQ.3 (.MTZ) data
     THE REFERENCE DATA IS A THREE-DIMENSIONAL LCF or MTZ DATA FILE.
     THIS OPTION IS MEANT FOR STRUCTURES THAT HAVE BEEN WELL
     WORKED OVER ALREADY -- E.G. PURPLE MEMBRANE.
        Input is on file with name HKLIN for LCF or MTZ file.

BUT           3  FC=.... SIGFC=.... PHCAL=.... FOM=....   ##(LCF CONTROL)
 or           3  LABIN AMP=... SIG=... PHASE=... FOM=...  ##(MTZ CONTROL)

     PROCEEDS ACCORDING TO NPROG.EQ.1, BUT REFINEMENT IS DONE AGAINST
     AMPLITUDE AND PHASE CURVE-FITTED DATA. THE PHASE ORIGIN IS REFINED
     AS WELL AS (if NTILT=T) THE TILTANGLE AND TILTAXIS. THIS REFINEMENT
     OF ORIGIN AND TILT IS CARRIED OUT SEPARATELY UNTIL THERE IS
     NO FURTHER CHANGE IN THE PARAMETERS.

 4  IFILM,TITLE                                              (I10,10A4)

 5  Filename -- e.g. SS1:[RH15]P4151.APH                          (A)

 6  NWGT                                                          (*)

 7  TAXA,TANGL,IORIGT                                             (*)

 8  ORIGH,ORIGK,STEP,WIN,SGNXCH,SCALE,ROT180,REVHK,CTFREV         (*)

 9  CS,KV,TILTH,TILTK                                             (*)

10  DRESMAX, DRESMIN (BLANK CARD GIVES 100.0,3.5)                 (*)

   Then the file of data contains data of the following kind
    ISER                                                        (*)
    IH,IK,A,P,IQ                                                (*)
    IH=900  (or EOF) --- THIS ENDS THE SET OF REFLECTIONS.

          ANY NUMBER OF FURTHER IMAGES SPECIFIED BY THE ABOVE CARDS CAN
          BE INCLUDED AT THIS STAGE.

11  IFILM<0  --- THIS ENDS DATA INPUT

12 TITLE --- TITLE FOR PLOT OUTPUT IF REQUESTED.            (20A4)
```

##

```
   ISPGRP - NUMBER OF SPACE GROUP AS BELOW
NPROG  - DETERMINES TYPE OF RUN
         IF =0, NORMAL SEQUENTIAL MERGING (OLD ORIGMERG).
         IF =1, READS IN PREVIOUSLY MERGED DATA O/P ON UNIT 3.
            IF =2, READS IN REFERENCE DATA FROM LCF FILE.
            IF =3, READS IN REFERENCE DATA FROM MTZ FILE.
NTILT  -  IF (F) NO CRYSTAL TILTANGLE OR TILTAXIS REFINEMENT.
          IF (T) CRYSTAL TILTANGLE AND TILTAXIS ARE REFINED.
   NBEAM  -  IF (F) NO BEAMTILT REFINEMENT.
             IF (T) BEAMTILT IS REFINED -- IN MILLIRADIANS.
   ILIST  - IF =1 PROGRAM LISTS EACH REFLECTION OTHERWISE
              ONLY THE PLOT OF RESIDUALS AND THE FINAL
              COMBINED LIST OF REFLECTIONS IS GENERATED
   ALNG   -  A AXIS IN ANGSTROMS for untilted crystal.
   BLNG   -  B AXIS IN ANGSTROMS       "        "   .
   WIDTH  -  THICKNESS OF UNIT CELL IN ANGSTROMS
   ANG    -  ANGLE BETWEEN A AND B - ONLY FOR P1 OR P2
   IPLOT  -  IF NOT 0, PLOT FINAL AMPLITUDE & PHASE CURVES
               ON CALCOMP PLOTTER
   MINRFL -  MINIMUM NUMBER OF POINTS REQUIRED FOR A CURVE
               TO BE PLOTTED
   IRUN   - RUN NUMBER, USED AS AN IDENTIFIER ON UNIT 3 O/P
   LHMIN  - MINIMUM H INDEX TO BE PLOTTED
   LHMAX  - MAXIMUM H INDEX TO BE PLOTTED
                 (PROGRAM STOPS AFTER LAST PLOT)
   IQMAX  - REFLECTION NOT USED FOR ORIGIN OR TILTANGLE
              REFINEMENT IF IQ>IQMAX
   IBOXPHS- SIZE OF PHASE ORIGIN SEARCH, (DEFAULT = 121)
   NREFOUT-  IF (F) NO OUTPUT OF REFERENCE PROJECTION DATA.
             IF (T) FILE IS CREATED WITH REFERENCE PROJECTION
                    DATA AT SAME ANGLE AS INPUT DATA.
   NSHFTIN-  IF (F) NO OUTPUT OF ORIGIN SHIFTED INPUT DATA
             IF (T) FILE IS CREATED FROM SHIFTED INPUT DATA
   IFILM  - INTEGER FILM IDENTIFIER
   TITLE  - DESCRIPTION OF FILM
   NIN    - UNIT NUMBER OF INPUT DATA STREAM * NOT USED NOW
   FILIN  - NAME OF FILE CONTAINING H,K,A,P,IQ DATA
   NWGT   - IF (T) THEN READ EXTRA FLMWGT DATA FOR EACH REFLECTION
            IF (F) THEN NO EXTRA WEIGHT DATA.
   ISER   - SERIAL NUMBER OF FILM ON UNIT NIN, MUST=IFILM.
   IH     - H INDEX OF REFLECTION
   IK     - K INDEX OF REFLECTION
   P      - PHASE OF REFLECION
   A      - AMPLITUDE OF REFLECTION
   IQ     - QUALITY OF REFLECTION
```

```
            TAXA   - ANGLE MEASURED FROM THE TILT AXIS TO THE ASTAR-AXIS,
                     MEASURED IN DIRECTION OF A TO B BEING POSITIVE.
            TANGL  - TILT ANGLE IN DEGREES
            IORIGT - IF IORIGT=1, ORIGIN REFINEMENT IS DONE WITH
                         WGT = 1.0 FOR EACH NEW SPOT.
            ORIGH  - INITIAL PHASE SHIFT FOR 1,0 -- IN DEGREES
            ORIGK  - INITIAL PHASE SHIFT FRO 0,1 --  "    "
            STEP   - STEP SIZE IN DEGREES FOR ORIGIN REFINEMENT
                     STEP = 0 ==> NO REFINEMENT
            WIN    - ZSTAR RANGE WITHIN WHICH SPOTS ARE COMPARED
                     FOR SCALING AND ORIGIN REFINEMENT
            SCALE  - MULTIPLIED BY AMPLITUDES BEFORE COMBINATION
                     IF EQUAL TO 0 SCALING IS AUTOMATIC
            SGNXCH - IF NOT EQUAL TO 0, FLIP AROUND A AXIS, USEFUL IN P121
            ROT180 - IF NOT=0, ROTATE 180 DEG ABOUT Z-AXIS, USEFUL IN P1,P3
            REVHK  - IF NOT = 0, H AND K ARE INTERCHANGED ON INPUT.
                     THIS IS A COSMETIC FEATURE TO FACILITATE INDEXING
                     DIFFICULT HIGHLY TILTED FILMS. NOTE THAT ALL OTHER
                     PARAMETERS, SUCH AS TAXA,TANGL MUST REMAIN CORRECT
                     W.R.T. THE ORIGINAL DIRECTIONS FOR H AND K.
          CTFREV - IF NOT = 0,
                   REVERSES SIGN OF STRUCTURE FACTOR BY ADDING 180 DEGS
                   TO THE PHASE. USEFUL FOR LOW DOSE IMAGES WHERE THERE
                   IS UNCERTAINTY ABOUT WHETHER IMAGE IS OVER-FOCUSSED
                   OR UNDER-FOCUSSED.
            CS     - SPHERICAL ABERRATION COEFFICIENT - USED TO GET
                     BEAMTILT ON RIGHT ABSOLUTE SCALE OF MILIRADIANS.
            KV     - MICROSCOPE VOLTAGE - USED TO CALCULATE WAVELENGTH.
            TILTH  - BEAMTILT IN DIRECTION OF ASTAR.
            TILTK  - BEAMTILT IN DIRECTION OF BSTAR.

##############################################################################

    OUTPUT IS MADE VIA
         UNIT   6 - LINEPRINTER
         UNIT   3 - MERGED DATA POINTS(H,K,ZSTAR,AMPL,PHASE,FILMNO,IQ CODE --
                    CAN BE USED BY ORIGREFN FOR FURTHER CYLES OF REFINEMENT.
         PLOT.PLT - PLOT FILE FOR PLOT OUTPUT.
         UNIT   2 - If requested, origin shifted H,K,0,AMP,PHASE of projection.
         UNIT   4 - If requested, H,K,0,REFAMP,REFPHASE for refdata projection.
         UNIT   9 - summary file with refined values of tilt,origin & beamtilt.

    INPUT IS MADE VIA
         UNIT   5 - CONTROL DATA
         UNIT  10 - NEW IMAGES TO BE MERGED, OR PREVIOUSLY MERGED DATASET
         HKLIN    - LCF FILE OF AMPLITUDES AND PHASES. (for NPROG.EQ.2)
         HKLIN    - MTZ FILE OF AMPLITUDES AND PHASES. (for NPROG.EQ.3)

##############################################################################
```

16. LATLINEK: Version 2.00 30-aug-00 RH

This is a program to do fitting of curves to either Intensity or F, Phi data for individual layer lines. Individual weights are used for F's and phases (or I's). Normally a trial set of A,B for each lattice line are input (optionally this can be calculated internally). This trial set is then refined to minimize the weighted least-squares error between F's and Phases.

Input parameters (unit 5):

TITLE 80 Character title for this data set

IPG Plane group number (1-17)

IPAT 0 for F & Phase 1 for Intensity data

AK,IWF,IWP AK = relative weights for phases with respect to the F's
IWF,IWP are flags to use individual weights for F's and Phases in input file:
-1 : use individual sigmas (1/sigma**2)
0 : set all weights = 1.0
1 : use individual weights
IWP= -2 : use individual sigmas; (wt=1/sigma**2);
: phase and sigma both input in degrees

ALAT,ZMIN,ZMAX,DELPLT
ALAT = lattice size in angstroms
ZMIN = minimum z* value expected for data set
ZMAX = maximum z* value expected for data set
DELPLT = z* interval for plotting
if DELPLT = 0.0, then no plotting

DELPRO,RMIN,RMAX,RCUT,PFACT
DELPRO = real-space or patterson-space sampling interval for profile function (in angstroms)
RMIN,RMAX lower,upper boundaries for profile function (angstroms)
in general RMIN = -RMAX
note, overall boundary width must be 2x as wide for Intensities compared to F,Phase
RCUT = distance from either boundary to point where tapering of profile is to start (in angstroms) see also PFACT
PFACT controls mode of tapering, starting RCUT inside of RMIN/RMAX and going towards RMIN/RMAX.
PFACT <= 0 then use linear drop off to zero at RMIN/RMAX
PFACT > 0 then use gaussian roll-off where PFACT = value of gaussian at RMIN/RMAX
(a value of .1 is reasonable)

IGUESS,BINSIZ
IGUESS = 0 to refine input set of lattice data
= 1 to generate a new set
BINSIZ = delta z* for binning observations
This is only used to generate the initial
guess, which is then refined against the
actual obsered data points.
(a value of .005 to .002 is reasonable)

NCYCLS,MPRINT Number of refinement cycles to perform.
If <0 then output initial guess.
If =0 then minimizer goes till end
else (25-50 is quite reasonable)
If MPRINT >0, print var/covar matrix
=0 do not

Data formats (all are free-format):

Observed data [logical unit = OBS] :
H, K, Zstar, Fobs, Phiobs, Weight on Fobs, Weight on Phiobs

If no Fobs for this Zstar you must set Fobs=-999.
If no Phiobs for this Zstar you must set Phiobs=-999.

For Intensity data:
Fobs actually = Iobs
Phiobs should be 0

It is assumed that the H,K are in the correct asymmetric
unit for the symmetry operators to be valid.
The data can be un-sorted on Zstar.

Initial guess for the lattice data [logical unit = GUESS] :
H, K, Zstar, AMP, PHASE

H,K must correspond to the H,K that is on the observed
data file. Data must be sorted in order of increasing Zstar
and MUST be in equal intervals of Zstar. The actual sampling
interval is not critical, as long as it is the same or finer
than the critical sampling interval of 1./(RMAX - RMIN)
If the plane group has an inversion-center along Zstar
then only Zstar >= 0 are allowed; the first value must
correspond to Zstar=0.

Output data [logical unit = OBS] :

H, K, Zstar, Fcalc, Phicalc, SigmaF, SigmaPhi, Figmerit
the figure of merit = cos(Sigmaphi)

Plots are generated on [logical unit = PLOT]

17. ALLSPACEA: Version 1.6 29-Sep-99 RH

Umbrella program to calculate internal phase residual in all 17 space groups from data on a single film. Can do the same thing within one film as ORIGTILT does between different films.

##

CARD INPUT

ON UNIT 'IN'
ANY NUMBER OF SPOTS WITH ANY INDEX (PRECEDED BY TITLE LINE)
H, K, AMPLITUDE, PHASE

ON UNIT 5

1. SYMM, ISPG(17) symmetry required, followed (if SYMM=SPEC) by up to 17 spacegroup numbers - end list of space groups with ##.

This first control card controls the space groups which are to be considered. For example, if axes are the same length and angle is near 90 degrees, then p4, p422, p4212 are sensible, as well as all lower symmetry. The permitted options are

ALL - all spacegroups
HEXA - all hexagonal + p2, c2
SQUA - all non-hexagonal
RECT - all rectangular, but not square nor hexagonal
OBLI - p2
TWO - p2
THRE - p3
SIX - p6
FOUR - p4
SPEC - specify spacegroups by a list of numbers.
- p1 is always considered to give statistical comparison

1a. List of spacegroup numbers specified separately (I3)

2. SEARCH,REFINE,TILT,NYC 3*(LOGICAL*1), I5 (* FORMAT)
IF TRUE(T) THEN APPROPRIATE OPERATION IS PERFORMED.
THE SEQUENCE OF OPERATIONS IS PERFORMED SEPARATELY, FOR EACH SPACE GROUP CONSIDERED, IN THE ORDER SHOWN.

3. ORIGH,ORIGK,TILTH,TILTK
STARTING ORIGIN PHASE SHIFT AND STARTING BEAM TILT.

4. STEP,ISIZE
PHASE-SHIFT STEP AND SIZE OF SEARCH AREA FOR PHASE ORIGIN GRID SEARCH.
IF GRID IS 121 X 121, A STEPSIZE OF 3 DEGREES WILL COVER WHOLE CELL.

5. A,B,GAMMA,RIN,ROUT,CS,REALKV
CELL DIMENSIONS AND RESOLUTION RANGE IN ANGSTROMS, SPHERICAL ABERRATION(in mm) AND MICROSCOPE OPERATING VOLTAGE (in KV, used to calcuate the wavelength).

6. ILIST,ROT180,IQMAX
   ILIST=T GIVES MORE DETAILED OUTPUT
   ROT180=1 ENABLES SAME CONVENTION AS OTHER PROGRAMS TO BE USED FOR
     P3 INDEXING CONVENTION - e.g. so that origin is same as in ORIGTILT.
   IQMAX is used to restrict the comparisons to spots with IQ<=IQMAX

```
######################################################################

   Table of phase comparisons to be made
      -  not comparable
      1  directly identical
      H  differ by 180 * H          JSIMPL  = number to compare directly
      K  differ by 180 * K          JSCREW   = number to compare + 180 * M
      HK differ by 180 * (H+K)       where M = H*JH180 + K*JK180


   SPACEGROUP  H=-h +h -h +k +k -k -k +h -h +k -k -h +h -h +h  JSIMPL
               H=                                 -k +k -k +k     JSCREW
 ref in
  prog # symb  K=+k -k -k +h -h +h -h -h +h -h +h +h -h +k -k         JH180
               K=                     -k +k -k +k                        JK180

  1   1   p1         -  -  -  -  -  -  -  -  -  -  -  -  -  -  -  -   0  0   -   -
  2   2   p2         -  -  1  -  -  -  -  -  -  -  -  -  -  -  -  -   1  0   -   -
  3   3b  p12        1  -  -  -  -  -  -  -  -  -  -  -  -  -  -  -   1  0   -   -
  4   "a   "         -  1  -  -  -  -  -  -  -  -  -  -  -  -  -  -   1  0   -   -
  5   4b  p121   K  -  -  -  -  -  -  -  -  -  -  -  -  -  -  -  -   0  1   -  180
  6   "a   "          -  H  -  -  -  -  -  -  -  -  -  -  -  -  -  -   0  1  180  -
  7   5b  c12        1  -  -  -  -  -  -  -  -  -  -  -  -  -  -  -   1  0   -   -
  8   "a   "         -  1  -  -  -  -  -  -  -  -  -  -  -  -  -  -   1  0   -   -
  9   6   p222   1  1  1  -  -  -  -  -  -  -  -  -  -  -  -  -   3  0   -   -
 10   7b  p2221  H  H  1  -  -  -  -  -  -  -  -  -  -  -  -  -   1  2  180  -
 11   "a    "    K  K  1  -  -  -  -  -  -  -  -  -  -  -  -  -   1  2   -  180
 12   8   p22121 HK HK 1  -  -  -  -  -  -  -  -  -  -  -  -  -   1  2  180 180
 13   9   c222   1  1  1  -  -  -  -  -  -  -  -  -  -  -  -  -   3  0   -   -
 14   10  p4     -  -  1  -  1  1  -  -  -  -  -  -  -  -  -  -   3  0   -   -
 15   11  p422   1  1  1  1  1  1  1  -  -  -  -  -  -  -  -  -   7  0   -   -
 16   12  p4212  HK HK 1  1  HK HK 1  -  -  -  -  -  -  -  -  -   3  4  180 180
 17   13  p3     -  -  -  -  -  -  -  -  -  1  -  1  -  -  -  -   2  0   -   -
 18   14  p312   -  -  -  -  -  -  1  -  1  1  -  1  -  -  1  -   5  0   -   -
 19   15  p321   -  -  -  1  -  -  -  1  -  1  -  1  -  1  -  -   5  0   -   -
 20   16  p6     -  -  1  -  -  -  -  -  -  1  1  1  1  -  -  -   5  0   -   -
 21   17  p622   -  -  1  1  -  -  1  1  1  1  1  1  1  1  1  -   11 0   -   -

   Notes:-
      1.  Compare all possible pairs of phases each with error E.
      2.  Error comparing 2 different reflections is   1.414 * E.
      3.  Error comparing reflections toits Friedel is   2.0 * E.
      4.  So Friedel comparisons should have less weight ????

   REFINEMENT OF PHASE ORIGIN AND BEAM TILT IN PROJECTION IMAGES.
    CONTAINS OPTIONS TO CARRY OUT :-
   (A) PHASE ORIGIN SEARCH, ENABLES BEST PHASE ORIGIN TO BE FOUND REGARDLESS
      OF HOW FAR FROM IT THE INITIAL ESTIMATE IS.
   (B) PHASE ORIGIN REFINEMENT. THIS CARRIES OUT LEAST SQUARES REFINEMENT
      TO MINIMISE PHASE RESIDUAL, ONCE THE PHASE ORIGIN MINIMUM IS NEAR.
      THE STARTING POINT CAN BE EITHER THE INPUT ORIGIN OR THE VALUES
      DETERMINED IN (A).
   (C) PHASE ORIGIN AND BEAM TILT REFINEMENT. FOUR PARAMETERS ARE REFINED
      HERE TO COMPENSATE FOR ALL IMAGE PARAMETERS. BEAM TILT CAUSES THE
      APPARENT ORIGIN TO MOVE ALONG A LINE WHEN SPOTS OF
      DIFFERENT RESOLUTION ARE CONSIDERED. THE STARTING POINT FOR PHASE
      ORIGIN IS THE OUTPUT FROM (A) OR (B), OR THE INPUT VALUES. THE
      STARTING POINT FOR THE BEAM TILT IS EITHER (0,0) OR THE INPUT VALUES.

      PERFORMS MINIMISATION (NOT LEAST SQUARES) OF THE RECIPROCAL
               SPACE DISTANCE ERROR
            L = SUM OF 2 * SIN(ABS(PHASEDIFF/2))
```

18. AVRGAMPHS: Version 1.5 10-Nov-95 RH

Input card data:-

Card 0	FLAG	(T or F) post ORIGTILTC ?
	FLAG allows merging of ORIGTILT files	
	with or without ctf values.	
Card 1	NSER,ZMIN,ZMAX	(*) serial number, z-range.
Card 2	IQMAX	(*) maximum IQ to use.
Card 3	A,B,GAMMA	(*) cell dimensions.

PROGRAM TO OBTAIN WEIGHTED AVERAGE PHASES FROM MERGED LIST
INPUT IS OUTPUT FROM ORIGMERG
OUTPUT TO INCLUDE EXPERIMENTAL RESIDUAL AND MERGED FOM

19. MAKETRAN: Version 1.07 29-Mar-00 RH

Create reference transform from MTZ file with given defocus.
This program reads in an MTZ file of diffraction amplitudes and phases from the experimentally determined and merged 3-D data from a 2-dimensional crystal, and writes out the transform of the projection of the structure in the direction, at the magnification, and modified by the requested CTF, for later use as a reference in cross-correlation with the digitised experimental image. The code is derived from a synthesis of bits of ORIGTILT, MASKTRAN, CTFAPPLY & EDMTZ.

Input cards:

CARD 1 : NPROG,ISHAPE,IAMPLIM,RAD
CARD 2 : NX NY DSTEP XMAG
CARD 3 : AX,AY,BX,BY, REVHK,SGNXCH,ROT180
CARD 4 : OX OY TX TY TAXA TANGL A B GAMMA
CARD 5 : RESMIN RESMAX resolution limits to be used in Angstroms
CARD 6 : DFMID1 DFMID2 ANGAST CS KV
CARD 7 : Output transform file name - mapformat, MODE=4 (complex reals)
CARD 8 : Output transform title to be put in image header.

Parameters describing reference data - MTZ format - SUBROUTINE GETSFS.
CARD 9 : ISPGRP,LFPZERO,SFACTOR,BFACTOR
CARD 10: LABIN F=AMP PHS=PHASE FOM=FOM ## -

NPROG - 0 for 2-D crystals
- 1 possible extensions to helical, icosahedral & single part.
ISHAPE - 1 hard edge circular holes
2 soft edge circular (Gaussian weight exp(-2) at edge)
3 hard edge square holes
IAMPLIM - T, limit spot amplitude to 2x average spot amplitude
F, no amplitude reduction
RAD - radius of circular hole or half-dege length of square hole
NX - Size of densitometered array (e.g. 2048 x 2048)
NY -
DSTEP - Densitometer step-size in microns.
XMAG - Precise magnification normally worked out from lattice
parameters and known cell dimensions.
AX,AY - Lattice parameters (from MMBOX) of (1,0) and (0,1)
BX,BY - in grid units.
SGNXCH - IF NOT EQUAL TO 0, FLIP AROUND A AXIS, USEFUL IN P121
ROT180 - IF NOT=0, ROTATE 180 DEG ABOUT Z-AXIS, USEFUL IN P1,P3

```
REVHK   - IF NOT = 0, H AND K ARE INTERCHANGED ON INPUT.
                THIS IS A COSMETIC FEATURE TO FACILITATE INDEXING
                DIFFICULT HIGHLY TILTED FILMS. NOTE THAT ALL OTHER
                PARAMETERS, SUCH AS TAXA,TANGL MUST REMAIN CORRECT
                W.R.T. THE ORIGINAL DIRECTIONS FOR H AND K.
OX,OY   - origin in degrees for (1,0) & (0,1)
TX,TY   - beamtilt in milliradians for (1,0) & (0,1)
TAXA    - Angle measured from the tilt axis to the A-axis,
          measured in direction of A to B being positive.
TANGL   - tilt angle in degrees
A       - cell dimensions and space group angle.
B       -   "
GAMMA   -   "
RESMIN,RESMAX  -   resolution limits to be used in Angstroms
DFMID1  - Defocus level (underfocus +ve). If DFMID2=DFMID1, image
DFMID2  -  is non-astigmatic. Otherwise, amount of defocus in two
           orthogonal directions, DFMID1 being defocus in direction
           ANGAST (degs) relative to X and Y of the Fourier transform.
CS      - Sperical aberration in mm.
KV      - Accelerating voltage in kilovolts
```

20. SCALIMAMP3D: Version 2.11 RH 19-Aug-99

Scales image amplitudes to selected reference data.
Program to scale up image amplitudes to restore the resolution-dependent fall off due to image blurring, radiation damage, temperature factor, static disorder, charging or any other source of power loss. Data will be scaled to a selected reference which has no resolution-dependent fall-off and which is hoped will have a similar amplitude distribution.

card input:

card 1: selected reference data, chosen from FF,BT,LZ,BR: RREF - (A2)
- FF - eldiff formfactors for IAM C,N,O average from Internl Tab Cryst.
- BT - Bacillus thuringiensis toxin cry3a - X-ray amplitudes to 2.5 A.
- LZ - tetragonal lyzozyme.
- BR - bacteriorhodopsin, average of p3 and orthorhombic crystal amps. only the BR selection allows anisotropic scaling to account for the likely orientation of helices perpendicular to membrane.

card 2: type of input data to be scaled:
NPROG,TWOFOLD,BXYMIN,BXYMAX,BZMIN,BZMAX - (*)
- NPROG=0, input is ORIGMERG o/p - H,K,Z,A,P,filmno,IQ,WT,B,CTF
- NPROG=1, input is AVRGAMPHS o/p - H,K,L,A,P,FOM
- NPROG=2, input is AVRGAMP o/p - H,K,L,A,SIGA
- if NPROG=1, TWOFOLD is active (T/F) for setting phase to 0/180

- if NPROG=0, scaling is via B-factors, with BMIN/MAX active
- BXYMIN/MAX minimum and maximum in-plane B-factors to apply
- BZMIN/MAX minimum and maximum vertical B-factors to apply

- if NPROG=1 or 2, scaling is in zones vs chosen reference data

```
card 3:  RESLIMXY, RESLIMZ, BEXTRA
          - resolution limits (Angstroms) in xy,z for SCALORIGTILT.

card 4: filename for data to be scaled        - (character*40)

card 5: cell dimensions and resolution for above: A,B,GAMMA,RESOL - (*)

    cards 4 and 5 can be repeated to produce up to 8 multiple plots if
    the primary purpose of the run is to produce graphical output from
    separate sets of projection data - only possible for AVRGAMPS data.

    INPUT :     - UNIT number is 11, filename from stream 5.
    OUTPUT:
          - output for CURVY on 'SCALIMAMP3D.DAT'         - unit 2
          - scaled up version of required data on  'OUT'  - unit 3
```

3.3.2 Electron diffraction pattern programs

1. BACKAUTOK: Version 3.00 15-Aug-00 RH

PROGRAM TO CALCULATE THE MEAN RADIAL DENSITY (BACKGROUND)
OF AN ELECTRON DIFFRACTION PATTERN - any size rectangular area.
The new version has options to carry out automatic centre
determination, and update of the header into the invisible IEXTRA
records used by the subsequent program PICKYCOR.

Plots three possible background raster choices for PICKYCOR
- only if IEXTRA entries in header are set for DX1,DY1,DX2,DY2
Plots radial background curve
Plots X-average, Y-average, and perimeter Y-average (YCOR)

Data input cards :

0.	IREF,IPLOT	if IREF.eq.'F' no automatic centring if IREF.eq.'T' centre is determined if IPLOT.eq.F' no plots done.
1.	CX,CY	Centre coords relative to centre of film
2.	NPLATE	Film number used to identify outputs
3.	TITLE	Title for same purpose
4.	NPNTS	smoothing over 2*NPNTS+1 in radial curve
5.	IRMAX,IRMIN	max and min limits for X,Y-average plots
6.	IRMAXC,IRMINC	max and min limits for YCORRECTION

Input files required and output files produced :

IN	files of the raw data
OUT	data corrected for radial background and y-correction
FORT2	radial background to be used in PICKPROFA
FORT4	y-correction to be used in PICKPROFA
PLOTBACK	plot output data, radial curve and X and Y variations

2. AUTOINDEXK: Version 3.0 15-Aug-00 RH

This program reads in a digitized electron diffraction pattern, to which
background correction has already been applied, searches for peaks,
averages the image areas centred on each peak, then performs a radial
spiral search until the two shortest base vectors are found.
These are the A- and B-axes.
In subroutine REINDEX, which can be a dummy subroutine, the base vector
indexing can be rearranged to fit with a crystal-specific scheme defined
by the user. For example, purple membrane hk requires I(4,3) >> I(3,4).
The lattice parameters together with suggested integration and
background raster sizes are put into the header records of the input file
and the output average picture file.
Output, for cosmetic examination only, is average picture near an average
spot, together with the assigned indexing, on OUT
There is also a plot file showing the selected rasters on PLOTOUT
For input, requires only the file name of the background-corrected
pattern, on IN

3. PICKAUTOK: Version 4.00 18-Aug-00 RH

derived from PICKYCOR much modified program for e.d. spot integration
FLAG TO SUPRESS EXCESSIVE PRINTOUT ADDED, TAC 21-NOV-85
NEW VAR TO DEFINE TILT ANGLE DIRECTION ON MICROSCOPE, TAC 19-NOV-84
NOTE:
****CONVENTIONS FOR TILTDIR APPLICABLE FOR 600 TO 1000 MM CAMERA
****LENGTH ON EM400 MICROSCOPE, WITH OBJECTIVE LENS CURRENT UNDERFOCUSSED.

NOW DOES A YCORRECTION TO REMOVE DENSITOMETER OD DRIFT (JMB) APPROX 1984.
WITH ADDITIONS TO DEAL AUTOMATICALLY W. TLTAXA,TLTANG 25.6.82.
READS RADIAL AVERAGE BACKGROUND CURVE WITH STANDARD DEVIATIONS
TESTS POINTS IN BACKGROUND RASTERS AGAINST MEAN AND STNDEV AT
APPROPRIATE RADIUS; REPLACES VALUE BY MEAN VALUE AT THIS RADIUS
IF DEVIATION IS MORE THAN 3*STNDEV; KEEPS COUNT OF NUMBER OF
SUCH POINTS -- MAY 82 .JMB.
NOW PLOTS RESIDUAL SPOT C.OF G. VECTOR ON UNIT 8, 14.1.81
OFFSET R**3 DISTORTION CORRECTION AND AUTOMATIC MAXRAD CUTOFF 14.1.81
B3 NOW SEARCHED WITHOUT OFFSET -MAY 82- MORE STABLE ALGORITHM.
PICKTILT WITH RADIAL BACKGROUND CORRECTION, 19.5.80
PICKOFF, JOYCE-LOEBL AND NIKON VERSION 29.11.79
LARGER DIMENSIONS AND RASTER, GREATER OVERLAP BETWEEN STRIPS, 3.12.79
MODIFIED FOR TILTED PATTERNS WITH BLURRED SPOTS IN ONE DIRN, 14.12.79
CORRECTS FOR CURVED EWALD SPHERE ROUGHLY, 20.1.81
CHANGED TO ADD *** TO LAST COLUMNS OF TITLE AND SOME EXTRA NUMBERS.
PROGRAM TO INTEGRATE SPOTS ON A LATTICE, STARTING FROM A RECTANGULAR
RASTER SCAN OF THE AREA . EG . OUTPUT FROM ROYAL OBSERVATORY SCANNER

DATA CARDS ARE

1. A,B,G,ANGDIS,SHRINK,TILTDIR,KV,LPRINT
   REAL SPACE CELL DIMENSIONS AND GAMMA ANGLE, ANGLE ON FILM
   PERPENDICULAR TO WHICH A SHRINKAGE BY FACTOR SHRINK IS TO BE
   APPLIED BEFORE CALCULATING FINAL TLTAXIS AND TILTANGLE.
   TILTDIR - DIRECTION OF TILT ON MICROSCOPE,
   -1 = CLOCKWISE
   +1 = COUNTERCLOCKWISE
   LPRINT - T=PRINT ALL REFLECTION INFORMATION
2. J,K
   LOOK-UP TABLE FOR OPTICAL DENSITY; LOOKUP(J)=K
   THIS IS LINEARLY INTERPOLATED FOR J=1,1500. THE FIRST CARD MUST
   HAVE J=1 AND THE LAST J=1500.
3. TITLE FOR LOOK-UP TABLE
4. NPLATE
   PLATE NUMBER
5. TITLE
   TITLE OF DIFFRACTION PATTERN, FOR USE ON OUTPUT FILE.
6. B1, B3
   RADIAL DISTORTION PARAMETERS, ONLY B3 USED CURRENTLY.
7. X0,Y0,

7a. TLTAXA,TLTANG
   COORDINATES OF CENTRE, POSITION OF TILTAXIS (ANGLE FROM TILTAXIS
   TO A-AXIS IN DIRECTION A TO B POSITIVE), SIZE OF TILTANGLE,
   TLTAXA,TLTANG OVERRIDE VALUES CALCULATED INTERNALLY, UNLESS = 0.
   NOTE-----TLTAXA HERE IS ANGLE BETWEEN TILTAXIS AND ASTAR ON FILM.

8. DX1,DY1,DX2,DY2
   POSITION OF (1,0) AND (0,1) RELATIVE TO CENTRE. IF ZERO, THESE
   ARE TAKEN FROM INPUT FILE HEADER.
9. ROUT,RIN,PRPMAX : 4-Apr-1992 now in Angstroms, converted to pixels.
   OUTER AND INNER RADII ; MAXIMUM PERPENDICULAR RESOLUTION FROM
   TILT AXIS FOR SPOTS TO BE INTEGRATED

```
   10. NXM,NYM,NSM,NXB,NYB,NSB,NPOS (TWICE),NTYPE
       NXMT,NYMT, ETC.
        PEAK AND BACKGROUND RASTERS AND POSITION OF BACKGROUND.
        THESE NUMBERS PUT IN TWICE IF IT IS A TILTED DIFFRACTION
        PATTERN, TO GIVE RASTER SIZE, ETC AT MOST BLURRED PART OF PATTERN.
        NPOS=1 IS AT CENTROID OF TRIANGLE, NPOS=2 IS TWICE AS NEAR SPOTS, ETC.
        NTYPE=0,OR 1 DETERMINES POSITION OF 6 BCKGROUNDS AS SHOWN IN
        OUTPUT OF BCKGROUND PROGRAM
      NTYPE=2 GIVES 4 BCKGROUNDS AT CENTRES OF LATTICE;
   11.  FRACT,ABSOL,XAMINE,NCYC,NCYC1
        REFLECTIONS WITH FRIEDEL DIFFERENCES GREATER THAN FRACT AND ABSOL
        ARE REJECTED.  WEAK REFLECTIONS ARE REJECTED FROM CENTRE OF GRAV.
        AND LATTICE PARAMETER CALCULATIONS BY A CRITERION USING XAMINE.
     NCYC=N FOR FIXED NUMBER OF CYCLES=N
     NCYC=0 MEANS GO STRAIGHT TO DATA ASSESSMENT USING INPUT PARAMETERS
     NCYC1=1 FOR PRINT ALL CENTERING RASTERS ON FIRST CYCLE
   12.  NELIM
        IF +VE, NUMBER OF REFLECTIONS TO BE EXCLUDED FROM LATTICE
        REFINEMENT; IF -VE, -NUMBER OF REFLECTIONS WHOSE RASTERS
        ARE TO BE DISPLAYED
   13.  NELH(I),NELK(I),I=1,8
        UP TO 8 INDICES OF REFLECTIONS TO BE EXCLUDED FROM REFINE; OR
        UP TO 8 INDICES OF REFLECTIONS TO BE DISPLAYED;
        OMIT THIS CARD IF NELIM=0

INPUT AND OUTPUT************************************************************

 UNIT 1 : INPUT DENSITOMETERED FILM ARRAY, any size
 UNIT 2 : OUTPUT OF INTEGRATED BACKGROUND SUBTRACTED INTENSITIES.
 UNIT 3 : INPUT RADIAL DENSITY CURVE FOR BACKGROUND CORRECTION.
 UNIT 4 : INPUT Y-AXIS DENSITOMETER DRIFT CURVE FOR BACKGROUND CORRECTION.
 UNIT 5 : INPUT DATASTREAM.
 UNIT 6 : OUTPUT DATASTREAM.
 UNIT 8 : PLOTTER OUTPUT OF SPOT POSNS. AND C.OF G. DEVIATIONS.
 UNIT 9 : INPUT header of image file with autoindexed lattice parameters
```

4. MERGEDIFF: Version 1.5 04-Dec-98 RH

VAX PROGRAM FOR ALL SEVENTEEN TWO-SIDED PLANE GROUPS.
ORIGINAL PROGRAM (SYMMETRY ETC.) S.D.FULLER 10.5.80
USED AFTER MUCH DEBUGGING IN EMBO COURSE 22.9.80
CONVERTED TO INTENSITIES AND S.D.'S ONLY (NO PHASES) RH 13.2.81
---- A USED TO STORE INTENSITY, P USED TO STORE DELTA-INTENSITY
NEW SORTING ROUTINE, SHLSRT, JMB1 14.7.82
TIDIED UP AND GENERALISED TO DO EVERYTHING NEEDED RH +JMB 7.9.82
L.S.CURVE FITTING AND S.D. CALCULATION JMB1 1982.
L.S.REFINEMENT OF TILTAXIS,TILTANGLE RH 14.9.82

IMPORTANT NOTE ##

1. THIS PROGRAM DOES DIFFERENCE COEFFS AND TWIN DETERMINATION IN P3.
2. THE MATRICES AND ONE STATEMENT IN ASYM HAVE BEEN CHANGED SO THAT THE STANDARD ASYMMETRIC UNIT IN P4,P3,P6 SPACE GROUPS HAS LATTICE LINES H,0 AND NOT 0,K PRESENT.

THIS VERSION IS SUPPOSED TO CARRY OUT ALL ACTIVITIES RELATED TO HANDLING ELECTRON DIFFRACTION INTENSITY DATA FROM 3D (TILTED) E.D. PATTERNS IN ANY TWO-DIMENSIONAL SPACE GROUP. IT CAN :-

1. READ IN AND PRODUCE A SORTED, MERGED LIST OF ROUGHLY SCALED DATA FROM ANY NUMBER OF FILMS, EITHER INDIVIDUALLY AND/OR FROM A PREVIOUSLY MERGED LIST.
2. FIT CURVES TO THE MERGED DATA AND PLOT THE WHOLE THING LATTICE LINE BY LINE, WITH THE POINTS,THE FITTED CURVE AND ITS S.D. THIS OPTION IS CURRENTLY DONE BY SEPARATE PROGRAM 'SYNCFIT' TAKING AS INPUT THE DATASET PRODUCED BY MERGHIGH ON UNIT 3
3. PERFORM PROPER SCALING (S.F. AND TEMPF) AGAINST A PREVIOUSLY CALCULATED SET OF CURVES.
4. THE INPUT IS TYPICALLY EXPECTED TO COME FROM PICKTILT (E.D. PATT. PROCESSING PROGRAM) AND OUTPUT TO GO STRAIGHT INTO THE NORMAL CRYSTALLOGRAPHIC SYSTEM.

##

CARD INPUT

0 NSER,TITLER (SER NO. AND TITLE FOR THIS JOB) (I10,10A4)

1 LIST,SORT,NFILE3,NFILE4,IGUIDE,LSUMMARY (IO CONTROL) (*)

2 LREF,LCURVES,BCURVES (REFERENCE DATA SPECS) (*)

3 SCFDET,TA_REFMT,DETWIN,MASK,LMODMSK (OPERATIONAL OPTIONS) (*)

4 ISPGRP,ALNG,BLNG,CLNG,WIDTH,ANG,RRESMAX (STR PARMS) (*)

5 LCF,LMODSIG,ORESMIN,ORESMAX,
AIMIN,AIMAX,DCUTOFF,LPRINT,CCRMAX (*)

5a TITLE IF LCF IS TRUE

```
 FOR EACH FILM TO BE PROCESSED...

   (i)    IFILM, ISUBTRACT, TITLE                                    (*)

   (ii)   NIN,TAXA,TANGL                                             (*)

   (iii)  SCALE,LBISO,TFPAR,TFPERP,
           SGNXCH,ROT180,HKREV,WIN,RESIN                             (*)

   (iv)   MASK(1),MASK(2),MASK(3),MASK(4),TP1,TP2,TP3,TP4            (*)

         (     LFILM,TITLET                                      (I5,18A4)
         (
 ON NIN  (     IH,IK,I,DELI                                      (2I5,2I6)
         (
         (     IH>=900  ---> ENDS THE SET OF REFLECTIONS.

    IFILM<0  ---> ENDS DATA INPUT

#########################################################################


                NSER   - SERIAL NUMBER AND TITLE OF THIS RUN, APPLIED TO
                TITLER - OUTPUT ON UNITS 3,4,6, AND 8,10(WHEN WRITTEN).

  FLAG MATRIX:
               FLAG/ SCFDET  DETWIN TA_REFMT LCURVES  LREF

       0               F       F       F       F       F
       1               F       F       F       F       T
       2               T       F       F       T       T
       3               T       F       T       T       T
       4               T       T       F       T       T
       5               T       T       T       T       T

       FLAGS: (T/F)
               LIST    : Program lists each reflection on input
                          otherwise only merged output on unit 3,4 is generat+
               SORT    : If F, no sorting and suppression of all outputs.
                          Note that this flag supercedes all others.
               NFILE3  : Sorted reflections output to FOR003.
               NFILE4  : Final list of combined reflections output to FOR004.
               IGUIDE  : Add guide points to output where curves extend to
                          higher resolution than data to be merged.
               LSUMMARY: Produce a summary file of merged film data.

               SCFDET  : Scale and temperature factor determination
               TA_REFMT: Tilt axis/angle refinement
               DETWIN  : Detwinning treatment (P3)
               MASK    : Global mask for determining twin proportions
               LMODMSK : Alter mask if one twin type < 0.0

               LREF    : Use reference data for comparisons
               LCURVES : Data read in from curve list vs merged list
               BCURVES : Use binary curves as opposed to ASCII encoded ones

                ISPGRP - NUMBER OF SPACE GROUP AS BELOW
                ALNG   -  A AXIS IN ANGSTROMS
                BLNG   -  B AXIS IN ANGSTROMS
                CLNG   -  C THICKNESS IN ANGSTROMS
                WIDTH  -  WIDTH OF UNIT CELL (ZSTAR COMPARISONS FOR SCALING)
                ANG    -  ANGLE BETWEEN A AND B - ONLY FOR P1
```

RRESMAX- MAXIMUM RESOLUTION CUTOFF FOR REFLECTION CONSIDERATION (Angstroms)

```
LCF    - Produce pre-LCF file for difference Fourier on
         channel 8 (T/F)
LMODSIG- Modify SIG values for output (increases lower limit)
ORESMIN- Associated minumum resolution cutoff
ORESMAX- Associated maximum resolution cutoff
AIMIN  - Associated minimum intensity
AIMAX  - Associated maximum intensity
DCUTOFF- Difference amplitude cutoff
LPRINT - Print Delta F's for low angle correl calc
CCRMAX - Correlation calc max resolution limit
```

Then for each input film:

```
IFILM  - INTEGER FILM IDENTIFIER
ISUBTRACT - new option 4.12.98 to allow possibility of
            subtraction of N0000 from specified film numbers
            to avoid duplicated films being confused as one
            film in later steps of processing
TITLE  - DESCRIPTION OF FILM

NIN    - UNIT NUMBER
TAXA   - ANGLE BETWEEN TILT AXIS AND A AXIS
         MEASURED IN DIRECTION OF A TO B BEING POSITIVE
         I.E. IF TAXA>0 THEN THE TILT AXIS IS CLOCKWISE
         FROM A.
TANGL  - TILT ANGLE IN DEGREES

SCALE  - MULTIPLIED BY AMPLITUDES BEFORE COMBINATION
         IF EQUAL TO 0 SCALING IS AUTOMATIC.
LBISO  - (T/F) flag for iostropic temperature factors.
TFPAR  - Temperature factor to be applied to input data.
TFPERP - Temperature factor to be applied to input data.
          PAR is parallel to tilt axis, PERP is
          perpendicular.  If isotropic temp factor
          desired, only TFPAR used.
SGNXCH - IF T, FLIP AROUND A AXIS(T/F). USEFUL IN P121.
ROT180 - IF T, ROTATE 180 DEGREES ABOUT Z-AXIS(T/F).
         USEFUL IN P1,P3 -- ONLY APPROPRIATE FOR IMAGES.
HKREV  - IF T, EXCHANGE H AND K AXES(T/F). THIS IS A COSMETIC
         FEATURE TO FACILITATE INDEXING OF DIFFICULT TILTED
         FILMS. NOTE THAT TLTAXA AND TLTANG MUST BE CORRECT
         W.R.T. THE ORIGINAL DEFINITIONS OF THE
         DIRECTIONS OF H AND K ON THE FILM.
WIN    - ZSTAR RANGE WITHIN WHICH SPOTS ARE COMPARED
         FOR SCALING

MASK   - Four values for detwinning mask.
BBIN   - Four values to specify twin proportions.
```

Then in each reflection file:

```
LFILM  - FILM NUMBER
TITLET - TITLE ON UNIT NIN (DATA). IF LFILM IS NOT EQUAL TO
         IFILM, THE SEARCH CONTINUES THROUGHOUT UNIT NIN.
```

```
               IH     - H INDEX OF REFLECTION
               IK     - K INDEX OF REFLECTION
               I      - INTENSITY OF REFLECTION
               DELI   - DELTA(S.D.) OF REFLECTION

##############################################################################

   INPUT IS MADE VIA
       UNIT  1 - IF REQUESTED, PREVIOUSLY MERGED DATA LIST
       UNIT NIN - NEW FILMS TO BE MERGED, NORMALLY UNIT 2
       UNIT  5 - CONTROL DATA
       UNIT  7 - PREVIOUSLY FITTED CURVES, STORED IN ASCII, IF REQUESTED
       UNIT  9 - (logical unit BCURVES) PREVIOUSLY FITTED CURVES IN BINARY FO+

   OUTPUT IS MADE VIA
       UNIT  3 - MERGED DATA POINTS IF REQUESTED (H,K,Z,INTENS,DELTA,FILMN)
       UNIT  4 - FINAL LIST OF COMBINED REFLECTIONS (FOR EXAMINATION)
                      (SIMILAR TO UNIT 3, BUT CLEARER FORMAT)
       UNIT  6 - LINEPRINTER
       UNIT  8 - PRE-LCF FILE IF DESIRED
       UNIT 10 - DELTA F VS S FORMATTED DATA, PRODUCED IF LCF=T
       UNIT 11 - Summary of film data, produced if LCF=T
       UNIT 12 - Summary of merged film data, produced if LSUMMARY=T

##############################################################################

     NUMBER   SPACEGROUP    ASYMMETRIC UNIT        REAL   IMAGINARY

          1          P1         H>=0

          2         P21         H,Z>=0              Z=0

          3         P12         H,K>=0              K=0

          4        P121         H,K>=0              K=0

          5         C12         H,K>=0              K=0

          6        P222         H,K,Z>=0            H=0
                                                    K=0
                                                    Z=0

          7       P2221         H,K,Z>=0          (0,2N,Z)  (0,2N+1,Z)
                                                    (H,K,0)
                                                    (H,0,Z)

          8      P22121         H,K,Z>=0            (H,K,0)
                                                   (2N,0,Z)  (2N+1,0,Z)
                                                   (0,2N,Z)  (0,2N+1,Z)

          9        C222         H,K,Z>=0            (H,K,0)
                                                    (H,0,Z)
                                                    (0,K,Z)

         10          P4         H,K,Z>=0            (H,K,0)

         11        P422         H,K,Z>=0            (H,K,0)
                                K>=H                (H,0,Z)
                                                    (0,K,Z)
                                                    (H,H,Z)

         12       P4212         H,K,Z>=0            (H,K,0)
```

		K>=H	(H,H,Z)	
			(2N,0,Z)	(2N+1,0,Z)
			(0,2N,Z)	(0,2N+1,Z)
13	P3	H,K>=0		
14	P312	H,K>=0	(H,H,Z)	
		K>=H		
15	P321	H,K>=0	(H,0,Z)	
		K>H	(0,K,Z)	
16	P6	H,K,Z>=0	(H,K,0)	
17	P622	H,K,Z>=0	(H,K,0)	
		K>=H	(H,H,Z)	

5. AVRGFDELF: Version 4.0 29-Dec-00 RH

PROGRAM TO OBTAIN AVERAGE deltaf's starting from DELTAF outputs from MERGEDIFF

input -

CARD 1.	NFNAT, NFDER	-	Number of films for native and derivati+ to be averaged and subtracted. NFNAT can be zero.
CARD 2.	ZMIN, ZMAX	-	minimum and maximum zstar for average.
CARD 3.	N1....NN	-	Fortran unit numbers for native data
CARD 3A.	WN1...WNN	-	Weights for native data (can be all 1.0)
CARD 4.	D1....DN	-	Fortran unit numbers for derivative data
CARD 4A.	WD1...WDN	-	Weights for derivative data.
CARD 5.	TITLE	-	Title to be used on output file on unit+
CARD 6.	SCALE	-	Overall scale factor

output - will be to UNIT 3, same format as input with 5 dummy numbers at e+ to maintain compatibility with Tom Ceska's EDLCFKPOS program.

6. SYNCFITP3: Version 1.2 05-Nov-98 RH

VERSION FOR P3; USES GUIDE POINTS FROM PREVIOUS CURVES
IF REQUIRED; THESE POINTS INCLUDED WITH DATA FOR LINE WITH
FILM NUMBER SET TO 0
FIT SYNC FUNCTIONS TO LATTICE LINES PRODUCED BY MERGHIGH
WITH OR WITHOUT PREPARATION OF INPUT DATA SET FOR PLOTTING
VERSION INCLUDES ESTIMATES OF ERRORS IN SYNC FUNCTION COEFFS
AND ERRORS IN FITTED CURVE. ALSO CALCULATES MERGING R-FACTORS
UNIT 2 USED FOR FITTED CURVES
THIS VERSION DOES NOT ELIMINATE NEGATIVE SYNC FUNCTION COEFFS
MISSING REGIONS OF THE LATTICE LINE ARE FILLED IN AS INTERNAL
GUIDE POINTS

THERE WILL BE AN OPTION WHICH WILL ALLOW PRINT OUT OF A COMPLETE
SET OF RECIPROCAL LATTICE AMPLITUDES IN A 500 ANGSTROM UNIT CELL FOR
SUBSEQUENT USE IN COMPUTING THE THREE-DIMENSIONAL STRUCTURE.

DATA SETS USED ARE:-

(1) LATTICE LINE DATA POINTS FOR CURVE FITTING
FORMAT OF DATASET:- TITLE RECORD,I10,10A4;
H,K,ZSTAR,AMP,DIFF,IFILM (2I3,F7.4,2F8.1,I6)
TERMINATED 100,100 ETC

(2) DATASET FOR NEW FITTED CURVES
H K 'L' INT SIG
FORMAT (2I4,3(2X,F8.1)); TERMINATED 100,100

(3) OUTPUT FORMATTED LIST OF SYNC FUNCTION COEFFICIENTS
H K; 'L' COEFF
FORMAT F8.1, F12.3

(10) PLOT DATA SET READY FOR PROGRAM PLOTCRVS
BINARY DATA SET- SEE SUBROUTINE POINTS FOR CONTENT OF THIS

```
  DATA CARDS ARE
  (1) IPLOT     (*)
  IF IPLOT=0, FITS SYNC FUNCTIONS AND COMPUTES R-FACTORS ONLY;
  IF IPLOT=1, FITS SYNC FUNCTIONS, COMPUTES R-FACTORS, AND
              PLOTS DATA POINTS AND FITTED CURVES
  (2) ACELL,BCELL,GAMMA       (*)
      2D UNIT CELL DIMENSIONS
  (3) CCELL   C-axis cell dimension for syn-function fit.
  (4) RESMAX,BSINC,SIGMIN,SIGMAX,SIGUID     (*)
      RESMAX; DATA DISCARDED IF (1/D**2) > RESMAX (IN ANGS**-2)
      BSINC;  APPLIES TEMP FACTOR EQUIVALENT TO 2*BSINC TO
              SINCS IN CURVE FITTING
      SIGMIN; MINIMUM SIGMA FOR CURVE FITTING
      SIGMAX; MAXIMUM SIGMA FOR CURVE FITTING
      SIGUID; SIGMA FOR INTERNAL GUIDE POINTS IS SIGUID*(AVERAGE
              SIGMA OF NEAREST DATA POINTS). SIGMA IS DOUBLED
              AS GUIDE POINTS GET FURTHER FROM DATA POINTS.
   (5) SSQFIX,SSQDAT      (*)
       IF SSQFIX=0.0, CALCULATE REQUIRED ERRORS SCALE FACTOR
       FOR EACH LINE AND COMPUTE OVERALL SCALE FACTOR THAT
       WILL BE NEEDED EVENTUALLY
       IF SSQFIX=1.0, USE PREVIOUSLY CALCULATED SCALE FACTOR
       FOR ALL LINES, SET BY SSQDAT
     ALL THESE HAVE DEFAULT VALUES IF SET AS 0.



   DATA SET IN PROGRAM BASED ON VALUE OF C THAT IS INPUT AS DATA:-
        WSTAR
        DZ
        WLHALF
        XMARGN
        SNCSTP
   IRFLMN;  MINIMUM NUMBER OF POINTS IN LATTICE LINE TO CURVE FIT
```

7. AVRGINTENS: Version 1.1 21-Mar-93 RH

PROGRAM TO OBTAIN WEIGHTED AVERAGE INTENSITIES FROM MERGED LIST
INPUT IS OUTPUT FROM TOM'S MERGDIFF PROGRAM
OUTPUT TO INCLUDE EXPERIMENTAL R-FACTOR

Control cards.

1. A,B,GAMMA Cell dimensions for statistics.
2. NSER,ZMIN,ZMAX Serial number on input file and zrange to use.

3.4 3-Dimensional helical programs:

1. HLXSEARCH: Version 2.0 12-Nov-00 RAC

The purpose of this program is to determine the tilt angle of the helix axis out of the plane normal to the direction of view and at the same time to position the phase origin on the particle axis. The user feeds the program with values of amplitude and phase for pairs of peaks in the computed transform. It then computes the sum of F*(phi1-phi2) over these pairs of related reflections. Values of (phi1-phi2) are corrected to allow for odd Bessel orders. They are also corrected for specified values of phase shift and tilt angle. The sum for each combination of phase shift and tilt angles is normalised by dividing by 360n and then scaled from 0 to 90. The normalised sums are output as an array.

Different indexing schemes may be tested in a single run, as described below. A separate residual array is output for each scheme.

DATA input on unit 5

1) TITLE (20A4)

2) OMEGAM,DOMEGA,NOMEGA,EXM,DEX,NEX,NNLAY,NOP,IDIM1,IDIM2 (free format)

OMEGAM,DOMEGA,NOMEGA
Tilt angle for searching:
starting angle in degrees
increment in degrees
no. of points in tilt search

EXM,DEX,NEX
X shift for searching:
starting X shift in angstroms
increment in angstroms
no. of points in X shift search

NNLAY
no. of different selection rules(Bessels)to be tried
up to 12

NOP
no. of pairs of reflections (le. 50)

IDIM1,IDIM2
transform dimensions

3a) Y(I),D(I),F(I),DPHI(I) (free format)
NOP of these pairs of cards

Y layer line spacing in transform Y grid steps

D spacing between reflection pair in transform X steps

F average value of amplitude(arbitrary scale) for the pair of reflections

DPHI (phase of left) - (phase of right) side reflection in degrees

3b) NLAY(I,J) (free format)
bessel order for the layer line in question,NNLAY
different trial values are allowed for each line

2. HLXDUMP: Version 2.00 12-Nov-00 RAC/JMS

Extracts lines of F and phi from transforms of helical particles produced by FFTRANS. The user specifies the location of the layer line in reciprocal space, its length and sampling frequency.

In general, the user will wish to have data at points in reciprocal space which do not correspond to the grid points calculated by FFTRANS, HLXDUMP assigns values to these points by bilinear interpolation. The transform is phase-shifted to bring its origin to the geometric centre of the box transformed (this position is stored on the disc area by BOXIM) before any interpolation is carried out. The results of the interpolation are of course only valid if the original sampling in reciprocal space is fine enough for the phases of the centred array to change slowly from point to point.

The program also corrects for tilts of the helix axis out of the plane normal to the direction of view. The effect of such a tilt is to intersect the cylindrical rings of Gn,l(R) on a chord not passing through the origin. As a result, Gn,l(R) are missed for very small values of R (this is called the eclipsed region). Gn,l(R) for larger values have the correct amplitude but the wrong phase; in addition the radii have been wrongly assigned. The program corrects the phase and reinterpolates along the line at evenly spaced intervals (selected by the user).

It is often found that the layer lines do not have their symmetry axis on the line through the origin which is normal to the layer lines. This problem seems to arise from a shear deformation of the object which manifests itself as a skewness of the transform. The user determines the angle of skewness of the pattern and sets SHEAR. The program centres the lines accordingly.

In addition, ORIGX, ORIGY often does not correspond to the projected axis of the particle. The user can bring the phase origin to the axis by adjusting XSHFT &/or YSHFT, which cause translations of the phase origin parallel to &/or normal to the layer lines respectively.

Note:
Near side means side nearest to the observer of the densitometered array. For this side, reflections from right-handed helices (positive n) are in the top left quarter of the transform, reflections from left-handed helices (negative n) in the top right quarter. Which side it corresponds to physically depends on the orientation of the film during densitometry By our conventions, the side of the particle next to the carbon support film is nearest to the electron beam, and the e.m. film is printed and densitometered emulsion up (same orientation as in the microscope during exposure), so the observer is put in the position of the electron beam, looking at the particle through the carbon.

Data Cards:

TITLE (10A4)

LLTOT,SAMPL,XSHFT,YSHFT,DELBR,ROT,SHEAR,TILT (*)

RMIN,RMAX,IDUMP,MERID,IZERO (*)

LLNO,NORD,YSP (*)

NL1,NL2,NR1,NR2 (*) This record only read in if IDUMP.GE.1

Items 4 (and 5 for IDUMP.NE.0) repeated for each layer line

TITLE identifies the particular choice of data.

LLTOT is the number of separate layer lines to be output.

SAMPL real space sample size in angstroms

XSHFT, YSHFT X & Y phase origin shift in real space steps.

DELBR - the required spacing between points at which the layer line is sampled, in reciprocal Angstroms. DELBR=0.0004 gives one sample/mm. on graphical output on printer.

ROT is the angle of the layer lines relative to the horizontal axes (in degrees). The angle is positive if the layer lines slope up to the right.

TILT tilt of the helix axis (in degrees), calculated by HLXSEARCH

SHEAR is the angle (in degrees) which the transform meridian makes
    with vertical axes. (Positive if meridian to left of vertical).
    N.B. Set equal to ROT if transform not sheared.

RMIN, RMAX limits for layer line plotting in reciprocal angstroms.
          Maximum range -0.2 to 0.2 rec Ang

IDUMP = 0 output graphed only
       = 1 output graphed & dumped to disc.
       = 2 output dumped to disc only

MERID = 0 both halves of meridional layer lines to both sides files
       = 1 only one half of meridionals to each side
       N.B. Set MERID=0 if you are going to use HLXSEPR to separate
             overlapping Bessels.

IZERO = 0 dumps all layer line data
       = 1 dumps only layer line data if NL1 and NL2 (or NR1 and NR2)
             are both non zero

LLNO layer line number

NORD bessel order for the layer line.

YSP Y intercept (in Y transform steps), where layer line crosses
   vertical axis.

NL1, NL2, NR1, NR2 specify the region of the line to be output. They are measured in units of DELBR from the layer line origin. NL1, NL2 are the nearest and furthest points from the origin, of the region of layer line to be output from the left-hand side. NR1, NR2 are the nearest and furthest points from the origin, of the region to be selected from the right-hand half of the layer line.
Note that the meridian corresponds to NL1=NR1=0.

FORMAT OF HLXDUMP OUTPUT:
HLXDUMP automatically separates the layer lines into halves and sorts the halves out into near and far side data, according to the signs of the NORD values. The output, which is read by HLXFOUR etc, has the following format:

TITLE, LLINFO, WTFAC, NORD, LLNO   (10A4,10A1,F10.3,2I5)

R, F, PHI   (3E10.3)

The last record is repeated for each point along the layer line.
The list of points is terminated by a blank record (i.e. R=0.0)
However, R=0.0 is not a terminator if it is on the first record after the title record.
Thus, if there are no points for a particular half layer line,the output at this position will consist of three records; the title record, followed by two blank records.

3. HLXFIT: Version 2.0 13-Nov-00 RAC

Program to determine the relative orientations of two different helical particles, by comparing the phases of corresponding points along the layer lines. The best relative radial scaling of the two images can also be determined.

The 'residual' calculated is:

sqrt(sum(F*(phi1-phi2')2)/sum(F))

where phi2' = phi2 - n dphi + 2pi Z dz

which is tabulated for each angle of rotation (dphi) about the z-axis, each axial shift (dz) and each radial scaling factor applied to the data for particle 2. Any data absent from the data set for particle 2, but present in the reference data set (particle 1) adds a penalty of F1*(90)2 to the residual sum, if IMISS is set to 1 (otherwise, missing data is simply ignored).

If particle 2 is thought to be upside-down relative to particle 1, phi2 is negated.

Data Cards:

FILREF (A)

LLMAX, CANG, DELBR, IPRINT, IMISS (*)

WT(L), L=1,LLMAX (*)

FILIN (A)

TITLE (20A4)

ISIDE, IPOLE (*)

PHIMIN, PHIMAX, DPHI (*)

ZMIN, ZMAX, DZED (*)

RSCMIN, RSCMAX, DRSC (*)

Items 4 to 9 may be repeated as many times as required, so that several data sets may be compared with the same reference (particle 1).

Note that each data set should have the same number of layer lines, in the same order. Dummy data should be inserted for missing layer lines (Title record + 2 blank records - see specification for HLXDUMP output).

FILREF file name for the reference particle.

LLMAX is the number of layer lines to be read in (le. 30)

CANG (in Angstroms), is the axial repeat

DELBR is the spacing of sample points along the layer lines (reciprocal angstroms).

IPRINT if = 1 layerline data printed ,if = 0 data not printed

IMISS if = 1 missing data penalty imposed, if = 0 missing data ignored

WT(I) weighting factors applied to the layer lines..LLMAX of them

FILIN file name for dataset 2, 3 etc.

TITLE for output to line printer

ISIDE = 0 if data 1 & data 2 both correspond to the same side (near or far) of the helix.
= 1 if they differ.

IPOLE is set to 0 if particles are to be compared in their initial polar orientations. If particle 2 is to be turned upside-down, set IPOLE = 1. Note that this inversion is carried out first, before any rotation about the helical axis or translation along the axis.

PHIMIN, PHIMAX specify the range of angles through which particle 2 is to be rotated about Z (anticlockwise rotation, when viewed down the axis corresponds to positive rotation angle).

DPHI the size of the steps between successive rotational orientations in which particle 2 is to be compared with the reference.Up to 12 steps

ZMIN, ZMAX, DZED specify (in Angstroms) the range and step size for the translations parallel to z which are to be tried. Up to 12 steps allowed

RSCMIN, RSCMAX define the range of scaling factors to be applied to distances along the layer lines of particle 2 data:

$$\frac{\text{R-distance of peak in transform 2}}{\text{R-distance of same peak in transform 1}}$$

DRSC is the step size in the radial scaling search - up to 10 steps.

4. HLXAVG : Version 2.0 13-Nov-00 RAC

Program for averaging different sets of layer line data. (Note : HLXFOUR is able to average the two sides of a single particle). The relative orientations of different particles are first determined using HLXFIT, which also supplies amplitude scaling factors if required.

Data for a difference Fourier can be produced, using scaling factors of appropriate signs.

Data sets can be modified for various purposes, e.g. changing the sampling distance (DELBR) of the layer lines, or changing the radial scale.

Data Cards:

TITLE (10A5)

LLMAX, NSIDE, CANG, DELBR, IPRINT (*)

FILIN (A)

ISIDE, IPOLE, PHISHF, ZSHIFT, RSCALE (*)

FSCAL(L), L=1,LLMAX (*)

items 3 to 5 are repeated for each data set (half transforms ?) to be included in the average.

Note that each data set should have layer lines in the same order, with no gaps. Dummy data should be inserted for missing layer lines (Title record, followed by 2 blank records - see specification for HLXDUMP output).

LLMAX is the total number of layer lines to be averaged (le.40).

NSIDE is the total number of data sets to be averaged.

CANG (in angstroms) is axial repeat distance

DELBR spacing of points sampled along the averaged layer lines - usually the same as the spacing in the individual data sets.

IPRINT if = 1 prints layer line data,otherwise does not

FILIN file name for input data set

ISIDE is set to 0 for 'near-side' data, to 1 for 'far-side' data.

IPOLE = 0 if data set is to be included in its initial orientation, = 1 it is to be turned upside-down before addition.

ZSHIFT and PHISHF define the shift (in A) in the positive z-direction & the rotation angle (in degrees) about the z-axis to be applied to the data set to bring the particle into the required common orientation.

RSCALE is a radial scaling factor to be applied to all radial distances along the layer lines, to bring all the data sets to the same size scale

FSCAL are relative scaling factors for the amplitudes on each layer line in case different data sets are on different scales etc.

5. HLXFOUR: Version 2.0 13-Nov-00 RAC

Program to carry out a Fourier-Bessel transformation of layer line data to produce a three-dimensional density map, which may be output as sectiions of various types.

The transformation is described by Klug, Crick & Wyckoff (Acta Cryst. 1968, 11, 199) and their conventions are adhered to - e.g. a positive value of n corresponds to a right-handed helix.
rho(r,phi,z) = 1/c * Sum over l & n (gnl(r)*exp(i(n*phi-2pi*l*z/c))

where

gnl(r) = exp(-i*n(PHI+pi/2)) * integral (Fl(R) * Jn(2pi*R*r) 2pi*R*dR

The input values of the transform (HLXDUMP output) are implicitly assigned to the plane PHI = +- pi/2 , where PHI is measured from the X-axis.

Input-output streams:

Input stream 1	layer line data	
Output stream 2	3-D map	OUT1
Output stream 3	Projection	OUT2
Output stream 4	File of g's for plotting	GOUT

Data Cards:

TITLE (10A4)

C, DELBR, RMAX, DELSR (*)

LLMAX, ISIDE, KOUT (*)

WT(L), L=1,LLMAX (*)

IHFH, IHFC, IHFV, IHFP, IHFZP, IQATOR, MAP, ITRFN (*)

Data for an artificial mean radial density distribution (g00(r)) is inserted here, if IQATOR = 1.

Followed by one or more sets of output parameters, in the following order :

PHIMIN, PHIMAX (*) if IHFH = 1

ZMIN, ZMAX, DELZED (*) horizontal sections, perpendicular to z-

---

RMIN, RMAX (*) if IHFC = 1

PHIMIN, PHIMAX, DELPHI (*) cylindrical sections, parallel to z-axis.

ZMIN, ZMAX, DELZED (*)

RMIN, RMAX (*) if IHFV = 1

PHIMIN, PHIMAX, DELPHI (*) vertical central sections at successive angles

ZMIN, ZMAX, DELZED (*)

XMIN, XMAX, DELX (*) if IHFP = 1

PHIMIN,PHIMAX (*) vertical parallel sections of constant x.

ZMIN, ZMAX, DELZED (*)

PHIMIN, MIND, DMIN (*) if IHFZP = 1

ZMIN, ZMAX, DELZED (*) single projection down z-axis.

C is the axial repeat distance of the helix in Angstroms.

DELBR is the spacing between samples along the layer lines, in reciprocal angstroms.

RMAX is the maximum radius for which little g's are calculated

DELSR is the spacing of points in the map,in the y direction. Points in the x direction are calculated at intervals of 2/3 DELSR, if IPLOT is set to 2, to be compatible with PLOTFOUR. If IPLOT = 0, samples in the x direction are at intervals of 5/6 * DELSR to give isometric output on the line printer (8 lines per inch).

LLMAX total number of layer lines read in

WT(L) weighting applied to each layer line (LLMAX of them)

NSP input unit number (layer line data)

ISIDE = 0 for nearside data, = 1 for farside data

IABS(KOUT) = 1 gives isometric line printer output only,

= 2 gives output map in standard format for TONE etc

= 3 gives output in standard format and line printer

If KOUT negative get listing of big G's

MAP = 1 outputs file of little g's for plotting with HLXGOUT

ITRFN .ne. 0 is supposed to apply a transfer function correction. NOT CHECKED!

RMIN,RMAX limits of radius in angstroms,RMAX must not exceed RMAX on item 2.

PHIMIN,PHIMAX limits in degrees of sector of map to be output

DELPHI spacing in degrees over which PHI is stepped

ZMIN, ZMAX are the axial limits for the map to be output

DELZED is the spacing in the axial direction of points in the map.

if IHFC=1, RMIN & RMAX are the inner and outer radial limits of the map. RMAX in this case should not be more than on card 2

6. HLXPROJ: Version 2.0 13-Nov-00 RAC

Reverse transforms selected layer line data, output by HLXDUMP, to synthesize a filtered projected image. The particle may be rotated about the helix axis to obtain views different from the original. The filtered images are output as numerical arrays on disc for plotting

Data Cards:

TITLE (20A4)

LLTOT, C, DELBR (*)

RMAX, DELSR, IRSTEP, IJUMP, NV (*)

WT(L), L=1,LLTOT (*)

PHI(IV), IV=1,NV (*)

ZMIN, ZMAX, DELZED, DMIN (*)

FILIN (A)

LLTOT = number of separate layer lines in a single data set.

C = axial repeat of helical particle

DELBR = spacing (dR) of data points along layer lines.

RMAX = maximum radius of particle

DELSR = radial separation between calculated density points in real space.

IRSTEP = intervals (in steps of DELBR) at which data are to be included the calculation.
If = 1, every point along the layer line is used,
if = 2, alternate points are included, etc.
The calculation may be very time-consuming if all layer line points are used to calculate points in a large filtered image array, and layer lines are often sampled much more finely than necessary, especially for this purpose.

IJUMP = option control: outputs one-sided filtered images for negative values,double-sided images for positive values.
+-1, prog thinks it is receiving 'near-side' data,
+-2, prog thinks data is 'far-side',
+-3, prog expects 'near-side' followed by far-side, on 2 separate files.

NV = number of different filtered images to be calculated from the data set showing views from different angles around the helix axis.

WT(L) = weighting factors for each layer line.

PHI(IV)'s are the required view angles in degrees.

ZMIN,ZMAX,DELZED = lower and upper values of axial distance z required for the filtered image, and the interval between sample points.

FILIN file name of layer line data set

Note : RMAX/DELSR * (ZMAX - ZMIN)/DELZED must not excced 50000
up to 40 layer lines
up to 200 steps / layer line
up to 20 views

7. HLXDYAD Version 1.0 04-Dec-00 JMS

Program to read in layer line data and set phases to 0 or 180.
Requires input and output filenames

8.HLXSEPDAT Version 2.0 13-Nov-00 RAC

This is a feeder program for HLXSEPR which copies layer line data from different views in known orientations(found in HLXFIT) to a direct access area. It assumes that the layer line data are sampled at the same spacing in each view.

Inputs on stream 2 with filenames specified in data
Output to direct access area on stream 3

Data cards :

NVIEW,LLMAX,DELBR,C,IREST (*)

NVIEW No. of "sides" to be input for this run
LLMAX No. of layer lines for each side
DELBR Layer line sampling in rec. Ang.
C Helical repeat in Angstroms
IREST 0 Not restart ie Starting new direct access area
1 Restart ie Adding data to existing area

Then for each side :

FILIN (A)
PHI,XSHIFT,YSHIFT,IPOLE (*)

FILIN Filename of data set containing layer line data for this side.
PHI Angle of view in degrees For reference particle near side has PHI=270, far side has PHI=90. Relative values of PHI found in HLXFIT then add to these. e.g. If HLXFIT gives a value -10 degrees for a second particle, corresponding PHI values for near and far sides will be 260 and 80 respectively.

XSHIFT Extra x-shift of origin in angstroms. Generally zero.
YSHIFT y-shift in angstroms. Used to refer all particles to common origin. Use value given by HLXFIT
IPOLE Used to invert particle in z-direction, if HLXFIT indicates this is necessary.
These last 3 variabled act on layer line data before it is written onto direct access data set

9.HLXSEPR: Version 2.00 13-Nov-00 RAC

Program to separate overlapping Bessels , using views of helix in different orientations. Uses LINFIL least squares package. The separated Bessel functions produced correspond to a "NEAR SIDE" set of transform values, ready to go into HLXFOUR.

Input layer line data on direct access file 2 , created by HLXSEPDAT program.
Output separated Bessel functions on stream 3 , in HLXFOUR format. Plot graphs of separated Bessels on printer.

Data cards:

TITLE (10A4) Title for separated data.

NVIEW,LLMAX,RADIUS,IGRAPH (*)

NVIEW No. of views (ie. sides)
LLMAX No. of layer lines in each view
RADIUS Radius of particle in angstroms - used for determining where Bessel contribution starts in transform.
IGRAPH Plot graphs of sep. Bessels if IGRAPH.NE.0

(RSCAL(NV),NV=1,NVIEW) (*)

RSCAL(NV),NV=1,NVIEW Radial scale factors from HLXFIT

Then for each layer line:

NL,NORD,(IORD(NO),NO=1,NORD) (*)

NL Layer line no.
NORD No. of different Bessel orders on layer line
IORD(NO),NO=1,NORD Bessel orders on layer line

FITWT(NV),NV=1,NVIEW (*) Amplitude weight factors for each view for this layer line. These are used to multiply the amplitudes on each layer line in each view before the separation is done.

Dimensions set for maximum no. of Bessels per layer line= 10, max no. of views = 32, max no of layer lines 20.

10.HLXLLOUT: Version 2.0 11-Nov-00 RAC

Program to select and graph standard format layer line data either with autoscaling for each layer line or on constant amplitude scale Layer line input on stream 1 (IN)

Data cards:

TITLE (10A4)
LLMAX,FSCA,FMAX,RMIN,RMAX,CANG (*)
IPLOT(I),I=1,LLMAX (*)

TITLE Title for plots (up to 40 chars)
LLMAX No. of layer lines to be input
FSCA Multiplying amplitude scale factor applied when data read from disc. Allows data set to be put on absolute scale.
FMAX Maximum amplitude overall on layer lines to be plotted, after FSCA has been applied.
If set to zero, then autoscaling used on each layerline.
RMIN,RMAX Radial range for plotting box (rec Ang.)

```
CANG     Helical repeat (Angstroms) to set ZSTAR
IPLOT(I) I=1,LLMAX  Plot particular layer line if 1, not if 0
```

11.HLXSIMUL: Version 2.0 13-Nov-00 RAC

Program to simulate projected image of helix for testing helical
reconstruction programs. Subunits built from arbitrary numbers
of spherical blobs of different size, position and density.
Single start helix specified by helical parameters DZ,DPHI.
Multi-start helix produced by putting more blobs into subunit,
related by appropriate rotational symmetry. The generated piece of
helix is centered in the z direction, which is vertical in TONE.
y axis is horizontal in TONE and x axis comes out towards observer.
Back or front of helix can be cut off and a linear ramp weighting
applied in order to simulate one sided or partially one-sided images.
Output standard image on stream 1 (OUT)
Present dimensions of output image are 256 x 512

DATA CARDS

(1) NBLOB,NUNIT,AXIS,DZ,DPHI,PHIROT,TILT,PZBACK,PZFRNT,IRAMP (*)
(2) RADH,RADS,Z0,PHI0,WT (*)
    (2) repeated NBLOB times.

NBLOB	Number of blobs per subunit
NUNIT	Number of subunits to be generated
AXIS	Y position of helix axis pixels (.LE.25 at present)
DZ	Z rise per subunit pixels
DPHI	Phi twist per subunit degrees
PHIROT	Rotation of whole helix about z axis degrees
TILT	Tilt of helix axis out of plane degrees Tilts about centre of helix about axis parallel to y. Positive TILT tilts top of particle towards observer.
PZBACK,PZFRNT	Back and front planes for windowing in pixels. Blobs lying outside these planes are omitted. If both set to zero there is no windowing.
IRAMP	0 Simple cut off by windowing planes 1 Cut off by window and linear ramp weighting of densities from 1 at front to 0 at back of window -1 Ramp weighting from 0 at front to 1 at back

For each blob in the subunit:

RADH	Radius from axis pixels
RADS	Radius of blob pixels
Z0	Z position of blob in first subunit pixels (generally zero)
PHI0	phi position of blob in first subunit degrees (measured from x-axis)
WT	Density weight

12.HLXFITT: Version 1.15 12-Jul-99 UNWIN

Program finds the common origin for a "test" and "reference" helical object, and calculates the relative amplitude and radial scales.

The common origin is determined by minimizing the phase residuals between reference datasets, according to:

phiF = sqrt(sum(|Fref|*dphi**2)/sum|Fref|)

Program also gives R-factors:

Rf = sum(||Fref| - |Ftest||)/sum|Fref|

Two alternative output files may be generated:

(a) new test dataset, oriented and radially scaled to fit the reference set

(b) "phase error" dataset, like (a) except that the phases output are the difference phases: phi(r) - phi(t)

equatorial data are omitted.

CNTFILE	- control data file
RDLFILE	- output file listing: Rf x 1000, phimin, zmin, rscalmin, phiF x 1000
NEWFILE	- new test dataset

Data cards in CNTFILE:

HLXTITLE	- image title
REFILE	- reference filename
NLL	- number of repeats (equivalent to llfact)
rep_dis	- repeat distance*NLL (A)
DELR1, DELR2	- layer-line sampling intervals (ref., test)
ACUT	- amplitude cutoff (% of max. amp. in ref.)
LLSPEC(I), WTSPEC(I) 6(I5.F5.1)	- up to 6 special layer-lines and weights
TFILE	- test filename
ISIDE	- 0 for near, 1 for far side
IPOLE	- 1 to rotate test helix by 180 degrees
PHIMID	- estimated phi value to search about (degrees)
DPHI	- search increment in phi
IPL	- no. of steps in phi (max. 8)
ZMID	- estimated z value to search about (A)
DELZ	- search increment in z
IZL	- no. of steps in z
RSCMID	- estimated rscal to search about
DRSC	- search increment in rscal
IRL	- no. of steps in rscal (max. 8)
IOUT	- 1 to write out NEWFILE

3.5 Rotational averaging AND filtering programs

1. RFILTIM: Version 2.0 04-Apr-00 RAC

Progam for filtering images with rotational symmetry. Using the Fourier transform of the image, the program finds the best position for the postulated rotational symmetry axis and then decomposes the transform into cylindrical harmonics about this origin. The program produces a rotational power spectrum, which is printed and displayed with CURVY. Those harmonics consistent with the postulated symmetry are then combined to produce a rotationally filtered image.
(Reference - Crowther and Amos J. Mol. Biol.(1971) 60,123-130.)

Input	Standard transform on stream 1 (IN)
Output	Filtered image on stream 2 (OUT)
Output	CURVY file on FOR003

CONTROL DATA

(1) HEADER (10A)

(2) N,NR,RSTEP,NLR,RSCAL (*)

(3) DXMIN,DXMAX,DELDX,DYMIN,DYMAX,DELDY,NBSTEP,NBMIN (*)

(4) ASCAL,BSCAL,PHI0,SCALE,JOPT,LGDUMP,NORM (*)

N	Rotational symmetry to be tested
NR	No. of annuli of data to be used from the transform
RSTEP	Spacing in transform steps of annuli
NLR	No. of radial steps in filtered image

RSCAL = Size of step in filtered image / Size of step in original densitometered image

DXMIN,DXMAX	Range of origin search in x direction measured in densitometer steps
DELDX	Interval of search in x direction in densitometer steps
DYMIN,DYMAX	Similarly for y direction
DELDY	
NBSTEP	No. of transform annuli to be binned into a band when printing residuals from origin search

NBMIN	No. of bands (of size NBSTEP) to be omitted when determining best origin. (First band i.e. low resolution data, is generally much the strongest and may be biased by gross stain distribution, in which case it should be omitted.)
ASCAL,BSCAL	Radial weighting factors in transform which may be used to increase artificially the strengths of the high frequencies. USE WITH CAUTION! Annulus number IR has a scale factor (ASCAL+IR*BSCAL) applied. For normal use set ASCAL=1.0, BSCAL=0.
PHI0	The filtered image is rotated PHI0 degrees relative to the densitometered image. Positive PHI0 rotates the image clockwise.
SCALE	Densities in the filtered image are multiplied by SCALE. SCALE=-1. inverts image contrast.
JOPT	0 g0 included in filtered image 1 g0 omitted from filtered image
LGDUMP	0 Do not dump gn's to disc file 1 Dump gn's to disc file (FORTRAN 10)
NORM	0 Do not normalise power spectrum 1 Normalise spectrum with power of N=0 term equal to 1

Current limitations:
- NR .LE. 40
- NLR .LE. 50
- Maximum image size transformed 256x256
- Maximum Bessel order 70
- Maximum of 15 different Bessel orders included in filtered image
- Maximum size of origin search 10x10 positions

2. ROTAV: Version 2.00 15-NOV-00 RAC

Rotational averaging of 2D image or 3D maps about z-axis.
in density space.
Will average 3-D map section by section
NB Rot. axis position measured from bottom LH corner
of TONE image as (0,0).

This is a general 2-D interpolation program that allows
the user to perform Rotations, Translations, Size
alterations and Re-sampling on a skewed or distorted
coordinate system.
The rotation from OLD axis to NEW axis is positive for
an anti-clockwise rotation.

Data input unit 5: all free format

ROTX
NSYM
AMAGX
XCEN,YCEN
NXB,NYB,IRAD
ICELL

Data map input 'IN', output map 'OUT'

3. IMROTRAN: Version 2.0 04-12-00 JMS

IMROTRAN is a program to rotate/ translate an image file (the relative file) and calculate a correlation coefficient wrt another image file (the reference file), then to output another image file of the average the reference file with the best fit of the relative file.

INPUT DATA:

(40A1) Input image file (reference file does not move)
(40A1) Input image file (relative file is rotated/translated)
(40A1) Output image file (average of above two)
(*) Theta1, Theta2, Thinc :
starting, finishing angles and increment in degrees. A +ve angle rotates relative file clockwise.
(*) Xtrans1, Xtrans2, Xinc :
starting, finishing translation in X and increment in pixels. A +ve value translates relative file to the right.
(*) Ytrans1, Ytrans2, Yinc :
starting, finishing translation in Y and increment in pixels. A +ve value translates relative file upwards.
(*) Rmax :
maximum radius (in pixels) over which the correlation coefficient is to be calculated.

3.5 General display programs

1. LASERTONE: TSH

Program converts MRC Image map format file to postscript format.

2. LASERTEXT: TSH

Program converts text file to postscript format.

3. HISTOK: Version 1.6 20-Nov-00 RH

Makes histogram of densities in an image.
Data unit 5 :
IQD (*) 0 Linear display
1 Logarithmic display

4. XIMDISP Version 16.4 01-Dec-00 JMS

Interactive graphics display program for manipulating digitized images and transforms. Main menu :

1 Re-scale image
2 Erase vectors
3 Hide zoom window
4 Modify zoom window
5 Hide menu/labels
6 Draw text string
7 Change colour table
8 Change cursor type
9 Enable pointer tracking
10 Draw another map
11 Display more sections
12 Average boxed densities
13 Box/Dump an area
14 Output/measure coordinates
15 Compute interactive FFT
16 Lattice refinement
17 Splinefit image

5.THREED:

Displays 2D array as simulated 3D contoured surface.

6. SURF: Version 1.2 04-Apr-00 RAC

ROTATES A MAP THROUGH SOME THETA AND PHI ANGLE, AND DISPLAYS
THE FRONT SURFACE AT SOME CONTOUR LEVEL WITH DEPTH CUEING.
FOR MORE DETAILS, SEE SEPARATE WRITE UP.

INPUTS: THETA,PHI,CLEVEL,FMAGF
THETA and PHI are the equatorial and azimuthal viewing angles. If THETA,PHI = 0,0 the map is viewed along the X axis, looking towards the origin. If 90,0 map is viewed along the Y axis, etc.

CLEVEL = contour level of map.

FMAGF = Magnification of output map.

INPUT AND OUTPUT MAPS ARE IN STANDARD MRC MAP/IMAGE FORMAT.

The outut of SURF should be run through LIGHT to give a shaded surface representation.

7. LIGHT: Version 1.1 04-Apr-00 RAC

ADDS ILLUMINATION CUEING TO A SURFACE IMAGE.
HAS FURTHER PROVISION FOR THE USE OF HIGHLIGHTS.

INPUTS:THETA,PHI,DEPTH,FDIF,NCOS,FSPEC

THETA,PHI are illumination angles. If THETA,PHI = 0,0 illumination is from viewing position. Theta positive gives illumination from th right, Phi positive gives illumination from above.
DEPTH gives ratio of lighting of back/front. If DEPTH = 0 Back is dark.
FDIF is fraction of reflected light that is diffuse.
NCOS is cosine power for specular reflection. Generally NCOS = 6. A higher power makes the surface more highly polished.
FSPEC is fraction of light in specular reflection. Any other light is only depth queued.

4.0 References to published papers

Crowther,R.A.,Henderson,R. and Smith,J.M. (1996)
J.Struct.Biol. 116,9-16

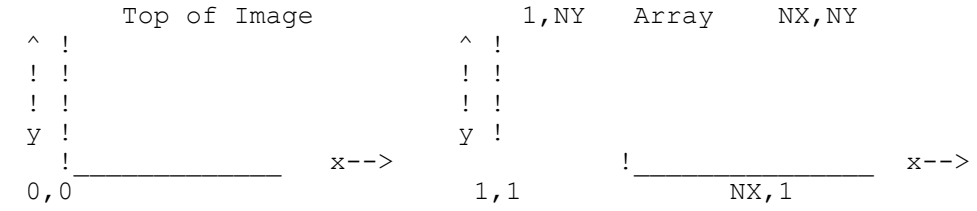
Program	Reference
ORIGTILT	Amos,L.A.,Henderson, and Unwin(1982) Prog.Biophys.Mol.Biol. 39, 183-231.
	Henderson,R.,Baldwin,Downing,Lepault and Zemlin (1986) Ultramicroscopy, 19, 147-178.
LATLINE	Agard,D,A. (1983) J.Mol.Biol. 167, 849-852
EMTILT	Shaw,P.J. and Hills,G.J. (1981) Micron 12, 279-282.
NIKSCN	Arndt,U.,Barrington-Leigh,Mallett and Twinn (1969) J.Phys.E. Sci.Instrum. 2,385-387.
SPLINEFIT	Egelman,E. (1986) Ultramicroscopy 19, 367-374.
SURF LIGHT	Vigers,G.P.A., Crowther,R.A. and Pearse,B.M.F. (1986) EMBO J. 5, 529-534. Vigers,G.P.A. (1986) PhD.Thesis Cambridge University.
QUADSERCHA LATLINE CCUNBENDC CTFREFINE CTFAPPLY	Henderson,R., Baldwin,Downing,Lepault and Zemlin (1986) Ultramicroscopy 19, 147-178.
TTMASK TTBOX TTREFINE	Henderson.R.,Baldwin,Ceska,Zemlin,Beckmann and Downing (1990) J.Mol.Biol. 213, 899-929.
BACKAUTO AUTOINDEX PICKAUTO SYNCFIT	Baldwin,J.M and Henderson,R.(1984) Ultramicroscopy,14,319-336.
MERGEDIFF	Ceska,T.A. and Henderson,R.(1990) J.Mol.Biol. 213, 539-560.
HLXFOUR HLXAVG HLXSEARCH HLXDUMP HLXFIT	DeRosier,D.J. and Moore,P.B.(1970) J.Mol.Biol. 52, 355-369.
HLXSEPDAT HLXSEPR	Crowther,R.A., Padron,R. and Craig,R. (1985) J.Mol.Biol.184, 429-439.
ICOSAHEDRAL VIRUSES	Crowther,R.A., DeRosier,D.J. and Klug,A. (1970) Proc.Roy. Soc. A317, 319-340. Crowther,R.A.(1971) Phil.Trans.Roy.Soc.B261, 221-230.
RFILTIM	Crowther,R.A. and Amos,L.A.(1971) J.Mol.Biol.60, 123-130.
XIMDISP	Judith M. Smith J. Struct. Biol., 125, Pages 223-228 (1999)

5. Documentation of IMAGE library

5.1 Higher-Level IMAGE File subroutines

These routine are designed to facilitate the rapid setup and manipulation of image-format files. Either Sequential access or Direct access I/O operations may be performed at any time.These routines will now also cope with map-format files.

In general, the X-Y origin is taken as 0,0 being in the lower-left corner of the image AND the first data point in the file (normally corresponding to array element 1,1).



The convention for FOURIER TRANSFORMS is that the transform of an image of dimensions NX x NY yields a transform of NX/2+1 x NY COMPLEX values. The origin of Fourier space is located at coordinates 0,NY/2 (disk coordinates, which would normally be 1,NY/2+1 in the FORTRAN array). In reciprocal lattice units:
X goes from 0 --> 0.5 and Y goes from -0.5 ---> (.5 - deltaY)

Upto 5 image files may be open at any one time!!

All higher-level image routines begin with the letter I. With the exception on the OPEN/CLOSE and Positioning routines a standard naming convention has been established.

The second 2 letters are chosen from the following.

- RD = Read
- WR = Write
- CL = Calculate
- CR = Create
- AL = Alter
- TR = Transfer
- RT = Return information

The last 3 letters are chosen from the following:

- CDN = Density limits (Complex numbers, ie uses Modulus)
- CEL = unit cell paramters
- CON = conversion to reals
- DEN = Density limits
- EXT = Extra information ("unused" header slots)
- HDR = Header
- LAB = Labels
- MOD = Mode
- ORG = Origin

SAM = Sampling information
SIZ = Size
SYM = Symmetry information
LIN = Line
SEC = Section
PAL = Part of Line
PAS = Part of Section

Specifications for higher-level image I/O routines:

File Set-Up Routines:

```
CALL IMOPEN(ISTREAM,NAME,ATBUTE)            Opens file NAME on ISTREAM

CALL IMCLOSE(ISTREAM)                       Closes file

CALL IRDHDR(ISTREAM,NXYZ,MXYZ,MODE,DMIN,DMAX,DMEAN)
                                    Read  header on input file

CALL IWRHDR(ISTREAM,TITLE,NTFLAG,DMIN,DMAX,DMEAN)
                                    Write header to output file

CALL ITRHDR(ISTREAM,JSTREAM)                    Transfer header from JSTREAM
                                    to ISTREAM (does not write!)

CALL ITRLAB(ISTREAM,JSTREAM)                    Transfer labels from JSTREAM
                                    to ISTREAM (does not write!)

CALL ITRCEL(ISTREAM,JSTREAM)                    Transfer CELL parmas  from
                                    JSTREAM to ISTREAM (no write!)

CALL ICRHDR(ISTREAM,NXYZ,MXYZ,MODE,LABELS,NL)   Create NEW header. The header
                                    is NOT written out. You must
                                    do a IWRHDR.
                                    In general, it is advised that
                                    one use ITRHDR followed by the
                                    appropriate alter calls such as
                                    CALL IALSIZ(....)   etc.
                                    This is preferred because all
                                    information is transferred by
                                    the transfer call.

CALL IALCEL(ISTREAM,CELL)                 Alter unit cell paramters

CALL IALCON(ISTREAM,FLAG)                 Alter conversion to reals.
                                    By default, all data is passed
                                    to the user as REALS or COMPLEX
                                    REALS, independent of storage mode
                                    on disk. This call allows this
                                    to be overridden.
                                    This should be used with CAUTION!!!
                                    FLAG = .TRUE.    conversion to REALS
                                    FLAG = .FALSE.    NO conversion!!!

CALL IALEXT(ISTREAM,EXTRA,ISTART,NEXTRA)        Alters  info in "unused"
                                    slot in header, starting
                                    at position ISTART.
                                    NEXTRA words are altered.
```

```
CALL IALLAB(ISTREAM,LABELS,NL)            Alters NL labels in header

CALL IALMOD(ISTREAM,MODE)                 Alter MODE on existing header

CALL IALORG(ISTREAM,XORIGIN,YORIGIN)            Alter XY origin information

CALL IALSAM(ISTREAM,MXYZ)                       Alter sampling information

CALL IALSIZ(ISTREAM,NXYZ,NXYZST)          Alter SIZE on existing header
                                    Note, the NXYZST is for your
                                    use ONLY. It is stored in the
                                    file header for interfacing with
                                    the X-ray programs, but all calls
                                    within the image package, are
                                    always taken relative to the
                                    start of each line, or section.

CALL IALSYM(ISTREAM,KSPG,KBS)                   Alters symmetry parameters
                                                KSPG is space group number
                                                KBS is number of bytes of
                                                symmetry data

CALL IALUVW(ISTREAM,IUVW)                       Alters matrix to permute
                                                cell  dimensions.
```

File Positioning Routine:

```
CALL IMPOSN(ISTREAM,NZ,NY)                Move to section NZ, line NY
                                    Default convetions are all
                                    numbers start at 0 !!!!
```

Line Read/Write Routines:

In all cases, ARRAY is a REAL or COMPLEX REAL data array.
All of these routines convert from/to Integer*2 as required.

```
CALL IRDLIN(ISTREAM,ARRAY,*LINE)           Read line  (NX points)

CALL IWRLIN(ISTREAM,ARRAY)                 Write line (NX points)


CALL IRDPAL(ISTREAM,ARRAY,NX1,NX2,*LINE)         Read  part line (NX1 - NX2)
                                    Data is always loaded into
                                    the FIRST element of ARRAY.
                                    After READ, pointer is at
                                    Start of next line.

CALL IWRPAL(ISTREAM,ARRAY,NX1,NX2)              Write part line (NX1 - NX2)
                                    from selected region in
                                    core onto disk.
```

Section Read/Write Routines:

In all cases, ARRAY is a REAL or COMPLEX REAL data array.
All of these routines convert from/to Integer*2 as required.

```
CALL IRDSEC(ISTREAM,ARRAY,*LINE)            Read  section

CALL IWRSEC(ISTREAM,ARRAY)                  Write section


CALL IRDPAS(ISTREAM,ARRAY,MX,MY,NX1,NX2,NY1,NY2,*LINE)
                                      Read  part of section
                                      After READ, pointer is at
                                      Start of next section.

CALL IWRPAS(ISTREAM,ARRAY,MX,MY,NX1,NX2,NY1,NY2)    Write  part of section
```

Other Useful Routines:

```
CALL ICLCDN(ARRAY,MX,MY,NX1,NX2,NY1,NY2,DMIN,DMAX,DMEAN)
                                      (Mod of Complex vals)
CALL ICLDEN(ARRAY,MX,MY,NX1,NX2,NY1,NY2,DMIN,DMAX,DMEAN)   (Real numbers)
                                      Calculates the MIN/
                                      MAX, & MEAN densities from
                                      the selected portion of
                                      ARRAY (assumed to be image!)
                                      NOTE: Only here does the
                                      counting start from 1.
CALL ICLLIM(ISTREAM,IXYZMIN,IXYZMAX,NXYZ)
                                      Prompts the user to supply
                                      area limit (0,0 lower left)
                                      and returns pixel limits
                                      # pixels, and user limits

IUNIT = IMUNIT(ISTREAM)                     Returns IUNIT which is
                                      compatible with the
                                      LOW-LEVEL routines.

CALL IRTCEL(ISTREAM,CELL)                   returns CELL(6)

CALL IRTEXT(ISTREAM,EXTRA,ISTART,NEXTRA)          Returns NEXTRA words extra
                                      slot in header, starting
                                      at position ISTART. There
                                      are 29 available words.

CALL IRTLAB(ISTREAM,LABELS,NL)              Returns LABELS(20,10)
                                      number of labels NL.

CALL IRTORG(ISTREAM,XORIGIN,YORIGIN)              Returns XY origin
                                      information

CALL IRTSAM(ISTREAM,MXYZ)                         Returns sampling information

CALL IRTSIZ(ISTREAM,NXYZ,MXYZ,NXYZST)             Returns SIZE info

CALL IRTSYM(ISTREAM,KSPG,KBS)                     Returns symmetry parameters
                                                  KSPG is space group number
```

	KBS is number of bytes of symmetry data
CALL IRTUVW(ISTREAM,IUVW)	Returns matrix to permute cell dimensions.

Variable Definitions: (ALL variables are INTEGER*4 or REAL!!)

ARRAY: A storage location for data transfer. NOTE ARRAY is either REAL*4 or COMPLEX*8 !!!!!

ATBUTE: File attribute specification. One of the following character strings must be given: 'NEW' 'OLD' 'RO' or 'SCRATCH'

DMIN/DMAX/ DMEAN: The minimum, maximum, & mean density values for this image.

EXTRA(29) An array (up to 29 long) or a storage location for holding the values for the EXTRA info slot in the header.

ISTART: A number between 1-29 to select the first element of the EXTRA info to transfer.

ISTREAM/ JSTREAM: A number between 1 and 12 used to select which file to use for READ/WRITE operations. A maximum of 5 files can be active at any one time.

IXYZMIN(3)/ IXYZMAX(3): Returned lower & upper pixel limits that correspond to user selected input range. (pixels have 0,0 at bottom left)

MODE: Defines data structure on disk:

0 = INTEGER*1	IMAGE	note:values between 127 & 255 stored as -128 to -1 but returned as their original values.
1 = INTEGER*2	IMAGE	
2 = REAL*4	IMAGE	
3 = INTEGER*2	FOURIER TRANSFORM	
4 = REAL*4	FOURIER TRANSFORM	

MX/MY: Dimensions of ARRAY. If transferred data size is smaller than MX,MY the remainder of the space will be set to 0. Note: MX correspons to the number of REAL numbers in the fast dimension of ARRAY. If MODE = 3 or 4 (Fourier Transform) MX MUST be multiplied by 2!!!

MXYZ(3): Specifies the number of columns, rows, & sections in the entire "unit cell" (can be identical to NXYZ).

LABELS(20,N) N = 1 - 10. This is a way to ititialize more than one text label when creating a new header. LABELS(20) is also permitted. Each label is 80 characters long (A4).

NAME: A character string specifying either the FILENAME or a LOGICAL name to associate with a given stream.

NEXTRA: A number bewteen 1-29 to select the number of EXTRA value to transfer.

NL: The number of LABELS being initialized (see LABELS, above).

NTFLAG: -1 no titles added to list.
0 to use TITLE as sole title on file (overwrites old title).
1 to add TITLE to end of list.
2 to add at top, pushing any other labels down.

NX1/NX2: Beginning & ending COLUMN numbers for data transfer. On reading these numbers are relative to NXTZST(1). For Fourier Transforms, these are taken as Complex Indicies!!!

NXYZ(3): Specifies the number of columns, rows, & sections in the current file (ie. fastest -> slowest changing).

NXYZST(3): Specifies the starting column, row and section number. Note, the NXYZST is for your use ONLY. It is stored in the file header for interfacing with the X-ray programs, but all calls within the image package, are always taken relative to the start of each line, or section. The start is ALWAYS denoted by 0.

NY: Line number for positioning pointer. This value is relative to NXYST(2)

NY1/NY2: Beginning & ending ROW numbers for data transfer. On reading these numbers are relative to NXTZST(2).

NZ: Section number for positioning pointer. This value is relative to NXYST(3)

TITLE(20) 80 character title. Written as dictated by NTFLAG.

XORIGIN/ YORIGIN: The X & Y image origin (generally used for relating phase origins).

*LINE LINE is a statement number to branch to on an END-OF-FILE error. Example: *99

5.2 image MAP Header Format

```
*        Length = 1024 bytes, organized as 56 LONG words followed       *
*       by space for 10 80 byte text labels.                             *
*                                                                        *
*       1       NX      number of columns (fastest changing in map)     *
*       2       NY      number of rows                                  *
*       3       NZ      number of sections (slowest changing in map)    *
*       4       MODE    data type :                                     *
*                       0       image : signed 8-bit bytes range -128   *
*                                       to 127                           *
*                       1       image : 16-bit halfwords                *
*                       2       image : 32-bit reals                    *
*                       3       transform : complex 16-bit integers     *
*                       4       transform : complex 32-bit reals        *
*       5       NXSTART number of first column in map (Default = 0)     *
*       6       NYSTART number of first row in map       "              *
*       7       NZSTART number of first section in map   "              *
*       8       MX      number of intervals along X                     *
*       9       MY      number of intervals along Y                     *
*       10      MZ      number of intervals along Z                     *
*       11-13   CELLA   cell dimensions in angstroms                    *
*       14-16   CELLB   cell angles in degrees                          *
*       17      MAPC    axis corresp to cols (1,2,3 for X,Y,Z)          *
*       18      MAPR    axis corresp to rows (1,2,3 for X,Y,Z)          *
*       19      MAPS    axis corresp to sections (1,2,3 for X,Y,Z)      *
*       20      DMIN    minimum density value                           *
*       21      DMAX    maximum density value                           *
*       22      DMEAN   mean density value                              *
*       23      ISPG    space group number 0 or 1 (default=0)           *
*       24      NSYMBT  number of bytes used for symmetry data (0 or 80)*
*       25-49   EXTRA   extra space used for anything  - 0 by default   *
*       50-52   ORIGIN  origin in X,Y,Z used for transforms             *
*       53      MAP     character string 'MAP ' to identify file type   *
*       54      MACHST  machine stamp                                   *
*       55      RMS     rms deviation of map from mean density          *
*       56      NLABL   number of labels being used                     *
*       57-256  LABEL(20,10) 10 80-character text labels                *
*                                                                        *
*       Symmetry records follow - if any - stored as text as in         *
*       International Tables, operators separated by * and grouped into *
*       'lines' of 80 characters (ie. symmetry operators do not cross   *
*       the ends of the 80-character 'lines' and the 'lines' do not     *
*       terminate in a *).                                              *
*                                                                        *
```

Data records follow.

5.3 Low-level random access subroutines

The LOW-LEVEL set of FORTRAN subroutines for doing either sequential or random access disk I/O with with variable record lengths are indicated below. The files are actually written as fixed-record direct-access files, but this is transparent to the user.

Note: IUNIT is NOT A Fortran Unit number, but an internal identifier

The calls provided are given below:

```
CALL QOPEN   (IUNIT,FILNAM,ATBUTE)          - Open file
[CALL QQOPEN  (IUNIT,FILNAM,ISTAT)          - Open file: use QOPEN]
CALL QCLOSE  (IUNIT)                        - Close file
CALL QMODE   (IUNIT,MODE,NMCITM)            - Change mode
CALL QREAD   (IUNIT,ARRAY,NITEMS,IER)       - Read nitems
CALL QREADI  (IUNIT,ARRAY,NITEMS,IER)       - Read nitems into integer array
CALL QREADR  (IUNIT,ARRAY,NITEMS,IER)       - Read nitems into real array
CALL QREADQ  (IUNIT,ARRAY,NITEMS,IER)       - Read nitems into complex array
CALL QREADC  (IUNIT,CHAR,IER)               - Read bytes into character var.
CALL QWRITE  (IUNIT,ARRAY,NITEMS)           - Write nitems
CALL QWRITI  (IUNIT,ARRAY,NITEMS)           - Write nitems from integer array
CALL QWRITR  (IUNIT,ARRAY,NITEMS)           - Write nitems from real array
CALL QWRITQ  (IUNIT,ARRAY,NITEMS)           - Write nitems from complex array
CALL QWRITC  (IUNIT,CHAR)                   - Write bytes from character var.
CALL QSEEK   (IUNIT,IREC,IEL,LRECL)         - Move to irec,iel
CALL QBACK   (IUNIT,LRECL)                  - Backspace 1 record
CALL QSKIP   (IUNIT,LRECL)                  - Skip 1 record
CALL QQINQ   (IUNIT,LFILNM,FILNAM,LENGTH) - Get filename and length
CALL QLOCATE (IUNIT,LOCATE)                 - Get position in file
CALL QRARCH (IUNIT, IOFFSET)                - set up number conversion
CALL QWARCH (IUNIT, IOFFSET)                - write conversion info
```

QSEEK calculates the location as (IREC - 1)*LRECL + IEL. Note: as in Fortran, addressing begins at 1 for both record & element
In these files, there are no true records: the use of "record length" and "record number" in QSEEK, QSKIP, QBACK is purely notional.
For QSEEK, any combination of IREC, IEL & LRECL which gives the same value of (IREC - 1)*LRECL + IEL is equivalent.

Where:

IUNIT = Variable returned by (Q)QOPEN to identify a file stream

FILNAM = file name for the stream (should be restricted to eight characters for CCP4 programs)

ATBUTE = File status for opening file
= 'UNKNOWN', 'SCRATCH', 'OLD', 'NEW', or 'READONLY'

ISTAT = File status on opening the file:

1,	'UNKNOWN'	open as 'OLD'/'NEW' check existence
2,	'SCRATCH'	open as 'OLD' and delete on closing
3,	'OLD'	file MUST exist or program halts
4,	'NEW'	create (overwrite) new file
5,	'READONLY'	self explanatory

NOTE: When using QQOPEN or QOPEN with ATBUTE = 'NEW' [ISTAT = 4], a check is made on the environment variable CCP4_OPEN - if this is set to UNKNOWN then the file is opened with attribute UNKNOWN rather than NEW to allow overwriting files that already exist.

```
 MODE   = Access mode = 0, BYTES
                      = 1, SHORT INT
                      = 2, (REAL) WORD
                      = 3, SHORT COMPLEX
                      = 4, COMPLEX
                      = 6, INTEGER

 NMCITM = No. of machine items (eg bytes) per element
 ARRAY  = Starting location for data storage in core
    NOTE: This should normally be an array of full-word fortran items
    (REAL or INTEGER) or double-word (COMPLEX) in the case that you
    want to transfer complex numbers (mode 4).  If necessary, unpack
    bytes using the routines provided in the library (or new ones).
    In particular, DON'T try to use BYTE or INTEGER*2 arrays, as these
    will likely cause alignment errors on RISC architectures.
 CHAR   = CHARACTER*n buffer for transfer
 NITEMS = Number of elements to transfer
 IER    = Error flag (0 = no error) else number of words transferred
 IREC   = Desired record number (starts at 1)
 IEL    = Desired element number within record (word) (starts at 1)
 LRECL  = Record length in elements

 No. of channels and buffer length in words set in #DEFINE statements

NOTE: use of QREAD/QWRITE is deprecated -- use QREAD<a>/QWRITE<a>
with a buffer of the correct type.
```