1 Introduction

Running d*TREK from the command line is, I think, relatively simple. The commands which are issued by the GUI's dtdisplay & dtprocess seem to be fairly simple, so I will record these and use as my baseline.

It looks like "indexing" will include 3 steps - spot finding by dtfind, indexing by dtindex and refinement (against the spots found in step no 1) in dtrefine. This gives a reasonably accurate orientation matrix, though I am not sure that it is completely accurate because some reflections are midding on the display!

In d*TREK it looks like most of the important information is kept in the d*TREK header file, which looks a lot like the ADSC SMV format header. This has all sorts of goniometry information in (boring) as well as some more useful stuff for instance the beam centre.

The initial header file can be created from the images with dtextract-header. This just reads in the image file and writes out an inital d*TREK header - this can then be used for the initial stages of the above processes.

2 Indexing

Spot picking for the indexing & refinement can be done off a number of images - and this gives a much better result.

3 Notes

Running d*TREK from the command line...

```
[prepare header]
dtextractheader image start.head
[update beam ctr] this is in pixels in start.head

dtfind start.head -seq 1 1 -sigma 3 -min 50 -filter 6 -out find.head
dtindex find.head dtfind.ref -maxresid 3.0 -sigma 5.0 -dps -nodiffs

... gives ...

FIND

dtfind:  Copyright (c) 1996 Molecular Structure Corporation
d*TREK version 9.5L -- Oct  4 2005
Command line:
 dtfind start.head -seq 1 1 -sigma 3 -min 50 -filter 6 -out find.head

     Header of file start.head successfully read.
A4_NONUNF_TYPE: >>Simple_mask<<
INFO in Cnonunf: using
```

```
     ../12287/12287_1_E1_001.img
     as the simple mask/nonunf file, was FirstScanImage.

     File ../12287/12287_1_E1_001.img successfully opened.
Min raw image pixel OK value in mask/nonunf/image file: 1


Command line string: >>-seq<<
Command line string: >>-sigma<<
Command line string: >>-min<<
Command line string: >>-filter<<
Command line string: >>-out<<

Resolution limits of an image are 979.65 to 1.37426
Resolution limits of peak search are 979.65 to 1.37426


dtfind: 2D method  used
...reading image ../12287/12287_1_E1_001.img...

     File ../12287/12287_1_E1_001.img successfully opened.
Find object listing:
     Sigma: 3
Resolution: 979.65 to 1.37426
   Minimum: 50
Circle lim: 1024, 1024, 0, 1448
  Rect lim: 20, 20, 2028, 2028
Spot wind.: 0, 0
Peak filt.: 6
Back. tile: 128, 128
 Seq. num.: 1, 1
Image dim.: 2048, 2048
   3D dump: 0
1339 preliminary spots found in 2D search with rotation angle 290.5 degs.

dtfind: There were 1074 spots found.
There were 1074 preliminary spots of which 4 were marked as saturated,
 or  0.37% of them.
Number of reflections written in 'dtfind.ref': 1074
dtfind: Spots written to dtfind.ref
dtfind - Wrote header file find.head

INDEX


dtindex:  Copyright (c) 1998, 1996 Molecular Structure Corporation
d*TREK version 9.5L -- Oct  4 2005
Command line:
 dtindex find.head dtfind.ref -maxresid 3.0 -sigma 5 -dps -nodiffs
```

```
     Header of file find.head successfully read.
Reflection list: dtfind.ref
Creflnlist::nRead with filename: dtfind.ref
INFO in Creflnlist::nRead, EOF after 1074 reflections read in
                                    (1074 total now in list).
Command line string: >>-maxresid<<
Command line string: >>-sigma<<
Command line string: >>-dps<<
Command line string: >>-nodiffs<<
INFO: deleted 0 reflns outside of resolution bounds.
      This leaves 1074 reflns for indexing.

INFO: 418 reflns deleted out of 1074 that might be in ice rings.
Max cell length allowed for reciprocal lattice vectors: 256.219


Method:     1D FFT with DPS algorithm
Out header: dtindex.head
Max cell:   256.219
Num vecs:   1000
Spacegroup: 0
Verbose:    1

Performing 1D FFT indexing (not cell reduction) with the DPS algorithm...see
  Steller, Bolotovsky, & Rossmann (1997) J. Appl. Cryst. 30, 1036-1040.

Max cell is:         256.219
Number of reflections/vectors used: 588
.................................
...refining best 30 directions and lengths...
.............................  done.
Number of vectors used for integer residual calculation: 588

     a      b      c  alpha   beta  gamma   Volume  Remarks #Indexed %Residual
=============================================================================
196.09  52.05  51.42  90.02 122.45 104.58   422661     Okay      435     0.265
 51.42 196.09  52.05 104.58  90.02 122.45   422661     Okay      435     0.265
 52.05  51.42 196.09 122.45 104.58  90.02   422661     Okay      435     0.265
 51.49 187.73  52.08 122.68  90.13  90.69   423682     Okay      432     0.268
187.73  52.08  51.49  90.13  90.69 122.68   423682     Okay      432     0.268
 52.08  51.49 187.73  90.69 122.68  90.13   423682     Okay      432     0.268
 51.42 196.09  73.15 123.80  45.36 122.45   422658     Okay      435     0.265
196.09  73.15  51.42  45.36 122.45 123.80   422661     Okay      435     0.265
 73.15  51.42 196.09 122.45 123.80  45.36   422661     Okay      435     0.265
196.09  52.05  73.15  44.66 123.80 104.58   422661     Okay      435     0.265
 52.05  73.15 196.09 123.80 104.58  44.66   422661     Okay      435     0.265
 73.15 196.09  52.05 104.58  44.66 123.80   422661     Okay      435     0.265
 73.15  51.50 187.74  90.69 113.13  45.40   423887     Okay      428     0.264
```

```
187.74  73.15  51.50  45.40  90.69 113.13   423887     Okay      428     0.264
 51.50 187.74  73.15 113.13  45.40  90.69   423887     Okay      428     0.264
187.73 196.09  51.43 122.45  90.70  34.89   422913     Okay      437     0.274
 73.15 187.71  52.06 122.67  44.67 113.16   422954     Okay      433     0.265
187.71  52.06  73.15  44.67 113.16 122.67   422954     Okay      433     0.265
 52.06  73.15 187.71 113.16 122.67  44.67   422954     Okay      433     0.265


Executing beam refinement with
beam search radius, acceptable shift radius: 10 9 ...
A4_NONUNF_TYPE: >>Simple_mask<<
INFO in Cnonunf: using
     ../12287/12287_1_E1_001.img
     as the simple mask/nonunf file, was FirstScanImage.

     File ../12287/12287_1_E1_001.img successfully opened.
Min raw image pixel OK value in mask/nonunf/image file: 1
Original (input header) beam center: [1030.0 1066.0]

First Pass.  Search dim0 in [1020 1040] dim1 in [1056 1076]
.........................................
Second Pass.  Search dim0 in [1036 1038] dim1 in [1061 1063]
Calculated pre-reduced cell solution is in agreement with detector beam center!
Original (input header) beam center: [1030.0 1066.0]
New      (calculated)   beam center: [1036.5 1061.4]
Header updated to reflect beam center change.

WARNING!: Beam position moved more than 5 pixels!
=======
INFO: Restart with adjusted beam center.
Max cell length allowed for reciprocal lattice vectors: 256.219


Method:     1D FFT with DPS algorithm
Out header: dtindex.head
Max cell:   256.219
Num vecs:   1000
Spacegroup: 0
Verbose:    1

Performing 1D FFT indexing (not cell reduction) with the DPS algorithm...see
  Steller, Bolotovsky, & Rossmann (1997) J. Appl. Cryst. 30, 1036-1040.

Max cell is:         256.219
Number of reflections/vectors used: 588
.................................
...refining best 30 directions and lengths...
.........................  done.
Number of vectors used for integer residual calculation: 588
```

a	b	c	alpha	beta	gamma	Volume	Remarks	#Indexed	%Residual
174.05	166.20	157.98	18.20	24.83	17.27	423646	Okay	394	0.060
166.20	157.98	174.05	24.83	17.27	18.20	423646	Okay	394	0.060
157.99	166.21	174.09	39.69	24.82	18.19	423539	Okay	392	0.060
158.00	166.21	73.10	102.74	89.98	18.19	423234	Okay	388	0.059
157.98	195.63	73.09	55.96	89.99	36.17	423560	Okay	395	0.061
157.98	166.21	51.67	90.00	90.09	18.20	423833	Okay	389	0.059
166.21	51.67	157.98	90.09	18.20	90.00	423834	Okay	389	0.059
51.67	157.98	166.21	18.20	90.00	90.09	423834	Okay	389	0.059
51.64	195.60	157.98	36.17	90.09	58.27	423209	Okay	385	0.059
157.98	51.64	195.60	58.27	36.17	90.09	423209	Okay	385	0.059
195.60	157.98	51.64	90.09	58.27	36.17	423209	Okay	385	0.059
51.66	157.99	174.06	24.83	107.28	90.08	423467	Okay	396	0.061
174.06	51.66	157.99	90.08	24.83	107.28	423468	Okay	396	0.061
157.99	174.06	51.66	107.28	90.08	24.83	423472	Okay	396	0.061
158.00	51.64	174.09	72.86	24.83	90.07	423231	Okay	383	0.059
174.09	158.00	51.64	90.07	72.86	24.83	423232	Okay	383	0.059
51.64	174.09	158.00	24.83	90.07	72.86	423231	Okay	383	0.059
73.09	157.99	51.66	90.08	45.23	89.99	423468	Okay	396	0.061
157.99	51.66	73.09	45.23	89.99	90.08	423468	Okay	396	0.061
51.66	73.09	157.99	89.99	90.08	45.23	423468	Okay	396	0.061
174.06	166.20	73.09	102.75	114.82	17.26	423434	Okay	396	0.061
174.10	166.21	73.09	102.75	65.16	39.69	423362	Okay	393	0.060
73.10	166.20	51.64	90.03	45.22	102.75	423344	Okay	393	0.060
166.20	51.64	73.10	45.22	102.75	90.03	423344	Okay	393	0.060
51.64	73.10	166.20	102.75	90.03	45.22	423345	Okay	393	0.060
51.66	73.09	195.63	55.96	58.26	45.23	423468	Okay	396	0.061
73.09	195.63	51.66	58.26	45.23	55.96	423468	Okay	396	0.061
195.63	51.66	73.09	45.23	55.96	58.26	423468	Okay	396	0.061
174.06	51.66	73.09	45.23	114.82	107.28	423468	Okay	396	0.061
73.09	174.06	51.66	107.28	45.23	114.82	423468	Okay	396	0.061
51.66	73.09	174.06	114.82	107.28	45.23	423468	Okay	396	0.061
73.09	174.09	51.65	72.88	45.23	65.16	423432	Okay	396	0.061
51.65	73.09	174.09	65.16	72.88	45.23	423432	Okay	396	0.061
174.09	51.65	73.09	45.23	65.16	72.88	423432	Okay	396	0.061

Least square fit to lattice characters...see
  Andrews & Bernstein (1988) Acta Cryst. A44, 1009-1018 and
  Paciorek & Bonin (1992) J. Appl. Cryst. 25, 632-637.
.....
.....
done.

Least-squares fit of reduced primitive cell to 44 lattice characters
sorted on decreasing (highest to lowest) symmetry.
Only solutions with residuals <=   3.0 are listed.

Soln num	LeastSq residual	Spgrp num*	Cent type	Bravais type Cell volume	a alpha	b beta	c gamma
7	0.190	75	P	tetragonal	51.796	51.796	157.982
				423844	90.000	90.000	90.000
9	0.166	21	C	orthorhombic	73.093	73.409	157.982
				847680	90.000	90.000	90.000
11	0.175	16	P	orthorhombic	51.669	51.923	157.982
				423839	90.000	90.000	90.000
12	0.064	5	C	monoclinic	73.691	73.168	157.982
				851816	90.000	90.141	90.000
12b	0.075	5	C	monoclinic	73.409	73.093	157.982
				847678	90.000	90.131	90.000
13	0.092	3	P	monoclinic	51.923	51.669	157.982
				423838	90.000	90.100	90.000
14	0.000	1	P	triclinic	51.669	51.923	157.982
				423834	89.900	89.915	89.753

*Suggested spacegroup number until systematic absences are examined.
...determining orientation angles...
.

Unit cell parameters and orientation angles

Num	Integer residual	a alpha	b beta	c gamma	Rot1	Rot2	Rot3
1	0.001	51.796	51.796	157.982	-75.915	20.479	-78.321
		90.000	90.000	90.000			
2	0.001	51.796	51.796	157.982	75.915	-20.479	101.679
		90.000	90.000	90.000			
3	0.001	51.796	51.796	157.982	104.085	20.479	-78.321
		90.000	90.000	90.000			
4	0.001	51.796	51.796	157.982	-104.085	-20.479	101.679
		90.000	90.000	90.000			
5	0.001	51.796	51.796	157.982	56.911	65.317	66.033
		90.000	90.000	90.000			

```
  6     0.001    51.796    51.796   157.982  -56.911  -65.317 -113.967
                 90.000    90.000    90.000

  7     0.001    51.796    51.796   157.982 -123.089   65.317   66.033
                 90.000    90.000    90.000

  8     0.001    51.796    51.796   157.982  123.089  -65.317 -113.967
                 90.000    90.000    90.000

================================================================================
The above table shows symmetry EQUIVALENT crystal orientation angles
for the indexing orientation.  All the solutions are equivalent for
the selected Bravais lattice.  The default selection usually has the
values closest to crystal orientation found in the input .head file or
the one where (|Rot1| + |Rot2| + |Rot3|) is a minimum.
Orientation angles choice 1 selected.

Crystal listing:

 Unit cell lengths:   51.7964   51.7964  157.9819
 Unit cell  angles:   90.0000   90.0000   90.0000
 Unit cell  volume: 423843.915
Orientation angles:  -75.9149   20.4794  -78.3208
         Mosaicity:     0.300
       Description: unknown

Spacegroup number: 75
             name: P4
Num. equiv. posns: 4
dtindex - Wrote header file dtindex.head

This works
----------

#!/bin/bash
export DTREK_PREFIX=infl
dtfind process.head -seq 1 2 -seq 59 60 -sigma 3 -min 50 -filter 6 \
-window 0 0 -out infldtfind.head

dtindex infldtfind.head infldtfind.ref -spacegroup 96 \
-maxresid 3.0 -sigma 5

dtrefine infldtindex.head infldtfind.ref -rej 1 1 2 -sigma 1 \
+CrysAll +DetAll -verbose 0 -go -verbose 1  -go

dtintegrate infldtrefine.head -window 0 0 -pad 1 \
-mosaicitymodel  1.000 0.000 -profit 50 7 -batch 1 4 -prerefine 2 -seq 1 60
```

```
dtscaleaverage infldtintegrate.head infldtprofit.ref \
-reject sigma 5.0 -reso 40 1.65 -scaleanom -errormodel  \
-reject fraction .0075 -batchscale -reqab spherical 4 3 infldtscale.ref
```

For the 1VPJ/12287 data set - phases ok. Have the following process.head file:

```
{
HEADER_BYTES= 2560;
A4_DETECTOR_DESCRIPTION=A4_ conversion;
A4_DETECTOR_DIMENSIONS=2048 2048;
A4_DETECTOR_SIZE= 209.72  209.72;
A4_DETECTOR_VECTORS=1 0 0 0 1 0;
A4_GONIO_NAMES=RotZ RotX/Swing RotY TransX TransY TransZ/Dist;
A4_GONIO_NUM_VALUES=6;
A4_GONIO_UNITS=deg deg deg mm mm mm;
A4_GONIO_VALUES=0.000 -0.002 0.000 0.000 0.000  170.000;
A4_GONIO_VECTORS=0 0 1 -1 0 0 0 1 0 1 0 0 0 1 0 0 0 -1;
A4_NONUNF_INFO=\$(FirstScanImage);
A4_NONUNF_TYPE=Simple_mask;
A4_OSC_RANGE= 1.0000;
A4_OSC_START= 290.0000;
A4_SPATIAL_BEAM_POSITION=1026.0 1065.0;
A4_SPATIAL_DISTORTION_INFO=1026.0 1065.0 0.10240 0.10240;
A4_SPATIAL_DISTORTION_TYPE=Simple_spatial;
A4_SPATIAL_DISTORTION_VECTORS=1 0 0 -1;
ADC=slow;
AXIS=phi;
BEAM_CENTER_X=105.10;
BEAM_CENTER_Y=101.05;
BIN=none;
BYTE_ORDER=little_endian;
CCD_IMAGE_SATURATION=65535;
CRYSTAL_GONIO_DESCRIPTION=Eulerian 3-circle;
CRYSTAL_GONIO_NAMES=Omega Chi Phi;
CRYSTAL_GONIO_NUM_VALUES=3;
CRYSTAL_GONIO_UNITS=deg deg deg;
CRYSTAL_GONIO_VALUES=0.000 0.000 0.000;
CRYSTAL_GONIO_VECTORS=1 0 0 0 1 0 1 0 0;
DATE=Sun Sep 26 14:01:35 2004;
DENZO_XBEAM=108.95;
DENZO_YBEAM=105.10;
DETECTOR_NAMES=A4_;
DETECTOR_NUMBER=1;
DETECTOR_SN=445;
DIM=2;
DISTANCE=170.0;
DTDISPLAY_ORIENTATION=-X+Y;
DTREK_DATE_TIME=11-Jul-2006 07:54:56;
```

```
DTREK_MODULE=unknown;
DTREK_VERSION=d*TREK version 9.5L -- Oct  4 2005;
PHI=290.000;
PIXEL_SIZE=0.102400;
ROTATION= 290.0000  291.0000  1.0000  5.0000  1.0000 0.0000 0.0000 0.0000 0.0000 0.0000;
ROTATION_AXIS_NAME=Omega;
ROTATION_FIELDS=RotStart RotEnd RotInc RotTime;
ROTATION_VECTOR=1 0 0;
SATURATED_VALUE=65535;
SCAN_FIELDS=RotStart RotEnd RotInc RotTime;
SCAN_ROTATION= 290.0000  291.0000  1.0000  5.0000  1.0000 0.0000 0.0000 0.0000 0.0000 0.0000
SCAN_ROTATION_AXIS_NAME=Omega;
SCAN_ROTATION_VECTOR=1 0 0;
SCAN_SEQ_INFO=1 1 0;
SCAN_TEMPLATE=../12287/12287_1_E1_???.img;
SIZE1=0;
SIZE2=0;
SOURCE_CROSSFIRE=0.0002 0.0002 0.0 0.0;
SOURCE_INTENSITY=1.0;
SOURCE_POLARZ=0.95 0 1 0;
SOURCE_SIZE=0.0 0.0 0.0 0.0;
SOURCE_SPECTRAL_DISPERSION=0.0002 0.0002;
SOURCE_VALUES=0 0;
SOURCE_VECTORS=0 0 1 0 1 0 1 0 0;
SOURCE_WAVELENGTH= 1.00000 0.97966;
TIME=5.0;
TWOTHETA=-0.002;
TYPE=unsigned_short;
UNIF_PED=1500;
WAVELENGTH=0.97966;
}

Only thing I changed was the beam centre (based on Labelit).
```

4 Plans

The best way to "wrap" d*TREK is probably through the header files, for instance having the "index" method write the initial header as input, then read the final header containing the indexing results. The actual text of the header could then be the "payload" of the result (in the same way as the mosflm matrix file etc.)

The results of the indexing are in a "cell" record in the header file - there is also the mosaic spread estimate in there.

In terms of processing, dtintegrate produces a header file - it may be worth recycling this later on to refine the parameters used in integration.

4.1 Initial Work

Looks like the input & output of all of the d*TREK processes will be the header files; a standard mechanism for reading, writing the header files could represent some standard functionality I want in a d*TREK Decorator - therefore define this.

4.2 Functionality

- [index] - if just a couple of images are available; use just dtfind, dtindex. if more frames are available define this to include a dtrefine step.
- [integrate] - if we have already refined then this is just integration, else it will include refinement.
- [scale] - scaling *via* scala or dtscaleaverage - need to find out how to do the former.

4.3 Wrappers

The following programs need wrappers:

- dtfind
- dtindex
- dtrefine
- dtintegrate
- dtscaleaverage

4.3.1 dtfind

4.3.2 dtindex

Input: -cell a b c alpha beta gamma -spacegroup 75
Output: get the cell etc. from header file.

5 Caveats

I am not sure that the statistics produced by dtscaleaverage are comparable to those from scala - the I/σ overall for 1vpj datasets (60 degree) was about 7, when the scala output gave the overall value of something like 12. Need to check this...

... however, the map calculated from the dataset looked ok; have not yet build into the data to get the final refinement statistics.

DTREK2SCALA (CCP4: Supported Program)

NAME

dtrek2scala - for conversion of integrated intensity and header files from D*TREK into multi-record mtz files

SYNOPSIS

dtrek2scala hklout foo_out.mtz [Keyworded input]

DESCRIPTION

The program DTREK2SCALA is used for converting reflection data files created by the program D*TREK. It uses the full goniometric description of the experiment (encoded in D*TREK header files) to generate a MTZ orientation blocks in the 'Cambridge' reference frame. The output is a multi-record MTZ file containing orientation blocks with the crystal and goniostat information: this file is suitable for input to SCALA for scaling
and is essentially equivalent to the output MTZ of MOSFLM.

The input files must be integrated or profile fitted intensity reflection files created by dtintegrate/dtprofit (e.g. dtprofit.ref) and the corresponding d*trek header file created by these programs (e.g. dtintegrate.head)

KEY WORDED INPUT

The various data control lines are identified by keywords with those available being:

ACCEPT , BATCH , BTITLE , CRYSTAL , FILE , HFILE , UGCB , LIMITS , SYMMETRY , REJECT , REINDEX , SCALE , SPLIT , TITLE , TOOFAR , NAME , PROCESS

ACCEPT n1 n2 n3 . . . (N.B. NOT WORKING!!!)

Set flags to accept reflections labelled with error flags n1,n2 etc (cf REJECT command below). MADNES sets a bit flag for each reflection for error conditions: this command (and REJECT) allow selection of which classes of reflection to accept. The flags are as follows:-

Flag Number	Default Setting	Error Condition
1	accept	Not found (ie weak)
2	accept	On YMS edge
3	accept	On ZMS edge
4	accept	On Phi edge

```
  5    reject      Too far from YMS
  6    reject      Too far from ZMS
  7    reject      Too far from Phi
  8    reject      Too big in YMS
  9    reject      Too big in ZMS
 10    reject      Too big in Phi
 11    reject      Background bad
 12    reject      Background sd bad
 13    reject      Negative sd
 14    accept      Fobs <= 0.0
 15    reject      Bad pixels
 16    reject      Overflow
```

BATCH <batch number> [<maximum batch number>]

Set BATCH number for output file. If the SPLIT option is used (qv), this will be the first batch number. Remember that batch numbers must be unique for all batches in an MTZ file. When reading multiple DTREK data reflection files a separate BATCH command must be used before each PROCESS keyword otherwise the program will not give the correct performance. Watch out if using the SPLIT option as well; batch numbers must be unique, and no check is made of this, so the starting batch number for each group must be sufficiently well separated. The optional maximum batch number may be used to avoid having a final batch with very few reflections in it.

BTITLE <title>

Set batch title for output MTZ file (defaults = file title TITLE)

CRYSTAL <crystal_number>

Set crystal number, a number defining a crystal which may contain a number of batches. This number is not currently used, but may be in future. The crystal number defaults to the first batch number.

FILE <filename>

Filename for d*trek reflection file. (default = dtprofit.ref).

HFILE <filename>

Filename for the d*trek header file after the integration/profile fitting stage. (default = dtintegrate.head) (see example).

LIMITS <Ymin> <Ymax> <Zmin> <Zmax>

Set limits on detector position Y,Z for reflection to be accepted This may be used to exclude reflections near the edge of the detector The

default is not to check detector position.

REINDEX <reindexing_rule>

Reindex data, according to a matrix specified in a similar way to symmetry operations

e.g. reindex k, h, -l
reindex h, -k, -h/2-l/2

Cell dimensions will be recalculated for the redefined cell. Be careful that the index transformation preserves the hand of the axes, ie that the matrix has a positive determinant. The program will not allow you to invert the hand (eg k,h,l is forbidden, k,h,-l is allowed). If the transformation leads to fractional indices for some cases (as in the 2nd example above), these reflections will be rejected. If the reindexing operations include translations, then the orientation data in the output file will not be strictly correct. Translations (eg h,k,l+1) can be useful if you have misindexed your crystal by eg 1 lattice point (usually along the spindle axis). However, in this case, you OUGHT to reprocess the data.

REJECT n1 n2 n3 . . .

Set flags to reject reflections labelled with error flags n1,n2 etc (cf ACCEPT command above).

SCALE <scale_factor>

Set output scale factor (default = 1.0). This can be adjusted to give intensities in a suitable range.

SPLIT <psi_range>

By default the actual oscillation range per image read from the header file is used to split the reflection into BATCHes. If <psi-range> is set then BATCHing is performed accordingly based on the requested psi range.

SYMMETRY <space-group name | space-group number | symmetry>

(compulsory)

Read the symmetry operations, specified as the name (eg P212121), the International Tables number, or as a series of SYMMETRY commands giving the symmetry operations (eg SYMMETRY X,Y,Z * -X,Y+1/2,-Z)

This last option is not recommended. The symmetry matrices are read from a standard file (logical name SYMOP), are printed, and are used to reduce the reflections to an asymmetric unit. The column M/ISYM in

the output file contains the number of the symmetry operation used to do this, odd numbers correspond to +hkl, even numbers to Bijvoet-related reflections -hkl. The asymmetric unit is selected according to the rule printed out with the symmetry

TITLE <Title>

Set file title for output MTZ file.

TOOFAR <Yshift> <Zshift> <Phishift>

Sets values for the maximum difference between calculated and observed position for a reflection to be accepted. Yshift and Zshift are in pixels, Phishift is in degrees. The default is not to do any checks on positional differences.

NAME PROJECT <pname> CRYSTAL <xname> DATASET <dname>

[Note that the keywords PNAME <pname>, XNAME <xname> and DNAME <dname> are also available, but the NAME keyword is preferred.]

Specify the project, crystal and dataset names for the output MTZ file. It is strongly recommended that this information is given. Otherwise, the default project, crystal and dataset names are "unknown", "unknown" and "unknown<ddmmyy>" respectively (where <ddmmyy> is the date, with no spaces).

The project-name specifies a particular structure solution project, the crystal name specifies a physical crystal contributing to that project, and the dataset-name specifies a particular dataset obtained from that crystal. All three should be given.

UGCB

If this keyword is present the D*TREK Goniostat matrix formed from the DATUM values given in the header keyword CRYSTAL_ORIENT_VALUES will be included into the UMAT written in to the mtz file batch header. The Goniostat datum values are consequently set to zero. The default behaviour is for the Goniostat orientation to be excluded from the UMAT. Scala versions before scala-3.1.4-beta (22 April 2002) will expect mtz files generated from DTREK2SCALA using the UGCB option because they make no use of the Datum values.

PROCESS

(compulsory)

Process the currently-defined input file (from FILE command or logical name MADHKL).

INPUT_FILES

D*TREK

D*TREK ASCII reflection file
A d*trek reflection file created by dtintegrate or dtprofit (usually called dtintegrate.ref or dtprofit.ref) must be specified using the FILE command (see example). If D*TREK is set to produce binary reflection files then you must first convert the binary file to ASCII using the D*TREK command

dtreflnmerge <input-file> <output-file> -text

The reflection file header provides a description of all the fields of the reflection file. The header should something like this otherwise the program may fail to convert correctly.

```
4 20 1
nH                  ; miller index
nK                  ; miller index
nL                  ; miller index
nBadFlag
fIntensity          ; profile fitted intensity
fSigmaI             ; sigma of profile fitted intensity
fOtherInt           ; integrated intensity
fOtherSig           ; sigma of integrated intensity
fObs_pixel0         ; vertical detector coordinate of reflection (Y)
fObs_pixel1         ; horizontal detector coordinate of reflection (Z)
fObs_rot_mid        ; observed reflection centroid
fObs_rot_width
fCalc_pixel0
fCalc_pixel1
fCalc_rot_mid
fResolution
fLPfactor           ; Lorentz and polarization correction factor
fCorrelation
sBatch              ; Batch number from integration
```

The relevant fields used by MADNES are described briefly. The reflections are listed sequentially in free format.

D*TREK header file
The d*trek header file contains a whole lot of information which allows you to find out just about anything about your experiment (assuming of course that you and the beamline software remembered to write the correct values to the image headers. In principle though, the important information about the experiment should be correct as it is necessary to correctly analyse your data and should therefore be available for reading by DTREK2SCALA. The following is a list of the

```
   d*trek header items used by DTREK2SCALA. If you encounter difficulties
   in converting your data then checking your d*trek header file may be a
   place to start. The d*trek header file can also be specified using the
   HFILE  command.  The file is named dtintegrate.head by default in both
   d*trek and in DTREK2SCALA.
CRYSTAL_GONIO_VALUES        Datum position on MGONAX
                            goniostat axes (degrees)
CRYSTAL_UNIT_CELL           Cell dimensions (A & degrees)
CRYSTAL_SPACEGROUP          space group number
CRYSTAL_ORIENT_VECTORS      Axis permutation from d*trek.
CRYSTAL_ORIENT_ANGLES       "missetting" angles (degrees)
APS1_GONIO_VALUES(6)        Crystal to detector distance (mm)
APS1_GONIO_VALUES(1,2,3)    detector tilts: DTAU(2) = theta
                            detector swing angle (degrees)
SOURCE_ORIENT_ANGLES        beam tilt angles (degrees)
CRYSTAL_MOSAICITY           reflection width (degrees)
SCAN_WAVELENGTH             wavelength (A)
SOURCE_SPECTRAL_DISPERSION  dispersion (delta lambda/lambda)
SOURCE_CROSSFIRE            synchrotron beam parameters:
                            gammaH, gammaV, Delcor, ?syn4?
                            scan axis number (1 -> MGONAX)
SCAN_ROTATION(1,2)          start and stop values of psi
                            (D*trek scan axes - usually Omega)  (degrees)
SCAN_ROTATION(3)            rotation width of each image (degrees)
SCAN_ROTATION(4)            time for each image (seconds)
CRYSTAL_GONIO_NUM_VALUES    number of crystal goniostat axes
CRYSTAL_GONIO_VECTORS       vectors defining the directions
                            of the MGONAX goniostat axes,
                            in the d*trek laboratory frame.
                            GONVEC(I,J),I=1,3 applies to the J'th axis
SOURCE_VECTORS(1,2,3)       idealized main beam vector
                            (anti-parallel to beam!), in d*trek
                            laboratory frame (excluding the
                            tilts parameterized by MU)
SOURCE_VECTORS(1,2,3)       main beam vector (anti-parallel
                            to beam!), in d*trek laboratory frame
                            (including the tilts parameterized by MU)
APS1_DETECTOR_DIMENSIONS    detector limits minimum, maximum Yms, Zms
APS1_GONIO_VECTORS          vectors defining detector rotations
APS1_DETECTOR_VECTORS       vectors defining detector translations
DTREFINE_RMS_MM             rms positional errors from last refinement
DTREFINE_RMS_DEG            rms rotational errors from last refinement
APS1_GONIO_VALUES(4,5)      detector offsets ccx, ccy
DTP_DTINTEGRATE_OPTIONS(11) number of images per batch used in dtintegrate

     New common block for d*trek specific things

SCAXIS                      scan axis
GONAX(3)                    names of the MGONAX goniostat axes
```

```
DETAX(3)                    names of the detector rotation angles
COMMENT                     crystal description

   N.B.  The  d*trek laboratory frame has X along the omega axis (towards
   base  plate  of  goniometer),  Z  antiparallel to the X-ray beam and Y
   completing a right-handed system. All rotations are right-handed. This
   information is encoded in GONVEC & SO, so these are used to define the
   frame.

OUTPUT_FILES

   HKLOUT  --  Multi-record MTZ file. Each batch has an orientation block
   as  defined  in  mtzlib.doc  for  area detectors. The columns for each
   reflection are
H K L       indices
M/ISYM      symmetry number, ie number of the Laue-group matrix used to reduce
this reflection to the asymmetric unit
BATCH batch number
I, SIGI intensity and standard deviation
IPR, SIGIPR intensity and standard deviation (in this case same as I, SIGI)
IERROR error flag from D*TREK
XDET,YDET detector coordinates of reflection (pixels)
XDET = Yms, YDET = Zms (ie Mosflm convention)
ROT rotation angle (degrees)
LP Lorentz and polarisation correction (d*trek only) LP

   This  file  must  be sorted on H K L M/ISYM BATCH before processing by
   SCALA. Several files may be sorted together by SORTMTZ.

EXAMPLES

   1. An example which runs on d*trek profile fitted reflection data
############### START EXAMPLE 1 ###################
dtrek2scala    hklout   junk.mtz    plot absplot  << eof
TITLE  Data processed with d*trek to 1.8A
SYMMETRY   20
CRYSTAL 1
BATCH 1
BTITLE  Crystal 1, run 1  # this title is for this batch only
FILE dtprofit_1.8A.ref
HFILE dtintegrate.head
PROCESS
eof
#
sortmtz HKLIN junk.mtz HKLOUT dtrek-data.mtz << EOF-sortmtz
#
# Sort keys since default keys are H K L
#
H K L M/ISYM
```

```
EOF-sortmtz
############### END EXAMPLE 1 ##################
```

2. An example which reads two reflection files dataset1.ref and dataset2.ref with there own header files.

```
############### START EXAMPLE 2 ##################
#!/bin/csh -f
#
set ident      = mydata
set title      = 'A crystal soaked in lots of alcohol'
set lowres     = 30
set highres    = 1.8
set resol      = "${lowres} ${highres}"
set residues   = 203
set spacegroup = P43212
set symmetry   = 96
set scr        = $HOME/tmp
#
#
dtrek2scala hklout ${ident}.mtz > ${ident}.dtrek2scala.log << EOF
TITLE $title
SYMMETRY $symmetry
CRYSTAL 1
BATCH 1
FILE dataset1.ref
HFILE dataset1.head
BTITLE CHI=0, PHI=0
PROCESS
BATCH 300
FILE dataset2.ref
HFILE dataset2.head
BTITLE CHI=30, PHI=0
PROCESS
EOF
#
sortmtz hklout ${ident}_sort.mtz > ${ident}_sort.log << EOF-sortmtz
H K L M/ISYM BATCH
${ident}.mtz
EOF-sortmtz
############### END EXAMPLE 2 ##################
```

AUTHOR

Based on the CCP4 program ABSURD. MTZ version May 1991 by Phil Evans and revised for use with D*TREK by Gwyndaf Evans.
DTREK2SCALA by Gwyndaf Evans (1998-2003).