

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 missing 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 initial 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, Bolotovskiy, & 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, Bolotovskiy, & 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	LeastSq	Spgrp	Cent	Bravais type	a	b	c
num	residual	num*	type	Cell volume	alpha	beta	gamma
7	0.190	75	P	tetragonal 423844	51.796 90.000	51.796 90.000	157.982 90.000
9	0.166	21	C	orthorhombic 847680	73.093 90.000	73.409 90.000	157.982 90.000
11	0.175	16	P	orthorhombic 423839	51.669 90.000	51.923 90.000	157.982 90.000
12	0.064	5	C	monoclinic 851816	73.691 90.000	73.168 90.141	157.982 90.000
12b	0.075	5	C	monoclinic 847678	73.409 90.000	73.093 90.131	157.982 90.000
13	0.092	3	P	monoclinic 423838	51.923 90.000	51.669 90.100	157.982 90.000
14	0.000	1	P	triclinic 423834	51.669 89.900	51.923 89.915	157.982 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 90.000	51.796 90.000	157.982 90.000	-75.915	20.479	-78.321
2	0.001	51.796 90.000	51.796 90.000	157.982 90.000	75.915	-20.479	101.679
3	0.001	51.796 90.000	51.796 90.000	157.982 90.000	104.085	20.479	-78.321
4	0.001	51.796 90.000	51.796 90.000	157.982 90.000	-104.085	-20.479	101.679
5	0.001	51.796 90.000	51.796 90.000	157.982 90.000	56.911	65.317	66.033

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 infltdtintegrate.head infltdtprofit.ref \
-reject sigma 5.0 -reso 40 1.65 -scaleanom -errormodel \
-reject fraction .0075 -batchscale -reqab spherical 4 3 infltdtscale.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).