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.