

Data collection & processing

Data acquisition → *images* → *intensities* (I, σ) → *amplitudes* (F, σ)

Pipelines & GUIs: DNA, XIA, ccp4i (others?)

CCP4 components:

- Mosflm new GUI
- Pointless determine spacegroup, match previous indexing
- (Scala)
- Truncate rewrite
 ? intensity statistics: twinning
- Experimental absorption correction

Pointless

Three distinct functions

- Determine Laue group & space group
- Match alternative indexing scheme to a reference merged dataset. Either exact (eg trigonal system) or accidental (eg $a \approx b$)
- Just reindex with specified operator and symmetry (most of the functionality of the REINDEX program)

Examples of running from command line

pointless file.mtz

pointless hklin file.mtz

determine likely Laue group & space group. All control input is optional

pointless hklin file.mtz hklout newfile.mtz

output data reindexed into "best" space group

pointless hklin file.mtz hklref referencefile.mtz hklout newfile.mtz

output data reindexed to best match with reference file, if there is a symmetry-related or accidental ambiguity

hklin may be merged or unmerged

hklref must be merged

pointless hklin file.mtz hklout newfile.mtz << eof

reindex -k,h,l

spacegroup P3121

eof

Reindex

Protocol for space group determination

1. From the unit cell dimensions, find the highest compatible lattice symmetry
2. Score each symmetry element belonging to lattice symmetry using all pairs of observations related by that element
3. Score combinations of symmetry elements for all possible sub-groups (Laue groups) of lattice symmetry group.
4. Score possible space groups from axial systematic absences

Example

Spacegroup: C 2 2 2 1

Cell: 43.68 71.92 89.20 90.00 90.00 90.00

The true space group C222₁

Lattice point group: P 6 2 2

Reindexing or changing symmetry

Reindex operator from input cell to lattice cell: [-1/2h-1/2k,-1/2h+1/2k,-l]

$$h' = (h \ k \ l) \begin{pmatrix} -0.5 & -0.5 & 0 \\ -0.5 & 0.5 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Lattice unit cell after reindexing: deviation 2.52 degrees

42.07 42.07 89.20 90.00 90.00 **117.45**

Possibly hexagonal
(within 3°! default tolerance is 2°)

Score each symmetry operator in P622

Rfactor (multiplicity weighted)

Correlation coefficient on E²
Z-score(CC)

Ne mt	Z-cc	CC	N	Rmeas		Symmetry & operator (in Lattice Cell)	
1	9.70	0.70	68480	0.211		identity	
2	9.39	0.68	88636	0.254	***	2-fold l	(0 0 1) {-h, -k, +l}
3	11.97	0.87	71371	0.205	***	2-fold	(1 -1 0) {-k, -h, -l}
4	0.54	0.04	74289	0.727		2-fold	(2 -1 0) {+h, -h-k, -l}
5	0.83	0.06	73108	0.709		2-fold h	(1 0 0) {+h+k, -k, -l}
6	11.91	0.86	71467	0.210	***	2-fold	(1 1 0) {+k, +h, -l}
7	0.46	0.04	75429	0.725		2-fold k	(0 1 0) {-h, +h+k, -l}
8	0.90	0.07	74008	0.701		2-fold	(-1 2 0) {-h-k, +k, -l}
9	2.09	0.15	158843	0.801		3-fold l	(0 0 1) {-h-k, +h, +l} {+k, -h-k, +l}
10	2.39	0.18	175498	0.852		6-fold l	(0 0 1) {-k, +h+k, +l} {+h+k, -h, +l}

Only the orthorhombic symmetry operators are present

A clear preference for Laue group Cmmm

Net Z(CC) scores are

$Z^+(\text{symmetry in group}) - Z^-(\text{symmetry not in group})$

Correlation coefficient & R-factor

Net Z(CC)
calculated in two ways

Likelihood

Cell deviation

Laue Group	NetZc	Zc+	Zc-	NetZa	Zs+	Za-	Lklhd	CC	Rmeas	Delta	ReindexOperator
= 1 C m m m ***	9.69	10.98	1.29	9.74	11.15	1.42	1.34	0.80	0.23	0.0	[h,k,l]
> 2 C 1 2/m 1 ***	8.39	11.97	3.58	6.47	11.97	5.50	1.10	0.87	0.21	0.0	[h,k,l]
> 3 C 1 2/m 1 ***	8.31	11.91	3.60	6.39	11.91	5.52	1.09	0.86	0.21	0.0	[-k,-h,-l]
4 P 1 2/m 1 **	5.63	9.39	3.76	3.29	9.39	6.10	0.66	0.68	0.25	0.0	[-1/2h+1/2k,-l,-1/2h-1/2k]
5 P -1 **	5.26	9.70	4.44	3.16	9.70	6.54	0.61	0.70	0.21	0.0	[1/2h+1/2k,1/2h-1/2k,-l]
6 P 6/m m m *	4.44	4.44	0.00	6.54	6.54	0.00	0.11	0.32	0.55	2.5	[-1/2h-1/2k,-1/2h+1/2k,-l]
7 P 6/m	0.03	4.47	4.44	-1.20	5.72	6.92	0.08	0.33	0.61	2.5	[-1/2h-1/2k,-1/2h+1/2k,-l]
8 C m m m	-0.41	4.16	4.57	-1.56	5.46	7.02	0.06	0.30	0.51	2.5	[1/2h-1/2k,-3/2h-1/2k,-l]
9 C m m m	-1.08	3.72	4.80	-1.60	5.43	7.03	0.05	0.27	0.52	2.5	[-1/2h-1/2k,-3/2h+1/2k,-l]
10 P -3 1 m	-1.25	3.73	4.98	-0.79	6.09	6.88	0.05	0.27	0.59	2.5	[-1/2h-1/2k,-1/2h+1/2k,-l]
11 P -3 m 1	-1.26	3.73	4.99	-0.83	6.07	6.90	0.04	0.27	0.59	2.5	[-1/2h-1/2k,-1/2h+1/2k,-l]
12 P -3	-2.71	2.09	4.79	-4.81	2.09	6.90	0.02	0.15	0.80	2.5	[-1/2h-1/2k,-1/2h+1/2k,-l]
13 C 1 2/m 1	-3.92	0.90	4.82	-6.04	0.90	6.93	0.01	0.07	0.70	2.5	[-3/2h-1/2k,-1/2h+1/2k,-l]
14 C 1 2/m 1	-4.00	0.83	4.83	-6.10	0.83	6.93	0.01	0.06	0.71	2.5	[1/2h-1/2k,-3/2h-1/2k,-l]
15 C 1 2/m 1	-4.37	0.54	4.91	-6.40	0.54	6.94	0.01	0.04	0.73	2.5	[-3/2h+1/2k,1/2h+1/2k,-l]
16 C 1 2/m 1	-4.46	0.46	4.92	-6.48	0.46	6.94	0.00	0.04	0.73	2.5	[-1/2h-1/2k,-3/2h+1/2k,-l]

Screw axis along 00l shows space group is C22₁

Screws detected by Fourier analysis of I/σ

Zone	Number	PeakHeight	SD	Probability	ReflectionCondition
1 screw axis 2(1) [c]	109	0.878	0.083	0.747	00l: l=2n

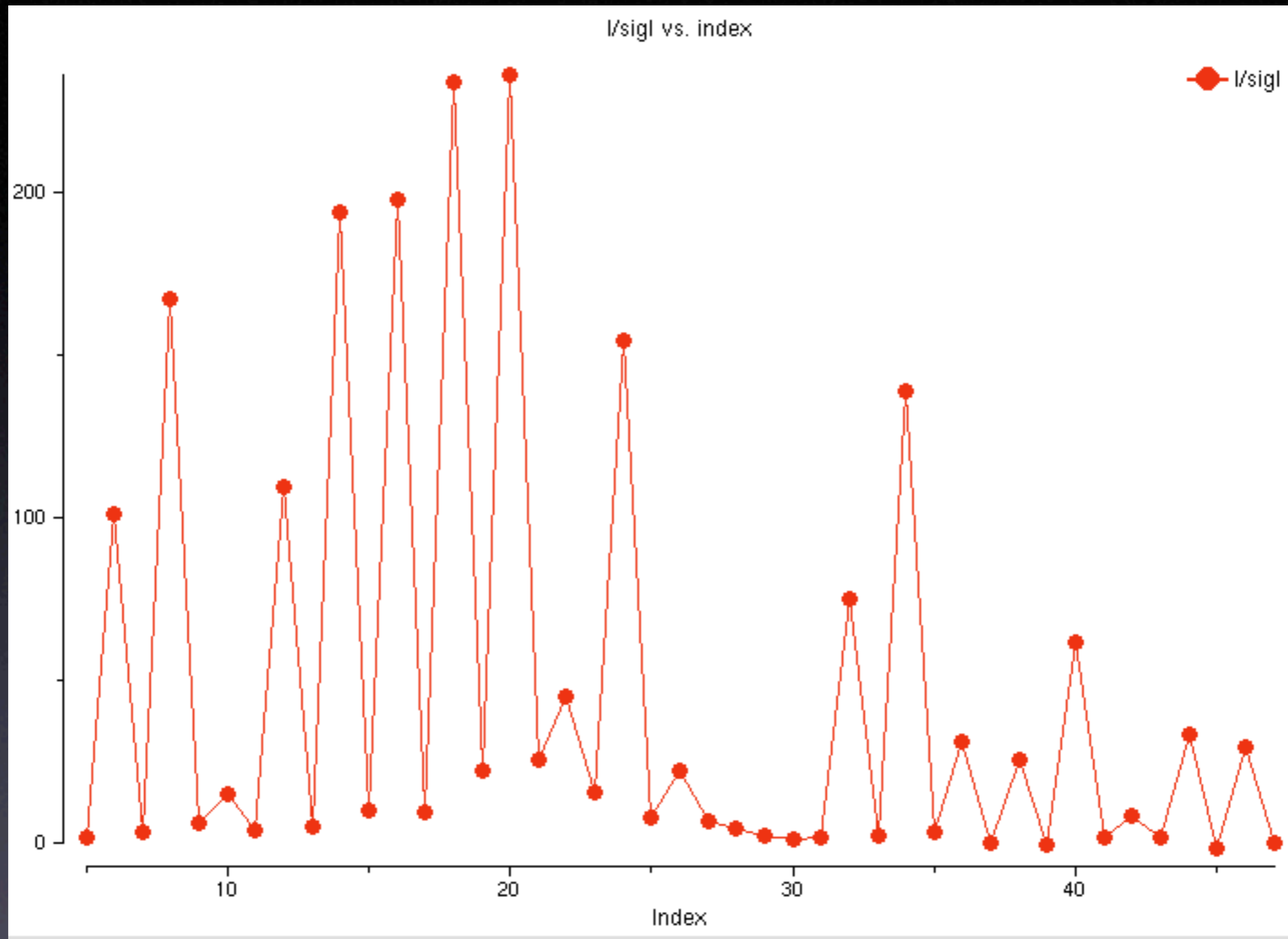
PeakHeight from Fourier analysis
 1.0 is perfect screw
 Probability of screw

'TotProb' is a total probability estimate (unnormalised)

'SysAbsProb' is an estimate of the probability of the space group based on the observed systematic absences.

'Conditions' are the reflection conditions (absences)

Spacegroup	TotProb	SysAbsProb	Reindex	Conditions
<C 2 2 21> (20)	1.063	0.747		00l: l=2n (zones 1)
..... <C 2 2 2> (21)	0.360	0.253		



Axial reflections $00l$ plotted as I/σ

Status

version 1.0.3 works(?) 28/03/2006

Dependencies:

cctbx

clipper

ccp4

<ftp://ftp.mrc-lmb.cam.ac.uk/pub/pre/pointless-1.0.3.linux>
[pointless-1.0.3.osxppc](ftp://ftp.mrc-lmb.cam.ac.uk/pub/pre/pointless-1.0.3.osxppc)
[pointless.html](ftp://ftp.mrc-lmb.cam.ac.uk/pub/pre/pointless.html)

Future

Ice rings/spots:

a powder ring has infinite rotational symmetry so it will fit any axis order. Plan to eliminate ice rings from statistics.

XML output for Graeme

ccp4i task

Scala rewrite (new program based on components from Pointless). Working title: Aimless