Data evaluation, integration and analysis I

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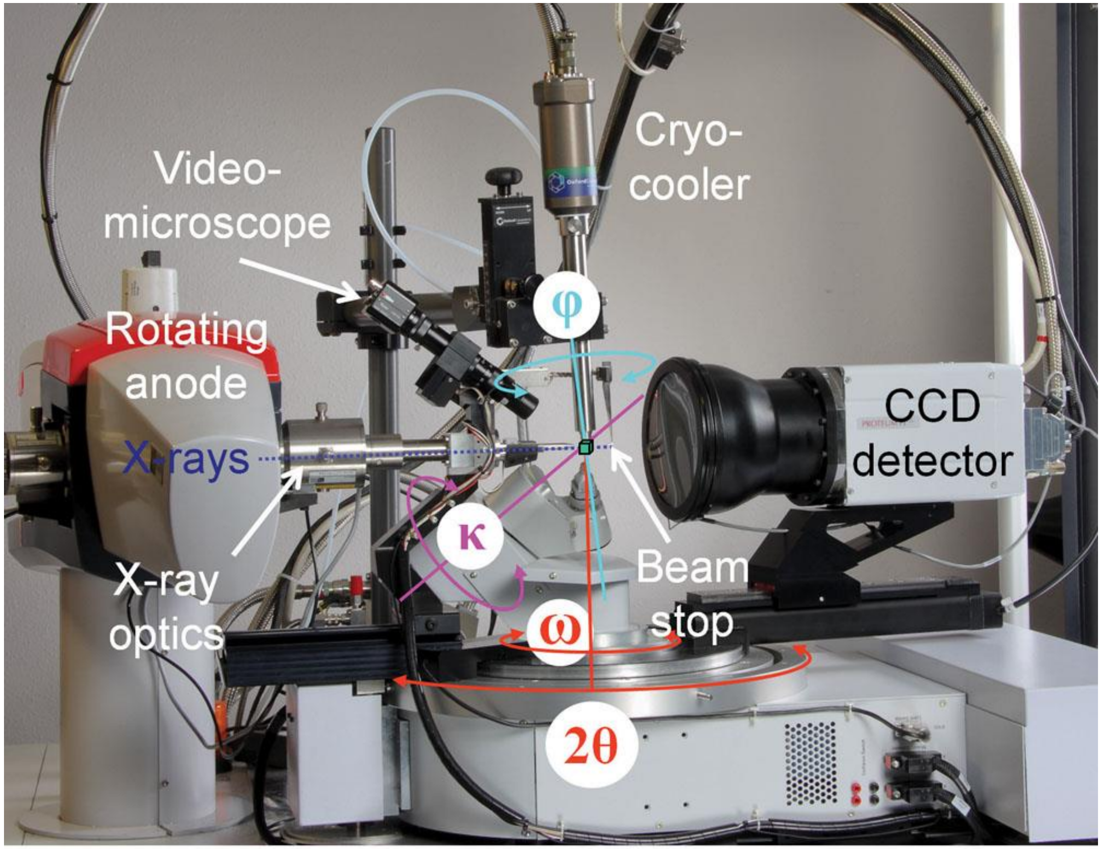
Content

Data processing with EVAL:

- Crystal orientation and goniometer
- Indexing
- Cell matrix refinement and metadata
- Reflection profiles and integration
- Intensities, corrections, scaling, merging
- Error estimates and contributions to esd
- Special cases:
  - Multiscan data
  - Twin lattices
  - incommensurate
  - Diffuse scattering

Diffractometer



EVAL

www.crystal.chem.uu.nl/distr/eval/

Eval Program Suite

Eval14 and eval15 are integration methods for single crystal X-ray diffraction on area detectors. Both methods use knowledge about the exact experimental setup.

- Eval14 applies boxsummation (BPB) with predicted reflection boundaries.
- Eval15 applies profile fitting with predicted reflection profiles

The eval15 method is described in:

> A.M.M. Schreurs, X. Xian and L.M.J. Kroon-Batenburg
> EVAL15: a diffraction data integration method based on ab initio predicted profiles
> *J. Appl. Cryst.* **43**, (2010) 70-82

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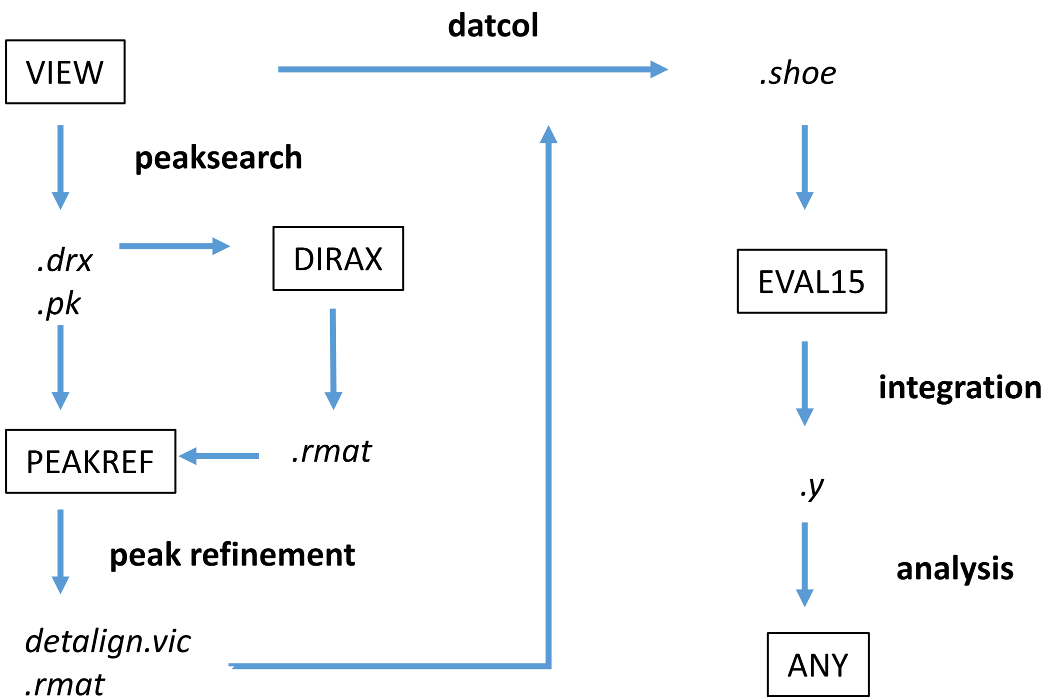
The eval14 method is described in:

> A.J.M. Duisenberg, L.M.J. Kroon-Batenburg and A.M.M. Schreurs
> An intensity evaluation method: EVAL-14
> *J. Appl. Cryst.* **36**, (2003) 220-229.

A reprint (Copyright © International Union of Crystallography *J. Appl. Cryst.* **36**, 220-229) can be found here (PDF file, 820 kb).

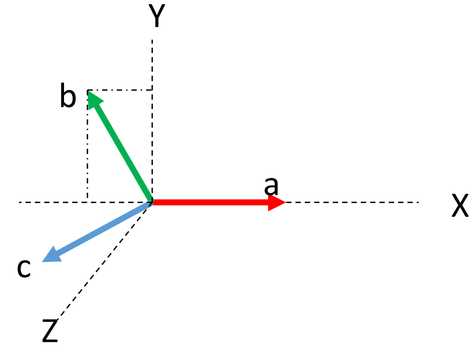
runs on Linux

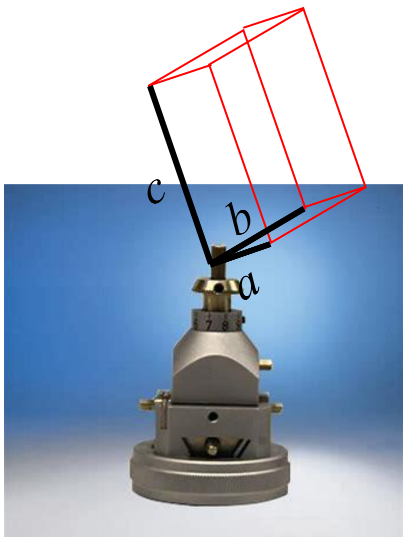
EVAL flow diagram



Lattice matrices and orientations

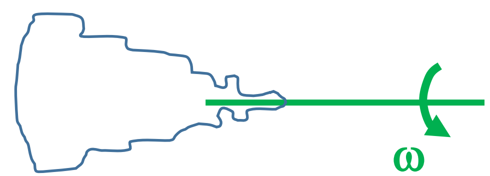
$$O=\begin{pmatrix} a & 0 & 0 \\ b\cos\gamma & b\sin\gamma & 0 \\ c\cos\beta & \dfrac{c(\cos\alpha-\cos\beta\cos\gamma)}{\sin\gamma} & \dfrac{V}{ab\sin\gamma} \end{pmatrix}$$

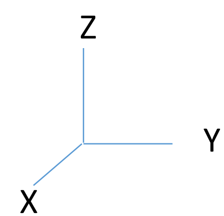




$$D = R_0 . O$$

$$R_\omega R_\chi R_\phi R_0 . O$$

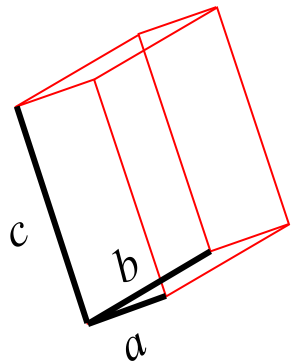


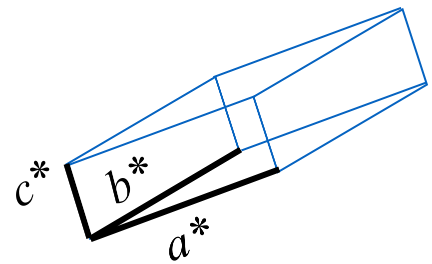


Laboratory Axes System

*often O^T is used as orthogonalization matrix

Crystal and reciprocal lattices





$$D$$

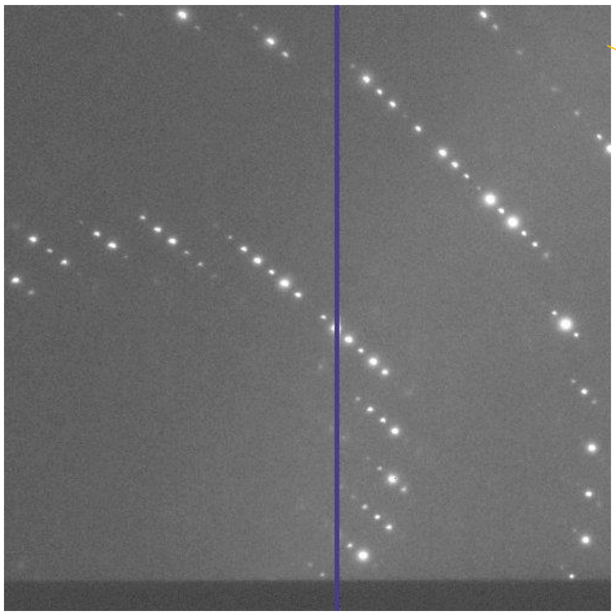
$$\begin{pmatrix} - & a & - \\ - & b & - \\ - & c & - \end{pmatrix}$$

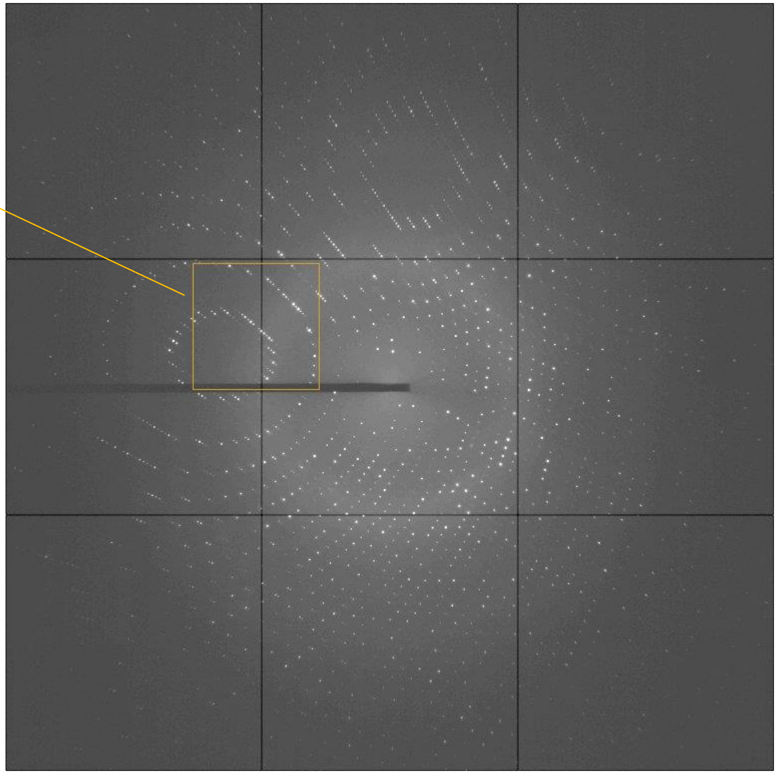
$$R = D^{-1}$$

$$\begin{pmatrix} | & | & | \\ a^* & b^* & c^* \\ | & | & | \end{pmatrix}$$

$$\mathbf{d}^*_{\mathbf{hkl}} = \boldsymbol{R}.\begin{pmatrix} h \\ k \\ l \end{pmatrix} = h\mathbf{a}^* + k\mathbf{b}^* + l\mathbf{c}^* = \frac{\mathbf{1}}{\boldsymbol{d_{hkl}}}$$

Thaumatin





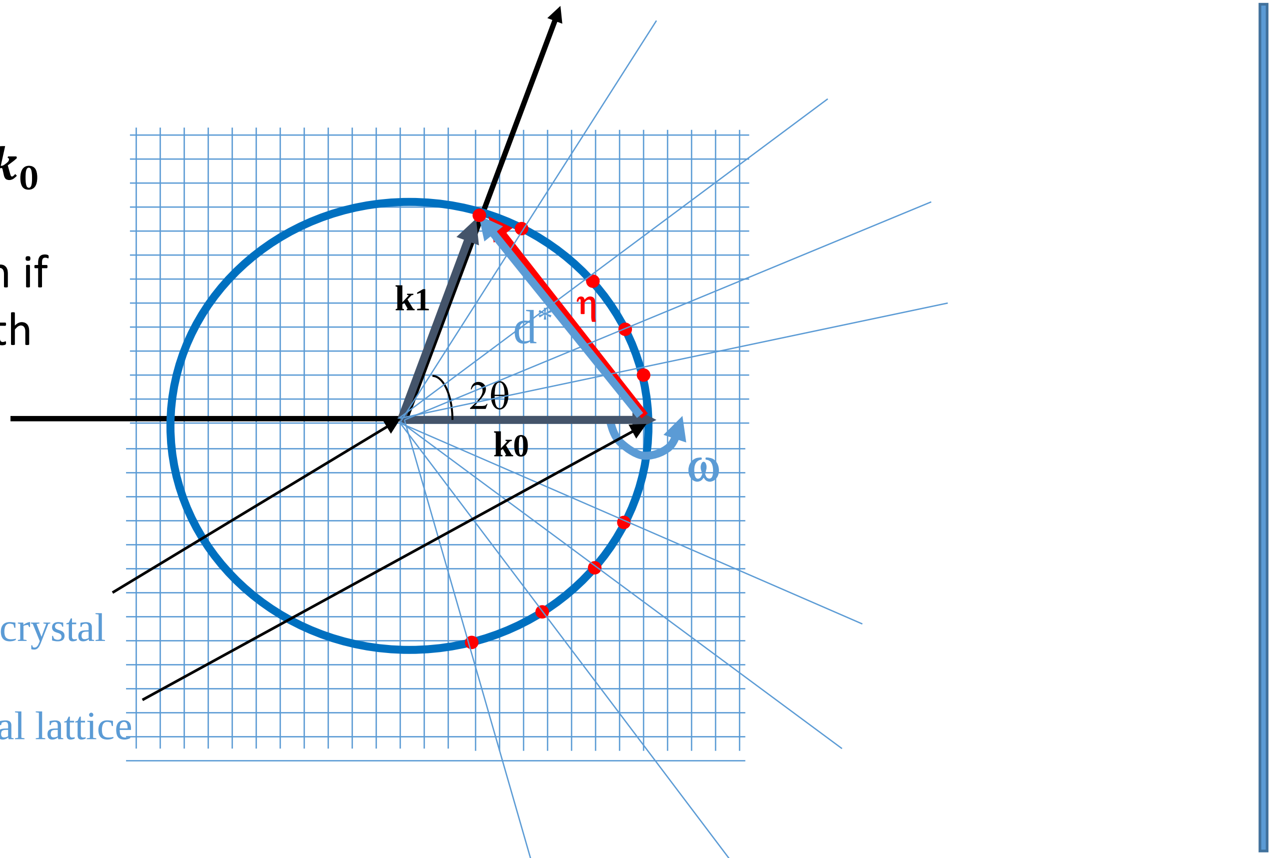
ADSC detector Diamond Light Source
Scan around horizontal spindle axis 0.5° increments

Ewald construction

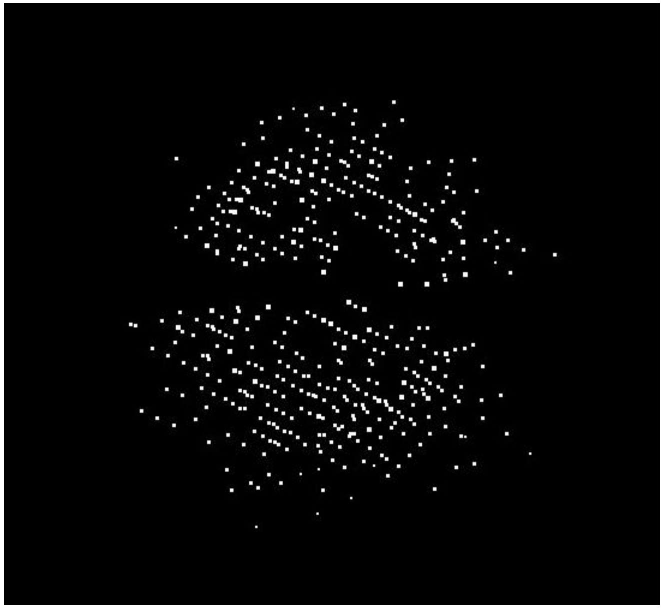
$$\boldsymbol{\eta} = \boldsymbol{k_1} - \boldsymbol{k_0}$$

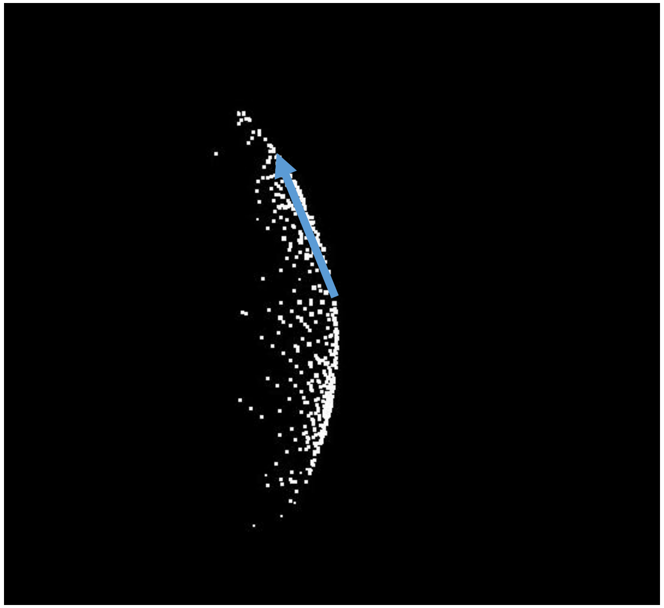
Bragg reflection if **d*** co-aligns with **η**

$|k_0| = 1/\lambda$



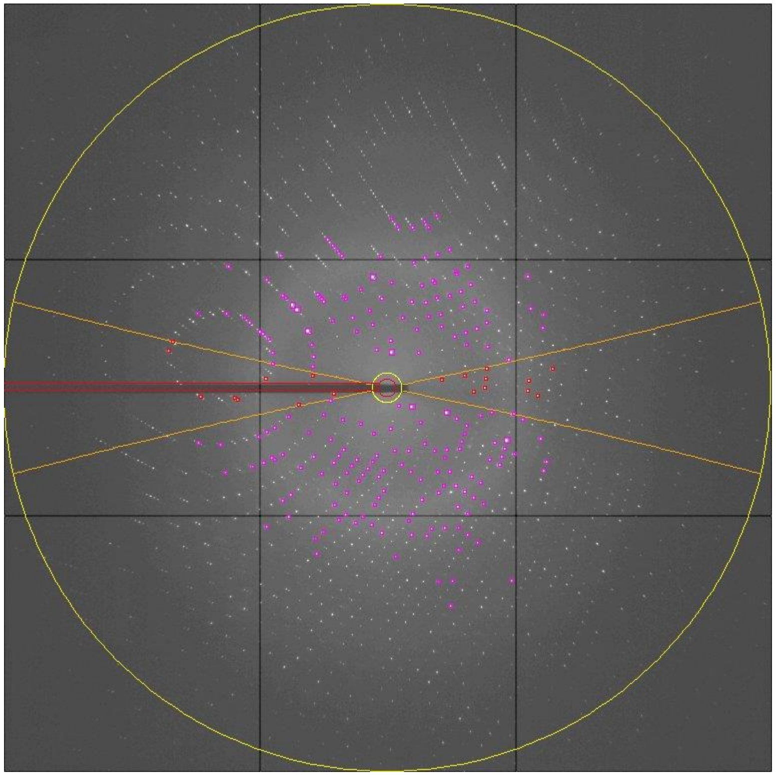
Ewald sphere





Indexing: find vectors d* and index these in (a*,b*,c*)

Indexing with Dirax



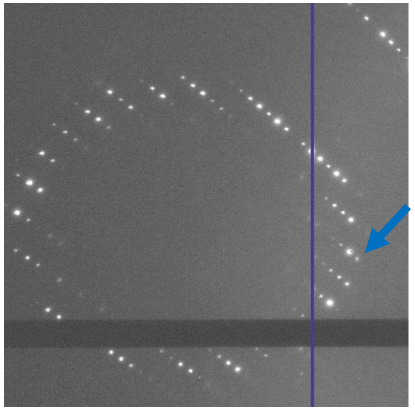
Peaks in 2D on the detector

d*

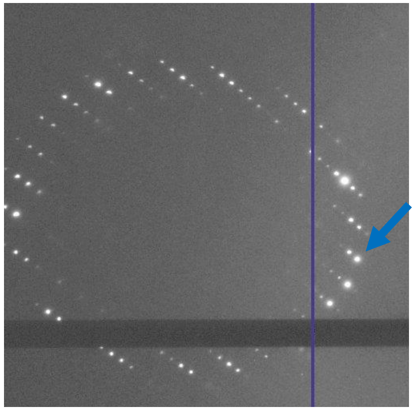
200 c-vectors from file pk2.drx.
Acl nH a b c alpha beta gamma Volume S
130 19 66.401 49.954 242.935 90.73 96.13 92.31 800438
126 17 45.308 57.681 238.449 96.49 87.23 103.79 601201
123 17 36.578 58.401 225.349 97.39 89.40 104.43 462223
119 111 81.498 172.526 204.769 98.93 95.47 89.79 2831121
116 118 56.728 57.489 150.502 90.88 91.66 90.99 490485
108 119 56.778 57.490 150.510 90.88 91.60 90.98 490958
90 107 56.772 57.550 150.147 89.25 91.89 89.01 490174
74 97 56.820 57.474 112.751 96.29 95.28 90.96 364300
Solutions limited by voltest

108 119 **56.778 57.490 150.510 90.88 91.60 90.98** 490958
selected ACL 108

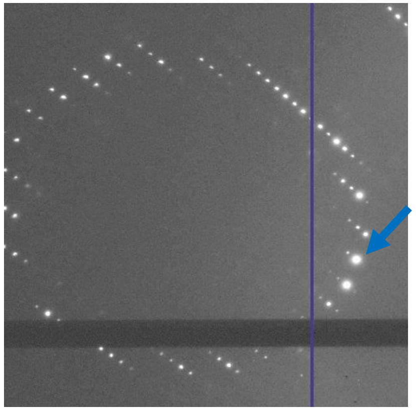
Indexing with Dirax



0-0.5°

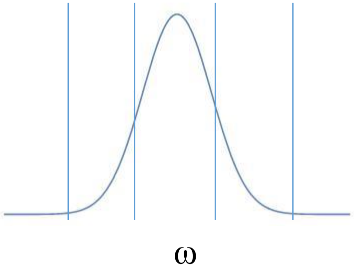


0.5-1.0°



1.0-1.5°

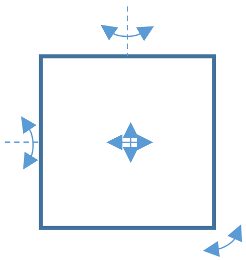
3D peak search over a range of 100°



DIRAX: **57.373 57.565 149.279 90.41 89.44 90.13** 492982

Peakref: Refining peak positions

		ref	current	initial	change	accumulate	shift	refl
D	a	Yes	57.64815	57.37284	0.27530	57.64815	0.11475	20152
	b	Con	57.64815	57.37284		57.64815	0.11513	20152
	c	Yes	149.61322	149.27934	0.33388	149.61322	0.29856	20152
	alpha	Fix	90.00000	90.41067		90.00000	0.20000	20152
	beta	Fix	90.00000	89.44347		90.00000	0.20000	20152
	gamma	Fix	90.00000	90.13022		90.00000	0.20000	20152
R_0	orx	Yes	0.79530	0.78922	0.00608	0.79530	0.00022	20152
	ory	Yes	0.59701	0.60462	-0.00762	0.59701	0.00022	20152
	ora	Yes	-51.16824	-51.19841	0.03017	-51.16824	0.20000	20152
	xtalx	No	0.00000	0.00000		0.00000	0.10000	20152
	xtaly	No	0.00000	0.00000		0.00000	0.10000	20152
	xtalz	Fix	0.00000	0.00000		0.00000	0.10000	20152
	zerodist	Yes	-0.16770	0.00000	-0.16770	0.16770	0.10000	20152
	zerohor	Yes	0.42149	0.00000	0.42149	0.01610	0.10000	20152
	zerover	Yes	-0.57659	0.00000	-0.57659	-0.46698	0.10000	20152
	detrotx	Yes	0.14871	0.00000	0.14871	0.14871	0.20000	20152
	detroty	Yes	0.27821	0.00000	0.27821	0.27821	0.20000	20152
	detrotz	Yes	0.36010	0.00000	0.36010	0.36010	0.20000	20152
	Vol		497210.97	491337.31	5873.66	497210.97		20152
residuals	mm		0.03903	0.70960	-0.67057	0.03903		20152
	mmAng	+	0.01495	0.28118	-0.26623	0.01495		20152
	rotoutside		0.03599	0.25945	-0.22346	0.03599		742
	rotinside		0.00000	0.00000	0.00000	0.00000		19410
	rotall	+	0.00133	0.09680	-0.09548	0.00133		20152
	res		0.01628	0.37799	-0.36171	0.01628		



Constrain Bravais lattice
Refine cell parameters

peaks from 100 images

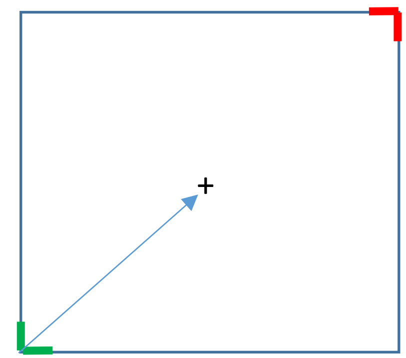
Refine instrumental parameters

pixel size 0.102 mm
scan width 0.5°

Metadata: image header

```
{
HEADER_BYTES=  512;
DIM=2;
BYTE_ORDER=little_endian;
TYPE=unsigned_short;
PIXEL_SIZE=0.1026;
BIN=2x2;
ADC=fast;
DETECTOR_SN=920;
DATE=Fri Jul 16 16:27:51 2010;
TIME=0.50;
DISTANCE=116.000;
OSC_RANGE=0.500;
PHI=0.000;
OSC_START=0.000;
TWOTHETA=0.000;
AXIS=phi;
WAVELENGTH=1.4880;
BEAM_CENTER_X=157.999;
BEAM_CENTER_Y=157.484;
CREV=1;
CCD=TH7899;
BIN_TYPE=HW;
ACC_TIME=1750;
UNIF_PED=1500;
IMAGE_PEDESTAL=40;
SIZE1=3072;
SIZE2=3072;
CCD_IMAGE_SATURATION=65535;
}
```

ASCII image header of ADSC detector at Diamond

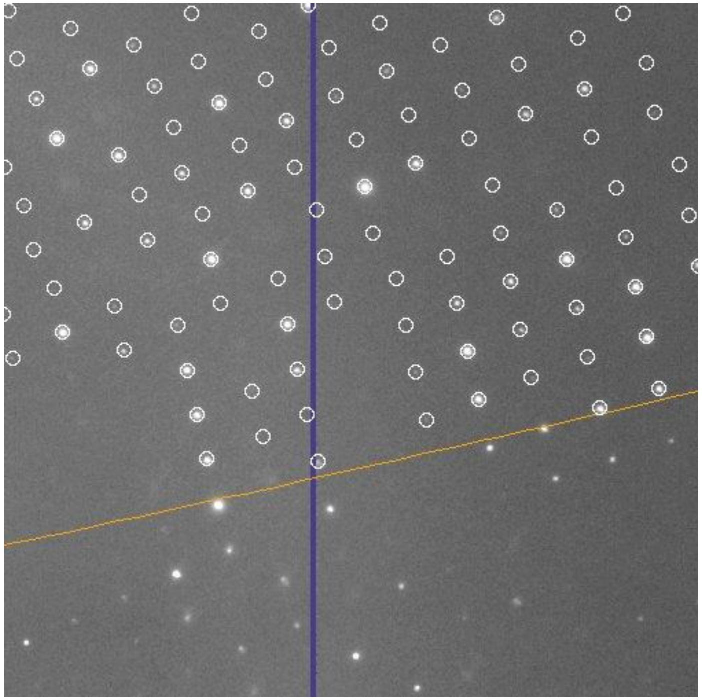


Center of incident beam in mm on detector

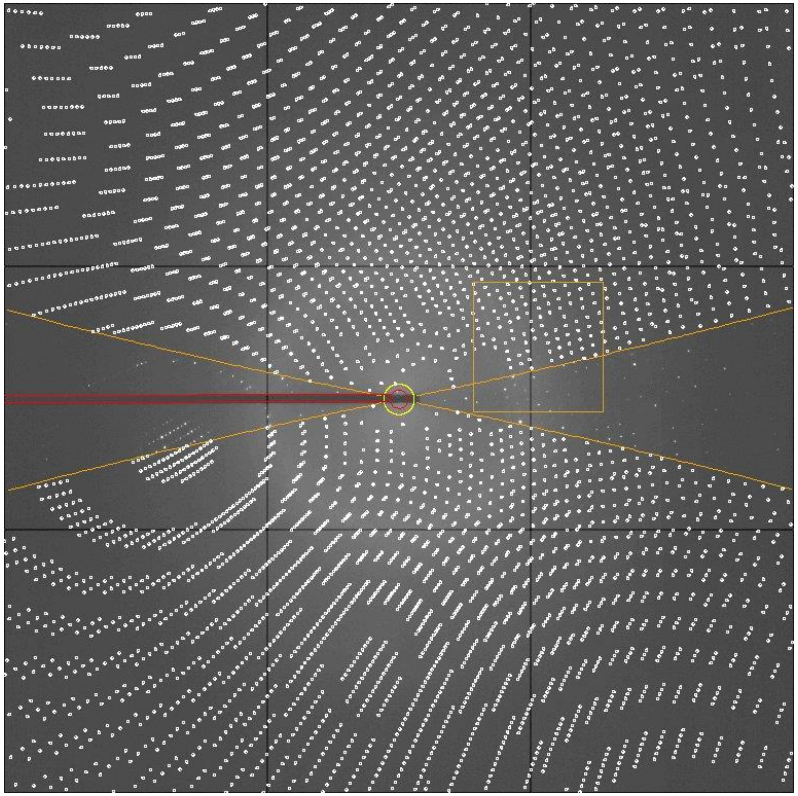
px= -(157.9/0.1026 -3072)=1533

py= -(157.48/0.1026-3072)=1537

VIEW: datcol

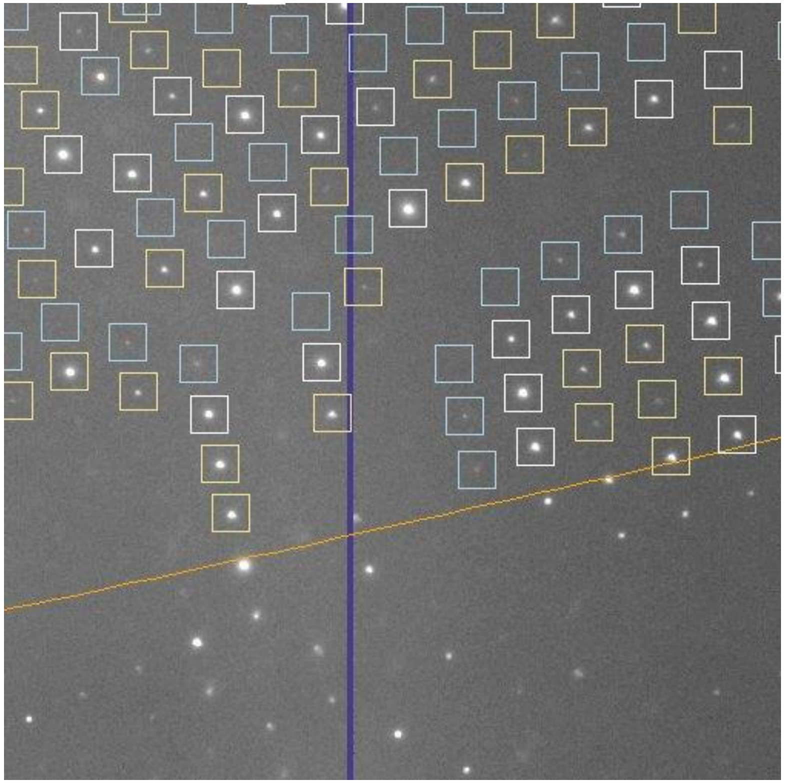


Frame 200



VIEW: datcol

Generation of shoeboxes
for integration with EVAL15



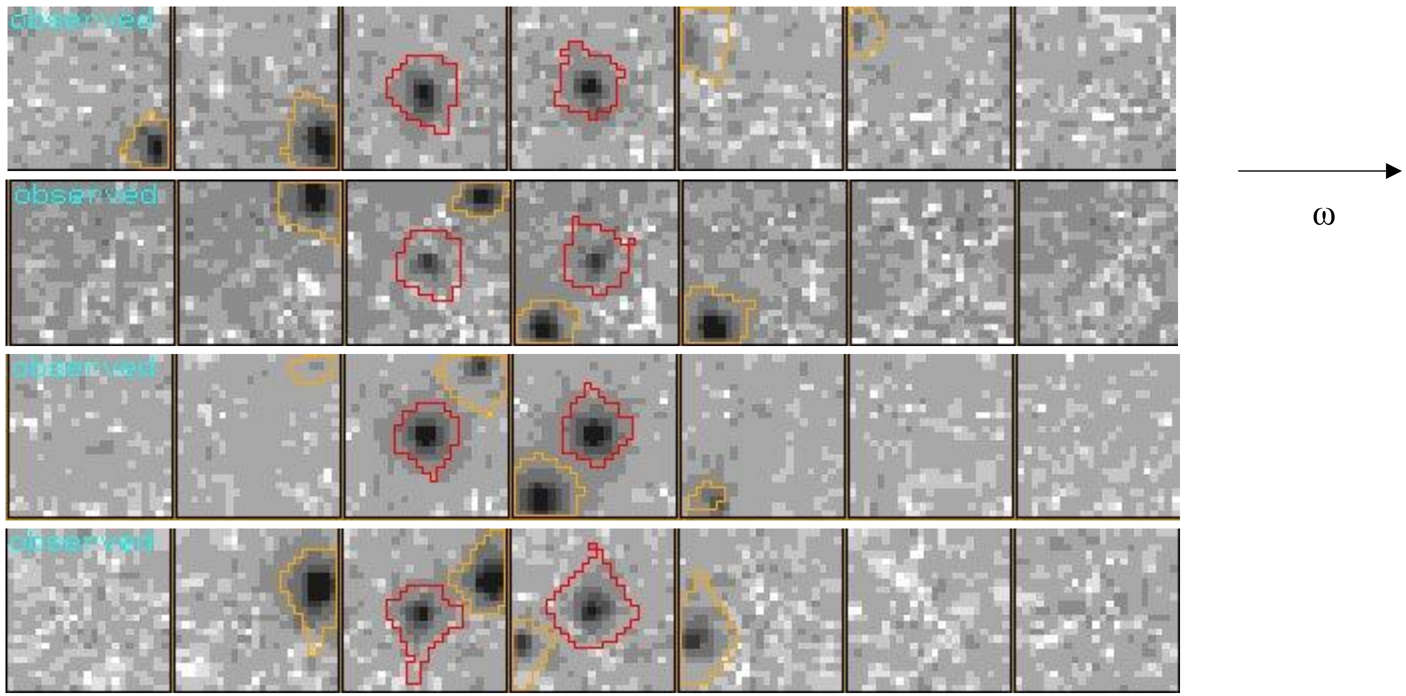
VIEW generated shoeboxes

hkl =(12, 11, 38)

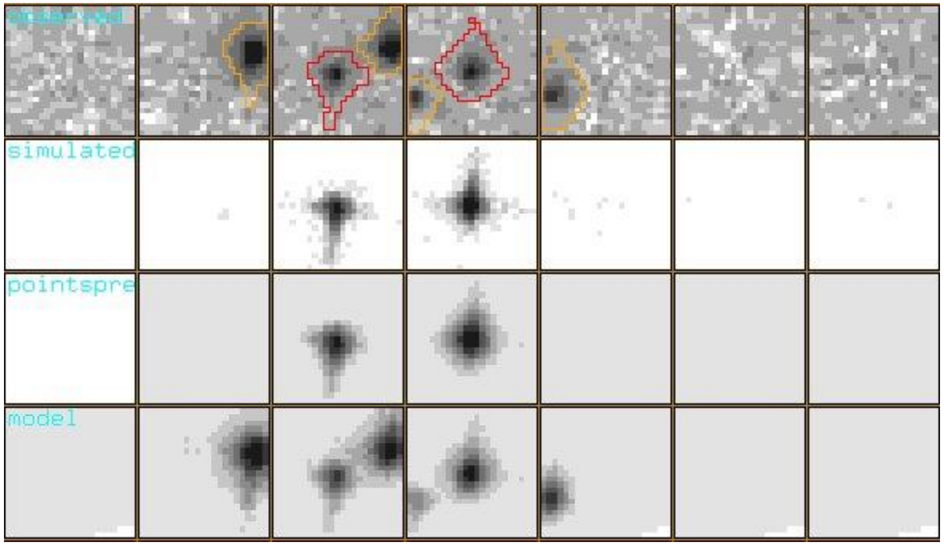
hkl =(17, -7, -16)

hkl =(14, -2, -27)

hkl =(21, 15, -17)



EVAL integration by SVD



ρ_i ← observed pixel intensities

model pixel intensities

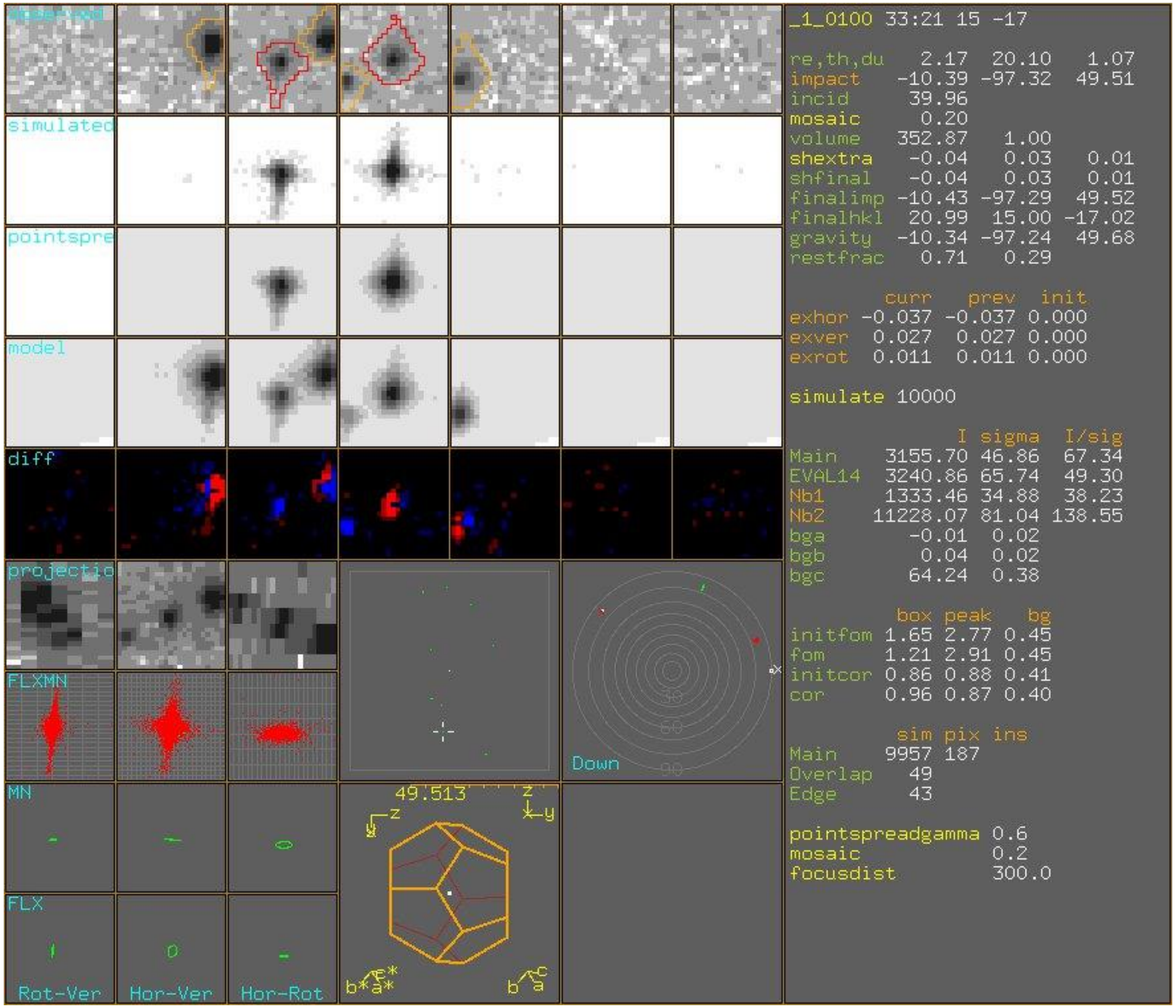
P_i

$$JP_i + \underbrace{ax_i + by_i + c}_{\text{background}} + \underbrace{J_{nb1}P_{i\,nb1} + ..}_{\text{neighbours}}$$

$$\chi^2 = \sum_{i=1}^{N} w_i \left[\rho_i - JP_i - \sum_{m}^{M} J_m P_{im} - ax_i - by_i - c \right]^2$$

Poisson statistics

$$I = J \sum_{i=1}^{N} P_i \qquad \sigma_i = \sqrt{\rho_i} \qquad w_i = \frac{1}{\sigma_i^2}$$



Corrected for Lorentz and polarization

χ

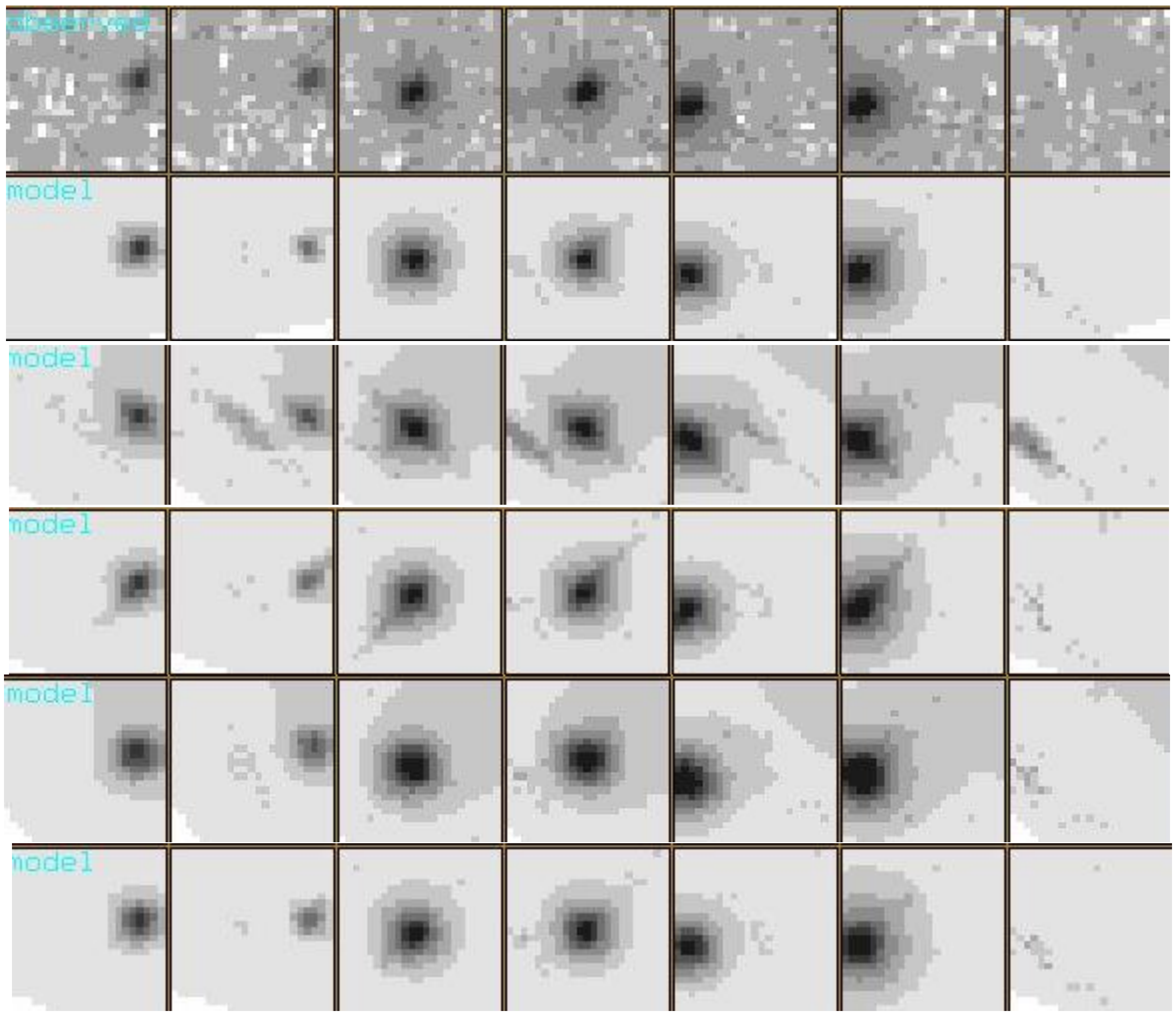
Data reduction

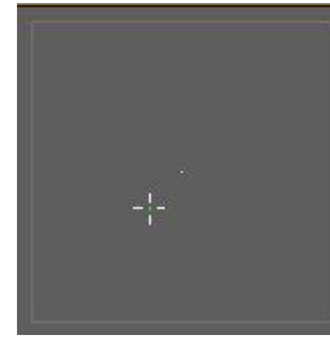
$$I \propto L(\eta)p(\eta)|F_{hkl}|^2$$

- Lorentz factor accounts for the relative time that a reciprocal lattice point spends on the Ewald sphere during the data collection
- Polarization factors accounts for incident beam polarization and polarization caused by reflection

After correction we get the squared structure factors:

$$|F_{hkl}|^2 = I/Lp$$





observed

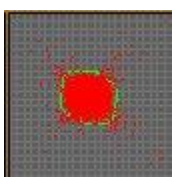
model

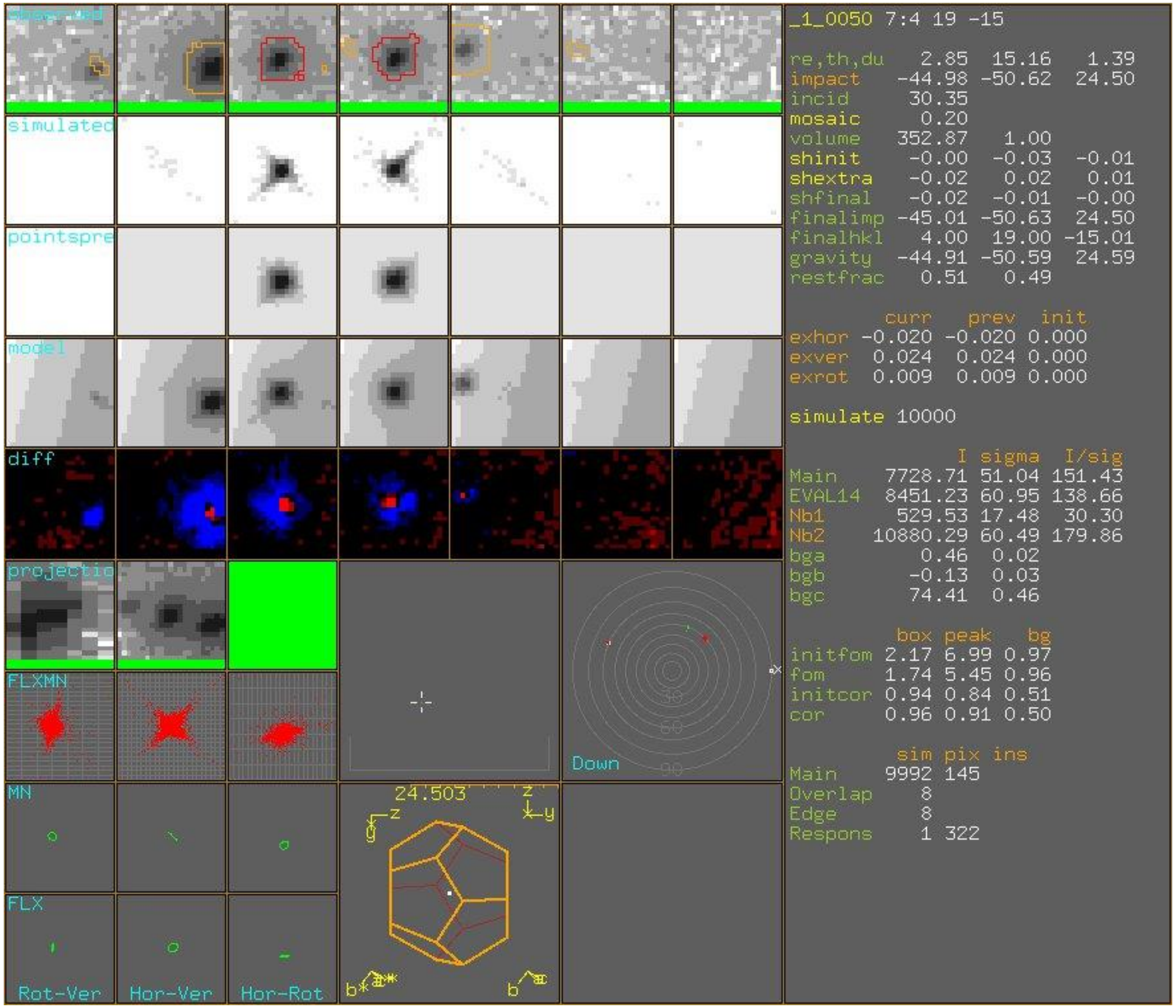
mosaic -> 0.5

$\sigma(\lambda)$ -> 0.002

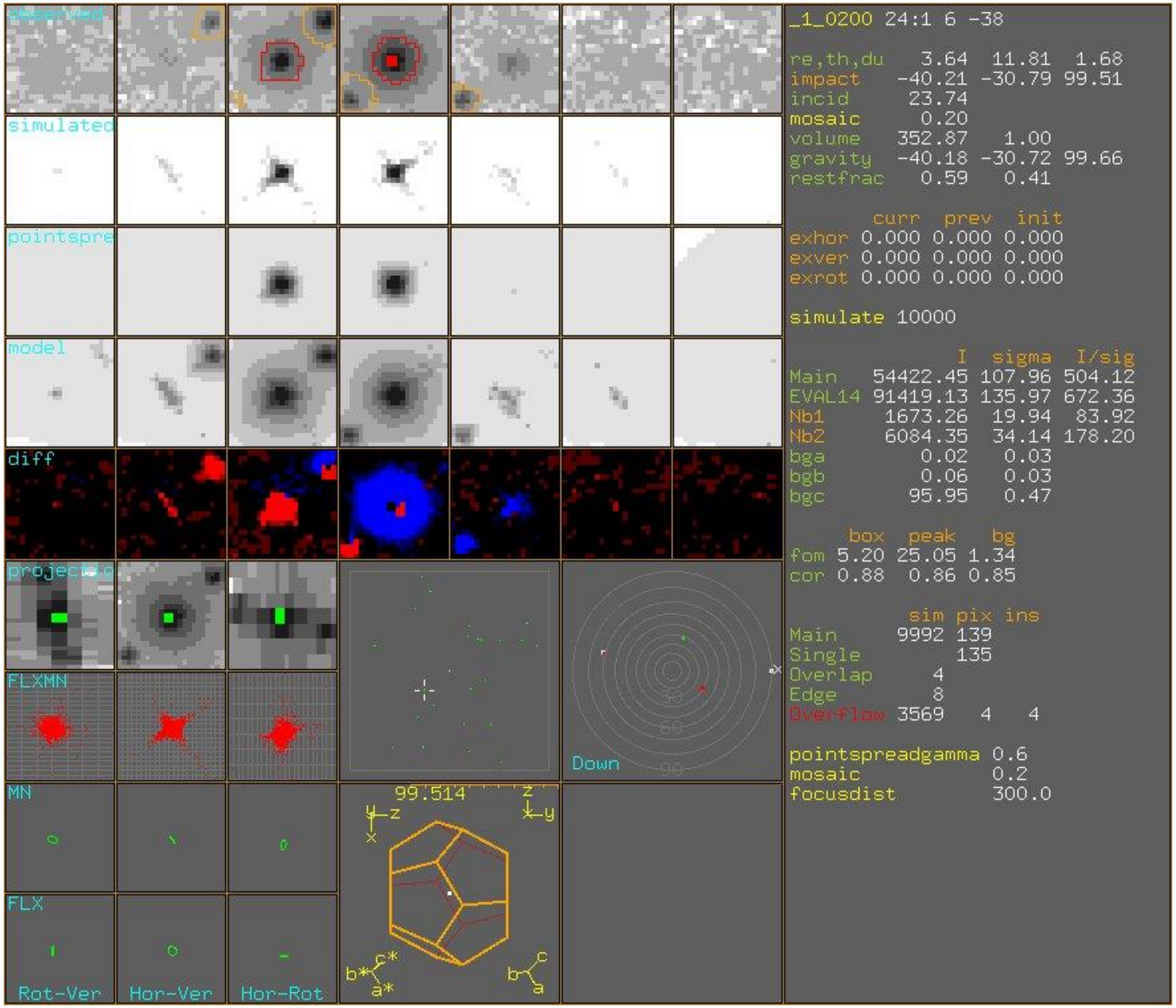
divergence -> 1.3 mrad

Xtal -> *2





Detector panel edge


simulated
pointspre
model
diff
FLXMN
MN
FLX
Rot-Ver
Hor-Ver
Hor-Rot
Down
99.514
_1_0200 24:1 6 -38
re,th,du 3.64 11.81 1.68
impact -40.21 -30.79 99.51
incid 23.74
mosaic 0.20
volume 352.87 1.00
gravity -40.18 -30.72 99.66
restfrac 0.59 0.41
curr prev init
exhor 0.000 0.000 0.000
exver 0.000 0.000 0.000
exrot 0.000 0.000 0.000
simulate 10000
I sigma I/sig
Main 54422.45 107.96 504.12
EVAL14 91419.13 135.97 672.36
Nb1 1673.26 19.94 83.92
Nb2 6084.35 34.14 178.20
bga 0.02 0.03
bgb 0.06 0.03
bgc 95.95 0.47
box peak bg
fom 5.20 25.05 1.34
cor 0.88 0.86 0.85
sim pix ins
Main 9992 139
Single 135
Overlap 4
Edge 8
Overflow 3569 4 4
pointspreadgamma 0.6
mosaic 0.2
focusdist 300.0

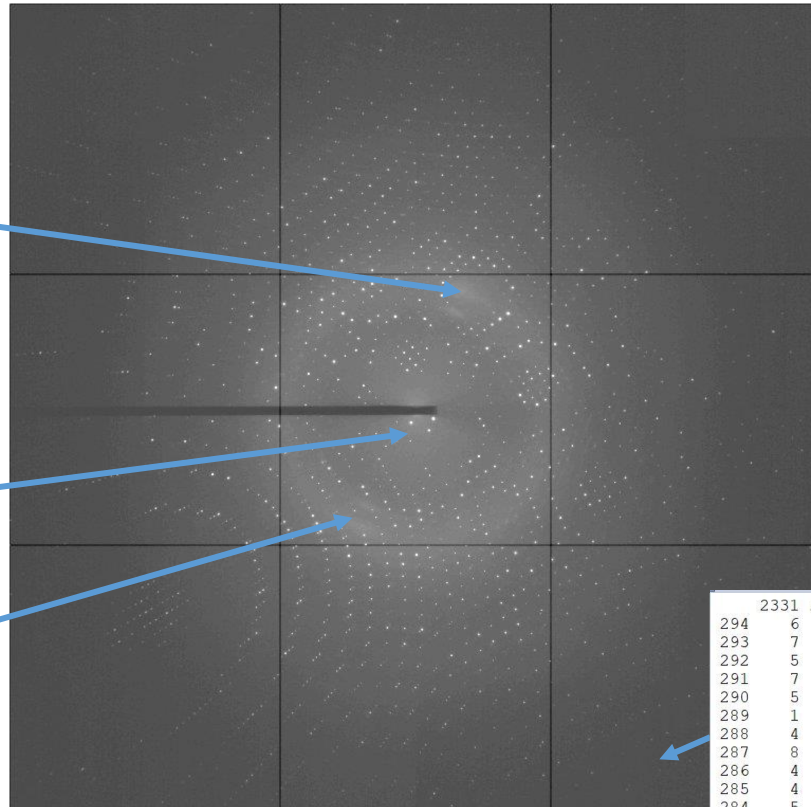
overflow

Background

fibre (nylon) loop

air scattering

crystal droplet (solvent)



From the image header:
Image pedestal=40
(base-line offset)
avoids having to store
negative numbers in 16 bits

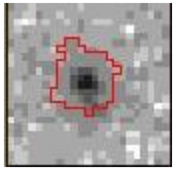
Dark current has been subtracted

	2331	2332	2333	2334	2335	2336	2337	2338	2339	2340	2341
294	6	8	9	5	3	6	8	4	4	2	5
293	7	7	6	4	5	0	4	0	2	6	6
292	5	1	0	1	3	1	3	2	6	7	5
291	7	4	5	-2	4	-1	5	7	10	6	3
290	5	4	4	1	11	6	10	8	1	2	2
289	1	4	6	4	9	0	3	4	8	6	4
288	4	5	5	14	7	3	6	3	6	3	2
287	8	4	8	9	9	6	9	2	3	5	4
286	4	6	6	7	3	3	5	2	3	7	6
285	4	3	7	5	3	2	4	3	5	7	5
284	5	6	7	5	-1	6	5	2	8	7	6

Range from 1 to 14 Most frequent: value=6 times=19
pixels: 114 Sum: 577 Mean: 5.06 Sigma: 2.38 (Sigma^2)/Mean: 1.12
pixels: 114 aBG -0.07 bBG -0.02 cBG 5.56 sigBG 2.39

Background and standard deviations of reflections

$$I_{net} = I_{bruto} - BG$$



$$I_{net} = J\sum_i P_i = \sum_i \rho_i - \sum_i (ax_i + by_i + c)$$

$$\sigma_I^2 = \sigma_{peak}^2 + \sigma_{BG}^2$$

According to Poisson statistics,
the higher the pixel intensities
the higher the background noise

Try to avoid background as much as you can

X-ray detectors

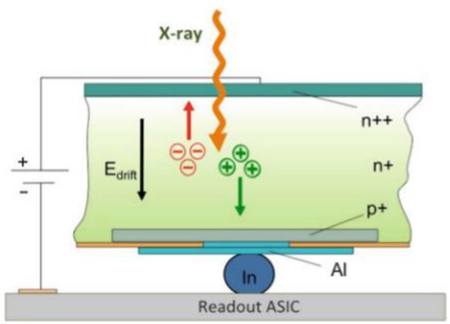
- Film and image plates
- Multiware array detectors
- CCD detectors
- Hybrid pixel detectors

photons xph $\xrightarrow{\text{phosphor}}$ light $\xrightarrow{\text{CCD}}$ e^- electrons $\xrightarrow{\text{amplifier}}$ V $\xrightarrow{\text{ADC}}$ image ADU's

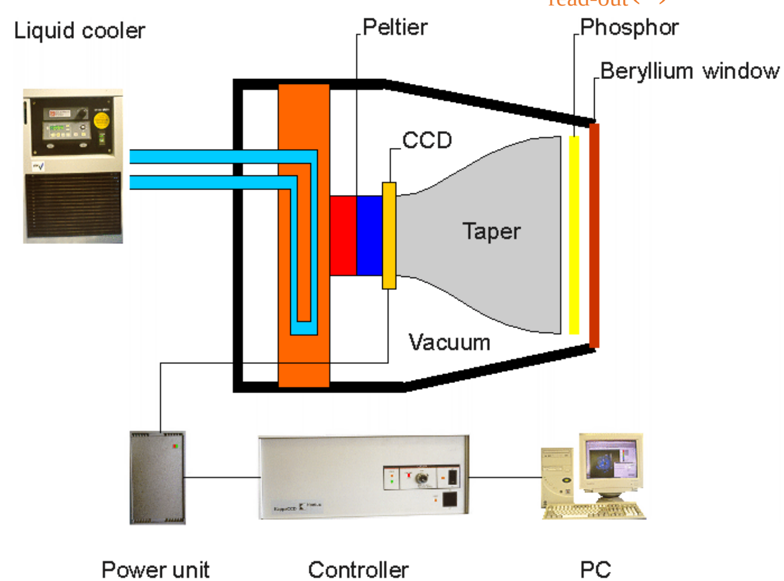
$\sigma(I)$ $\sigma(I)$ $\sigma(I)$

$\sigma_{\text{dark-current}}(t)$

$\sigma_{\text{read-out}}(n)$



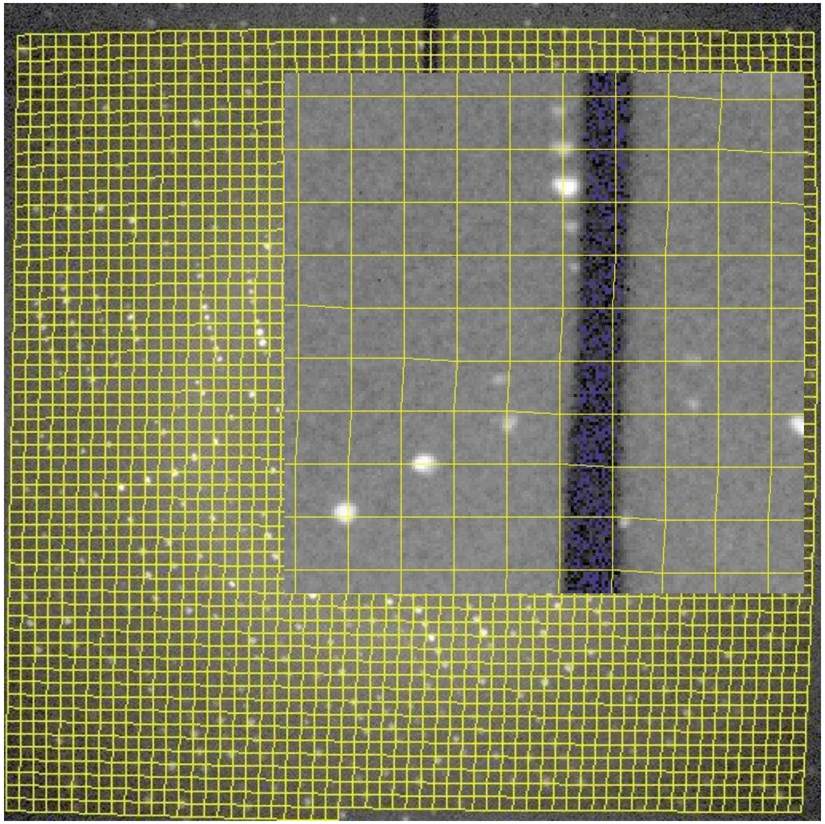
Silicon sensor pixel



Almost no point spread
No electronic noise and dark current
No read-out noise

Unwarping images

Pixels on the CCD detectors are distorted, largely due to the fibre optic taper.
The equipment's software will have a distortion table that maps every pixel in the image file to the true position on the detector.
If you want to take the images away from the equipment, you'd better unwarp the images.

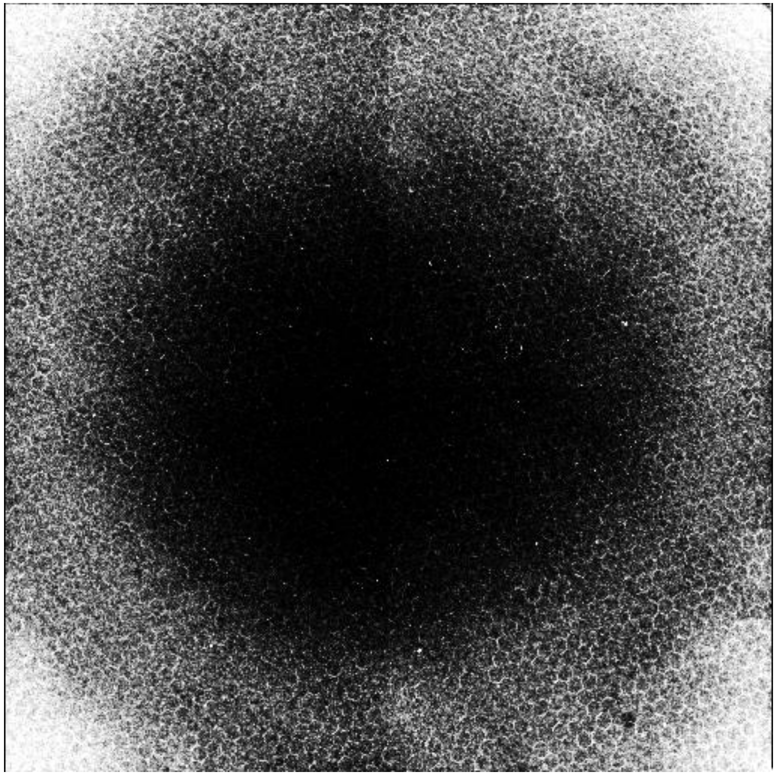


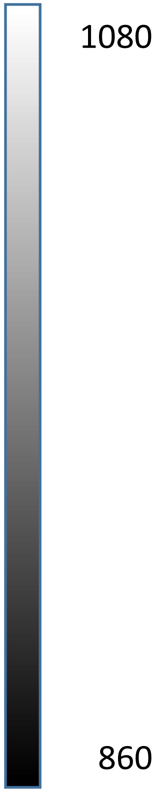
Flood field

Non-uniformity correction image of CCD detector

In the centre larger phosphor thickness
Calibrated with homogeneous scatterer

Platinum 135 CCD





ANY: analysis

```
pg 4/mmm
pointgroup set to 4/mmm
nPg=16 (h,k,l) (k,-h,l) (-h,-k,l) (-k,h,l) (h,-k,-l) (-k,-h,-l) (-h,k,-l) (k,h,-l)
(-h,-k,-l) (-k,h,-l) (h,k,-l) (k,-h,-l) (-h,k,l) (k,h,l) (h,-k,l) (-k,-h,l)
RebuildDB ok centric=on

Completeness and Rmerge for Shells
Forbid: EDGEVER EDGEHOR EDGEROT BADUNIF OVERFLOW MAXSHIFT
Allow: GOOD WEAK NEGATIVE
Require: NONE
theta from 0.0 to 27.709
```

Sh	Theta	Reso	Meas	Equi	Obs	Mis	Lost	Total	Perc	Cum	Uni1	Uni2+	Nrsym	Redun	Rsym	Rmeas	Rpim	Chi2
1	12.46	3.447	43845	6609	50454	18	522	50994	98.9	98.9	25	3666	47609	12.99	0.066	0.069	0.019	637.25
2	15.78	2.736	41851	8787	50638	0	0	50638	100.0	99.5	2	3487	47107	13.51	0.087	0.090	0.024	313.74
3	18.14	2.390	41134	9696	50830	0	2	50832	100.0	99.6	0	3448	47370	13.74	0.113	0.117	0.031	189.00
4	20.04	2.172	40382	10650	51032	0	0	51032	100.0	99.7	0	3430	47237	13.77	0.106	0.110	0.029	188.12
5	21.66	2.016	39182	11526	50708	0	0	50708	100.0	99.8	0	3394	46466	13.69	0.109	0.114	0.031	72.70
6	23.09	1.897	38388	12382	50770	0	0	50770	100.0	99.8	0	3379	46058	13.63	0.121	0.126	0.034	50.32
7	24.38	1.802	37693	13007	50700	0	0	50700	100.0	99.8	0	3360	45594	13.57	0.136	0.141	0.038	30.55
8	25.57	1.724	37410	13852	51262	0	0	51262	100.0	99.9	0	3394	45715	13.47	0.154	0.160	0.044	25.30
9	26.68	1.657	36203	14329	50532	0	0	50532	100.0	99.9	0	3336	44613	13.37	0.174	0.181	0.049	22.72
10	27.71	1.600	26893	23925	50818	0	0	50818	100.0	99.9	0	3349	33563	10.02	0.200	0.211	0.066	17.08
	27.71	1.600	382981	124763	507744	18	524	508286	99.9	99.9	27	34243	451332	13.18	0.094	0.098	0.027	161.28

```
Resolution 45.663-1.6 (1.657-1.6)
Rsym 0.094 (0.2) Rmeas 0.098 (0.211) Rpim 0.027 (0.066)
Reflections 451359 (33563) Unique 34270 (3349) Completeness 99.893 (100.0) Redundancy 13.18 (10.022)
```

σ_I^2 from Poisson statistics

$$\chi^2 = \frac{\sum (I - \langle I \rangle)^2}{\sum \sigma^2} \approx 1 \quad ??$$

ANY: analysis

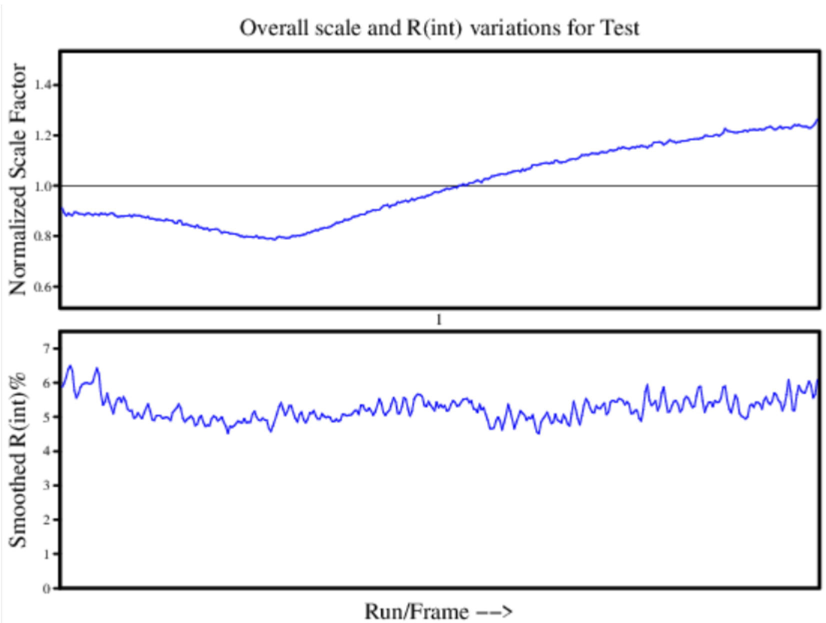
Intensity distribution for Shells, unmerged and merged
Forbid: EDGEVER EDGEHOR EDGEROT BADUNIF OVERFLOW MAXSHIFT
Allow: GOOD WEAK NEGATIVE
Require: NONE

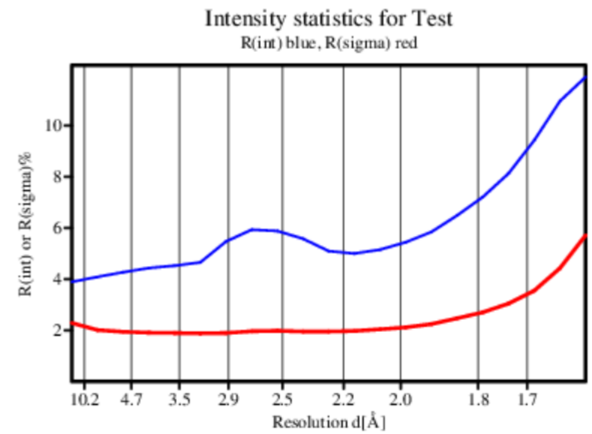
Sh	Theta	Reso	N	<I>	<s>	<I/s>	Nmerge	<I>	<s>	<I/s>	cc1/2	cc*	npair
1	12.46	3.447	47634	601.48	2.28	206.72	3691	641.34	12.65	55.49	0.998	0.999	3666
2	15.78	2.736	47109	390.19	2.38	127.40	3489	389.65	9.90	38.08	0.997	0.999	3487
3	18.14	2.390	47370	197.47	2.04	76.98	3448	198.03	6.54	29.17	0.994	0.999	3448
4	20.04	2.172	47243	165.13	2.10	63.20	3430	165.93	5.04	31.67	0.995	0.999	3430
5	21.66	2.016	46460	129.79	2.09	49.81	3394	129.67	4.11	30.06	0.995	0.999	3394
6	23.09	1.897	46061	94.66	2.04	37.99	3379	95.05	3.34	27.06	0.994	0.998	3379
7	24.38	1.802	45591	61.65	1.96	26.23	3360	62.53	2.46	23.60	0.993	0.998	3360
8	25.57	1.724	45719	45.77	2.00	19.62	3394	46.59	2.08	20.62	0.990	0.998	3394
9	26.68	1.657	44609	34.83	2.09	14.52	3336	35.53	1.78	17.82	0.990	0.997	3336
10	27.71	1.600	33563	27.44	2.24	10.91	3349	27.97	2.09	12.82	0.975	0.994	3349
	27.71	1.600	451359	181.55	2.12	65.69	34270	184.43	5.10	28.95	0.998	0.999	34243

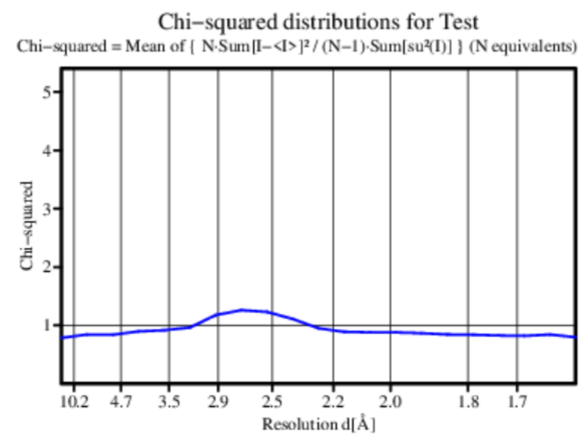
Merged I/σ

Next: scaling and error model for esd

SADABS: scaling

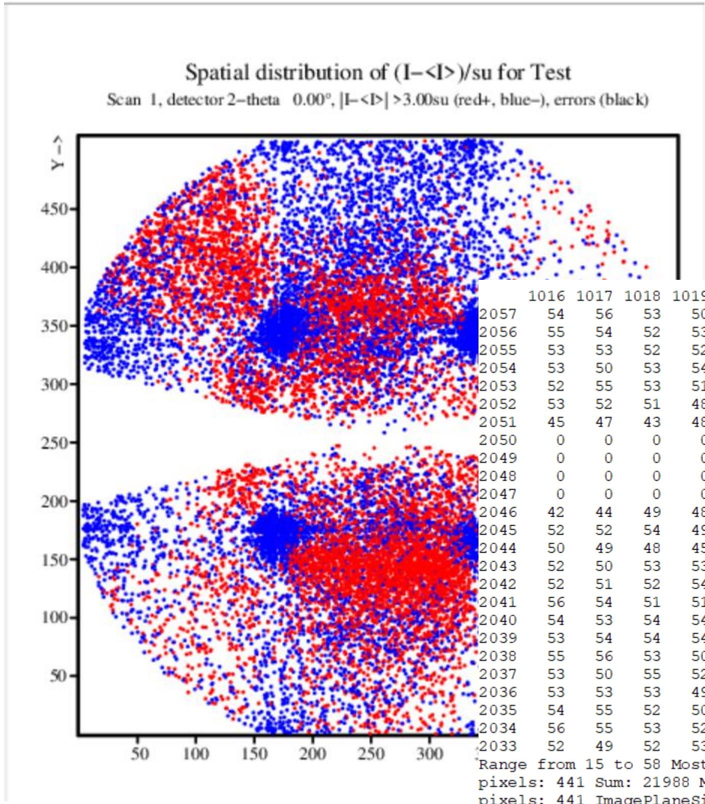


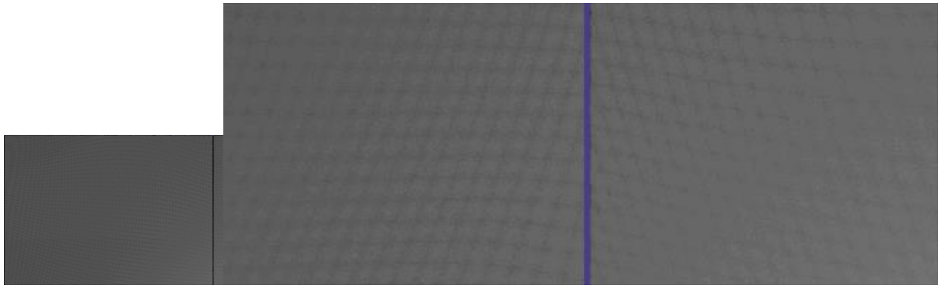




Bruker propriety software

Detector systematic errors





	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040
2057	54	56	53	50	48	49	48	0	0	0	0	36	48	52	53	53	53	49	50	52	53	54	51	53	54
2056	55	54	52	53	48	50	45	0	0	0	0	33	50	54	53	53	52	52	45	49	50	52	51	53	55
2055	53	53	52	52	51	49	44	0	0	0	0	33	50	53	53	53	52	50	51	51	49	54	52	53	52
2054	53	50	53	54	49	45	45	0	0	0	0	29	47	50	52	50	51	52	50	49	53	52	53	51	54
2053	52	55	53	51	52	47	49	0	0	0	0	32	40	49	45	50	50	52	51	48	51	49	52	52	53
2052	53	52	51	48	50	47	43	0	0	0	0	15	38	44	43	48	44	48	44	43	42	48	48	51	50
2051	45	47	43	48	42	43	31	0	0	0	0	19	40	47	44	40	47	45	44	45	43	44	45	42	48
2050	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2049	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2048	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2047	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
2046	42	44	49	48	50	43	33	0	0	0	0	40	40	25	31	34	33	31	40	38	36	33	36	31	40
2045	52	52	54	49	50	48	45	0	0	0	0	17	39	44	43	43	44	49	51	45	44	44	49	47	43
2044	50	49	48	45	52	52	53	0	0	0	0	33	50	48	47	49	49	50	52	51	45	51	52	50	50
2043	52	50	53	53	53	54	49	0	0	0	0	41	47	45	46	45	51	48	50	53	49	48	52	51	51
2042	52	51	52	54	52	53	49	0	0	0	0	42	49	47	51	52	54	51	52	52	53	54	50	53	53
2041	56	54	51	51	54	52	49	0	0	0	0	43	52	52	49	50	53	53	52	54	53	51	55	55	55
2040	54	53	54	54	49	53	48	0	0	0	0	44	53	53	54	50	51	55	56	54	51	53	55	54	55
2039	53	54	54	54	52	52	53	0	0	0	0	45	51	52	53	53	53	54	52	54	54	56	51	54	56
2038	55	56	53	50	52	52	52	0	0	0	0	46	52	53	54	52	54	55	56	55	56	54	56	54	56
2037	53	50	55	52	53	52	53	0	0	0	0	43	53	52	54	54	53	54	54	53	55	54	56	56	55
2036	53	53	53	49	53	55	47	0	0	0	0	44	51	52	53	54	56	54	54	55	55	53	57	54	54
2035	54	55	52	50	47	51	51	0	0	0	0	42	52	51	51	54	54	56	56	57	56	57	55	54	54
2034	56	55	53	52	53	52	49	0	0	0	0	40	51	52	53	53	55	55	58	57	57	56	57	58	57
2033	52	49	52	53	50	53	48	0	0	0	0	39	53	52	51	52	55	53	54	55	54	55	56	58	56

```
Range from 15 to 58 Most frequent: value=53 times=67
pixels: 441 Sum: 21988 Mean: 49.86 Sigma: 5.99 (Sigma^2)/Mean: 0.72
pixels: 441 ImagePlaneSigma npx=441 npp=184 aBG 0.04 bBG -0.24 cBG 52.08 sigBG 5.71
```

Error model

True standard deviations can be described by second order polynomial in I *

$$\sigma^2 = bgnoise^2 + \sigma_p^2 + (gI)^2$$

Random noise

Systematic

Read-out noise
Dark current
Incoherent scattering

= I

From Poisson statistics

Instrument errors:

- Error in pixel size
- Profile error
- Counting error
- Inhomogeneity phosphor
- Radiation damage

SADABS: $$\sigma^2 = K[\sigma_I^2 + (g\langle I\rangle)^2]$$

*Popov & Bourenkov Acta Cryst D59 (2003) 1145

Statistics after scaling

Completeness and Rmerge for Shells
Forbid: EDGEVER EDGEHOR EDGEROT BADUNIF OVERFLOW MAXSHIFT SADABS
Allow: GOOD WEAK NEGATIVE
Require: NONE
theta from 0.0 to 27.709

Sh	Theta	Reso	Meas	Equi	Obs	Mis	Lost	Total	Perc	Cum	Uni1	Uni2+	Nrsym	Redun	Rsym	Rmeas	Rpim	Chi2
1	12.46	3.447	42278	8176	50454	18	522	50994	98.9	98.9	25	3666	45535	12.42	0.044	0.046	0.013	0.88
2	15.78	2.736	39330	11308	50638	0	0	50638	100.0	99.5	2	3487	43608	12.51	0.051	0.053	0.014	1.10
3	18.14	2.390	37346	13484	50830	0	2	50832	100.0	99.6	1	3447	42251	12.26	0.059	0.061	0.017	1.23
4	20.04	2.172	39188	11828	51016	0	16	51032	100.0	99.7	1	3428	45323	13.22	0.052	0.054	0.015	0.98
5	21.66	2.016	38348	12360	50708	0	0	50708	100.0	99.8	0	3394	45050	13.27	0.051	0.053	0.014	0.89
6	23.09	1.897	37636	13134	50770	0	0	50770	100.0	99.8	0	3379	44744	13.24	0.056	0.058	0.016	0.88
7	24.38	1.802	37061	13639	50700	0	0	50700	100.0	99.8	0	3360	44531	13.25	0.065	0.067	0.019	0.86
8	25.57	1.724	36689	14573	51262	0	0	51262	100.0	99.9	0	3394	44525	13.12	0.077	0.080	0.022	0.84
9	26.68	1.657	35308	15224	50532	0	0	50532	100.0	99.9	0	3336	43204	12.95	0.093	0.097	0.027	0.83
10	27.71	1.600	25987	24815	50802	0	16	50818	100.0	99.9	5	3343	32099	9.60	0.115	0.121	0.039	0.84
	27.71	1.600	369171	138541	507712	18	556	508286	99.9	99.9	34	34234	430870	12.59	0.052	0.055	0.015	0.93

Sh	Theta	Reso	N	<I>	<s>	<I/s>	Nmerge	<I>	<s>	<I/s>	cc1/2	cc*	npair
1	12.46	3.447	45560	184.07	12.56	14.16	3691	191.78	4.31	47.76	0.999	1.000	3666
2	15.78	2.736	43610	123.88	8.54	13.60	3489	119.40	2.41	45.99	0.999	1.000	3487
3	18.14	2.390	42252	63.44	4.49	12.65	3448	62.20	1.34	42.10	0.998	1.000	3447
4	20.04	2.172	45330	52.73	3.81	12.23	3429	52.24	1.07	43.36	0.999	1.000	3428
5	21.66	2.016	45044	41.57	3.11	11.37	3394	41.19	0.87	40.60	0.999	1.000	3394
6	23.09	1.897	44747	30.25	2.40	10.44	3379	30.25	0.68	37.36	0.999	1.000	3379
7	24.38	1.802	44528	19.67	1.78	8.91	3360	19.94	0.51	32.16	0.999	1.000	3360
8	25.57	1.724	44529	14.57	1.53	7.68	3394	14.85	0.44	27.66	0.998	0.999	3394
9	26.68	1.657	43200	11.07	1.42	6.35	3336	11.32	0.41	22.78	0.997	0.999	3336
10	27.71	1.600	32104	8.83	1.41	5.19	3348	9.02	0.51	15.55	0.994	0.998	3343
	27.71	1.600	430904	56.56	4.20	10.41	34268	56.77	1.29	35.74	0.999	1.000	34234

$$\sigma^2 = K[\sigma_I^2 + (g\langle I\rangle)^2]$$

Fitted in SADABS to minimize χ^2