

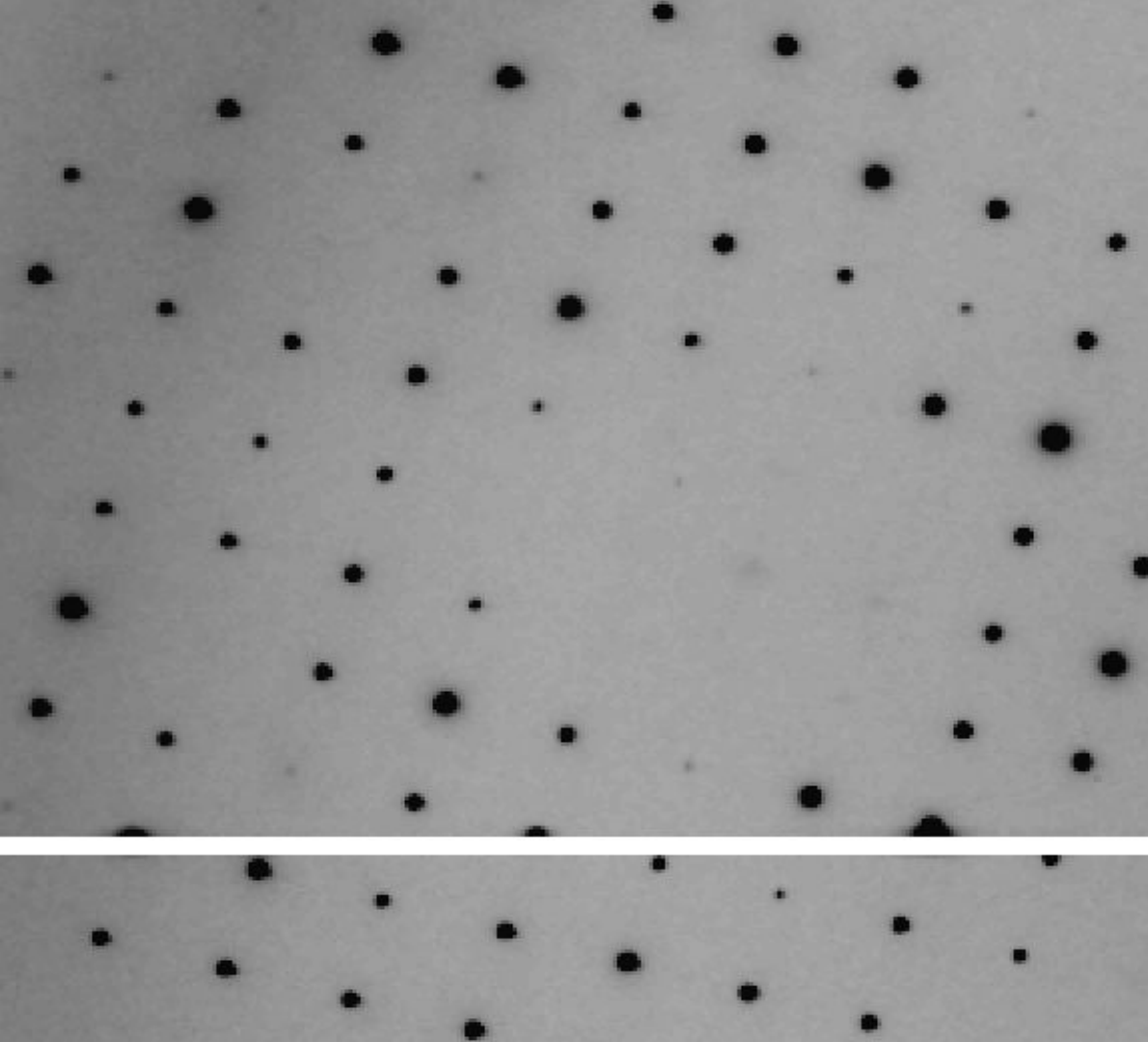
Data processing with DIALS



James Parkhurst

Institut Pasteur de Montevideo/CCP4 workshop, Uruguay,
November 2017

**What are we doing and why are we
doing it?**



Compute the intensity of each Bragg spot in a set of diffraction images

$$|F_{hkl}| = \sqrt{\frac{K I_{hkl}}{Lp}}$$

K = constant for given crystal

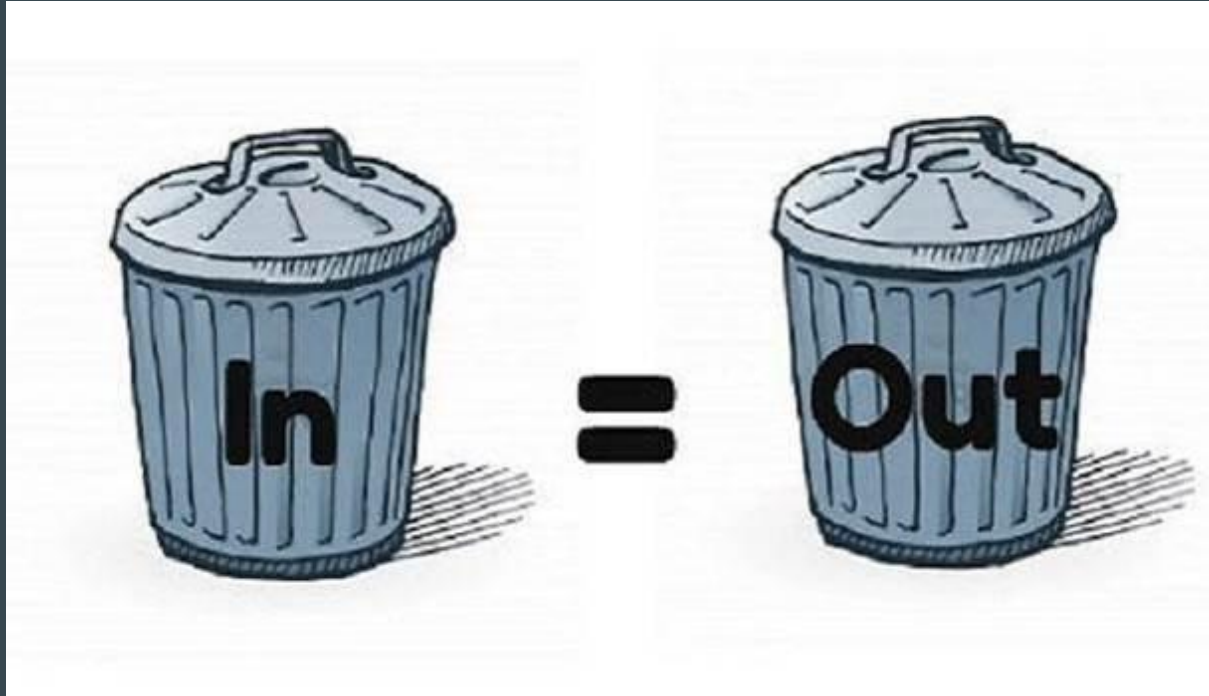
L = Lorentz factor

p = polarization factor

$$\rho(x, y, z) = \frac{1}{V} \sum_h \sum_k \sum_l F_{hkl} e^{-2\pi i(hx + ky + lz)}$$

Electron density at every point in the cell depends on the intensity of every reflection. We need to measure our intensities as well as possible!

Warning: garbage in, garbage out



Data collection is the last experimental stage; if you collect bad data you are stuck with it! Data processing programs won't be able to rescue you!

DIALS overview

Acknowledgements

research papers

Acta Crystallographica Section D
**Biological
Crystallography**
ISSN 0907-4449

XDS

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The usage and control package *XDS* for 1 described in the con include automatic di range and recogniti Moreover, the limita number of correction pixel contents have t been restructured fo and completeness of measurement.

1. Functional speci

The program package developed for the re recorded on a plana monochromatic X-ra *XDS* accepts a : rotation images fro and multiwire area metrics and produce: of the reflections occ way. The program as positive amount of c incident beam and cr imposes no limitati directions of the rot oscillation range cov

research papers

Acta Crystallographica Section D
**Biological
Crystallography**
ISSN 0907-4449

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The finer things in

X-ray diffraction images from sensitive detectors can be cha depending on whether the rotati is greater than or less than the c The expectations and consequen and thin images in terms of spa X-ray background and $I\sigma(I)$ software suite for processing (introduced, and results from d those from another popular pac

1. Introduction

Two-dimensional position-sensitive for many years in X-ray diffract ular, data from crystals of mac oligonucleotides and their cor acquired with an area detector obsolete), a multi-wire system recently commercialized char coupled to a phosphor-coated fit detectors, the crystal, centered in oscillated around a single axis th $\sim 2.0^\circ$, while counts from diffrac for a specified time. At the en detector is read out and the cou two-dimensional array with each to a distinct position on the c

research papers

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Crystallography**
ISSN 0907-4449

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The integrati

The objective of any produce from a set of with their associated uncertainties), togeth crystal unit-cell param reliable, but should i intervention. The pro three stages. The first parameters and the o parameters may indic: The second step is to r parameters and also l known as post-refiner images, which consists reflections on each in intensity of each reflex out while simultaneou parameters. Basic fea each of these three st with reference to the |

1. Introduction

The collection of mac gone dramatic advanc advent of two-dimensi and CCDs, crystal cry monochromatic and

Centre National de la Recherche Scientifique
Université Paris-Sud

Laboratoire pour l'Utilisation du Rayonnement Electromagnétique

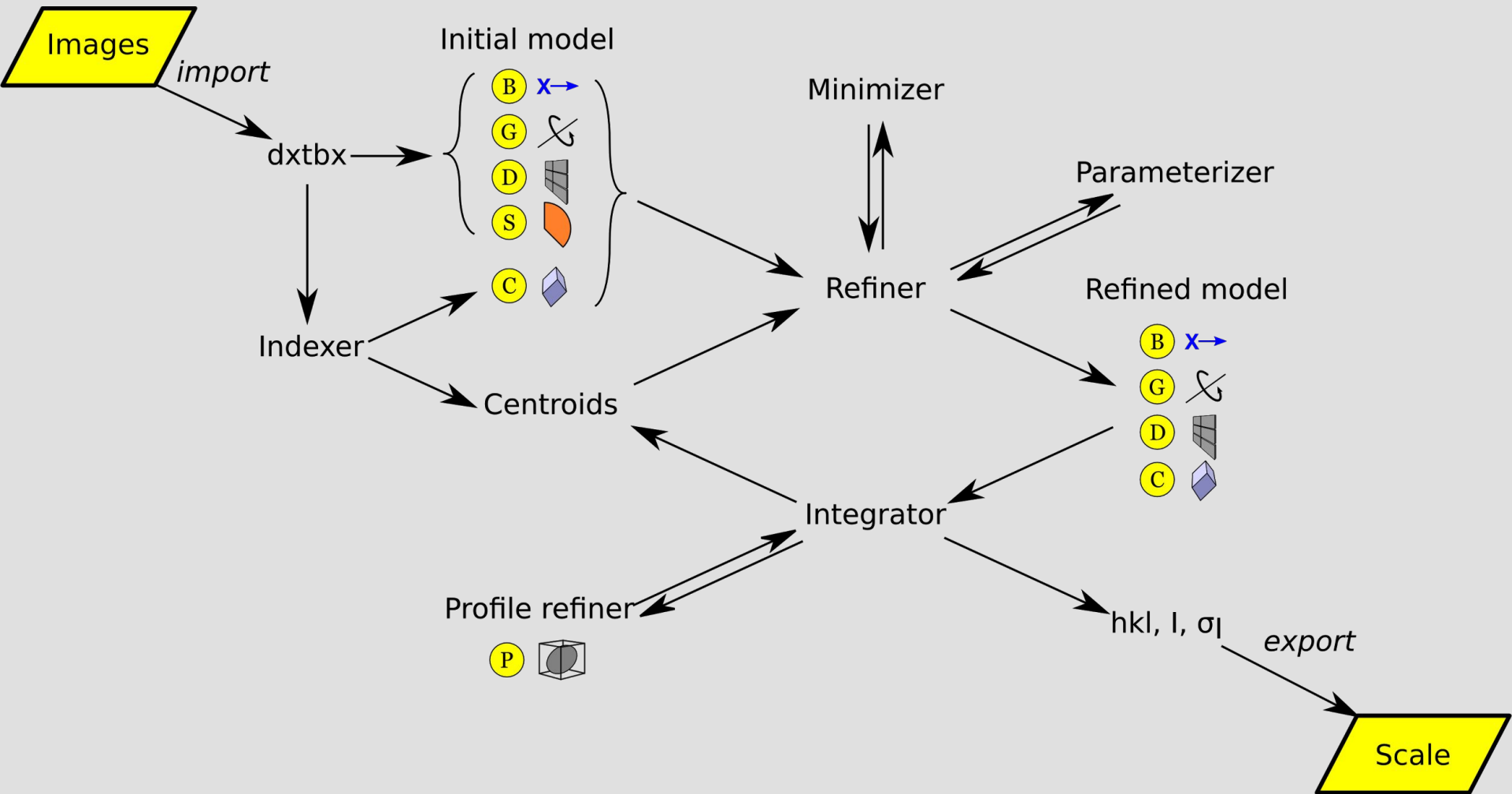
Proceedings

of the EEC Cooperative Workshop

on Position-Sensitive Detector Software

(Phases I & II)

held at L.U.R.E. from May 26 to June 7, 1986.



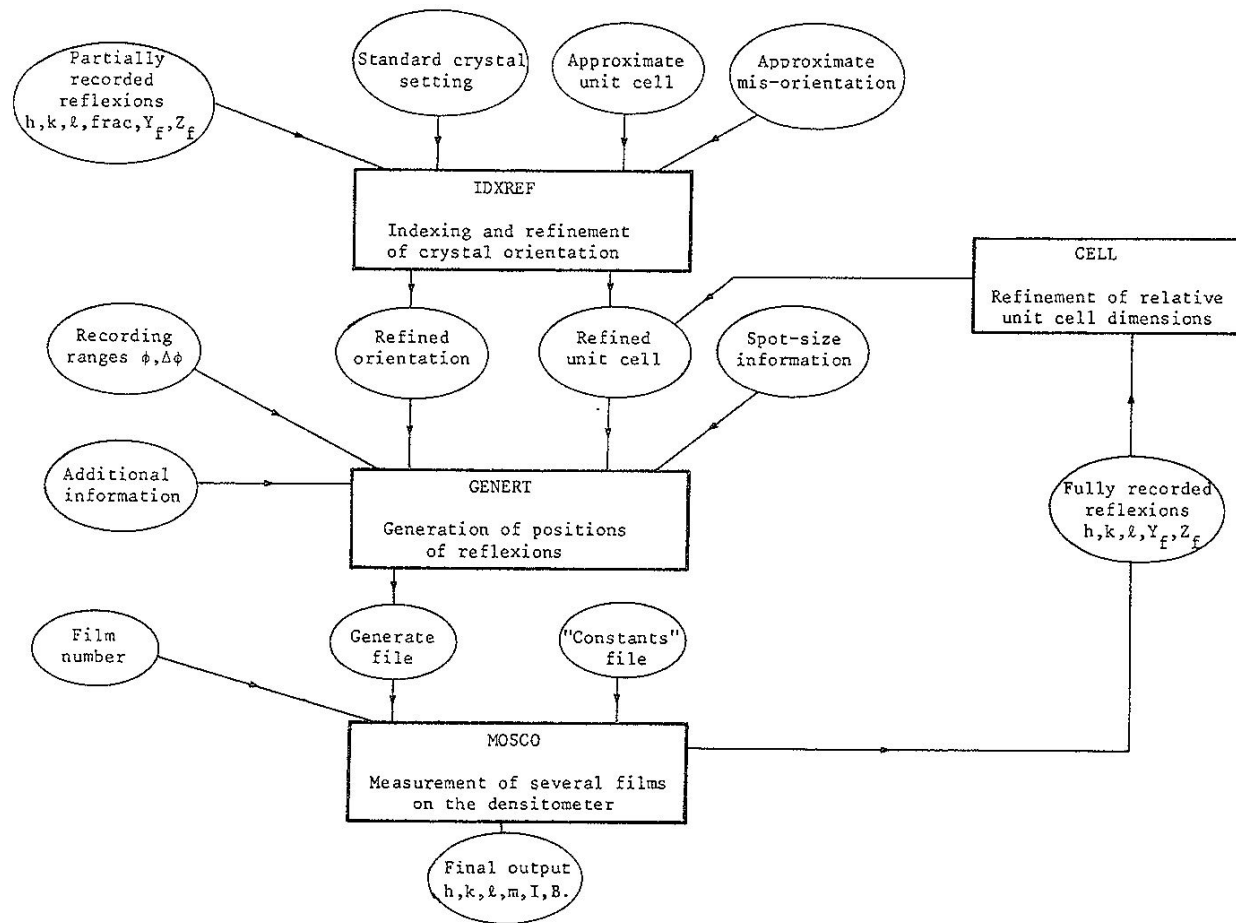
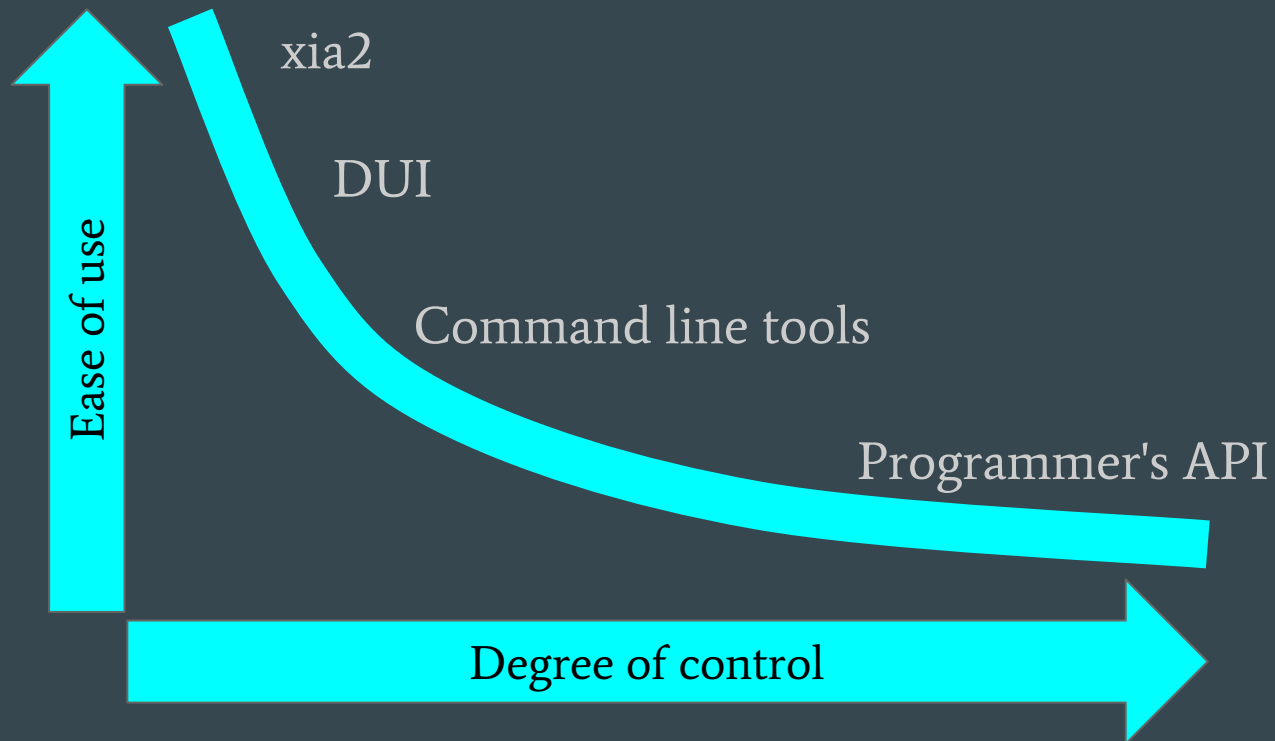


Fig. 10.1. Simplified flow-diagram of the Cambridge system, showing the inter-relationship of the component programs, IDXREF, GENERT, MOSCO and CELL.

Philosophy: toolbox



Philosophy: levels of interaction



xia2 -dials \${data_directory}

```
For AUTOMATIC/DEFAULT/NATIVE
High resolution limit          1.36    6.08    1.36
Low resolution limit          53.92   53.92   1.40
Completeness                   99.8    99.9    97.8
Multiplicity                   5.3     4.9     3.1
I/sigma                        11.7    26.8    2.2
Rmerge                         0.061   0.026   0.370
Rmeas(I)                       0.075   0.032   0.521
Rmeas(I+/-)                    0.075   0.032   0.495
Rpim(I)                        0.032   0.014   0.279
Rpim(I+/-)                     0.042   0.018   0.326
CC half                        0.999   0.998   0.818
Wilson B factor                8.913
Anomalous completeness        97.5    100.0   77.3
Anomalous multiplicity        2.6     3.1     1.8
Anomalous correlation         0.005   0.204  -0.019
Anomalous slope               0.955   0.000   0.000
Total observations             292123  3747    12262
Total unique                   55480   768     3919
Assuming spacegroup: P 41 21 2
Other likely alternatives are:
P 43 21 2
Unit cell:
57.781  57.781 149.995
90.000  90.000  90.000
```

DIALS/XIA2 in CCP4 I2

CCP4-7.0.037 Project Viewer: General

File Edit History Utilities Projects Help

Task menu View in Coot View in CCP4mg Export MTZ Help Bibliography Clone job Run Run on server

Job list Project directory

Job/File

- 4 xia2/dials
- ↖ 3 xia2/dials
- ↖ 1 xia2/dials

Import merged data, sequences, alignments or coordinates

Integrate X-ray images

- xia2** Automated integration of images with DIALS using xia2
DIALS Select a directory containing images and integrate them
- xia2** Automated integration of images with XDS using xia2
XDS Select a directory containing images and integrate them
- Integrate images with Mosflm**
Launch iMosflm and capture output

X-ray data reduction and analysis

Experimental phasing

Bioinformatics including model preparation for Molecular Replacement

Molecular Replacement

Model building and Graphics

Refinement

Ligands

Validation and analysis

Export and Deposition

Reflection data tools

Coordinate data tools

Developer tools

Future: DIALS GUI (currently in development)

The screenshot displays the DIALS GUI interface. On the left is a 'History Tree' showing a sequence of operations: import, find_spots, index, refine_bravais_settings, reindex { P 4 }, refine, integrate, reindex { C 2 2 21 }, and another index operation. The 'Integrate' panel in the center features a 'Stop' button, a 'DIALS integrate' button, and an 'Integrate' section with 'Simple' and 'Advanced' tabs. The 'Advanced' tab is active, showing settings for 'integration.profile.fitting' (True), 'integration.background.algorithm' (median), and 'integration.mp.nproc' (4). Below this is a table of experimental parameters:

Beam		Crystal			Scan		Detector			
X (mm)	Y (mm)	a	b	c	Image Range	1	540	Distance (mm)	265.07	
211.01	205.36	57.78	57.78	150.0	oscillation	0.15	Exposure time	0.07	Number of panels	1
Wavelength (Å)	0.97625	α	β	γ	strong spots	116048	Indexed spots	114682	refined spots	102414
		90.0	90.0	90.0	prof int spots	0	sum int spots	0	Pixel size	X (mm) Y (mm)
									0.172	0.172
		Space Group	P 4							
		Orientation (deg)	rot X	rot Y	rot Z					
			147.95	64.42	53.15					

On the right, the 'Image View' shows a diffraction image with a grid of panels and green spots. A status bar at the bottom indicates 'X: 157, Y: 419, I: -1'. A footer note reads 'Click the Dials icon to run >> refine'.

Main DIALS programs

```
dials.import  
dials.find_spots  
dials.index  
dials.refine_bravais_settings  
dials.refine  
dials.integrate  
dials.export_mtz
```

More than 50 other dials.* commands

Then onwards into the CCP4 data processing pipeline:
POINTLESS → AIMLESS → CTRUNCATE...

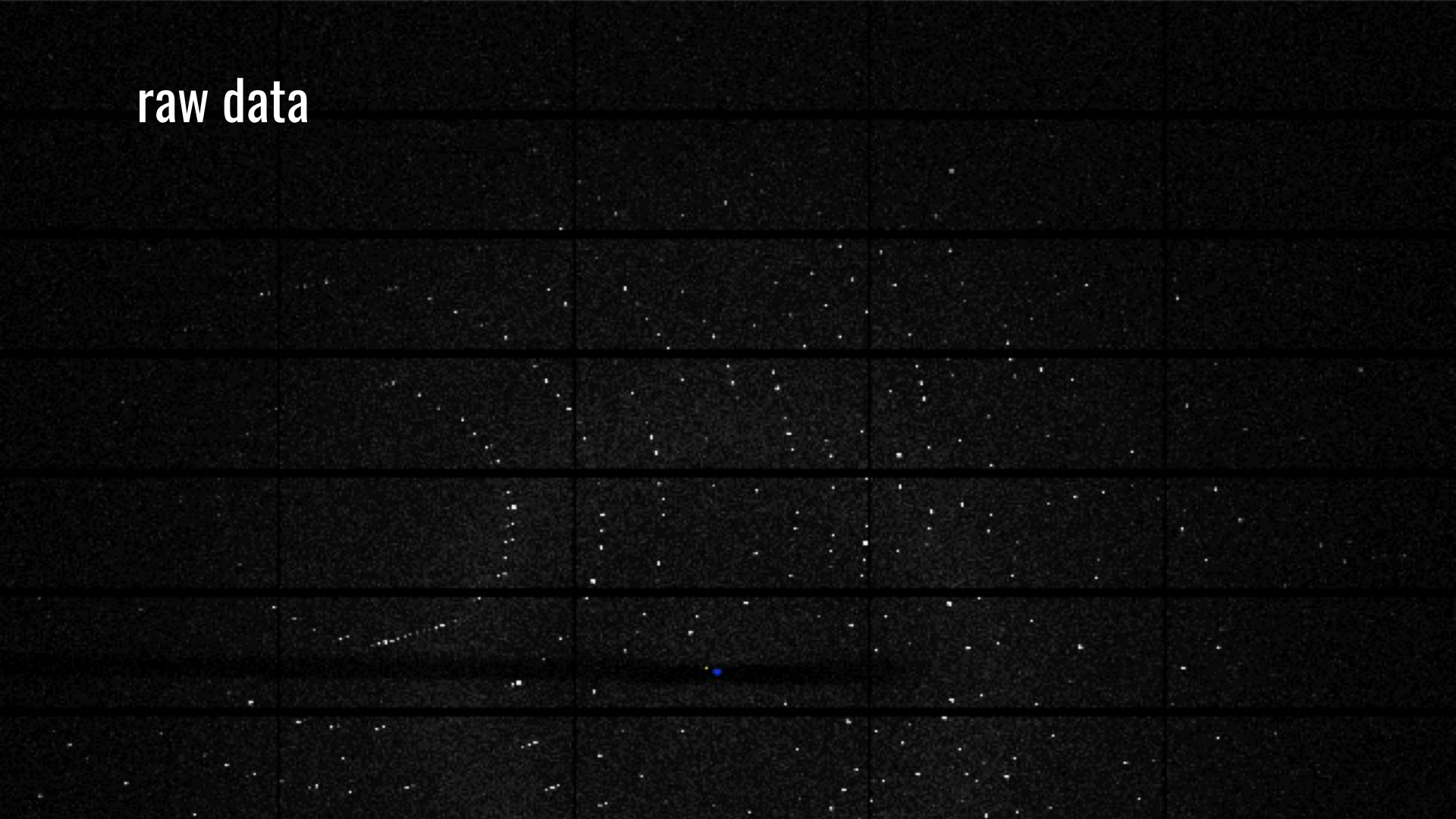
DIALS on the command line

```
$ dials.import ${data_directory}/th_8_2_0*.cbf
$ dials.find_spots datablock.json nproc=8
$ dials.index datablock.json strong.pickle
$ dials.refine_bravais_settings experiments.json indexed.pickle
$ dials.reindex indexed.pickle change_of_basis_op=a,b,c
$ dials.refine bravais_setting_9.json reindexed_reflections.pickle outlier.algorithm=tukey
  use_all_reflections=true scan_varying=true output.experiments=refined_experiments.json
$ dials.integrate refined_experiments.json refined.pickle outlier.algorithm=null nproc=4
$ dials.export_mtz integrated.pickle refined_experiments.json hklout=integrated.mtz
$ pointless hklin integrated.mtz hklout sorted.mtz > pointless.log
$ aimless hklin sorted.mtz hklout scaled.mtz > aimless.log << eof
  resolution 1.3
  anomalous off
eof
$ ctruncate -hklin scaled.mtz -hklout truncated.mtz -colin '/*/*/[IMEAN,SIGIMEAN]' > ctruncate.log
```

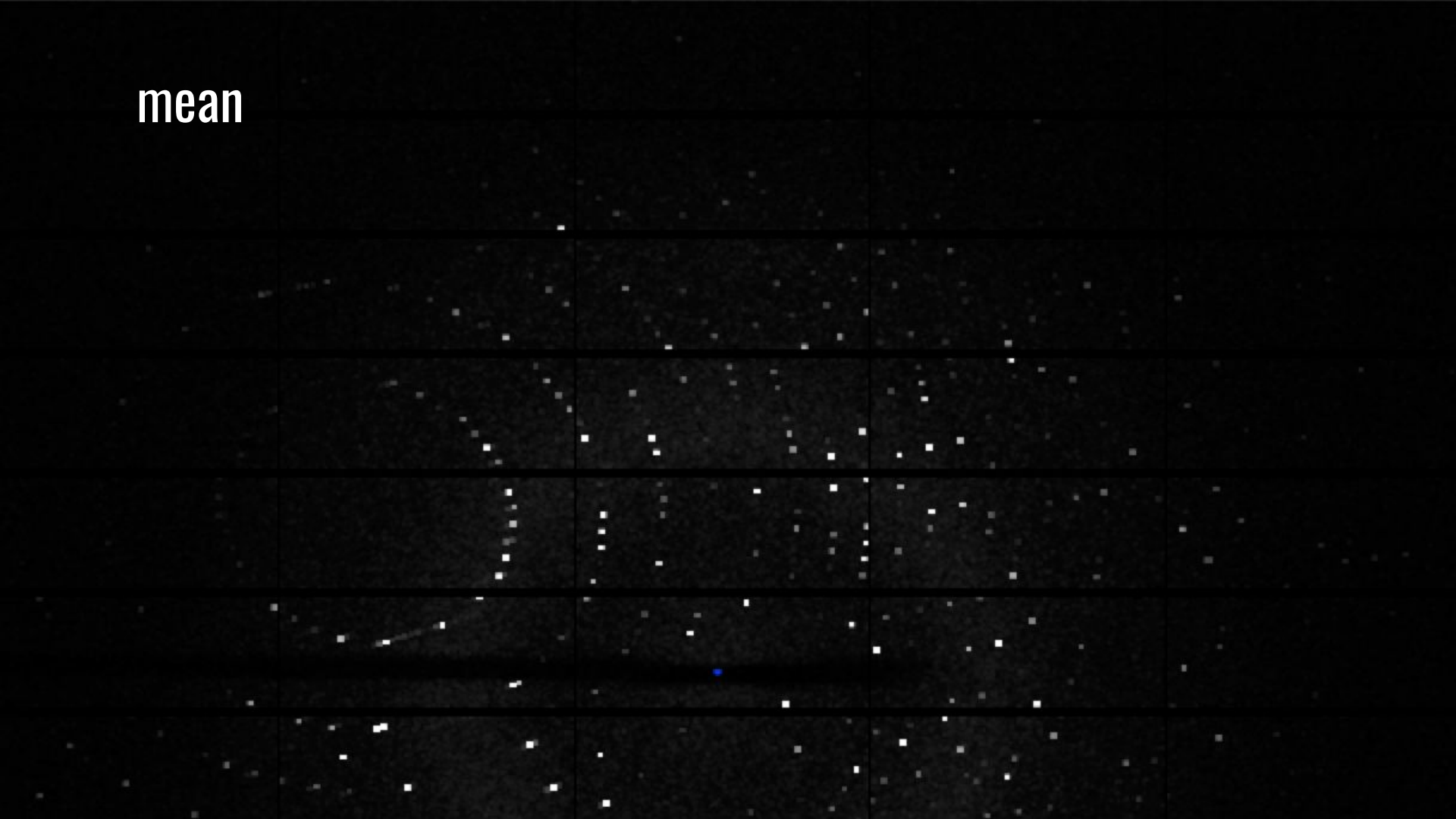
Who needs a GUI?

Spot finding

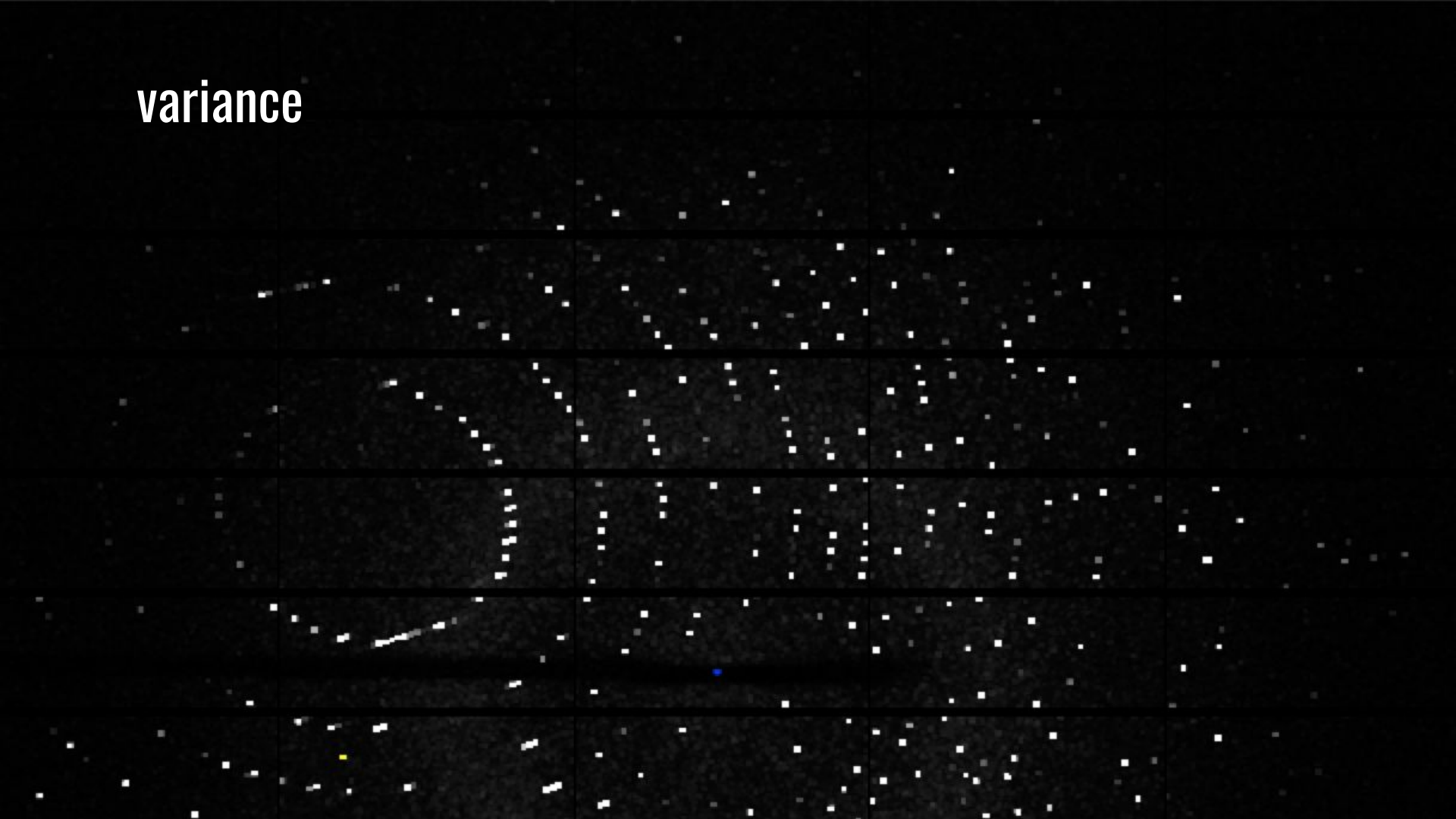
raw data



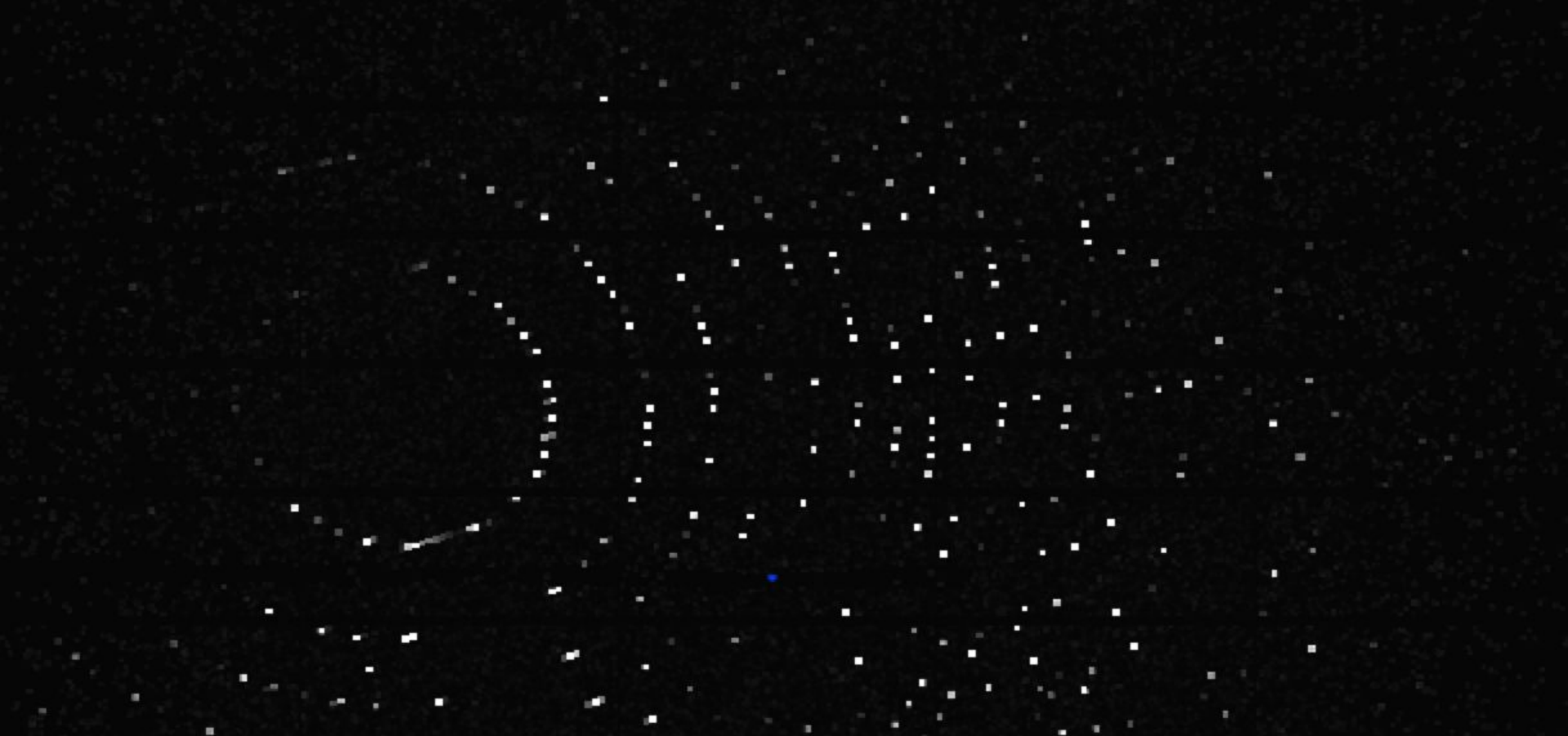
mean



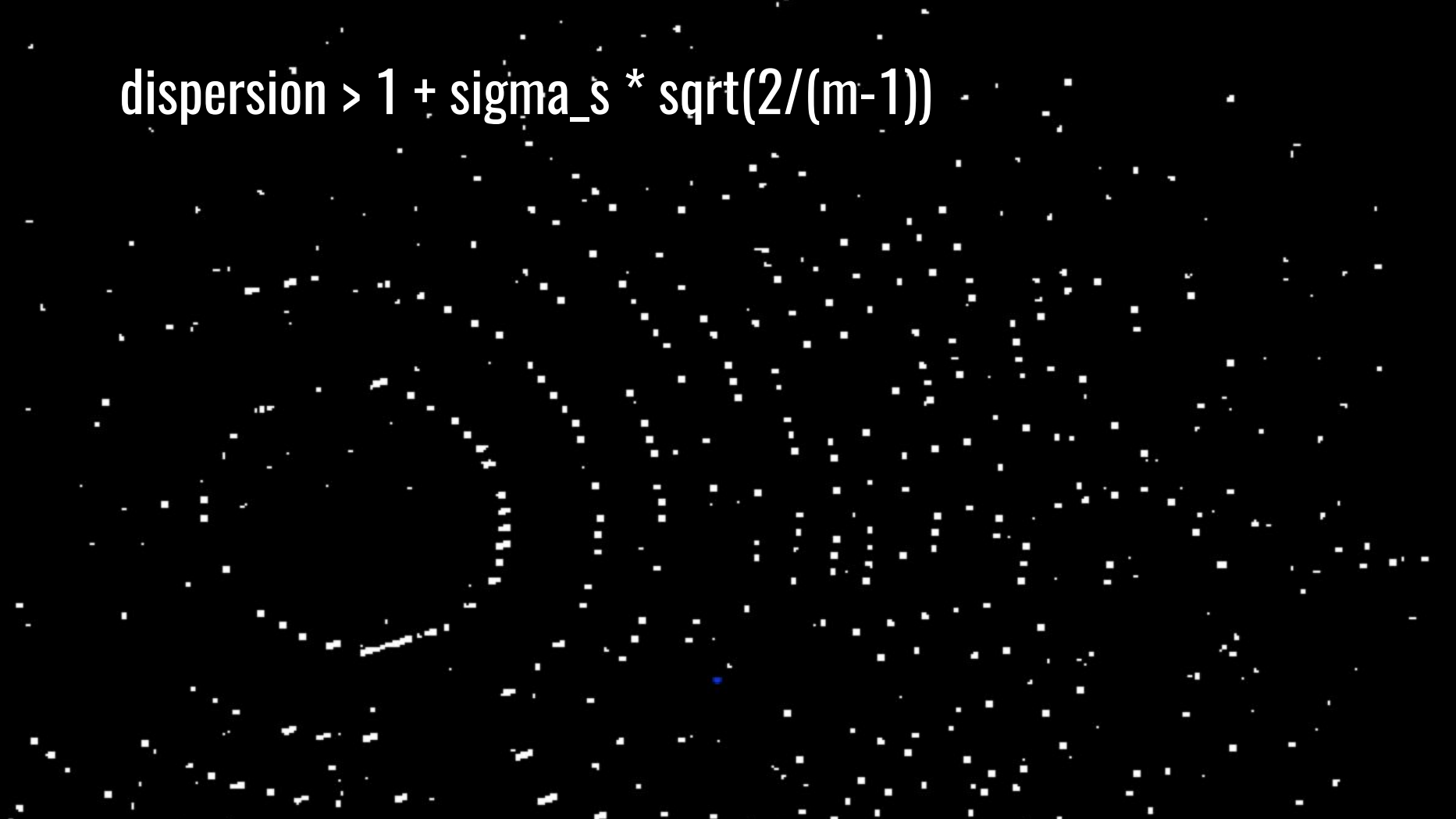
variance



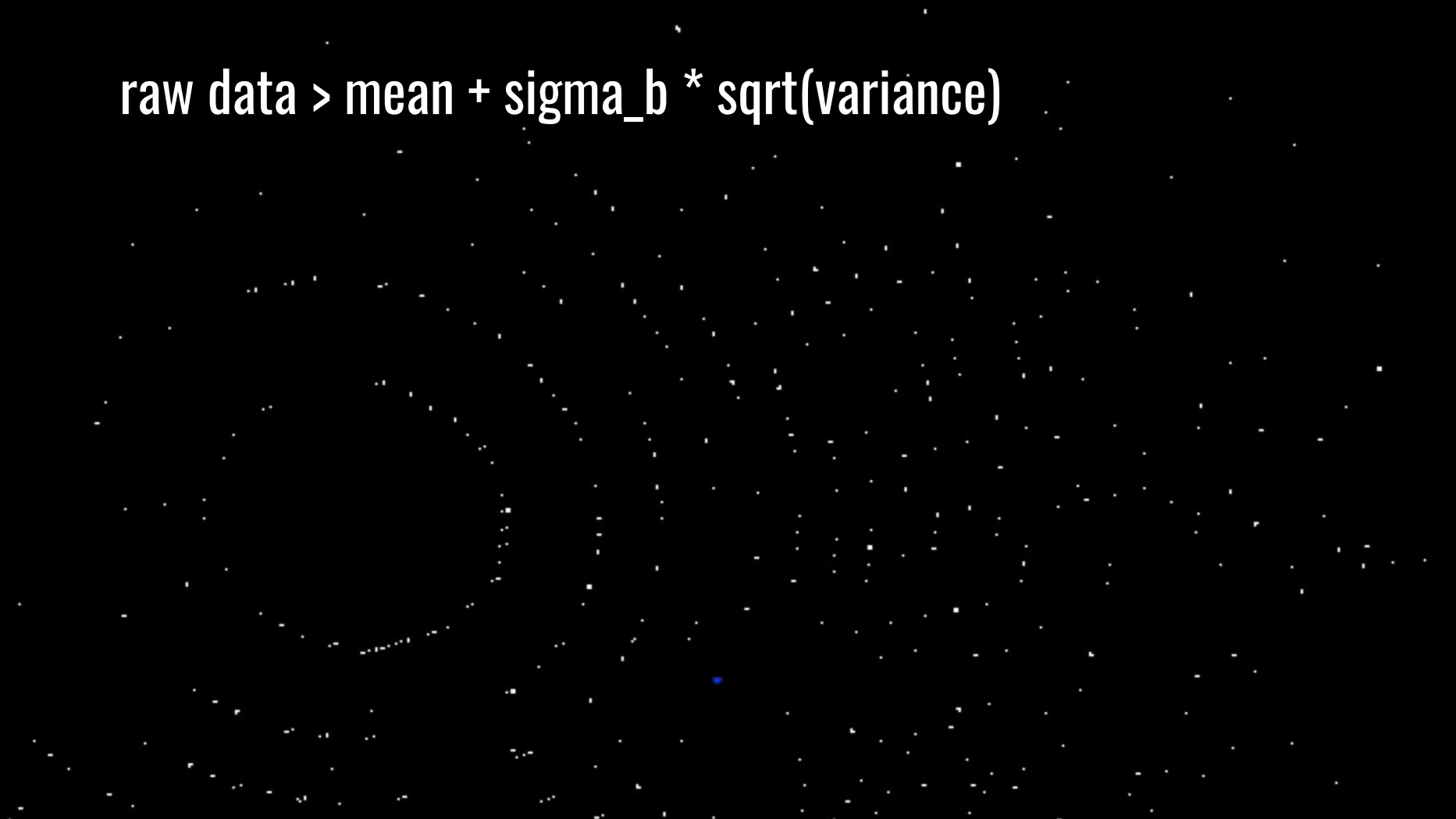
dispersion = variance / mean



dispersion $> 1 + \sigma_s * \sqrt{2/(m-1)}$



raw data > mean + sigma_b * sqrt(variance)



./saturn/lyso_00001.img

Load file Save As... Image: lyso_00001.img [1] Previous Next Jump to image: 1

Settings

Zoom level: 100%

Color scheme: grayscale

Brightness: 100

Show resolution rings Show ice rings

Mark beam center Mark centers of mass

Spot max pixels Spot all pixels

Draw reflection shoebox Show predictions

Show hkl

Sigma background 6.0

Sigma strong 3.0

Global Threshold 0.0

Min. local 2

Gain 1.0

Kernel size 3 3

Click and drag to pan; middle-click and drag to plot intensity profile, right-click to zoom

Default spot finding parameters are often not suitable for CCD images

Image is from Rigaku Saturn 92 detector

./saturn/lyso_00001.img

Load file Save As... Image: lyso_00001.img [1] Previous Next Jump to image: 1

Settings

Zoom level: 100%

Color scheme: grayscale

Brightness: 100

Show resolution rings Show ice rings

Mark beam center Mark centers of mass

Spot max pixels Spot all pixels

Draw reflection shoebox Show predictions

Show hkl

Sigma background 6.0

Sigma strong 10.0

Global Threshold 0.0

Min. local 2

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Kernel size 3 3

Click and drag to pan; middle-click and drag to plot intensity profile, right-click to zoom

Default spot finding parameters are often not suitable for CCD images

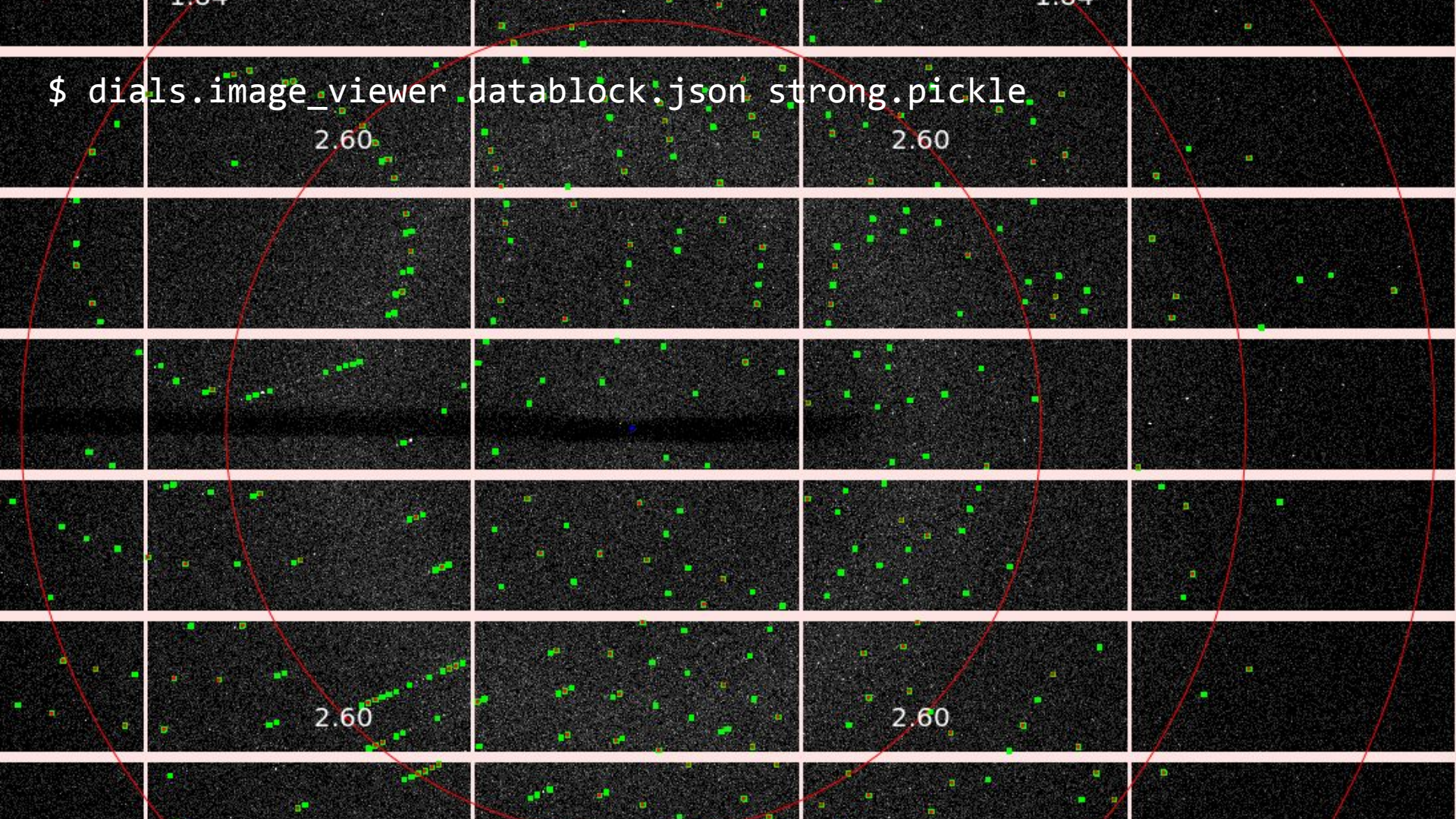
\$ dials.image_viewer datablock.json strong.pickle

2.60

2.60

2.60

2.60



Indexing

dials.index

Map centroids to reciprocal space,
analyse for periodicity and
determine basis vectors for the
reduced cell

- Choice of method:
 - 1D FFT (DPS)
 - 3D FFT - **default**
 - new real space grid search algorithm
- Optionally provide known unit cell and space group

```
$ dials.index datablock.json strong.pickle
Found max_cell: 199.1 Angstrom
Setting d_min: 3.89
```

```
RMSDs by experiment:
```

Exp	Nref	RMSD_X (px)	RMSD_Y (px)	RMSD_Z (images)
0	4049	0.2881	0.25838	0.17767

```
Final refined crystal models:
```

```
model 1 (114690 reflections):
```

```
Crystal:
```

```
Unit cell: (57.804, 57.782, 150.027, 90.009, 89.991, 89.990)
```

```
Space group: P 1
```

```
U matrix: {{ 0.3455, -0.2589, -0.9020},
            { 0.8914,  0.3909,  0.2292},
            { 0.2933, -0.8833,  0.3659}}
```

```
B matrix: {{ 0.0173,  0.0000,  0.0000},
            {-0.0000,  0.0173,  0.0000},
            {-0.0000,  0.0000,  0.0067}}
```

```
A = UB: {{ 0.0060, -0.0045, -0.0060},
          { 0.0154,  0.0063,  0.0015},
          { 0.0051, -0.0153,  0.0024}}
```

```
Saving refined experiments to experiments.json
Saving refined reflections to indexed.pickle
```

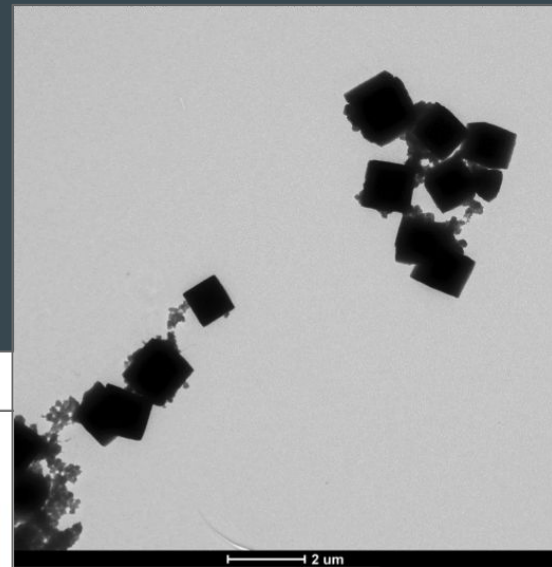
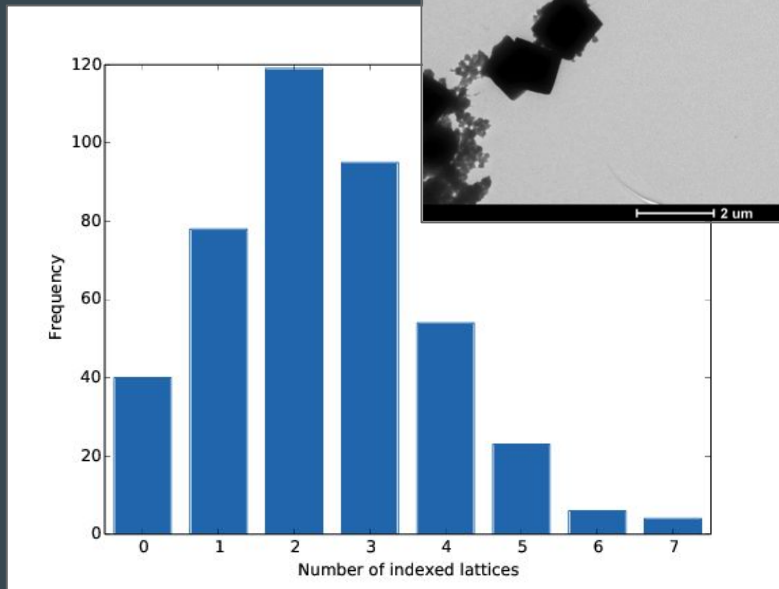
dials.index

DIALS contains an indexing algorithm that is very successful at identifying multiple lattices

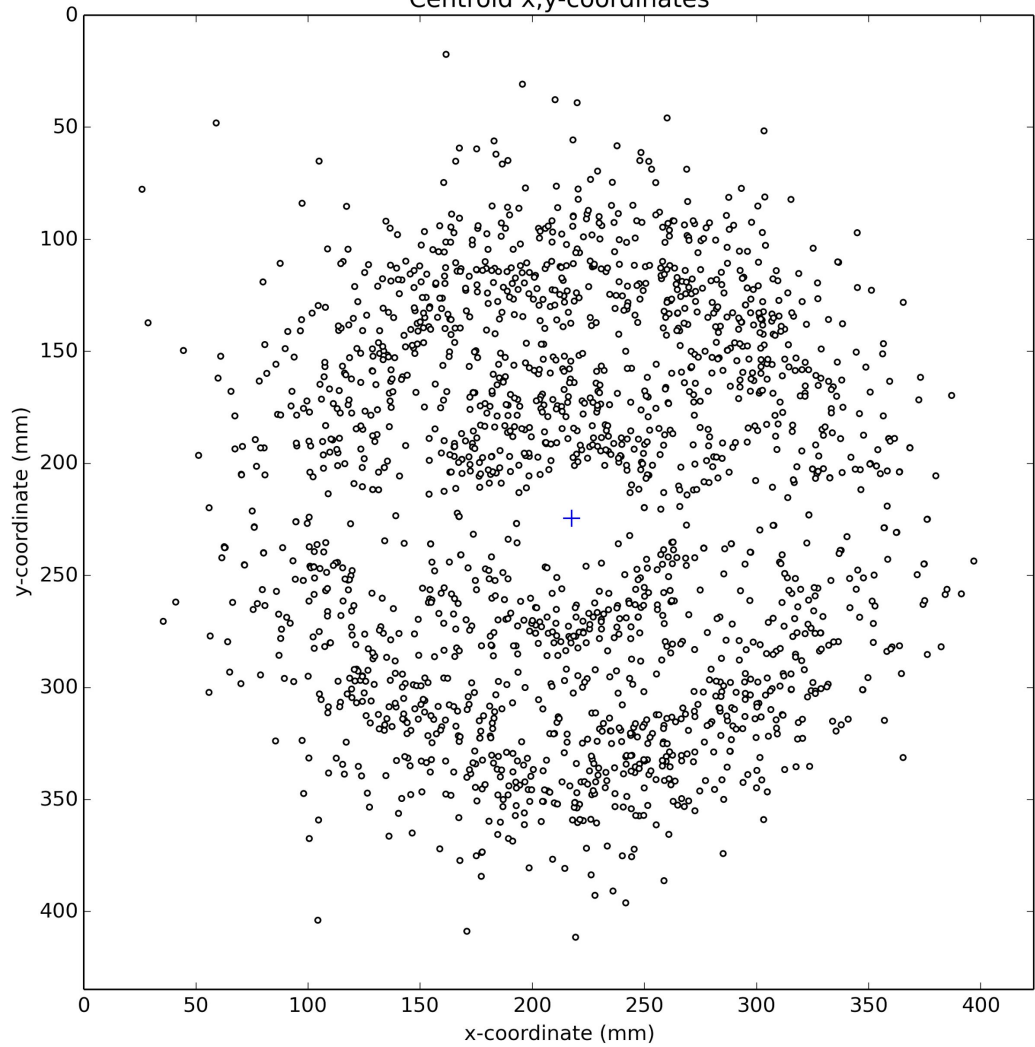
This even works when lattices diffract equally well, and only a narrow wedge of data is available

As additional lattices are found, joint refinement reduces correlations between crystal and detector parameters

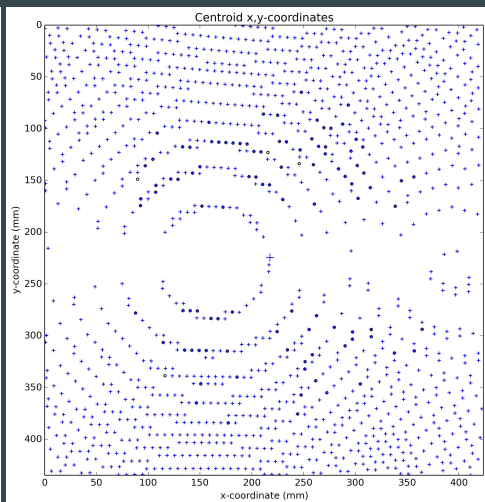
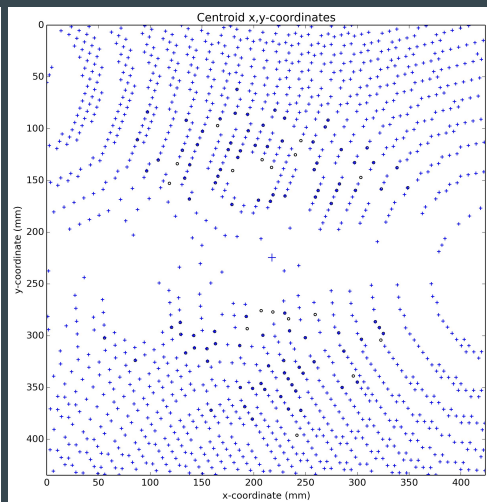
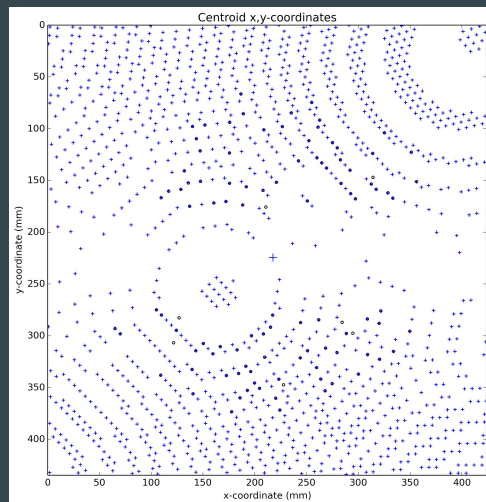
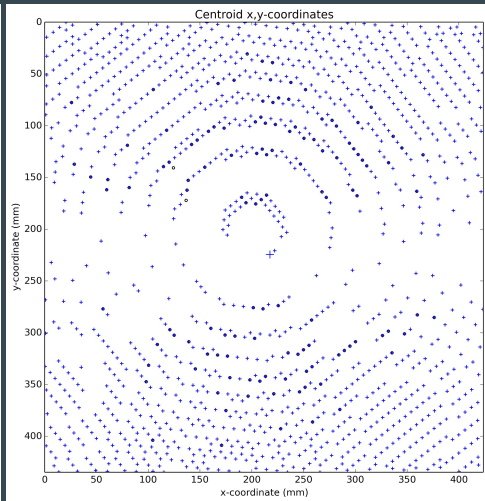
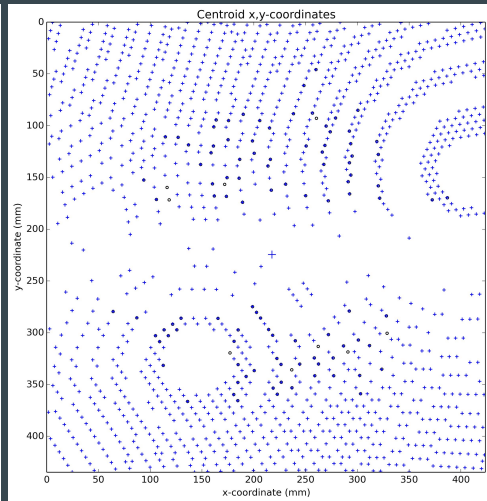
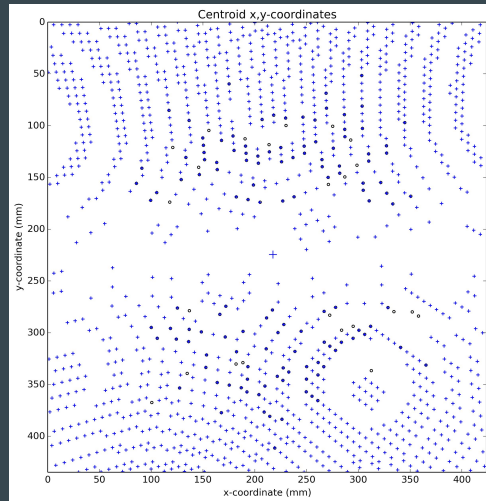
R. Gildea et al. (2014) Acta Cryst. D70, 2652-66



Centroid x,y-coordinates



1° wedge of data
1858 spots



6 lattices identified

dials.reciprocal_lattice_viewer

```
$ dials.reciprocal_lattice_viewer  
Usage: dials.reciprocal_lattice_viewer [options] datablock.json reflections.pickle
```

Options:

```
-h, --help          show this help message and exit  
-c, --show-config  Show the configuration parameters.  
-a ATTRIBUTES_LEVEL, --attributes-level=ATTRIBUTES_LEVEL  
                   Set the attributes level for showing configuration  
                   parameters  
-e EXPERT_LEVEL, --expert-level=EXPERT_LEVEL  
                   Set the expert level for showing configuration  
                   parameters  
-v                 Increase verbosity
```

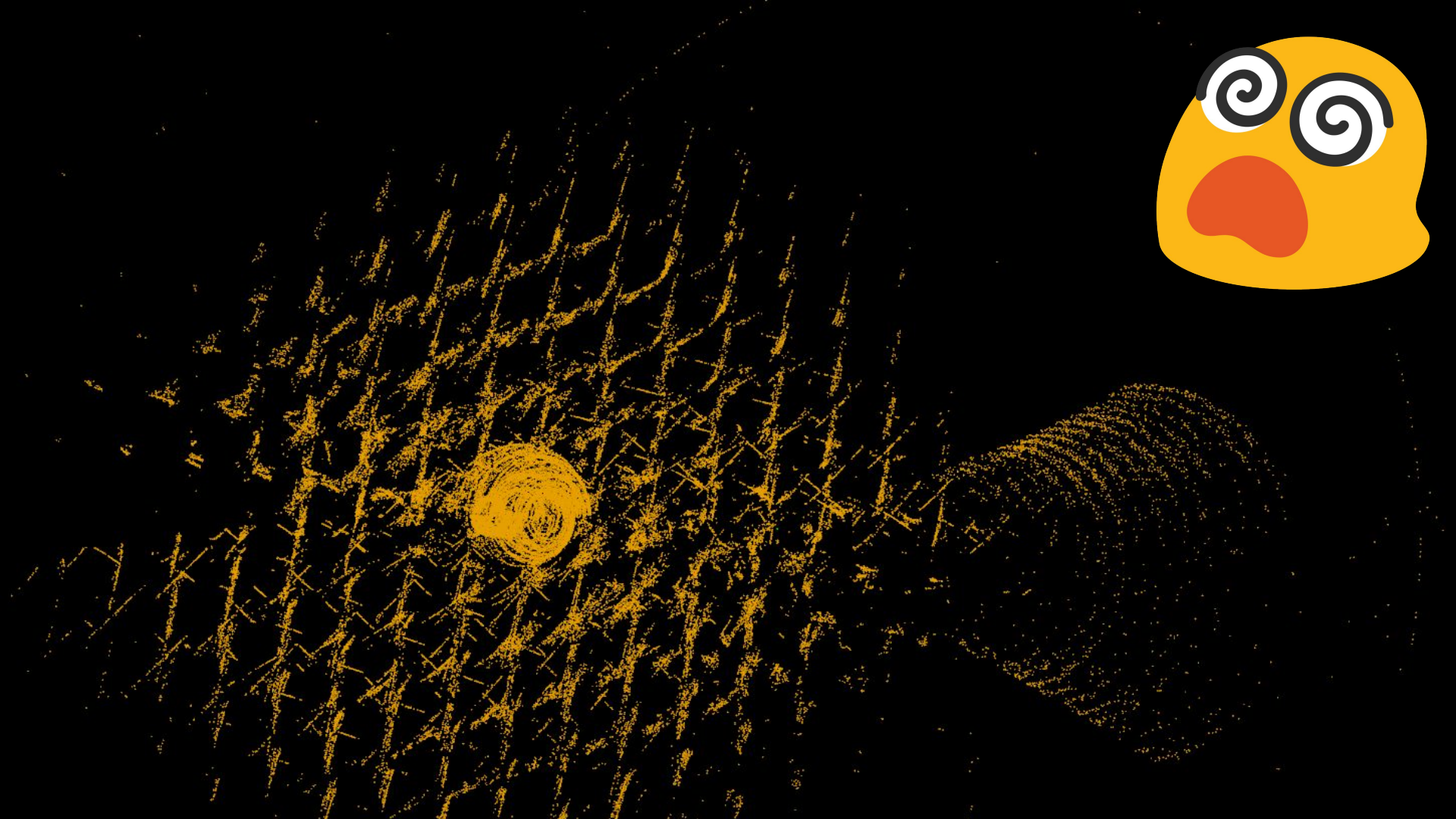
Visualise the strong spots from spotfinding in reciprocal space.

Examples:

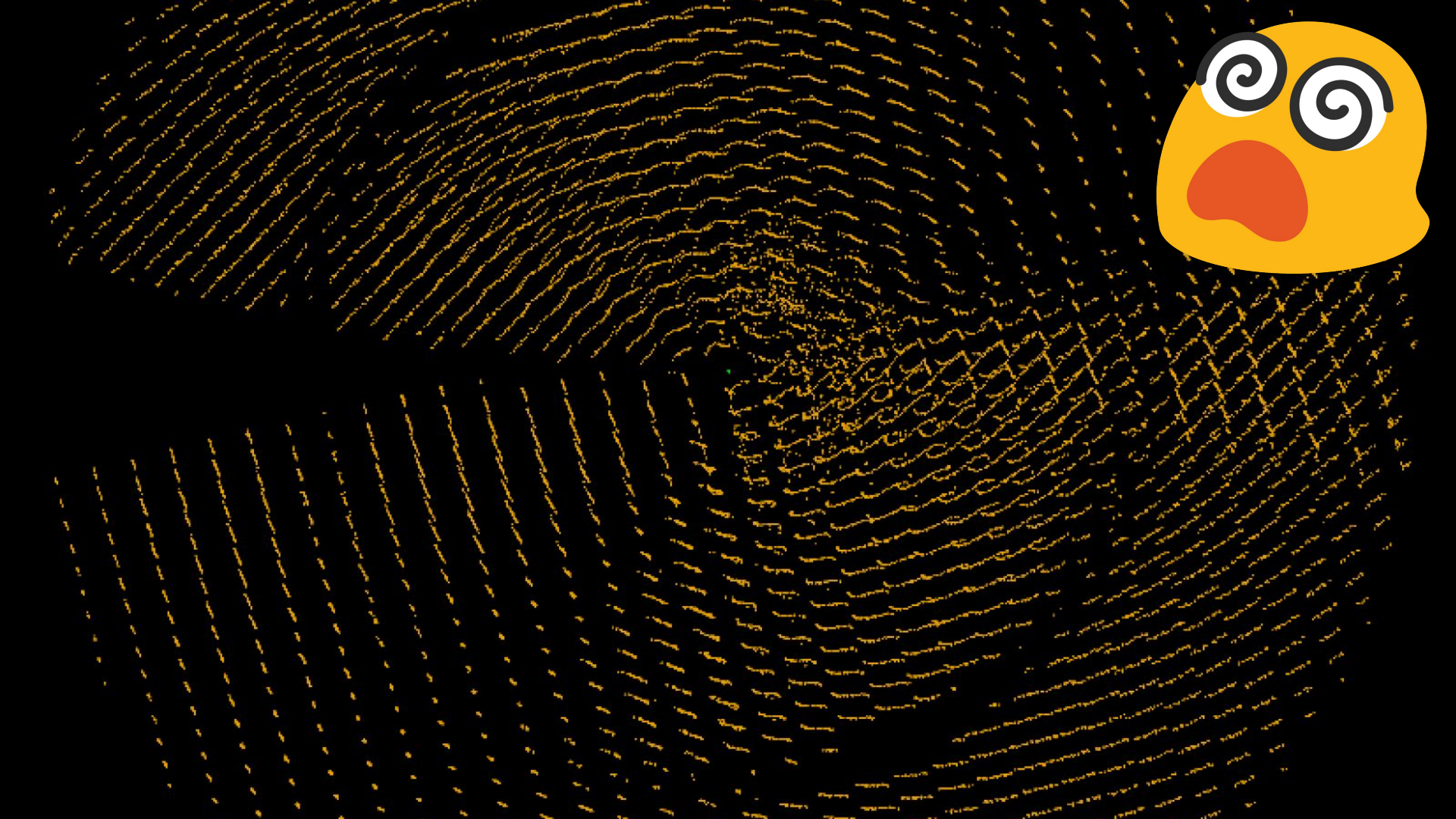
```
dials.reciprocal_lattice_viewer datablock.json strong.pickle
```

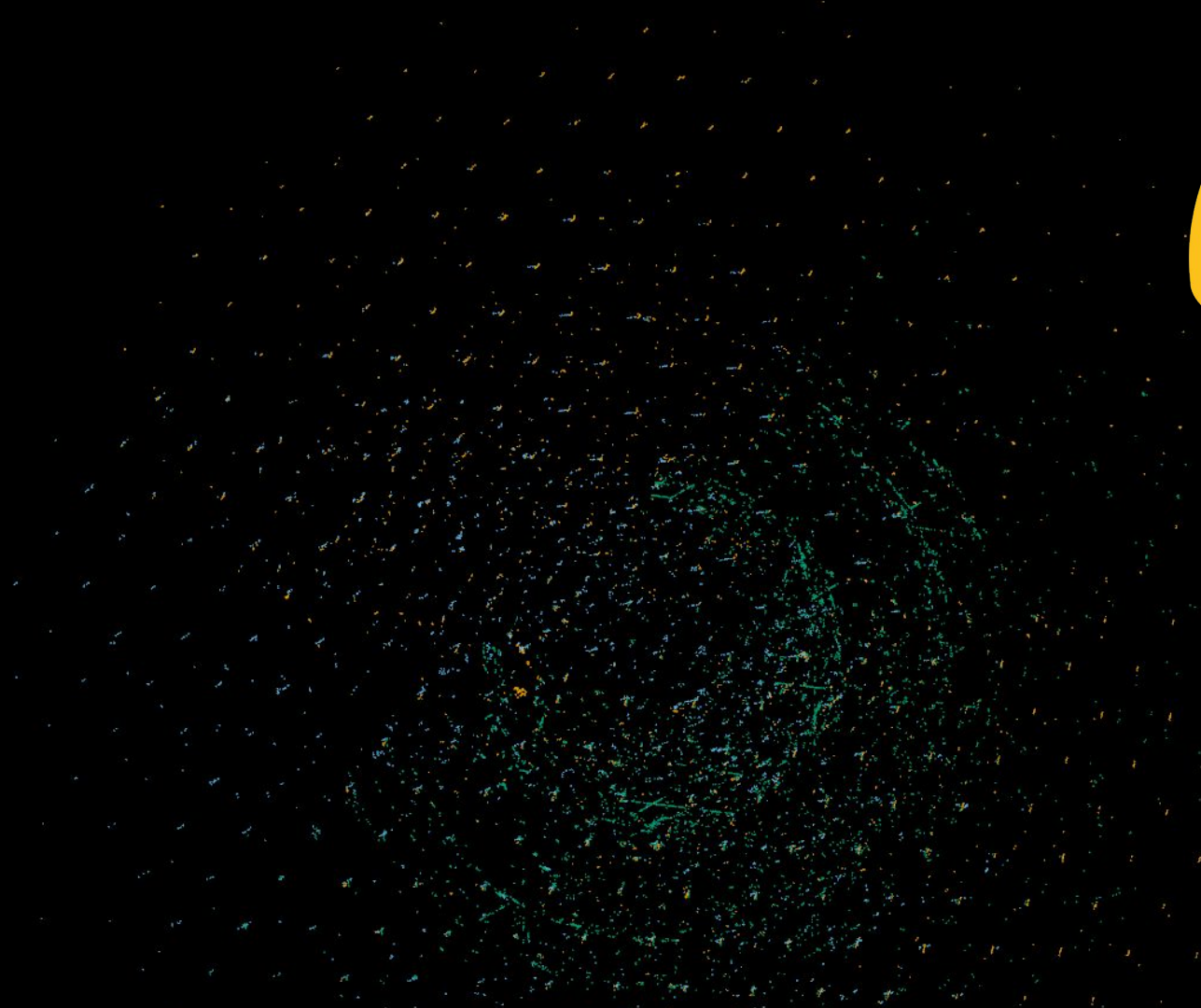
```
dials.reciprocal_lattice_viewer experiments.json indexed.pickle
```

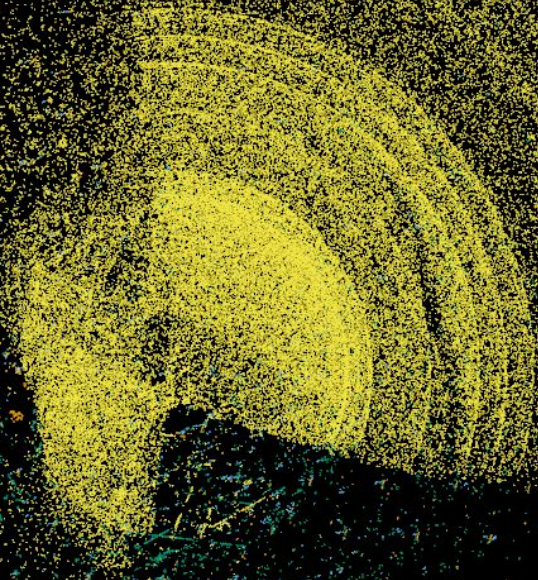












dials.refine_bravais_settings

- After indexing, look for lattice symmetry
- All compatible Bravais lattices are tested
- Metric fit score, refined RMSD and symmetry element CCs are reported
- The user chooses which solution to take further

```
$ dials.refine_bravais_settings experiments.json indexed.pickle
```

```
-----  
Solution Metric fit  rmsd  min/max cc #spots lattice                unit_cell  volume  cb_op  
-----  
*  9  0.0311 0.063 0.800/0.857  8099  tP  57.78  57.78 150.00  90.00  90.00  90.00  500867  a,b,c  
*  8  0.0311 0.063 0.800/0.969  8099  oC  81.72  81.73 150.01  90.00  90.00  90.00 1002008  a-b,a+b,c  
*  7  0.0272 0.061 0.969/0.969  8099  mC  81.73  81.74 150.03  90.00  89.99  90.00 1002365  a-b,a+b,c  
*  6  0.0311 0.062 0.805/0.805  8099  mC  81.73  81.72 150.02  90.00  89.99  90.00 1002012  a+b,-a+b,c  
*  5  0.0154 0.061 0.800/0.906  8099  oP  57.79  57.76 149.99  90.00  90.00  90.00  500672  a,b,c  
*  4  0.0147 0.060 0.821/0.821  8099  mP  57.77  57.80 150.01  90.00  90.02  90.00  500853  -b,-a,-c  
*  3  0.0154 0.060 0.906/0.906  8099  mP  57.80  57.78 150.02  90.00  89.98  90.00  500945  a,b,c  
*  2  0.0152 0.061 0.800/0.800  8099  mP  57.78 150.01  57.80  90.00  89.99  90.00  500925  b,c,a  
*  1  0.0000 0.060          -/-  8099  aP  57.80  57.78 150.03  90.01  89.99  89.99  501086  a,b,c  
-----
```

```
* = recommended solution
```


dials.refine_bravais_settings

- After indexing, look for lattice symmetry
- All compatible Bravais lattices are tested
- Metric fit score, refined RMSD and symmetry element CCs are reported
- The user chooses which solution to take further

```
$ dials.refine_bravais_settings experiments.json indexed.pickle
```

```
-----  
Solution Metric fit  rmsd  min/max cc #spots lattice                unit_cell volume  cb_op  
-----  
      5    3.7053 1.048 0.199/0.438  1792      oP  11.52  13.51  29.38  90.00  90.00  90.00  4571  a,b,c  
      4    3.7053 1.001 0.438/0.438  1755      mP  13.43  11.55  29.30  90.00  91.40  90.00  4543 -b,-a,-c  
      3    3.7038 1.033 0.287/0.287  1811      mP  11.47  29.43  13.46  90.00  88.93  90.00  4542 -a,-c,-b  
*     2    0.1091 0.065 0.199/0.199  1929      mP  11.63  13.55  30.14  90.00  93.69  90.00  4739  a,b,c  
*     1    0.0000 0.060      -/-    1890      aP  11.63  13.55  30.15  89.94  93.70  90.06  4742  a,b,c  
-----
```

```
* = recommended solution
```

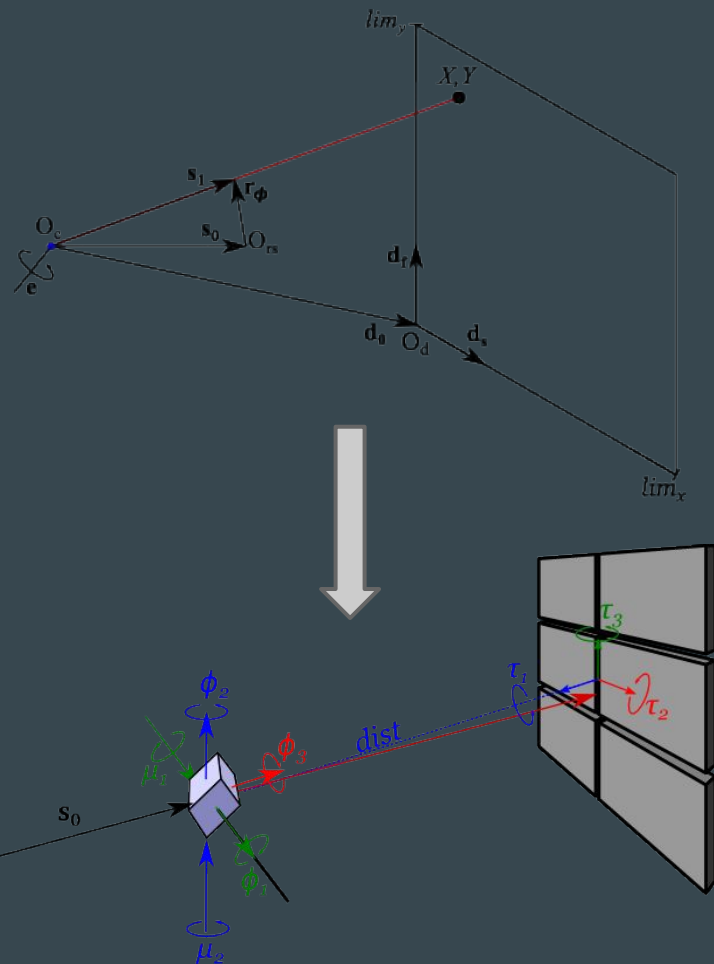
Refinement

dials.refine

Parameterise the reflection prediction equation,
 minimise the squared differences between predictions
 (X_c, Y_c, ϕ_c) and observations (X_o, Y_o, ϕ_o)

Model	State	Parameters
Beam	\mathbf{s}_0	2 orientation angles (μ_1, μ_2) 1 length of \mathbf{s}_0 (ν , wavenumber)
Crystal orientation	\mathbf{U}	3 orientation angles ($\varphi_1, \varphi_2, \varphi_3$)
Crystal unit cell	\mathbf{B}	6 elements of the metrical matrix \mathbf{G}^*
Detector	\mathbf{d}	3 translations (Dist, t_1, t_2) 3 rotation angles (τ_1, τ_2, τ_3)

18 parameters in the $P1$ case. Usually ν and μ_1 are fixed



dials.refine

We approach this as a traditional non-linear least squares problem

Keep simple and robust by using the positional residual only (no post-refinement)

Do refinement globally, using strong spot data from the whole scan

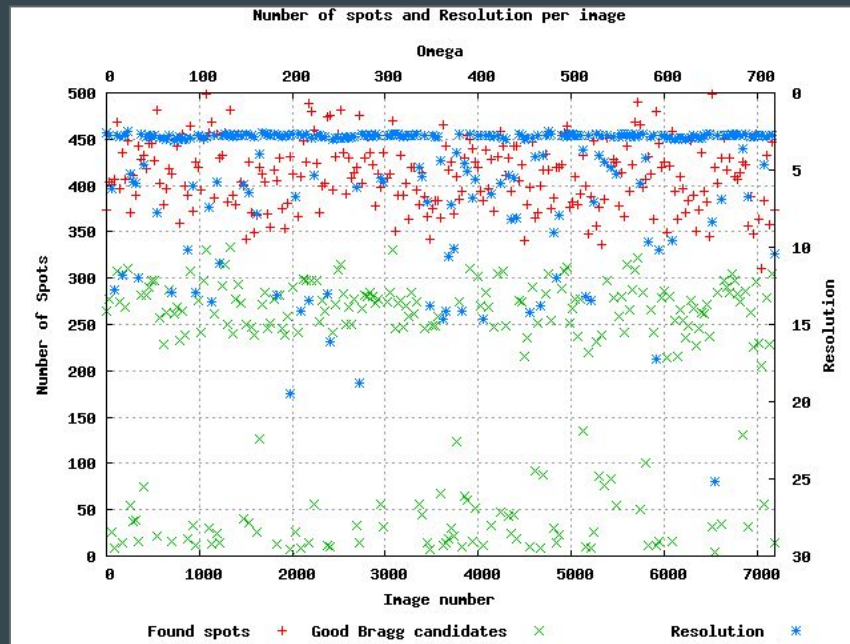
How do we model a crystal that changes during the data collection?

The crystal orientation and the unit cell may change due to

- sampling of different mosaic blocks during data collection
- crystal "slippage" (unlikely for cryo-cooled samples)
- radiation damage

dials.refine: example

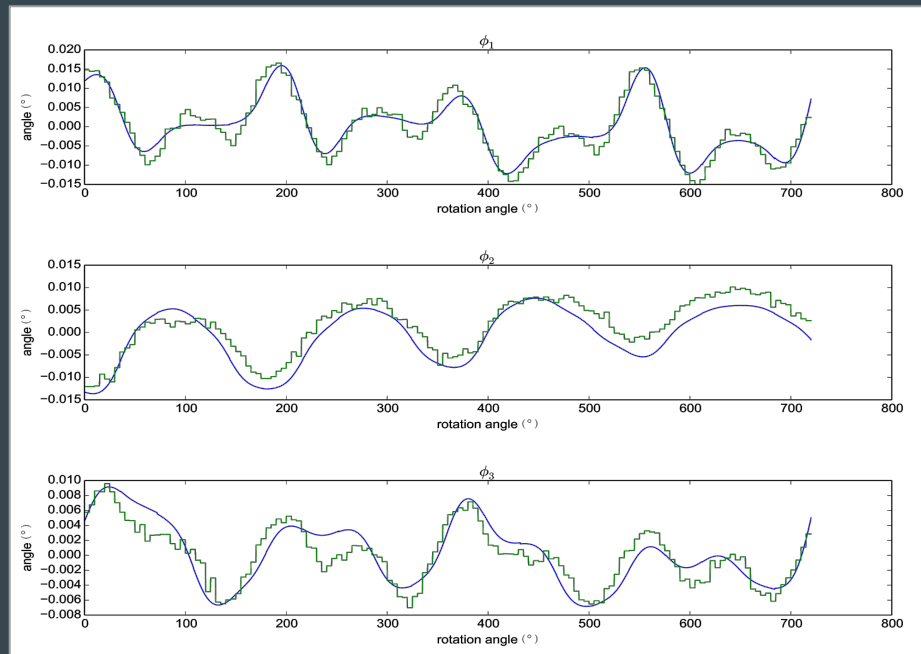
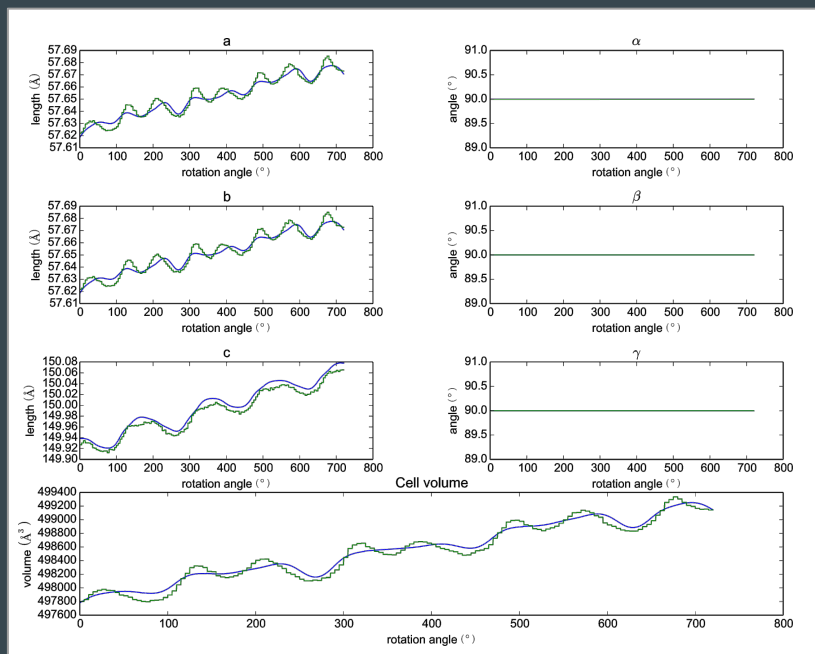
720° of tetragonal thaumatin data collected at 0.1°/image, 40Hz, 3% transmission at DLS I03



Scan-varying refinement

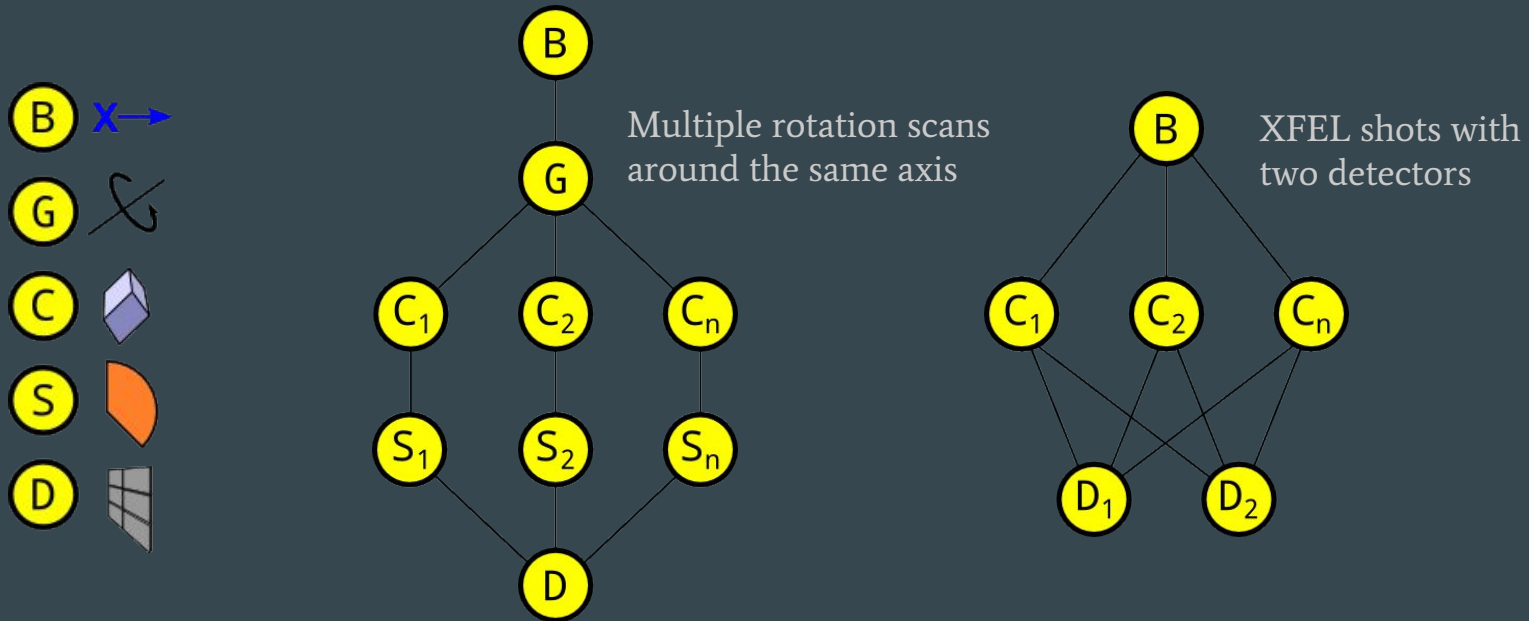
Global, scan-varying refinement with a Gaussian smoother inspired by AIMLESS

117 parameters in total: 6 detector, 1 beam, 22 "samples" of 3 crystal orientation and 2 unit cell parameters



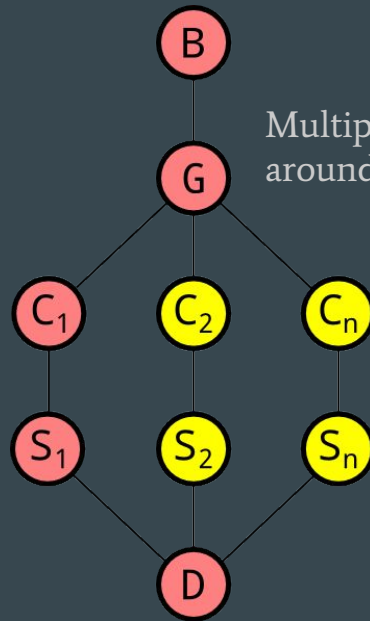
Multiple experiments

- Global refinement across datasets that share some models
- Typical use cases involve multiple crystals

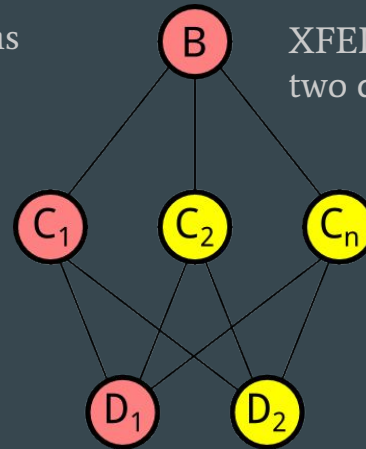


Multiple experiments

- Global refinement across datasets that share some models
- Typical use cases involve multiple crystals



Multiple rotation scans
around the same axis

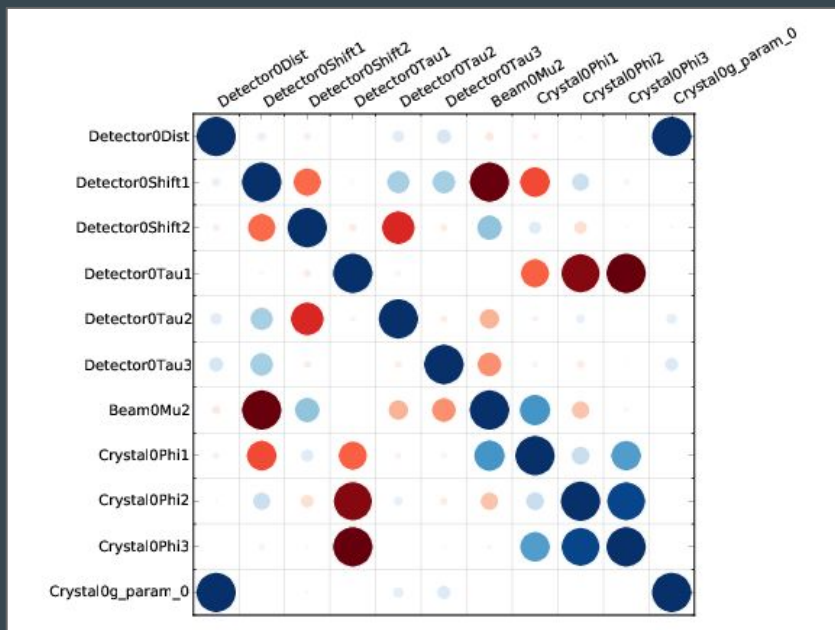


XFEL shots with
two detectors

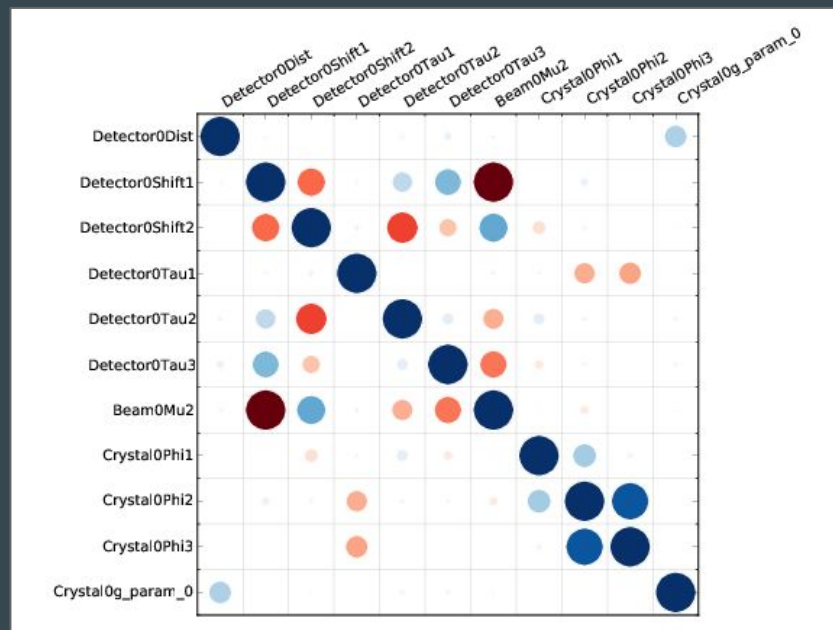
Multiple experiments

Cubic polyhedrin crystals, 1° scans

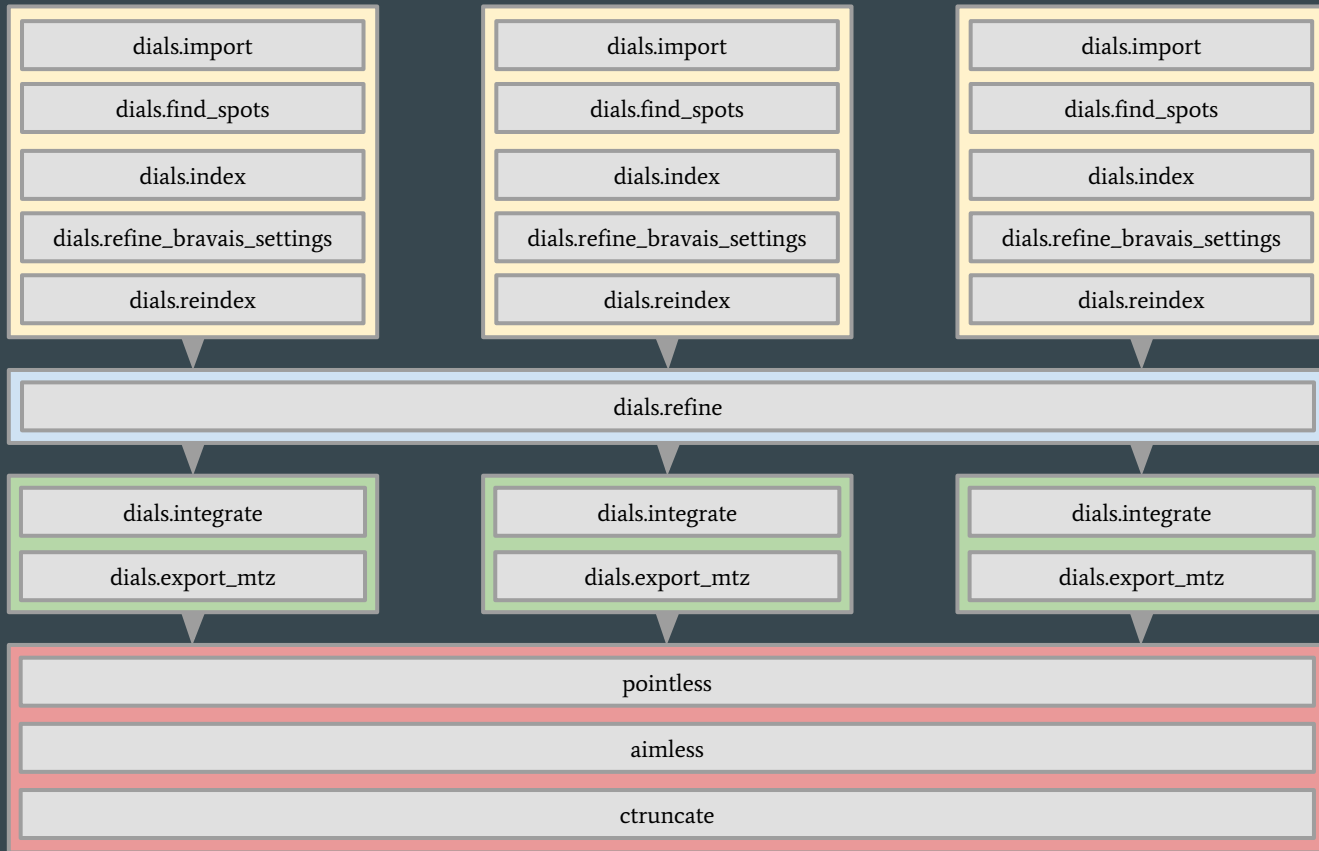
One lattice



5 sweeps (16 lattices)

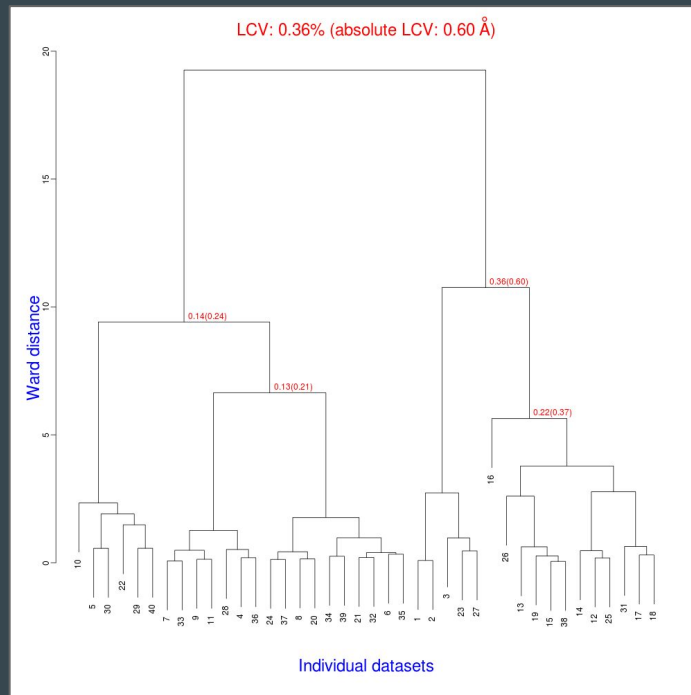
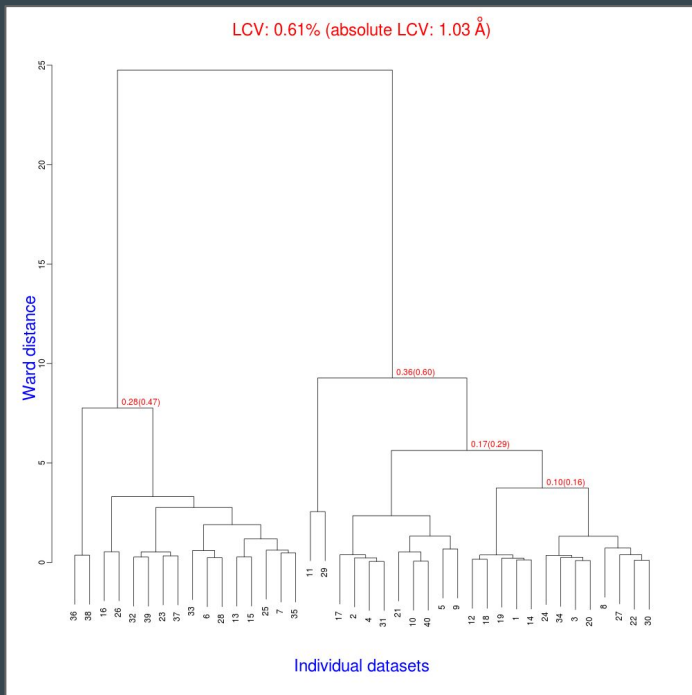


Joint refinement



Multiple experiments

Use joint refinement as a preparatory step for BLEND



TehA data. See *Acta Cryst. D71* (June 2015) for original analysis

Integration

Tasks in dials.integrate

Calculate the bounding box parameters from strong reflections



Predict the positions of reflections on the images

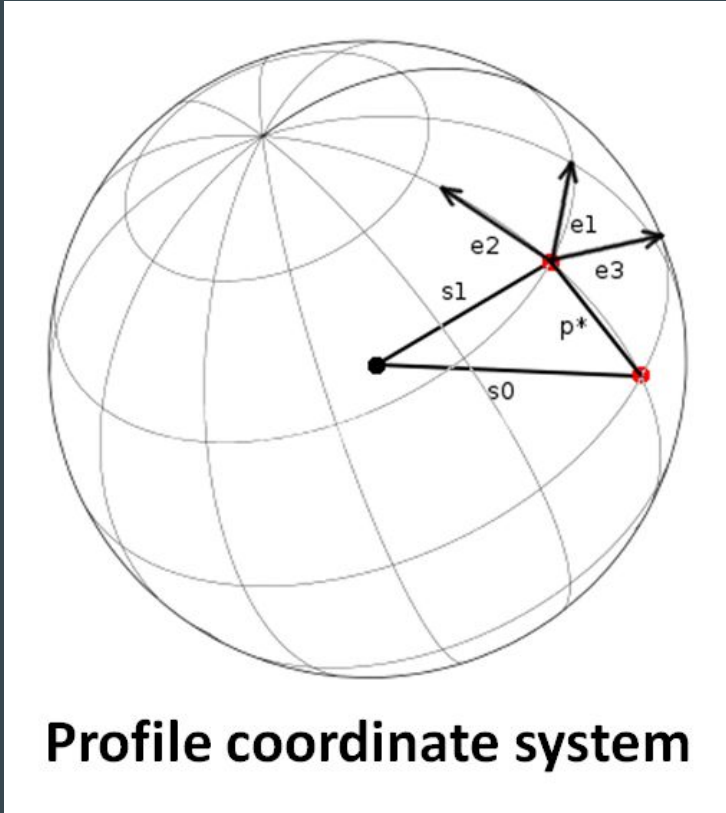


Build reference profiles across all images



Integrate the reflections and save output

Computing reflection shoeboxes



Use the kabsch model of a normal distribution on the surface of the Ewald sphere

- Corrects for geometrical distortions
- Makes spots appear to have taken shortest path through Ewald sphere
- Model assumes a Gaussian profile in Kabsch coordinate system

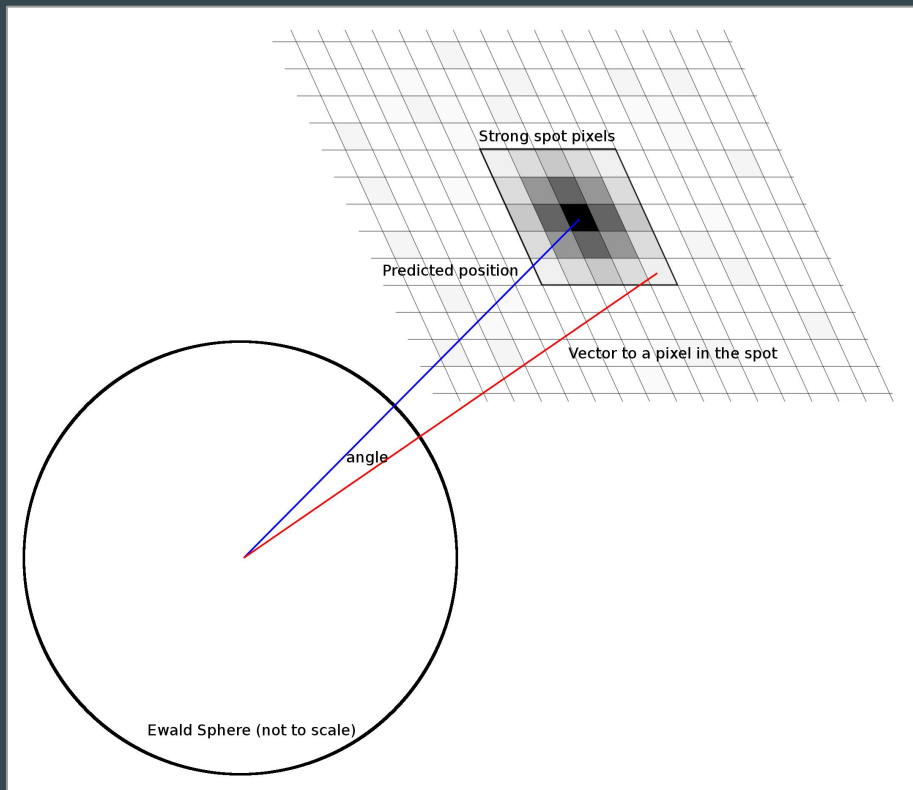
$$\exp\left(\frac{-\epsilon_1^2}{2\sigma_D^2}\right) \exp\left(\frac{-\epsilon_2^2}{2\sigma_D^2}\right) \exp\left(\frac{-\epsilon_3^2}{2\sigma_M^2}\right)$$

2 parameters:

σ_D - roughly "beam divergence"

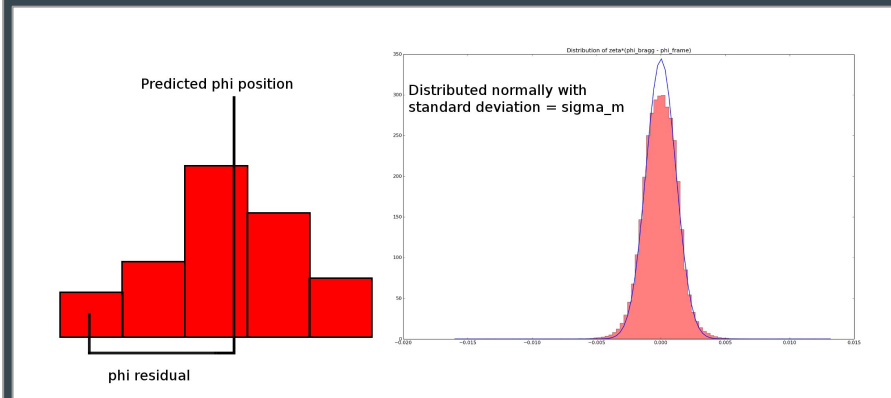
σ_M - roughly "mosaicity"

Computing reflection shoeboxes

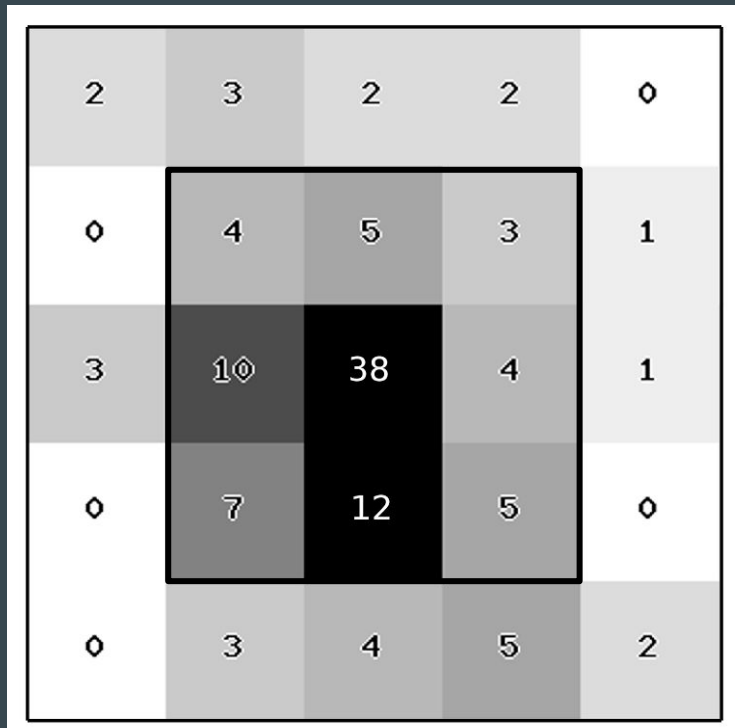


σ_D is calculated from the spread of angles between the predicted diffracted beam vector and the vector for each strong pixel in the spot

σ_M is calculated by maximum likelihood method assuming a normal distribution of phi residuals for each strong pixel in the spot



Integration



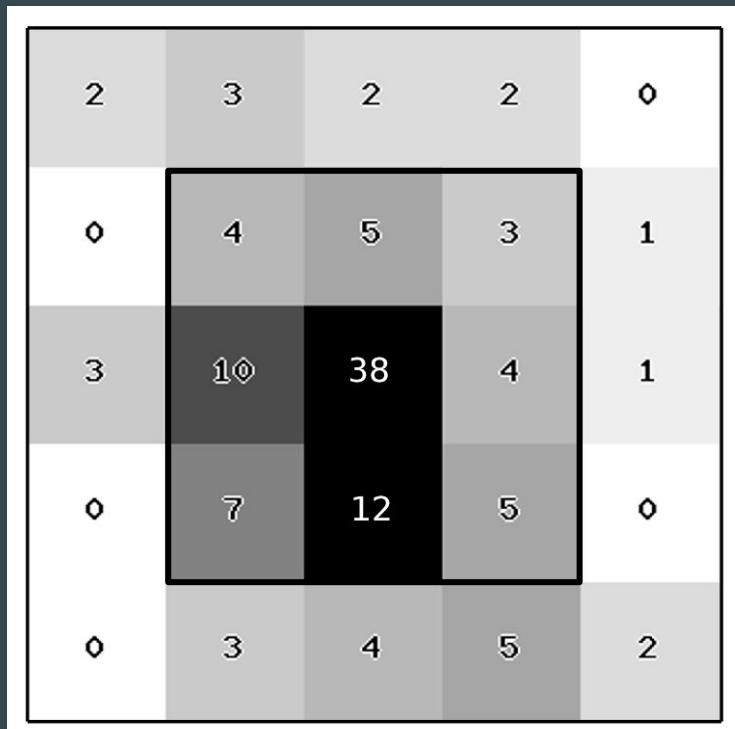
Summation integration: estimate the reflection intensity by summing the counts contributing to the reflection and subtracting the background

$$I = \text{SUM}(\text{Counts} - \text{Background})$$

Profile fitting: fit a known profile shape to the reflection to estimate the intensity

Need to estimate background under reflection peak

Background determination



Don't know background in signal region so estimate from the surrounding pixels

Background = MEAN(Background Counts)

Background = $(2+3+2+2+0+0+1+3+1+0+0+0+3+4+5+2) / 16$

Background = 2.5

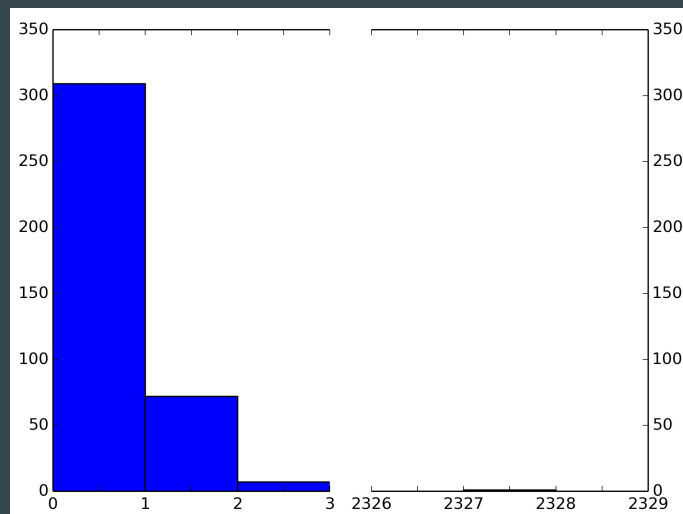
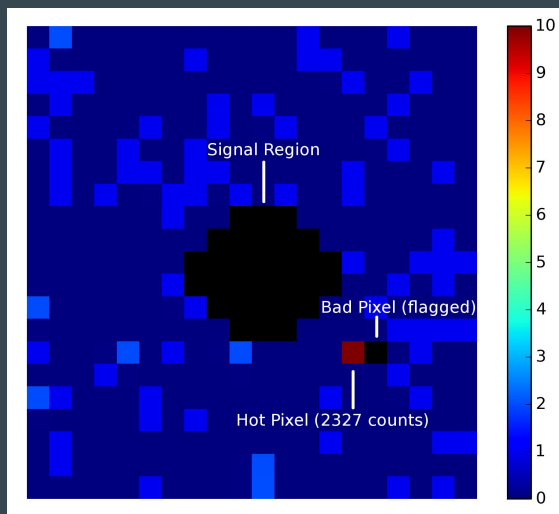
$I = \text{SUM}(\text{Counts} - \text{Background})$

$I = 4+5+3+10+38+4+7+12+5 - 9*2.5$

$I = 88 - 22.5$

$I = 65.5$

Background outlier pixels



	With Hot Pixel	Without Hot Pixel
<i>Mean</i>	6.20	0.22
<i>Variance/Mean</i>	2237.90	0.926

~1 for Poisson
distribution

Background modelling with outlier pixels

DIALS has multiple options for outlier pixel handling

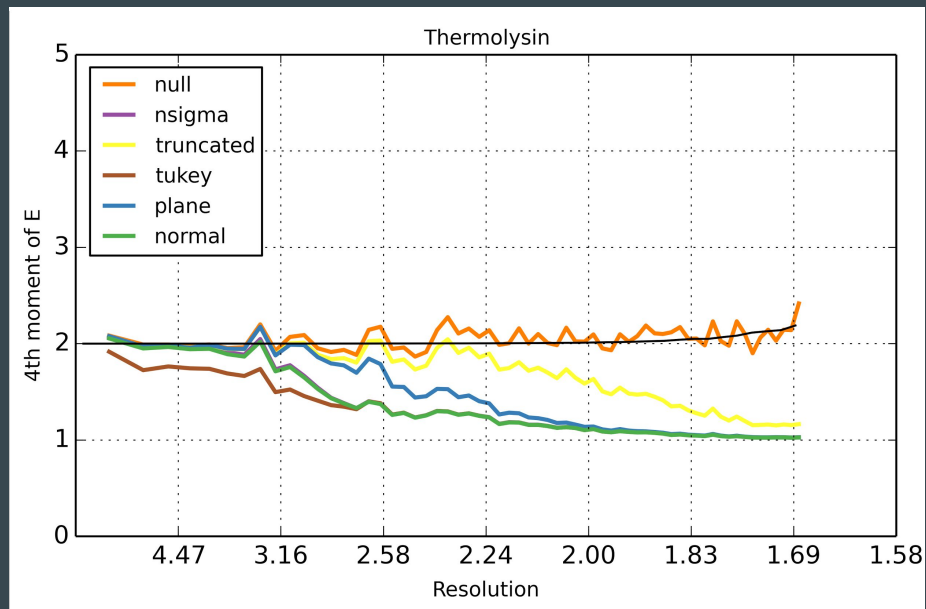
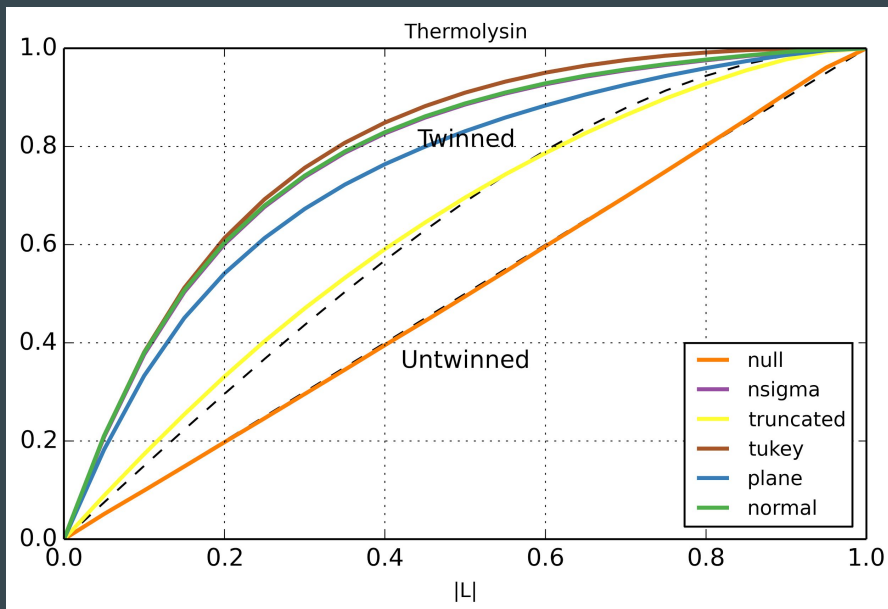
- Truncated - removed percentage of high and low valued pixels
- Normal - remove pixels above and below 3 STD around the mean
- Tukey - remove pixels based on interquartile range
- Plane - compute a plane and remove pixels based on deviation from plane (based on published mosflm algorithm)
- Normal - iteratively remove high valued pixels until they are approximately normally distributed (based on published XDS algorithm)

However, these methods assume a normal distribution and result in biases intensity estimates (particularly for low background)

Default algorithm in DIALS used a GLM algorithm

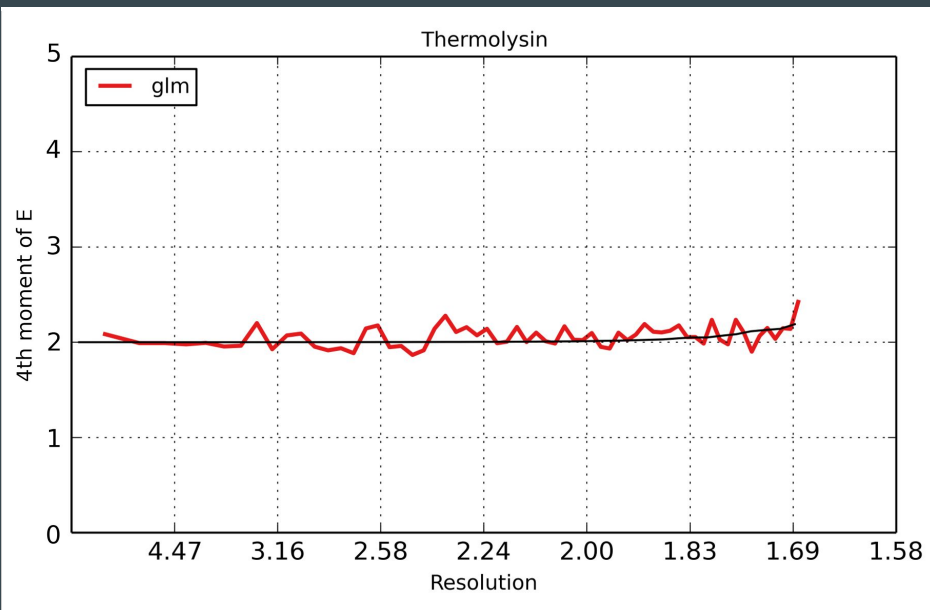
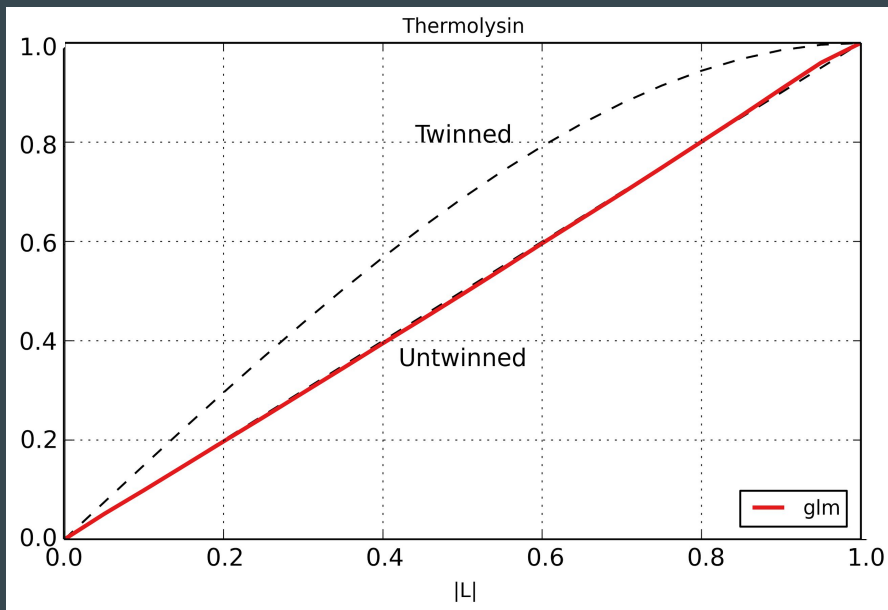
- assumes a Poisson distribution of pixel counts.
- Provides an unbiased estimate of the reflection background

Bias in background determination



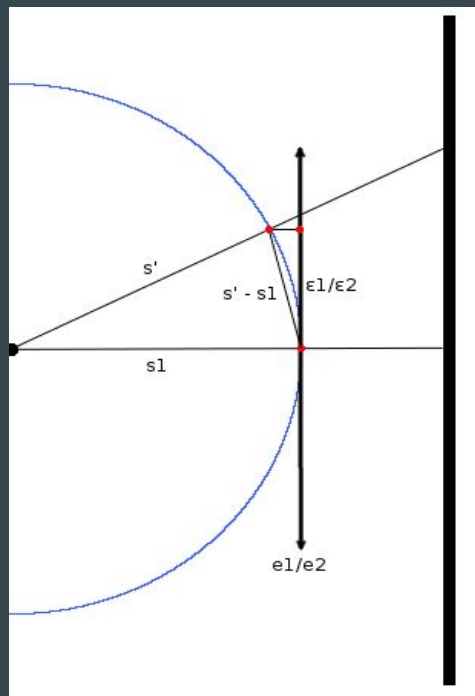
These methods all introduce bias. Background is *underestimated*. Integrated intensities are *overestimated*.

Bias in background determination

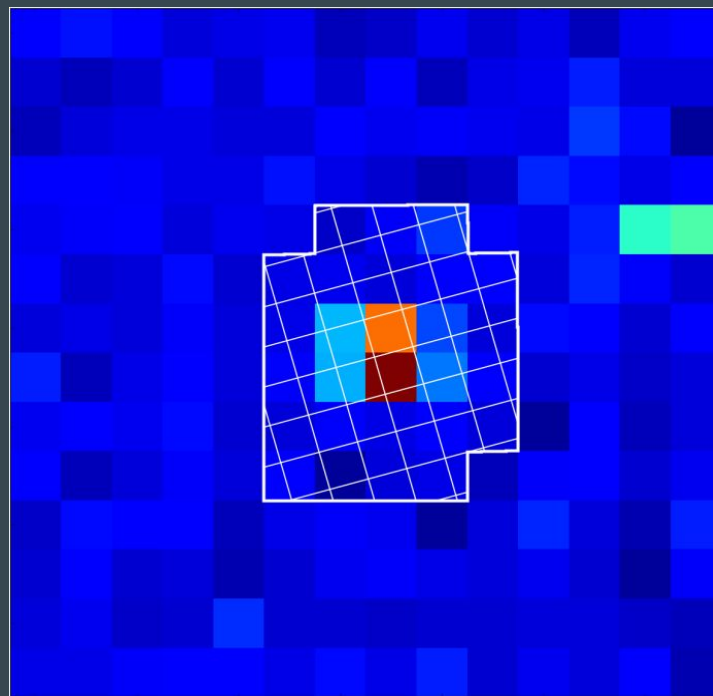


Using a Poisson GLM instead of a least-squares fit removes the bias and still allows outlier rejection

3D profile fitting pixel gridding

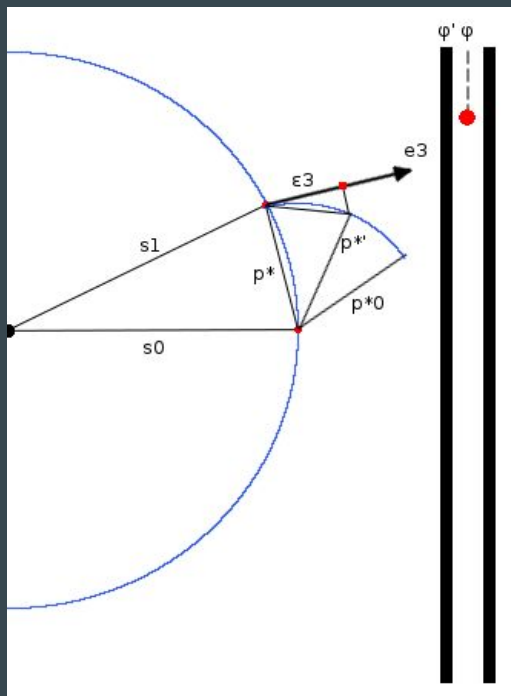


Pixels are mapped to the Ewald sphere.

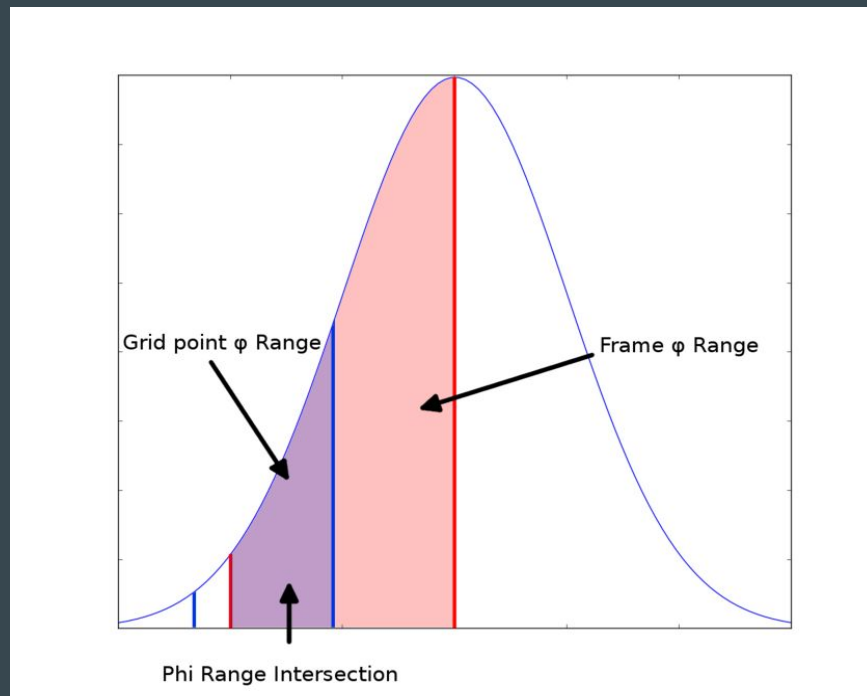


Counts are redistributed to Ewald sphere grid by computing fractional overlap of each pixel and Ewald sphere grid point

3D profile fitting phi gridding

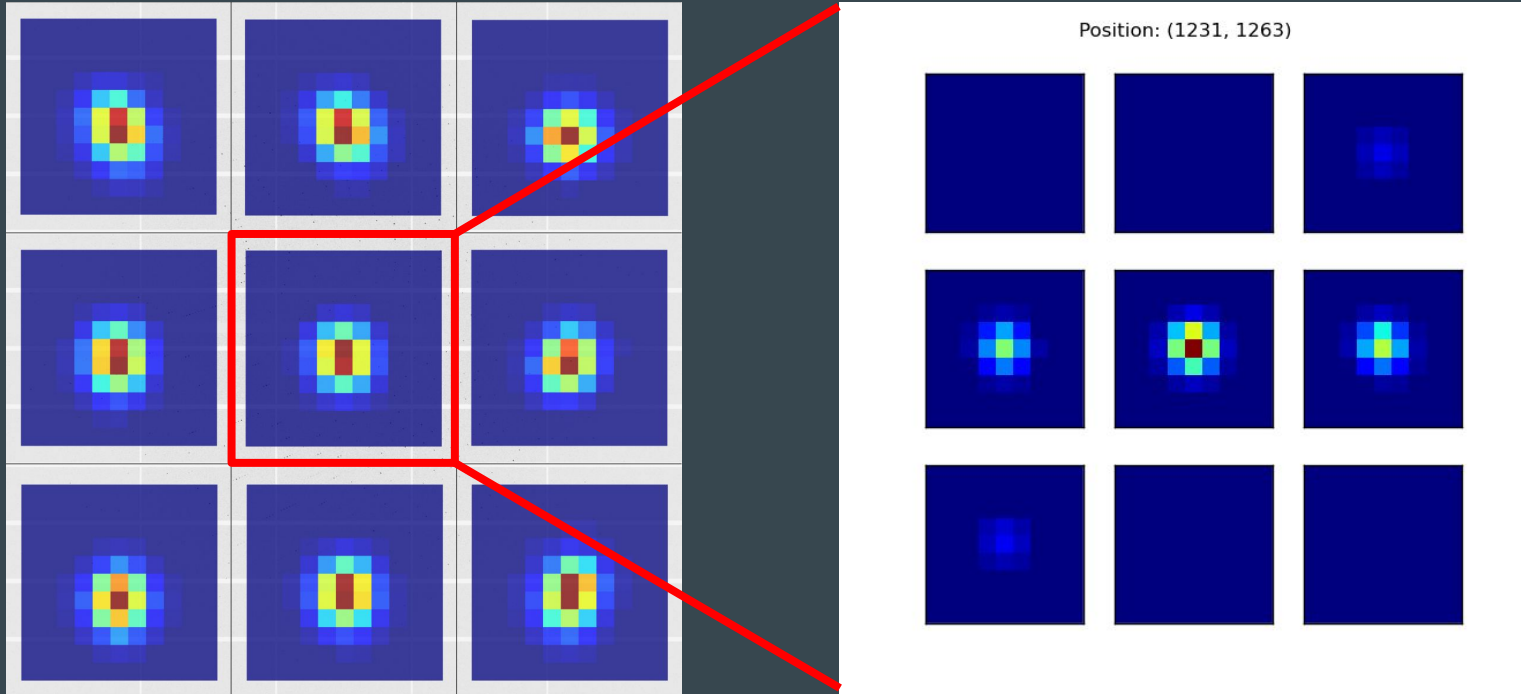


Frames are transformed to make reflection appear as if it took the shortest path through the Ewald sphere



Counts on each image are distributed by finding the angular overlap between each grid point and each image and integrating over the intersection

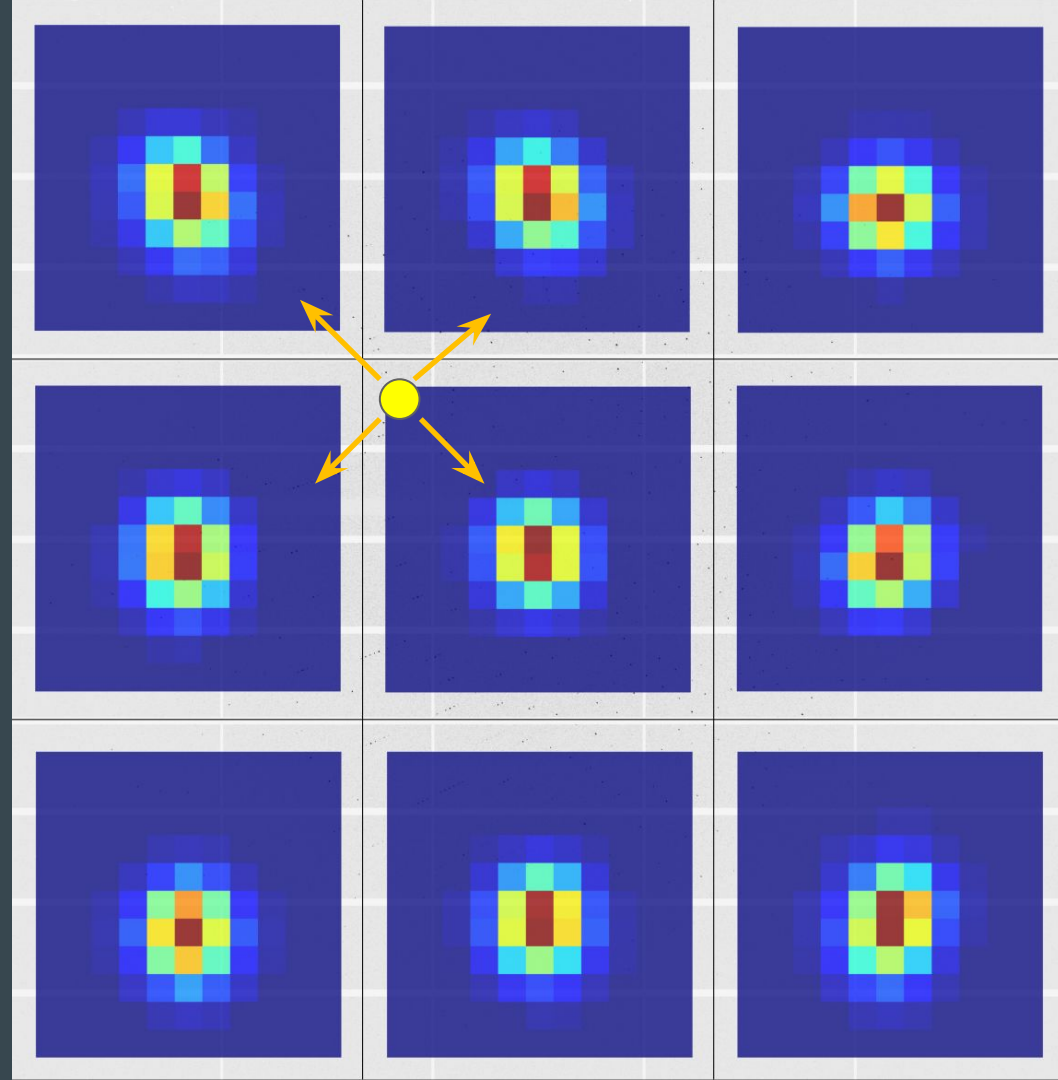
Building reference profiles



- Building reference profiles - detector space
- **DIALS** constructs a number of reference profiles using a rectangular grid on the detector

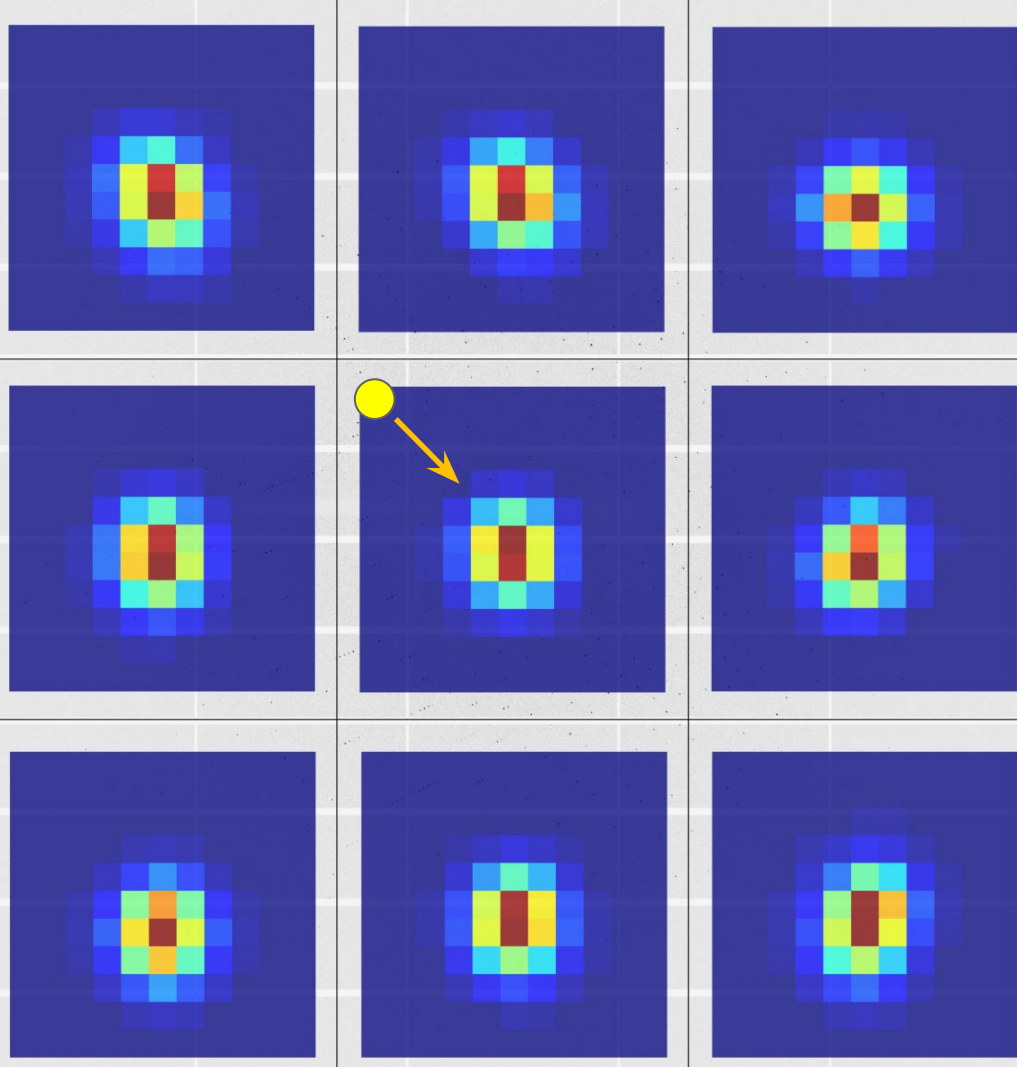
Building reference profiles

Each strong spot contributes to building the profile at adjacent grid points

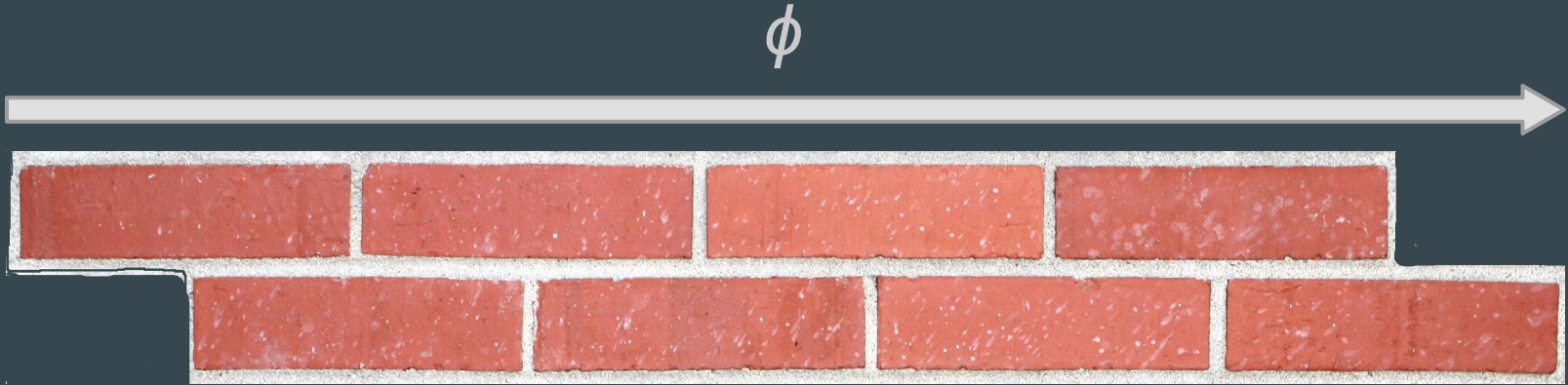


Fitting reference profiles

Each reflection is fitted against its closest reference profile



Fitting reference profiles



Profile for reflection at position x derived from average of strong reflections in block with centre nearest x

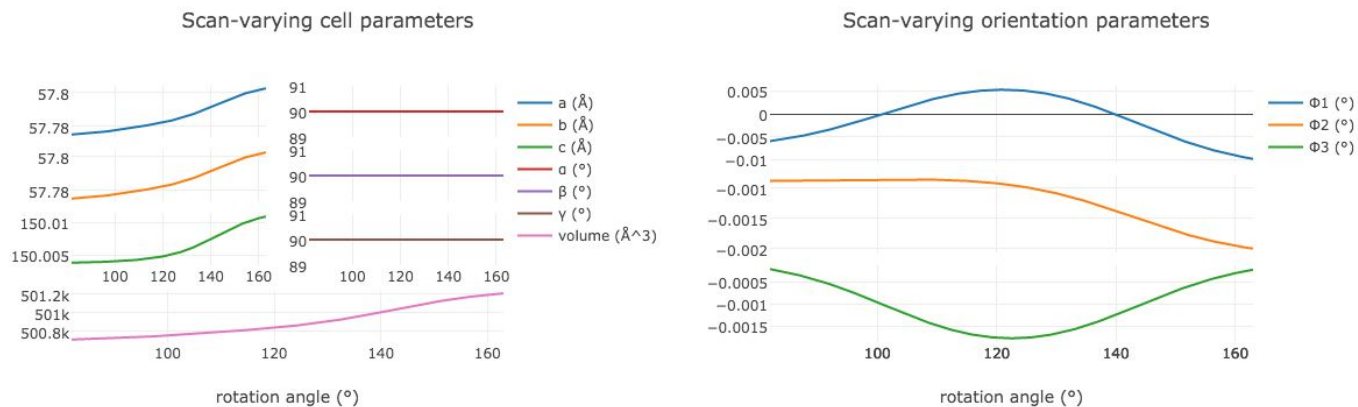
dials.report

Experiments

Crystal:	Space group:	P 4 (No. 75)	Unit cell:	(57.785 57.785 150.006 90.000 90.000 90.000)
U matrix:	$\begin{pmatrix} 0.3455 & -0.2590 & -0.9020 \\ 0.8913 & 0.3911 & 0.2292 \\ 0.2935 & -0.8831 & 0.3660 \end{pmatrix}$		B matrix:	$\begin{pmatrix} 0.0173 & 0.0000 & 0.0000 \\ -0.0000 & 0.0173 & 0.0000 \\ -0.0000 & 0.0000 & 0.0067 \end{pmatrix}$
A = UB:	$\begin{pmatrix} 0.0060 & -0.0045 & -0.0060 \\ 0.0154 & 0.0068 & 0.0015 \\ 0.0051 & -0.0153 & 0.0024 \end{pmatrix}$			
A sampled at 541 scan points			Average unit cell:	(57.786 57.786 150.006 90.000 90.000 90.000)

Experimental geometry

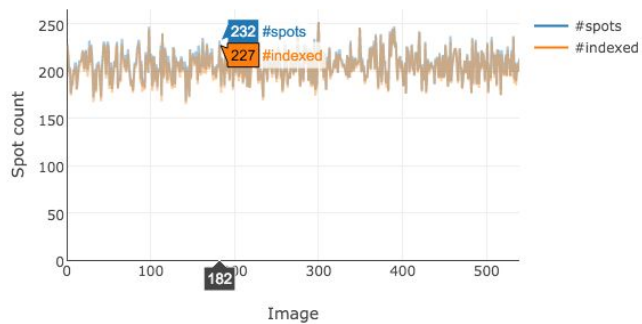
Analysis of scan-varying crystal model



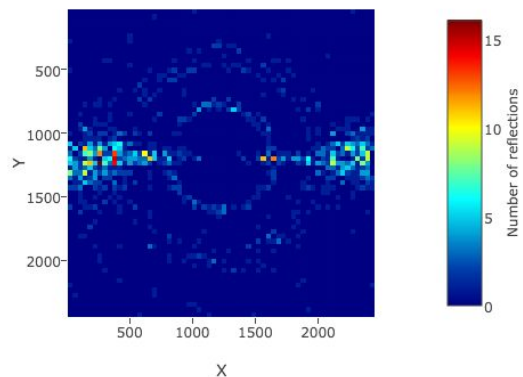
Analysis of strong reflections



Spot count per image

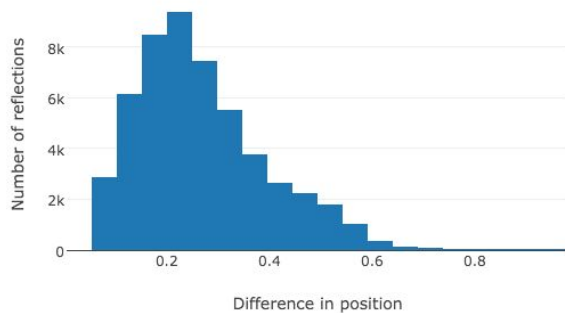


Number of unindexed reflections binned in X/Y

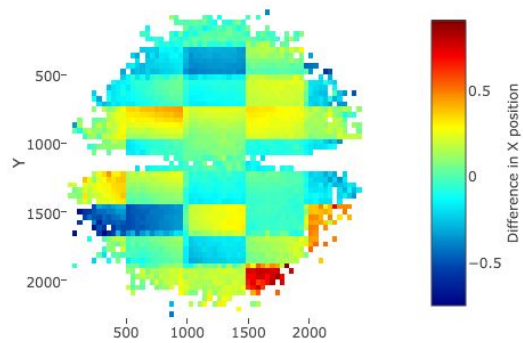


Analysis of reflection centroids

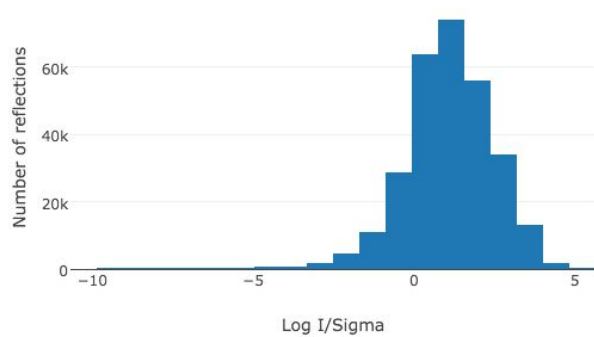
Difference between observed and calculated centroids



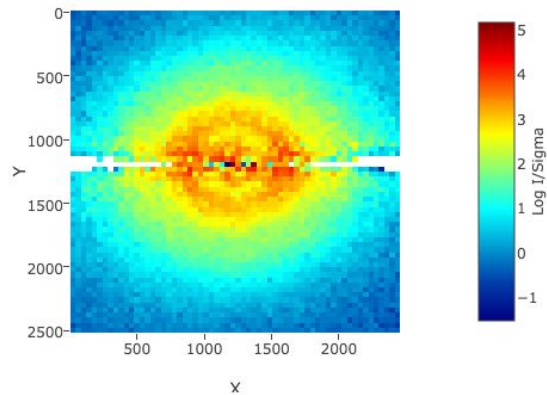
Difference between observed and calculated centroids in X



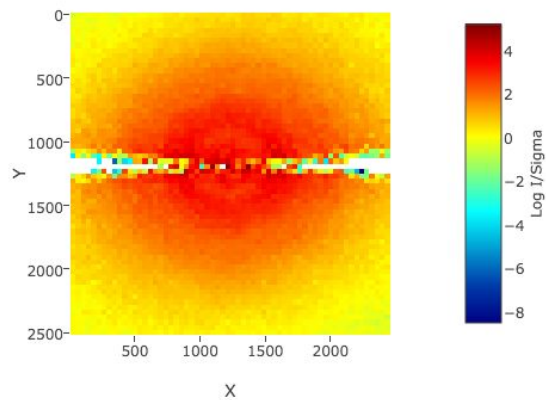
Log I/Sigma histogram



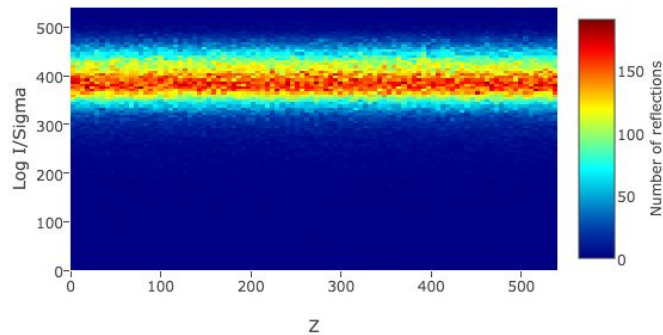
Distribution of $I(\text{sum})/\text{Sigma}$ vs X/Y



Distribution of $I(\text{prf})/\text{Sigma}$ vs X/Y



Distribution of I/Sigma vs Z



DIALS

Diffraction Integration for Advanced
Light Sources

Navigation

[About](#)

[Installation](#)

[Getting started](#)

[Documentation](#)

[Publications](#)

[Links](#)

[License](#)

Processing in Detail

Introduction

DIALS processing may be performed by either running the individual tools (spot finding, indexing, refinement, integration, exporting to MTZ) or you can run `xia2 -dials`, which makes informed choices for you at each stage. In this tutorial we will run through each of the steps in turn, checking the output as we go. We will also enforce the correct lattice symmetry.

Tutorial data

The following example uses a Thaumatin dataset collected using beamline I04 at Diamond Light Source which is available for download from [DOI 10.5281/zenodo.10271](https://doi.org/10.5281/zenodo.10271)

Import

The first stage of step-by-step DIALS processing is to import the data - all that happens here is that the image headers are read, and a file describing their contents ([datablock.json](#)) is written. It's worth noting that if this file is changed subsequent processing can use this.

```
dials.import data/th_8_2_0*cbf
```

The output just describes what the software understands of the images it was passed, in this case one sweep of data containing 540 images.

The following parameters have been modified:

```
input {  
  datablock = <image files>  
}
```

```
-----  
DataBlock 0  
  format: <class 'dxtbx.format.FormatCBFMiniPilatusDLS6MSN100.FormatCBFMiniPilatusDLS6MSN100'>  
  num images: 540  
  num sweeps: 1  
  num stills: 0  
-----
```

Writing datablocks to datablock.json

Find Spots



Quick start guide

If you don't like reading manuals and just want to get started, try:

```
xia2 -2d /here/are/my/images
```

or:

```
xia2 -3d /here/are/my/images
```

or:

```
xia2 -dials /here/are/my/images
```

(remembering of course `-atom X` if you want anomalous pairs separating in scaling.) If this appears to do something sensible then you may well be home and dry. Some critical options:

Option	Usage
<code>-atom X</code>	tell xia2 to separate anomalous pairs i.e. $I(+)$ \neq $I(-)$ in scaling
<code>-2d</code>	tell xia2 to use MOSFLM and Aimless
<code>-3d</code>	tell xia2 to use XDS and XSCALE
<code>-3dii</code>	tell xia2 to use XDS and XSCALE , indexing with peaks found from all images
<code>-dials</code>	tell xia2 to use DIALS and Aimless

If this doesn't hit the spot, you'll need to read the rest of the documentation.

Navigation

[Getting started](#)

[Using xia2](#)

[Installation](#)

[Introductory example](#)

[Insulin tutorial](#)

[Program output](#)

[Parameters](#)

[Comments](#)

[History](#)

[Acknowledgements](#)

[Release notes](#)

[License](#)

Summary

- DIALS used routinely for automated data processing via xia2
- XIA2 is the “friendly” DIALS user interface for synchrotron data, and is bundled with DIALS
- Software available from <http://dials.github.io/> under BSD license
- Binary releases available for Mac and Linux
- DIALS 1.6 is included in CCP4 7.0 (including Windows)
- GUI is currently in development

Acknowledgements

DIALS East

Gwyndaf Evans, Graeme Winter, David Waterman, James Parkhurst, Richard Gildea, Luis Fuentes-Montero, Markus Gerstel, Melanie Vollmar

DIALS West

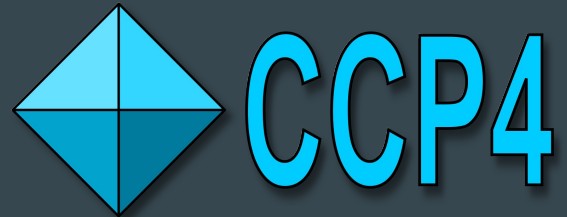
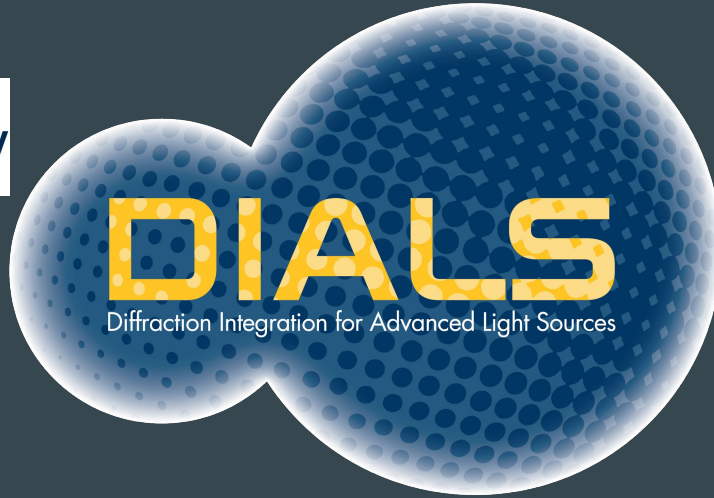
Nick Sauter, Aaron Brewster, Tara Michels-Clark, Iris Young

Lots of other people

Garib Murshudov, Andrew Leslie, Phil Evans, Harry Powell, Takanori Nakane

DIALS East – Diamond / CCP4





Thanks for listening!



<https://dials.diamond.ac.uk>

