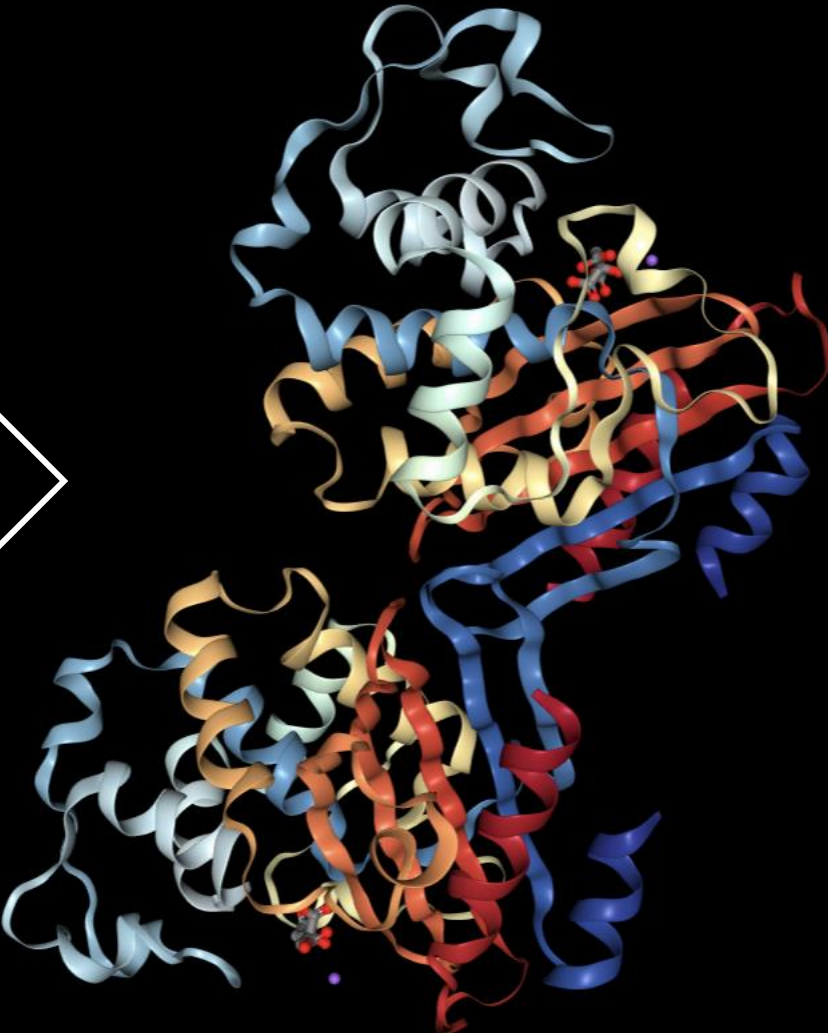
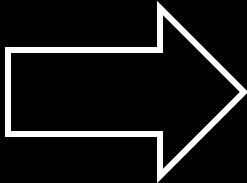
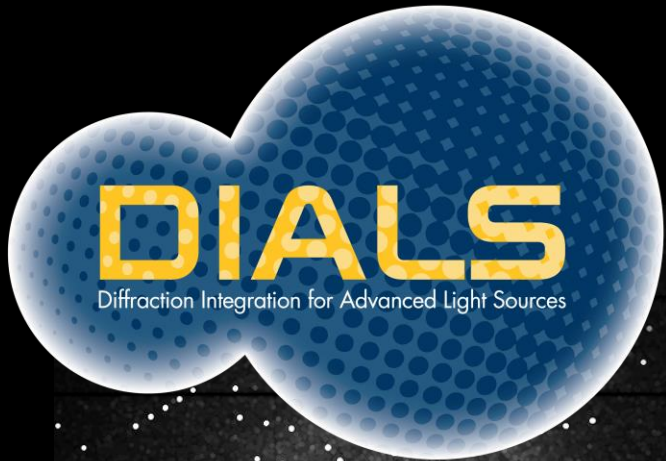


# DIALS for Neutron and Laue Diffraction

Early Science on the NMX Macromolecular Diffractometer, 26 August 2024

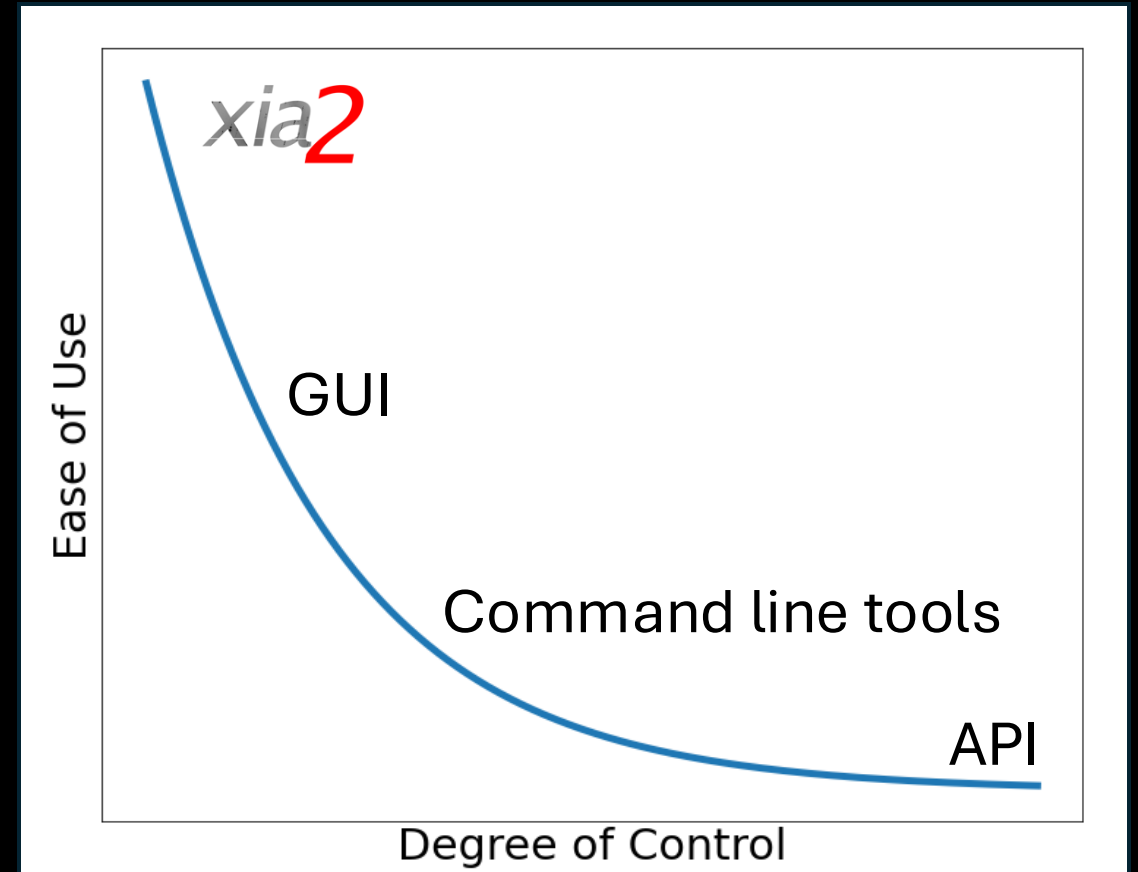
David McDonagh





# Philosophy

- Designed to be modular and extensible
- Focus on code sustainability





# History

## Funding



2011

2024



## Developers

# Developers

- Over 50 contributors worldwide



# DIALS Today

- Supports (almost) all X-ray instruments worldwide
- Multiple workshops given internationally per year
- Embedded in multiple synchrotrons
- Deployed as part of the CCP4 suite

Journal of  
Applied  
Crystallography

ISSN 1600-5767



STRUCTURAL  
BIOLOGY



STRUCTURAL  
BIOLOGY



STRUCTURAL  
BIOLOGY

ISSN 2059-7983



STRUCTURAL  
BIOLOGY

## *dxtbx*: the diffraction experiment toolbox

James M. Parkhurst,<sup>a</sup> Aaron S. Brewster,<sup>b</sup> Luis Fuentes-Montero,<sup>a</sup> David G.  
***DIALS*: implementation and evaluation of a new  
integration package**

## Electron diffraction data processing with *DIALS*

Max T. B. Clabbers,<sup>a</sup> Tim Gruene,<sup>b</sup> James M. Parkhurst,<sup>c</sup> Jan Pieter Abrahams<sup>a,b</sup> and

***xia2.multiplex*: a multi-crystal data-analysis  
pipeline**

Diffraction-geometry refinement in the *DIALS*  
framework

## Laue-DIALS: open-source software for polychromatic X-ray diffraction data

Rick A. Hewitt\*<sup>1,(a)</sup> Kevin M. Dalton\*<sup>2,3,1,(b)</sup> Derek Mendez<sup>4</sup> Harrison K. Wang<sup>1,5</sup>

PROTEIN|SCIENCE

Tools for Protein Science | Open Access |

## DIALS as a toolkit

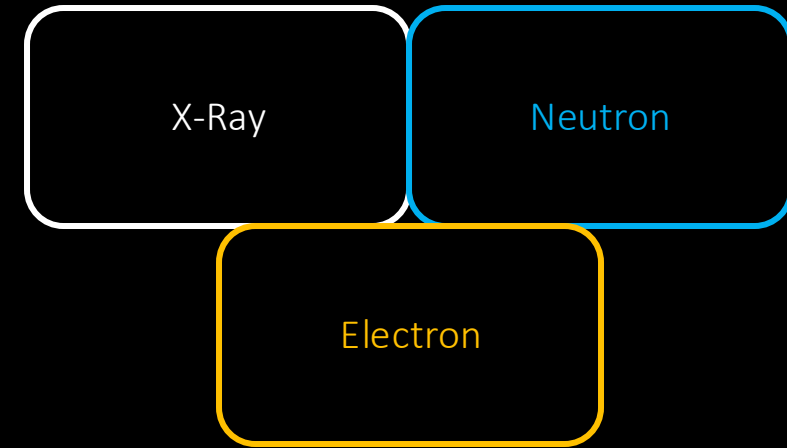
Graeme Winter , James Beilsten-Edmands, Nicholas Devenish, Markus Gerstel, Richard J. Gildea,  
David McDonagh, Elena Pascal, David G. Waterman, Benjamin H. Williams, Gwyndaf Evans

First published: 08 November 2021 | <https://doi.org/10.1002/pro.4224> | Citations: 21

**Funding information:** FP7 Research Infrastructures, Grant/Award Number: 283570; National Institute of  
General Medical Sciences, Grant/Award Numbers: GM095887, GM117126; Wellcome Trust, Grant/Award  
Numbers: 202933/Z/16/Z, 218270/Z/19/Z

# Beyond X-rays

- Diffraction patterns can be obtained from multiple sources
- These all reveal complimentary information
- Different sources have resulted in different developer communities
- These boundaries create friction for users



# Beyond X-rays

2011



2024

X-ray Rotational  
Experiments

Serial  
Crystallography

Electron  
Diffraction

Neutron  
Diffraction

Laue Diffraction

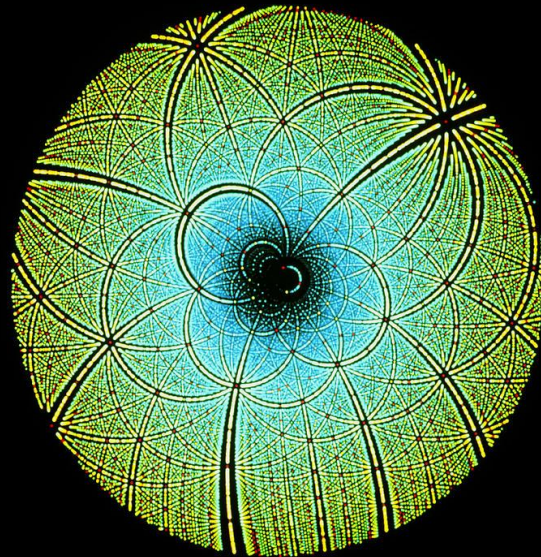
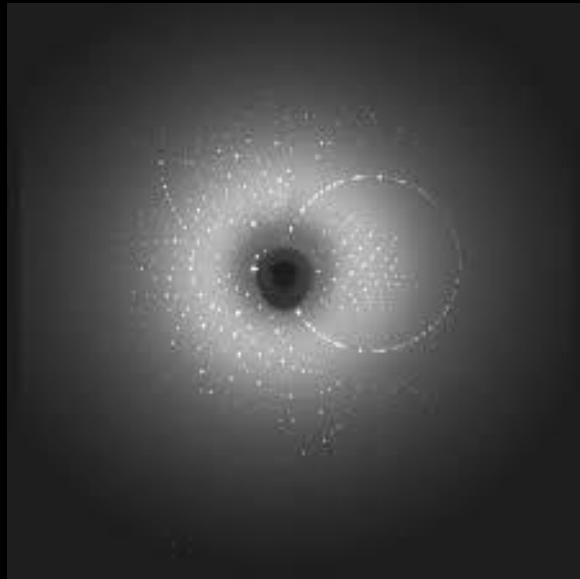


# Motivation

- Increasing demand for neutron macromolecular crystallography data



- Typical for users to also have X-ray data
- Demand for other polychromatic sources in the wider community



# The Work

- Adapt DIALS for polychromatic sources
- Laue prediction / refinement
- New integration algorithms
- Custom scaling pipeline
- Modern interface tailored to neutrons

# The Work

- Adapt DIALS for polychromatic sources
- Laue prediction / refinement
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Neutron time-of-flight  
Laue

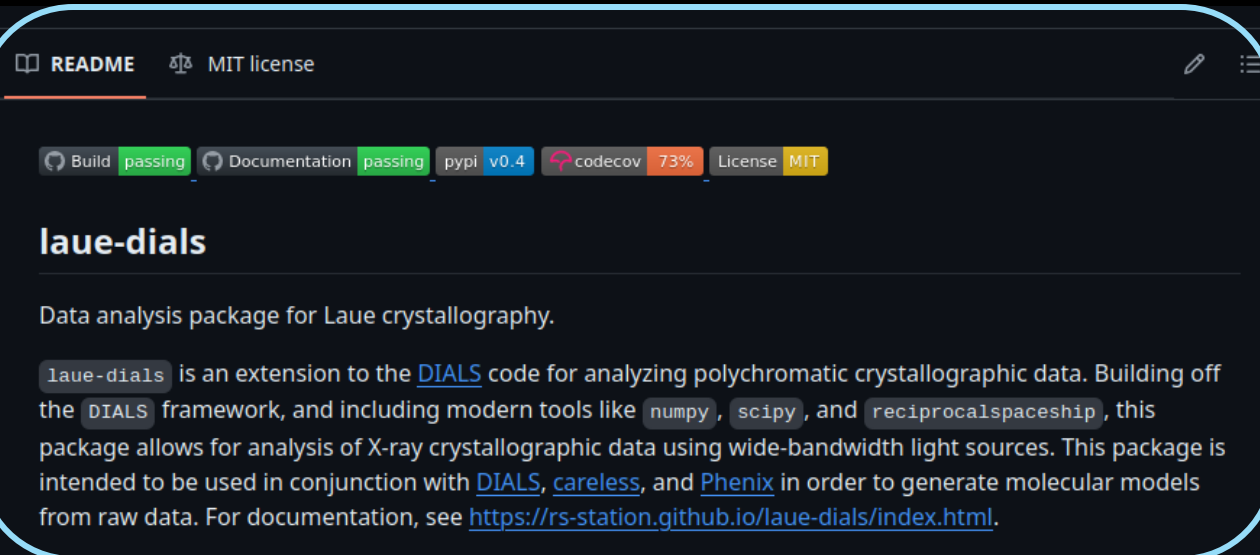
X-ray Laue

# The Work

- Adapt DIALS for polychromatic sources
- Laue prediction / refinement
- New integration algorithms
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- Modern interface tailored to neutrons

Neutron time-of-flight  
Laue

X-ray Laue



The screenshot shows the GitHub repository page for 'laue-dials'. At the top, there are links for 'README' and 'MIT license'. Below that, there are several status badges: 'Build passing', 'Documentation passing', 'pypi v0.4', 'codecov 73%', and 'License MIT'. The main heading is 'laue-dials' followed by the description 'Data analysis package for Laue crystallography.' The text below explains that 'laue-dials' is an extension to the 'DIALS' code for analyzing polychromatic crystallographic data, building on the 'DIALS' framework and including modern tools like 'numpy', 'scipy', and 'reciprocalspaceship'. It states that the package allows for analysis of X-ray crystallographic data using wide-bandwidth light sources and is intended to be used in conjunction with 'DIALS', 'careless', and 'Phenix' to generate molecular models from raw data. A link to the documentation is provided: <https://rs-station.github.io/laue-dials/index.html>.

## Laue-DIALS: open-source software for polychromatic X-ray diffraction data

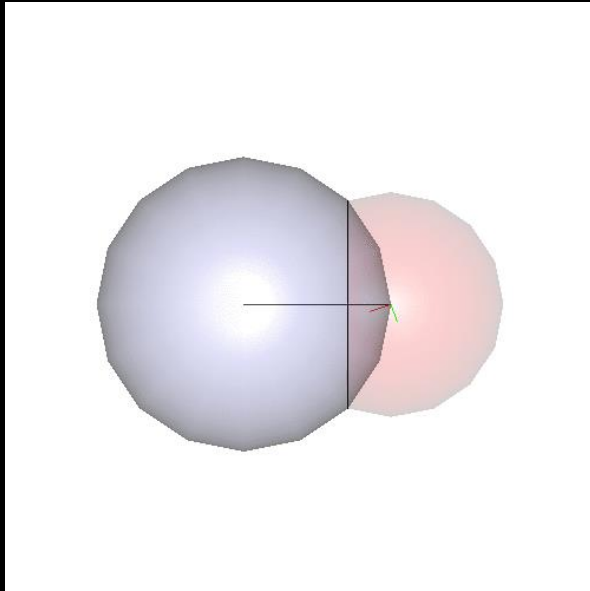
Rick A. Hewitt<sup>\*,1,a)</sup> Kevin M. Dalton<sup>\*,2,3,1,b)</sup> Derek Mendez,<sup>4</sup> Harrison K. Wang,<sup>1,5</sup>  
Margaret A. Klureza,<sup>6</sup> Dennis E. Brookner,<sup>1</sup> Jack B. Greisman,<sup>1</sup> David McDonagh,<sup>7</sup>  
Vukica Šrajer,<sup>8</sup> Nicholas K. Sauter,<sup>9</sup> Aaron S. Brewster,<sup>9,c)</sup> and Doeke R. Hekstra<sup>1,10,d)</sup>

<sup>1)</sup>*Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA 02138*

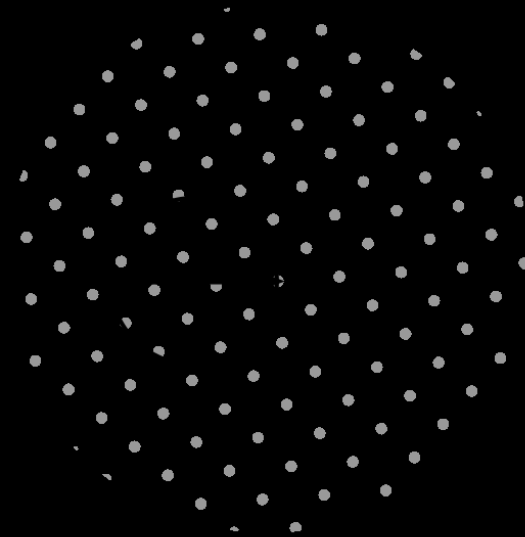
<sup>2)</sup>*Linac Coherent Light Source, SLAC National Accelerator Laboratory, Menlo Park, 94025, CA, USA*

# The Work

- Adapt DIALS for polychromatic sources
- Laue prediction / refinement
- New integration algorithms
- Custom scaling pipeline
- Modern interface tailored to neutrons



• Rotation scan



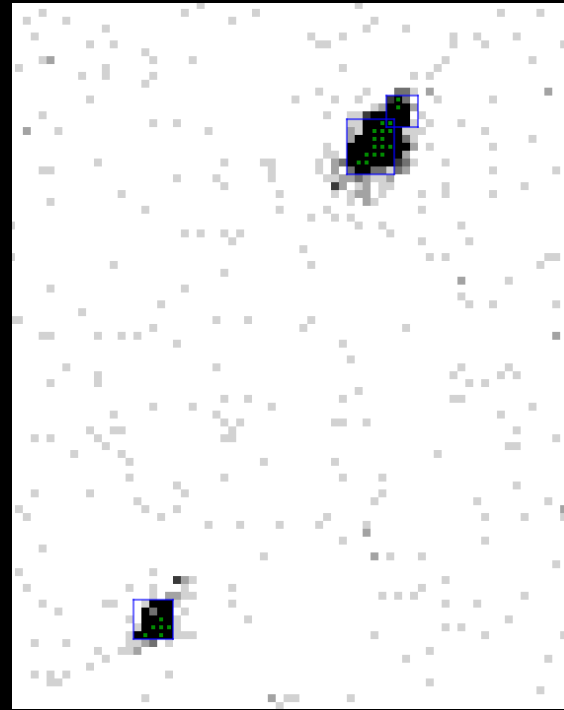
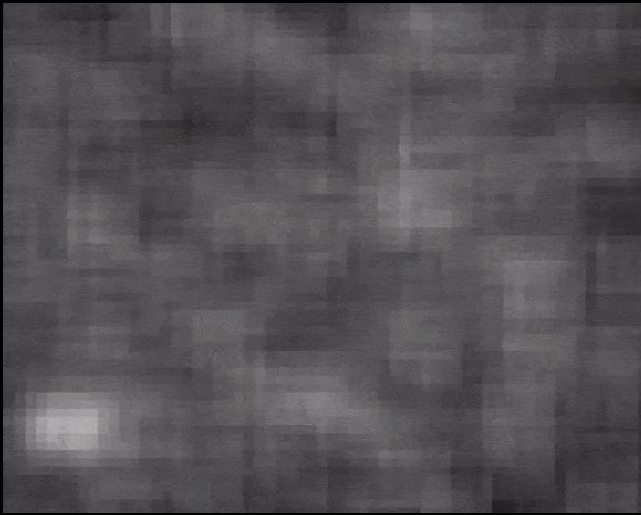
• Wavelength scan



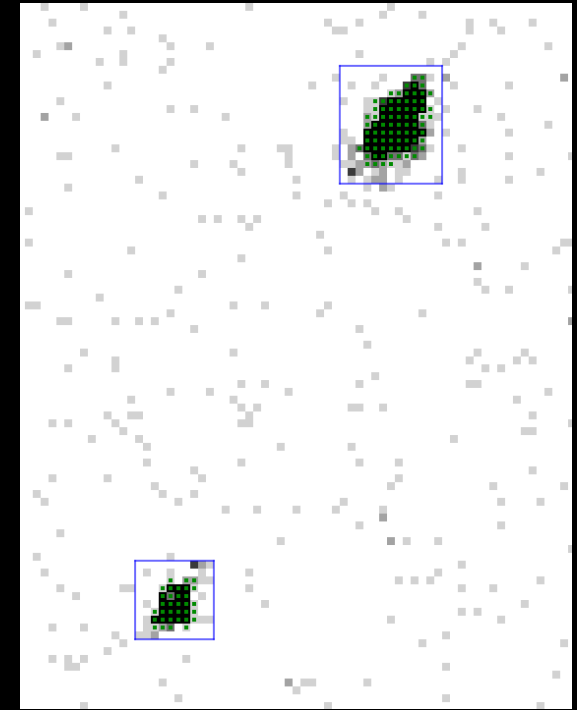
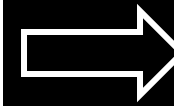
# Spot Finding



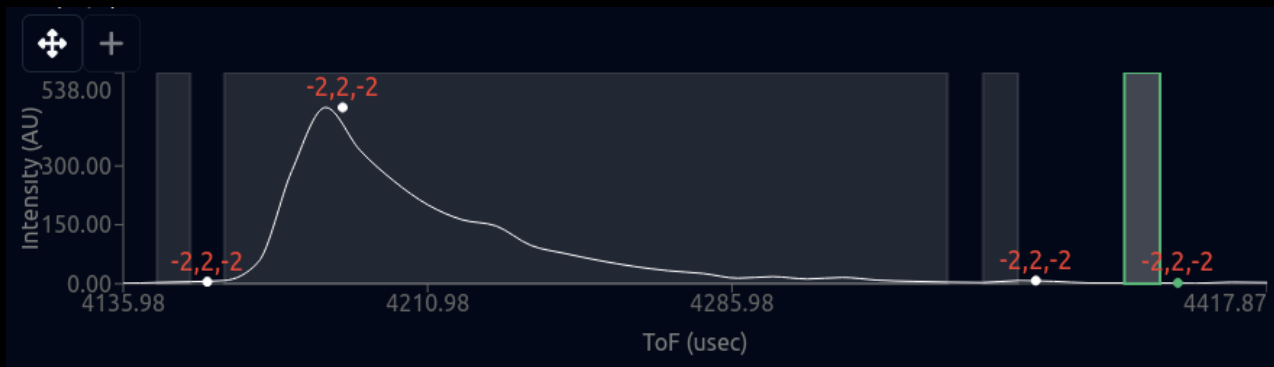
- Multiple algorithms: dispersion, dispersion-extended, radial profile
- Work well for ToF data but weak data requires tinkering



dispersion



dispersion-extended



- ToF profiles require specific post processing

# Indexing



- For neutron time-of-flight Laue data, wavelengths are known
- For X-ray Laue data these must be estimated
- Algorithms: 3D FFT, 1D FFT, real space grid search, pink indexer

 **FOUNDATIONS ADVANCES**  
ISSN 2053-2733

**research papers**

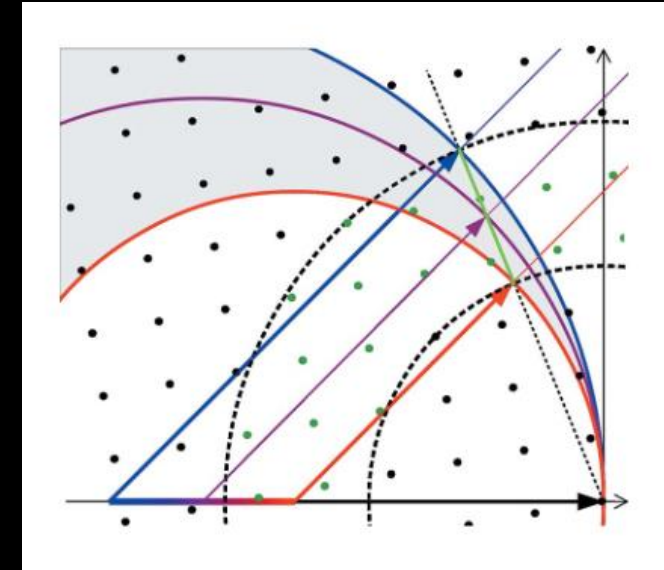
## *pinkIndexer* – a universal indexer for pink-beam X-ray and electron diffraction snapshots

Yaroslav Gevorkov,<sup>a,b,\*</sup> Anton Barty,<sup>a</sup> Wolfgang Brehm,<sup>a</sup> Thomas A. White,<sup>a</sup> Aleksandra Tolstikova,<sup>a,c</sup> Max O. Wiedorn,<sup>a,c,d</sup> Alke Meents,<sup>a</sup> Rolf-Rainer Grigat,<sup>b</sup> Henry N. Chapman<sup>a,c,d</sup> and Oleksandr Yefanov<sup>a</sup>

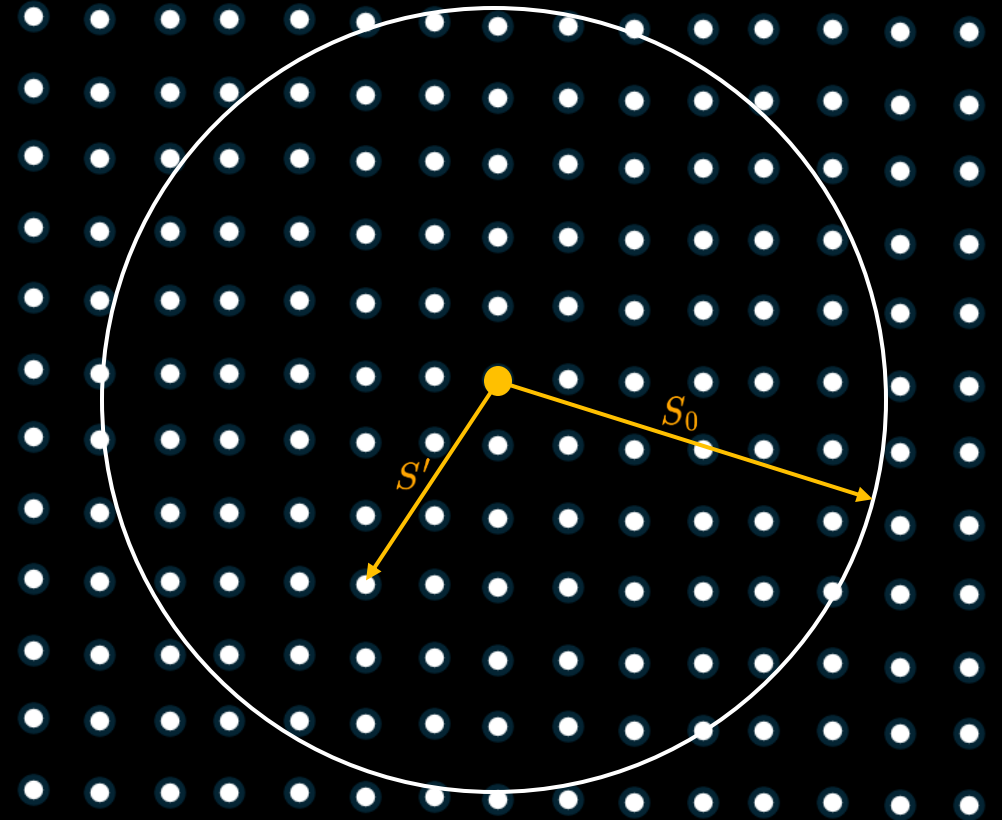
<sup>a</sup>Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron DESY, Notkestraße 85, 22607 Hamburg, Germany, <sup>b</sup>Vision Systems, Hamburg University of Technology, 21071 Hamburg, Germany, <sup>c</sup>Department of Physics, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany, and <sup>d</sup>The Hamburg Center for Ultrafast Imaging, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany. \*Correspondence e-mail: yaroslav.gevorkov@desy.de

Received 2 September 2019  
Accepted 18 November 2019

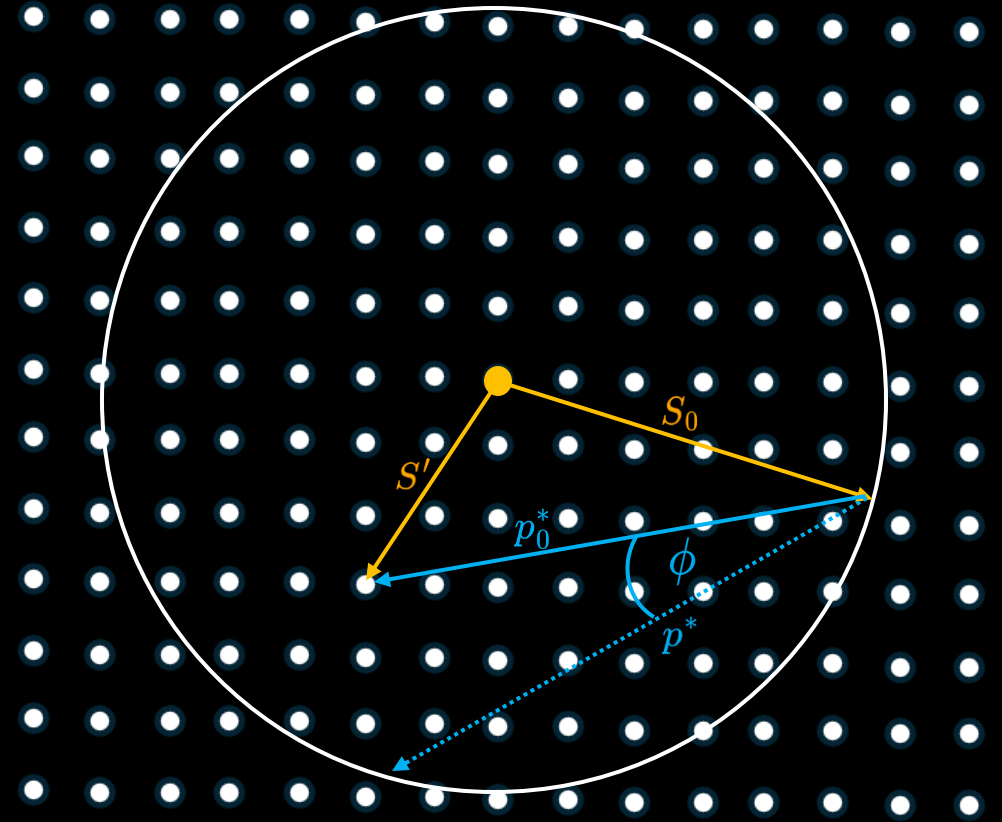
Edited by A. Altomare, Institute of Crystallography - CNR, Bari, Italy



# Laue Refinement



# Laue Refinement

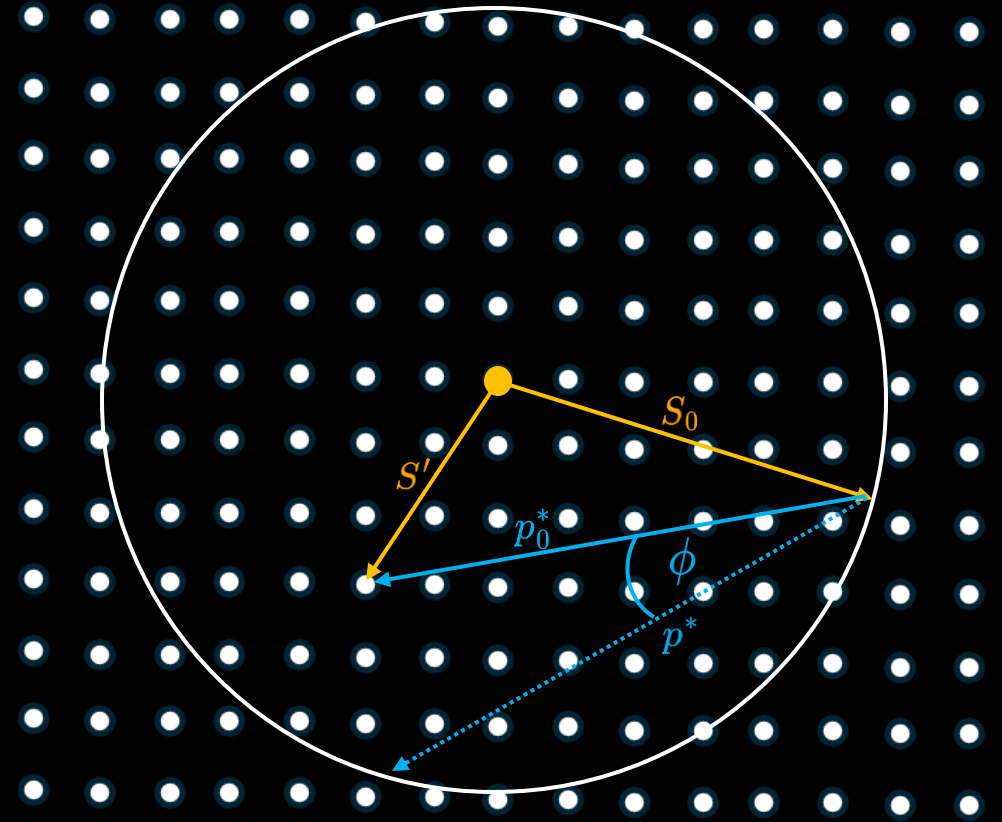


# Laue Refinement



- Diffraction condition

$$p^* \cdot p^* + p^* \cdot 2S_0 = 0$$





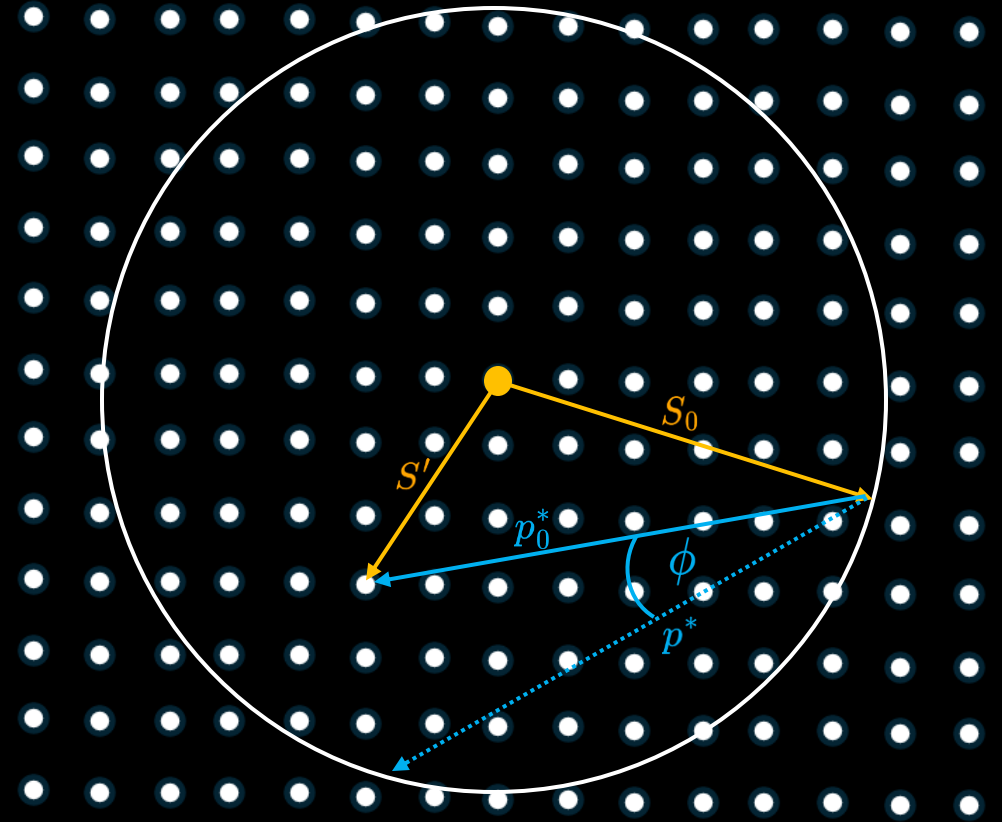
# Laue Refinement



- Diffraction condition

$$p^* \cdot p^* + p^* \cdot 2S_0 = 0$$

$$\lambda = -2 \frac{\hat{S}_0 \cdot p_0^*}{p_0^* \cdot p_0^*}$$



# Laue Refinement



- Diffraction condition

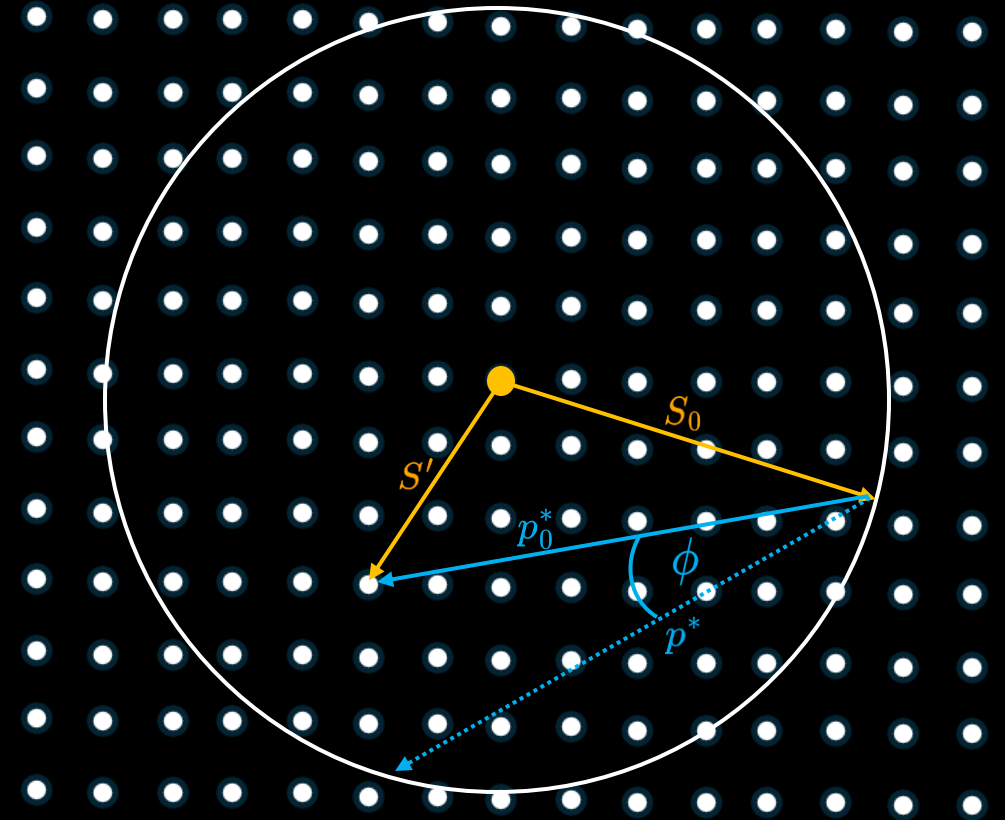
$$p^* \cdot p^* + p^* \cdot 2S_0 = 0$$

$$\lambda = -2 \frac{\hat{S}_0 \cdot p_0^*}{p_0^* \cdot p_0^*}$$

- Cost function

$$L = \frac{1}{2} \sum_{i=1}^n w_{i,X} (X - X_{obs})^2 + w_{i,Y} (Y - Y_{obs})^2 + w_{i,\lambda} (\lambda - \lambda_{obs})^2$$

$$\frac{\partial L}{\partial p} = \frac{1}{2} \sum_{i=1}^n w_{i,X} \frac{\partial X}{\partial p} (X - X_{obs})^2 + w_{i,Y} \frac{\partial Y}{\partial p} (Y - Y_{obs})^2 + w_{i,\lambda} \frac{\partial \lambda}{\partial p} (\lambda - \lambda_{obs})^2$$



# Laue Refinement



- Diffraction condition

$$\mathbf{p}^* \cdot \mathbf{p}^* + \mathbf{p}^* \cdot 2\mathbf{S}_0 = 0$$

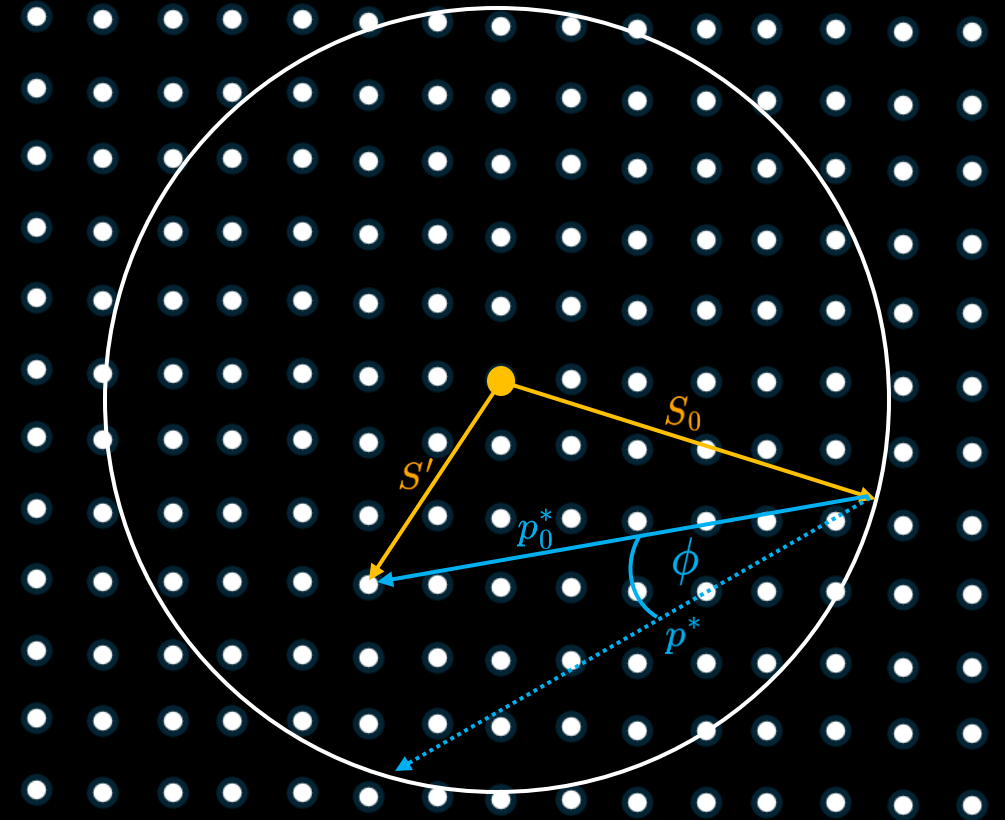
$$\lambda = -2 \frac{\hat{\mathbf{S}}_0 \cdot \mathbf{p}_0^*}{\mathbf{p}_0^* \cdot \mathbf{p}_0^*}$$

- Cost function

$$L = \frac{1}{2} \sum_{i=1}^n w_{i,X} (X - X_{obs})^2 + w_{i,Y} (Y - Y_{obs})^2 + w_{i,\lambda} (\lambda - \lambda_{obs})^2$$

$$\frac{\partial L}{\partial p} = \frac{1}{2} \sum_{i=1}^n w_{i,X} \frac{\partial X}{\partial p} (X - X_{obs})^2 + w_{i,Y} \frac{\partial Y}{\partial p} (Y - Y_{obs})^2 + w_{i,\lambda} \frac{\partial \lambda}{\partial p} (\lambda - \lambda_{obs})^2$$

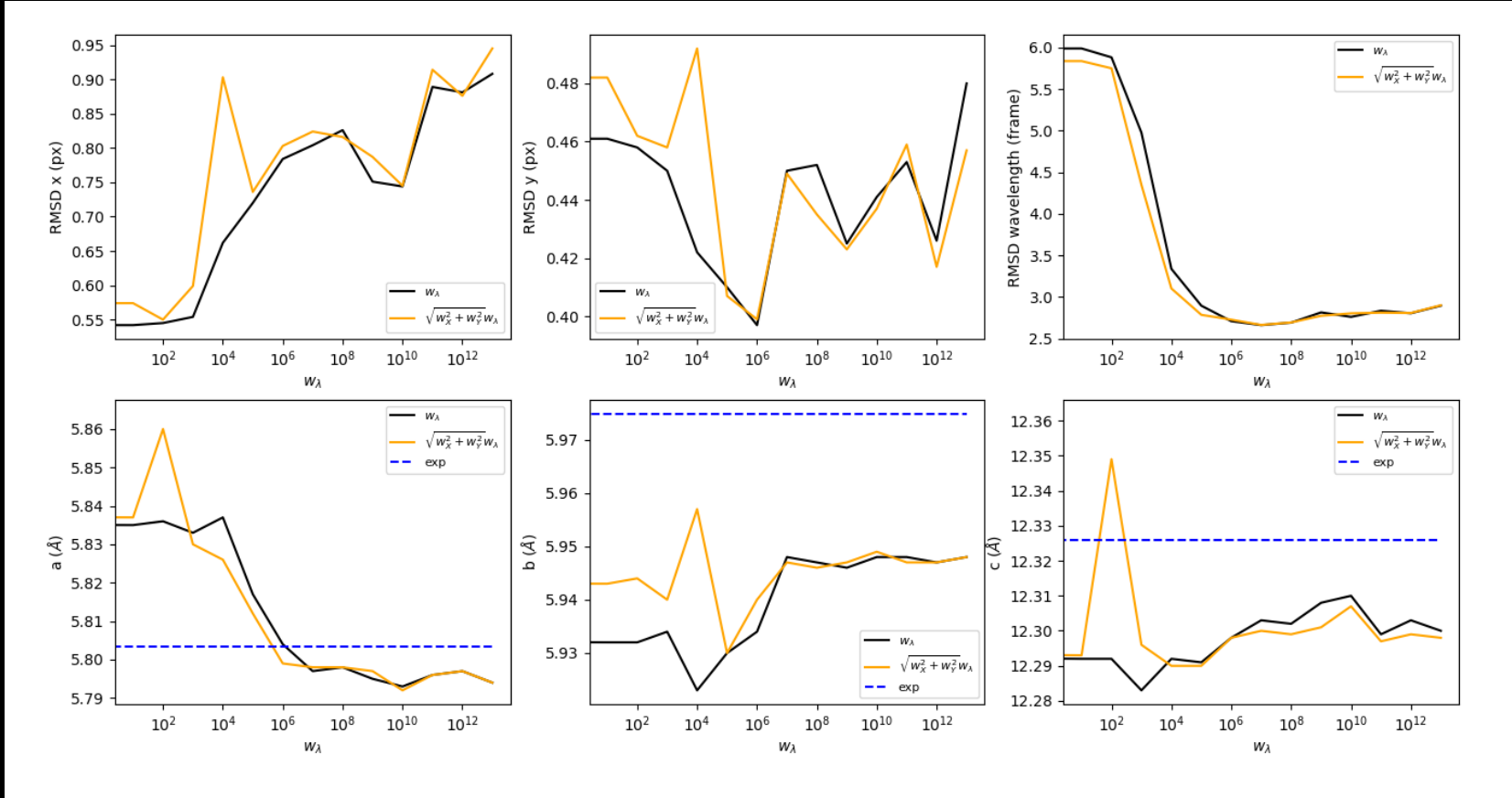
$$\frac{\partial \lambda}{\partial p} = -2\hat{\mathbf{S}}_0 \left( \frac{\frac{\partial \mathbf{p}_0^*}{\partial p} |\mathbf{p}_0^*|^2 - 2\mathbf{p}_0^* \frac{\partial \mathbf{p}_0^*}{\partial p} \cdot \mathbf{p}_0^*}{|\mathbf{p}_0^*|^4} \right)$$



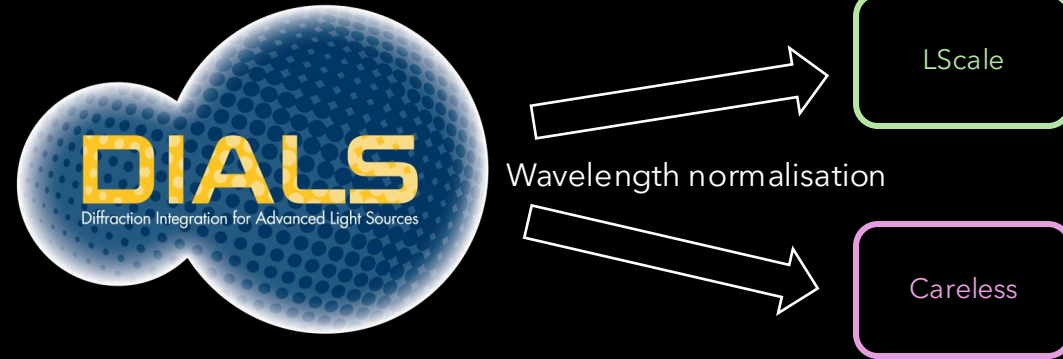
# Laue Refinement



$$L = \frac{1}{2} \sum_{i=1}^n w_{i,X}(X - X_{obs})^2 + w_{i,Y}(Y - Y_{obs})^2 + w_{i,\lambda}(\lambda - \lambda_{obs})^2$$



# Scaling Pipeline



K.M Dalton, J. B. Freisman, D. R. Hekstra, A unifying Bayesian framework for merging X-ray diffraction data. Nature Comms., 13, 2022.

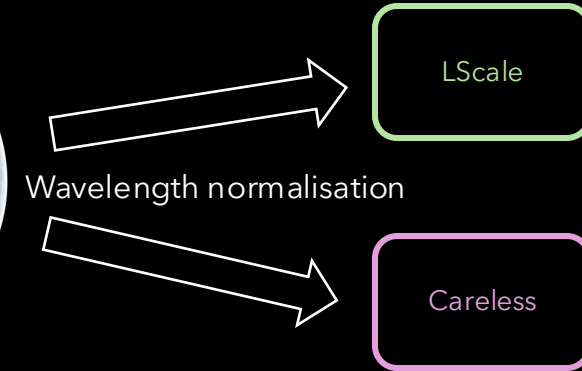
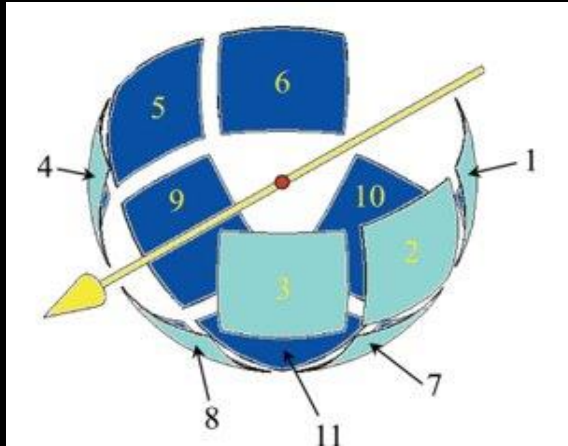
S. Artz, J.W. Campbell, M. M. Harding, Q. Hao, J. R. Helliwell, LSCALE – the new normalization, scaling and absorption correction program in the Daresbury Laue software suite. J. Appl. Cryst., 32:554-562, 1999.



# Scaling Pipeline



SXD



- Wavelength range: 0.2 - 10 Angstroms

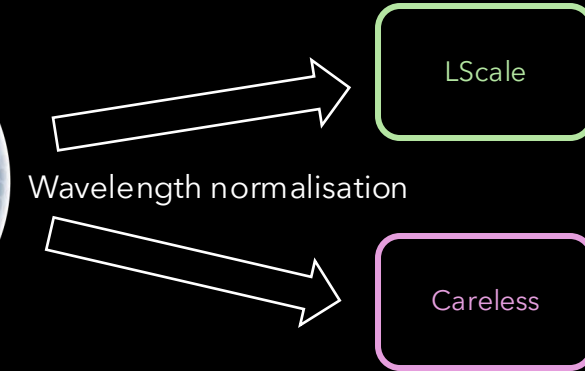
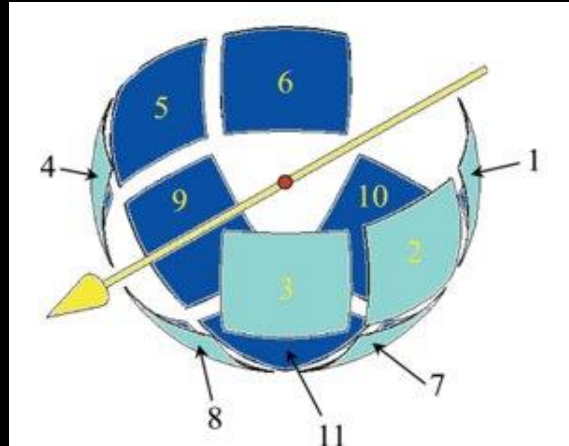
K.M Dalton, J. B. Freisman, D. R. Hekstra, A unifying Bayesian framework for merging X-ray diffraction data. Nature Comms., 13, 2022.

S. Artz, J.W. Campbell, M. M. Harding, Q. Hao, J. R. Helliwell, LSCALE – the new normalization, scaling and absorption correction program in the Daresbury Laue software suite. J. Appl. Cryst., 32:554-562, 1999.

# Scaling Pipeline



SXD



- Wavelength range: 0.2 - 10 Angstroms
- Vanadium run to correct for the incident spectrum
- Empty run to correct for the Vanadium background
- Spherical absorption correction for every shoebox pixel

K.M Dalton, J. B. Freis man, D. R. Hekstra, A unifying Bayesian framework for merging X-ray diffraction data. Nature Comms., 13, 2022.

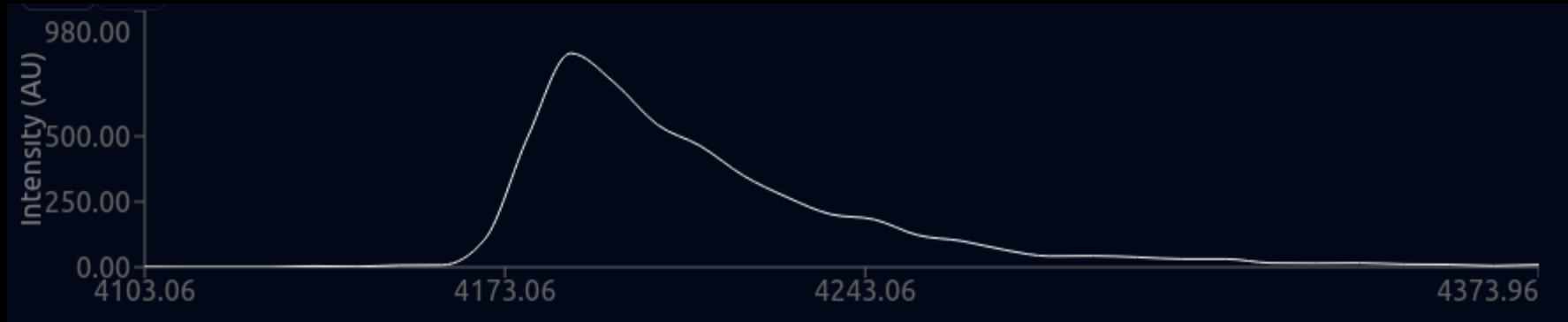
S. Artz, J.W. Campbell, M. M. Harding, Q. Hao, J. R. Helliwell, LSCALE – the new normalization, scaling and absorption correction program in the Daresbury Laue software suite. J. Appl. Cryst., 32:554-562, 1999.

C.W Dwiggs Jnr, Rapid Calculation of X-ray absorption correction factors for spheres to an accuracy of 0.05%. Acta. Cryst. A., A31: 395-396, 1975.

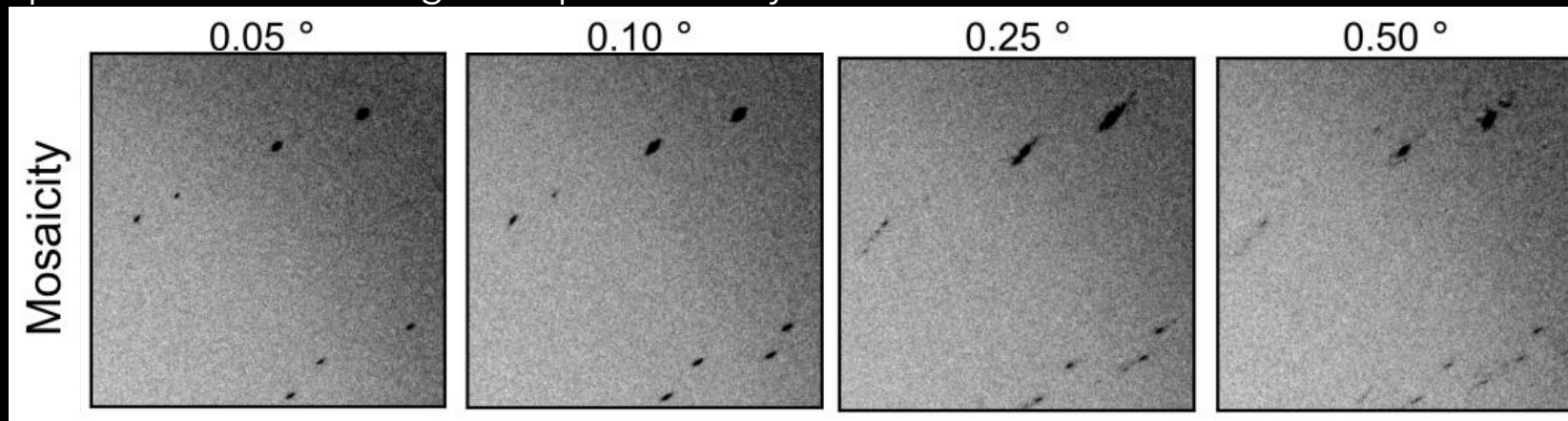
# Laue Integration



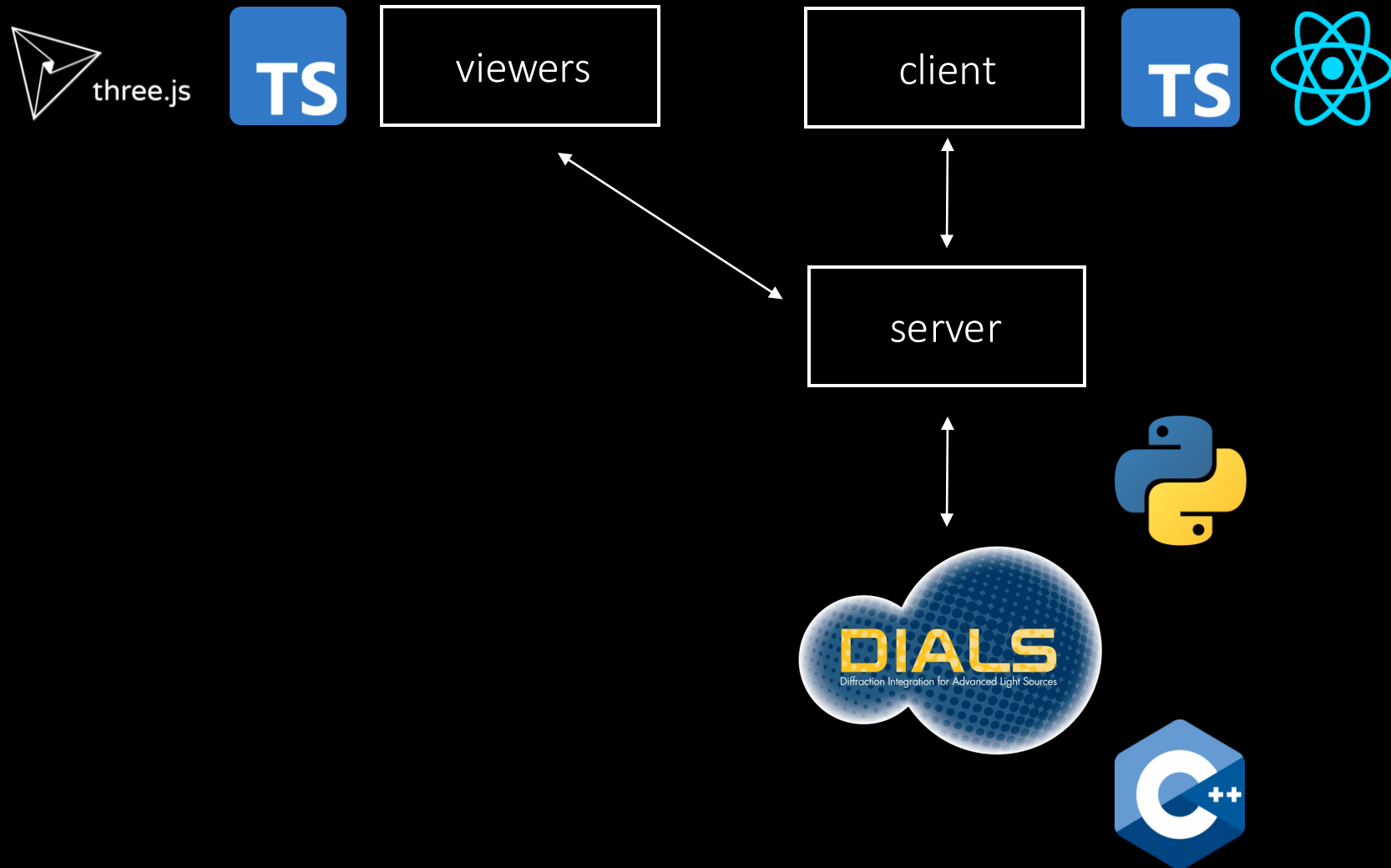
- Neutron time-of-flight Laue peaks have asymmetric profiles
- Algorithms: 1D profile fitting, 3D profile fitting, XDS profile fitting



- Elliptical profiles used for elongated spots in X-ray Laue data



# Interface



# Interface

Active files... ▼

Reflection Table Save

**\* Experiment** Reciprocal Lattice Experiment Planner Integration Profiler Reciprocal Space

Import Find Spots Index Refine Integrate

Browse... No files selected. Documentation

Using Local Server

Advanced Options

See Documentation for full list of options

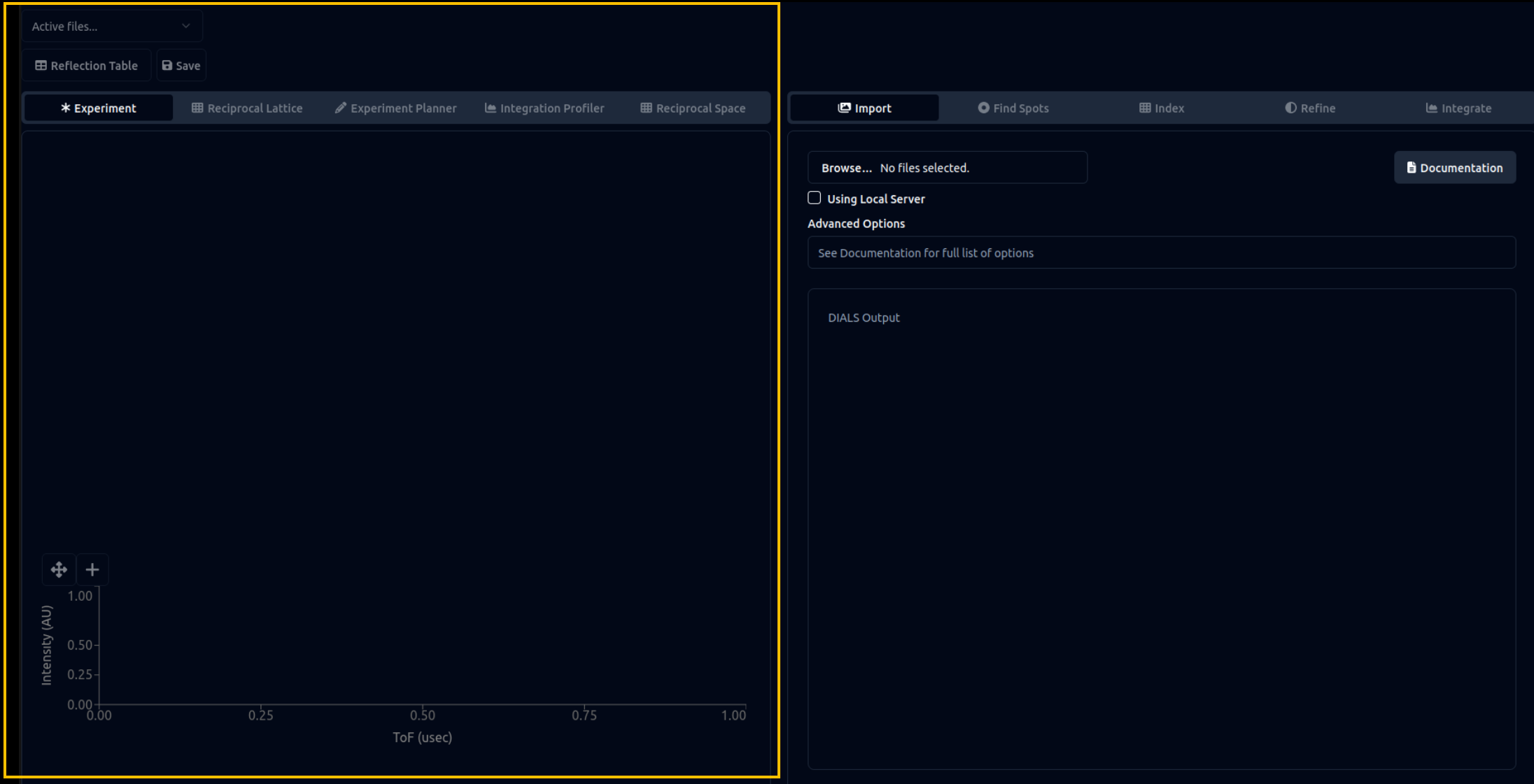
DIALS Output

Intensity (AU)

ToF (usec)



# Interface



- The state of your experiment

# Interface



- The state of your experiment

Import Find Spots Index Refine Integrate

Browse... No files selected. Documentation

Using Local Server

Advanced Options

See Documentation for full list of options

DIALS Output

- Actions applied to your experiment

# Interface: Importing Data

long\_x\* Instrument: NMX Experiment: Simulated Rubredoxin

Reflection Table Save

\* Experiment Reciprocal Lattice Experiment Planner Integration Profiler Reciprocal Space

Import Find Spots Index Refine Integrate

long\_x\* Documentation

Advanced Options

See Documentation for full list of options

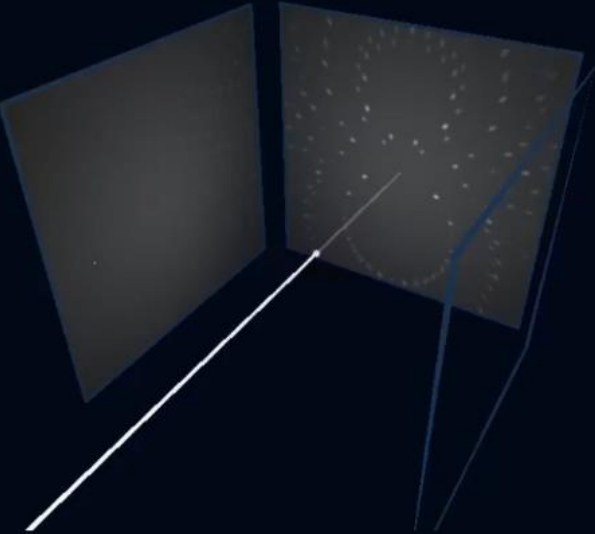
DIALS (2018) Acta Cryst. D74, 85-97. <https://doi.org/10.1107/S2059798317017235>  
DIALS 3.dev.1162-gf3f717693  
The following parameters have been modified:

```
input {
  experiments =
}
```

Format:

```
template: /home/davidmcdonagh/work/anmx/long_x20_100_out.h5:1:100
template: /home/davidmcdonagh/work/anmx/long_x40_100_out.h5:1:100
template: /home/davidmcdonagh/work/anmx/long_x70_100_out.h5:1:100
template: /home/davidmcdonagh/work/anmx/long_x90_100_out.h5:1:100
num images: 400
sequences:
still: 0
sweep: 4
num stills: 0
```

Writing experiments to imported.expt



03 (579, 193)

Intensity (AU)

ToF (usec)

92819.46 107819.46 122819.46 151703.31

2492.07 300.00 650.00 0.00

# Interface: Spot Finding



# Interface: Indexing

long\_x\* Instrument: NMX Experiment: Simulated Rubredoxin  
Identified 1743 reflections (67.24% indexed)  
Unit Cell: a: 34.753 b: 35.891 c: 44.595  $\alpha$ : 90.0  $\beta$ : 90.0  $\gamma$ : 90.0 SG: P2ac2ab

Reflection Table Save

\* Experiment Reciprocal Lattice Experiment Planner Integration Profiler Reciprocal Space

Import Find Spots Index Refine Integrate

Run Detect Symmetry Documentation

Indexing Algorithm: fft3d Outlier Algorithm: auto

Initial Space Group: P212121 Initial Unit Cell: 34.406, 35.273, 44 hkl Tolerance: 0.3 Optimize Detector Panels Separately:

Advanced Options  
See Documentation for full list of options

```
{ 1.0000, -0.0003, 0.0001}  
B matrix: {{ 0.0288, 0.0000, 0.0000},  
{ 0.0000, 0.0279, 0.0000},  
{ 0.0000, 0.0000, 0.0224}}  
A = UB: {{-0.0000, 0.0000, 0.0224},  
{-0.0000, -0.0279, 0.0000},  
{ 0.0288, -0.0000, 0.0000}}
```

Imageset	# indexed	# unindexed	% indexed
0	304	140	68.5
1	268	103	72.2
2	276	142	66
3	324	185	63.7

Saving refined experiments to indexed.expt  
Saving refined reflections to indexed.refl

# Interface: Planning and Applying Symmetry

sxd\_nacl\_run\_13.nxs

Instrument: SXD Experiment: NaCl sphere 6mm diameter RT j:14,14 (33298)  
Identified 497 reflections (61.37% indexed)

Unit Cell: a: 4.029 b: 4.033 c: 4.051  $\alpha$ : 91.255  $\beta$ : 119.302  $\gamma$ : 119.047 SG: P1

Reflection Table Save

\* Experiment Reciprocal Lattice Experiment Planner Integration Profiler Reciprocal Space

Import Find Spots Index Refine Integrate

Run Detect Symmetry Documentation

Indexing Algorithm: fft3d  
Outlier Algorithm: auto

Initial Space Group: None Initial Unit Cell: None hkl Tolerance: 0.3  
Optimize Detector Panels Separately:

Advanced Options  
See Documentation for full list of options

model 1 (305 reflections):  
Crystal:  
Unit cell: 4.029, 4.033, 4.051, 91.255, 119.306, 119.047  
Space group: P 1  
U matrix:  $\begin{pmatrix} 0.7864 & -0.2704 & 0.5554 \\ 0.4104 & -0.4433 & -0.7969 \\ 0.4617 & 0.8546 & -0.2376 \end{pmatrix}$   
B matrix:  $\begin{pmatrix} 0.2482 & 0.0000 & 0.0000 \\ 0.1378 & 0.2836 & 0.0000 \\ 0.1981 & 0.1027 & 0.3011 \end{pmatrix}$   
A = UB:  $\begin{pmatrix} 0.2679 & -0.0197 & 0.1672 \\ -0.1171 & -0.2076 & -0.2400 \\ 0.1853 & 0.2180 & -0.0715 \end{pmatrix}$

Imageset	# indexed	# unindexed	% indexed
0	305	191	61.5%

Saving refined experiments to indexed.expt  
Saving refined reflections to indexed.refl

04 [40, 46]

02 (39, 2)

Intensity (AU)

ToF (usec)

842.40

500.00

250.00

0.00

500.50

5500.50

10500.50

18988.24

3, -6, 3

2, -4, 2

1, -2, 1



# Interface: Integration Profiling

sxd\_nacl\_run\_14.nxs

**Instrument:** SXD **Experiment:** NaCl sphere 6mm diameter RT j:14,14 (33298)  
Identified 497 reflections (61.37% indexed)

**Unit Cell:** a: 4.029 b: 4.033 c: 4.051  $\alpha$ : 91.255  $\beta$ : 119.301  $\gamma$ : 119.046 SG: P1

\* Experiment
Reciprocal Lattice
Experiment Planner
Integration Profiler
Reciprocal Space

03 (8, 11)

Method: 1D Profile Fit

Summation: 1D 3D

$I/\sigma$ : 44.42 44.19

ToF Bounding Box Size (frames): 10

A: 200  $\alpha$ : 0.4  $\beta$ : 0.4  $\sigma$ : 10 Calculate

Legend: ○ intensity ○ background ○ profile

02	20	(0, -2, 4)	(16, 63)	(19, 63)	4.347	3073.910
02	18	(0, -1, 1)	(18, 63)	(19, 65)	4.690	10133.311
03	8	(2, -2, 4)	(12, 13)	(13, 13)	0.303	653.494
03	10	(3, -3, 1)	(32, 7)	(33, 6)	0.323	696.639
03	9	(4, -5, -1)	(53, 8)	(53, 7)	0.326	705.040
03	8	(3, -4, 4)	(17, 34)	(17, 34)	0.391	843.930
03	6	(4, -5, 0)	(48, 19)	(49, 19)	0.391	843.930
03	15	(4, -5, 1)	(41, 27)	(42, 26)	0.408	880.094
03	41	(2, -2, 2)	(21, 13)	(22, 13)	0.423	912.322
03	47	(1, -1, 3)	(8, 11)	(9, 11)	0.445	960.967
03	22	(2, -2, 1)	(29, 10)	(30, 9)	0.475	1024.412
03	8	(3, -4, -1)	(59, 9)	(59, 8)	0.460	994.167
03	10	(4, -6, 2)	(42, 47)	(43, 47)	0.485	1045.086
03	16	(4, -6, 0)	(62, 35)	(62, 33)	0.489	1055.578
03	7	(2, -3, 4)	(9, 38)	(9, 38)	0.492	1061.925
03	7	(4, -6, 1)	(52, 43)	(53, 42)	0.506	1092.048
03	37	(3, -4, 2)	(31, 37)	(32, 37)	0.537	1157.193
03	71	(3, -4, 0)	(53, 25)	(53, 24)	0.580	1250.971
03	22	(3, -5, 3)	(29, 58)	(30, 57)	0.583	1258.491

Scroll to top

# Status: Beta testing

- Send me data!



SXD  
LMX



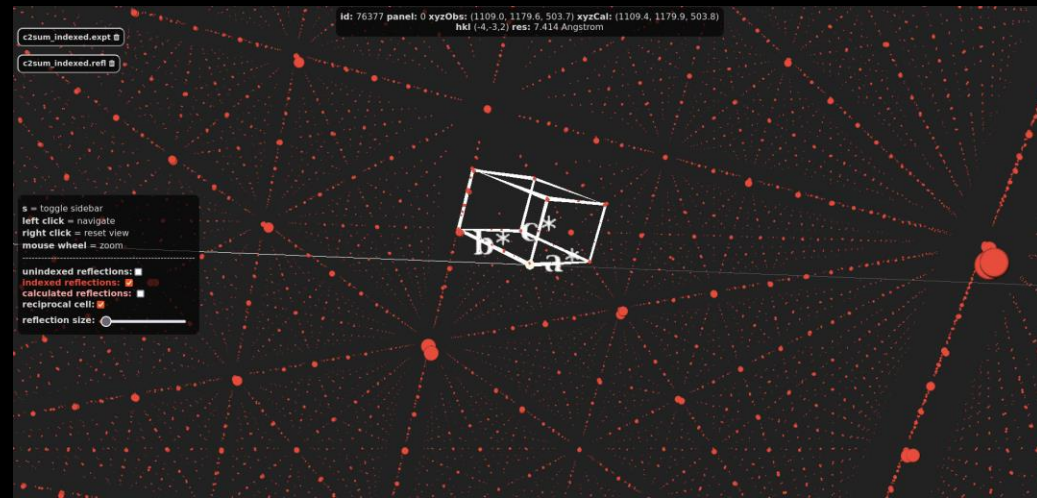
MANDI



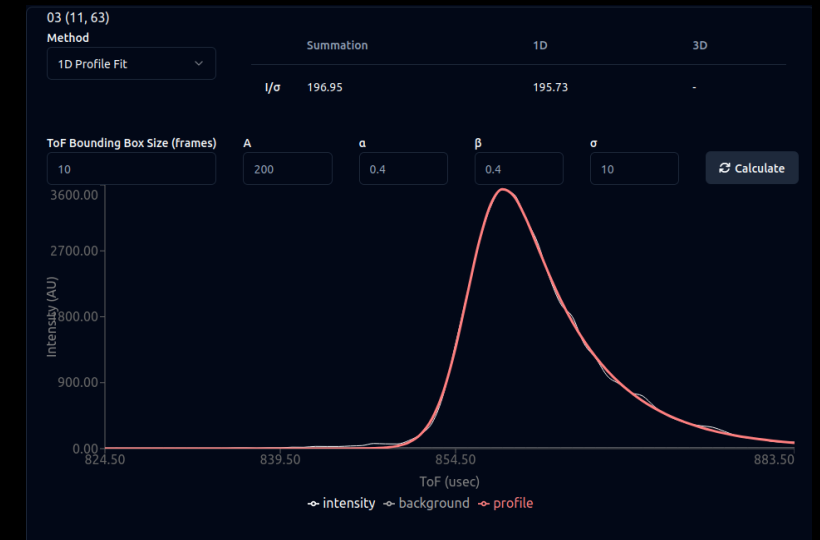
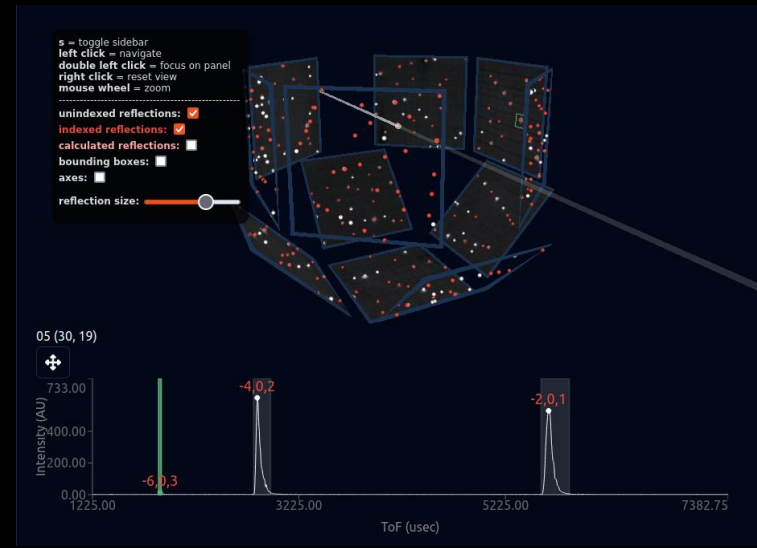
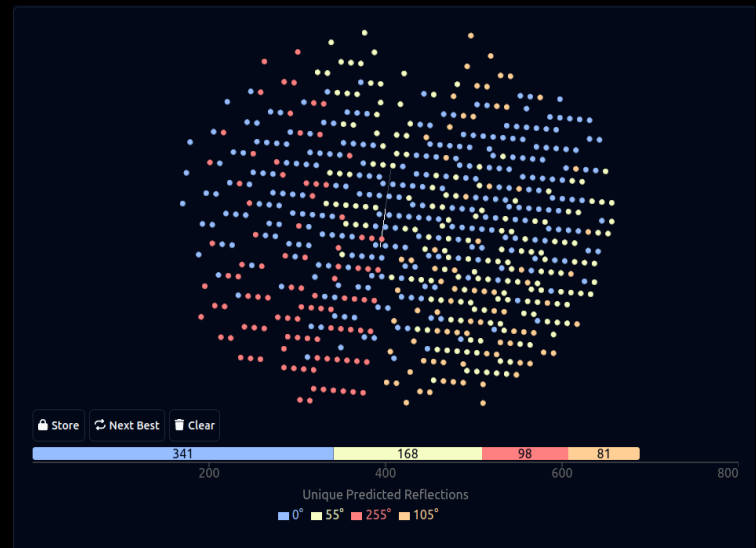
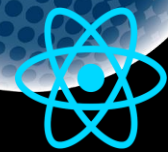
NMX



X-ray Laue



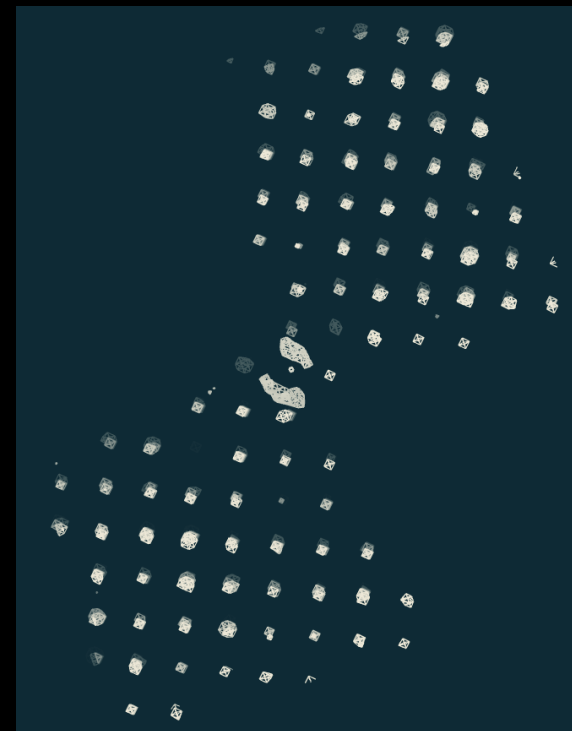
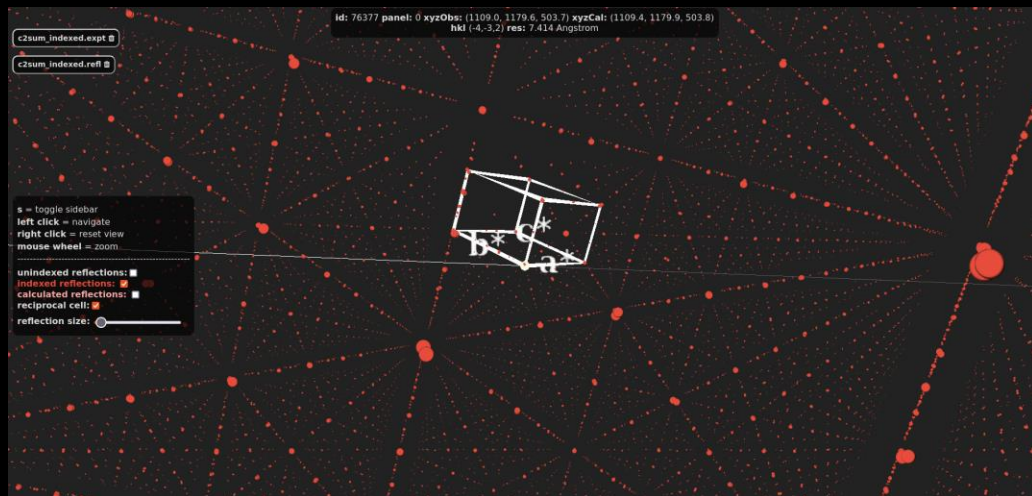
three.js



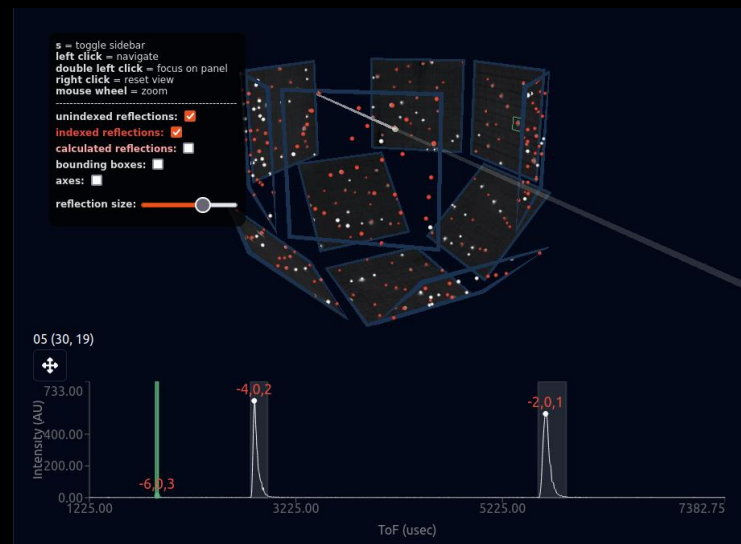
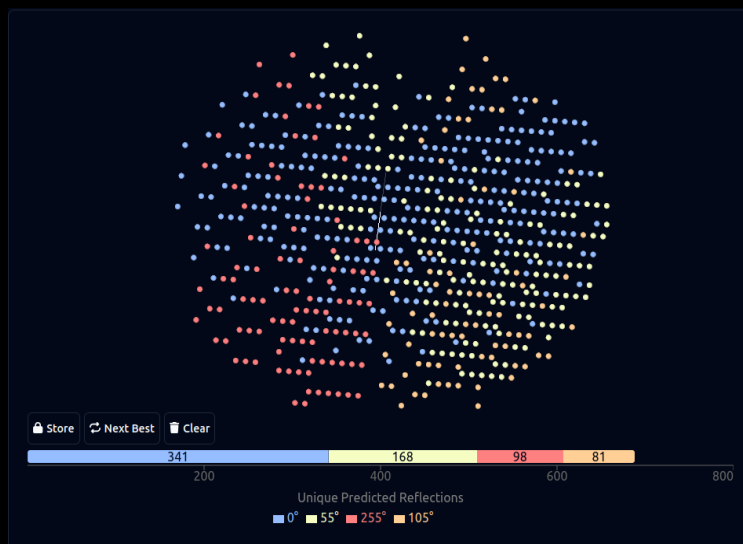
# Status: Beta testing

- Send me data!

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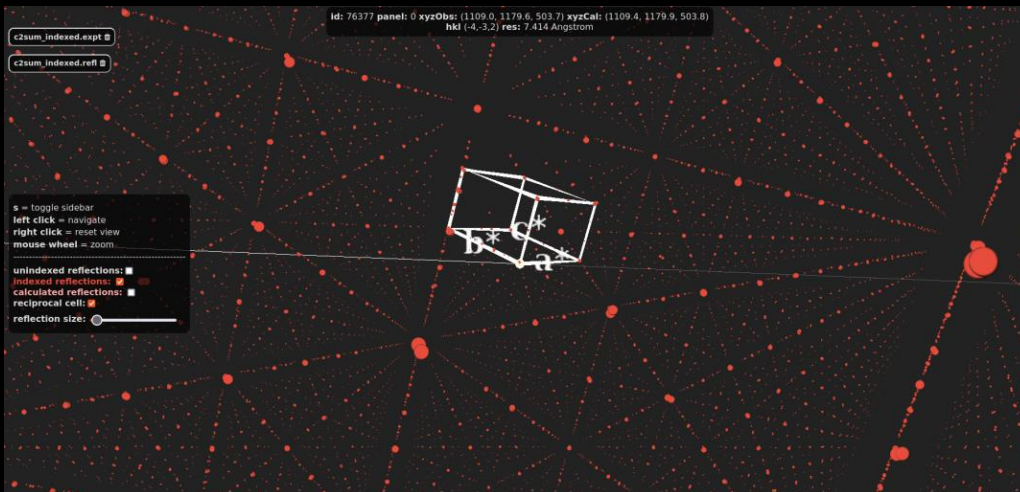
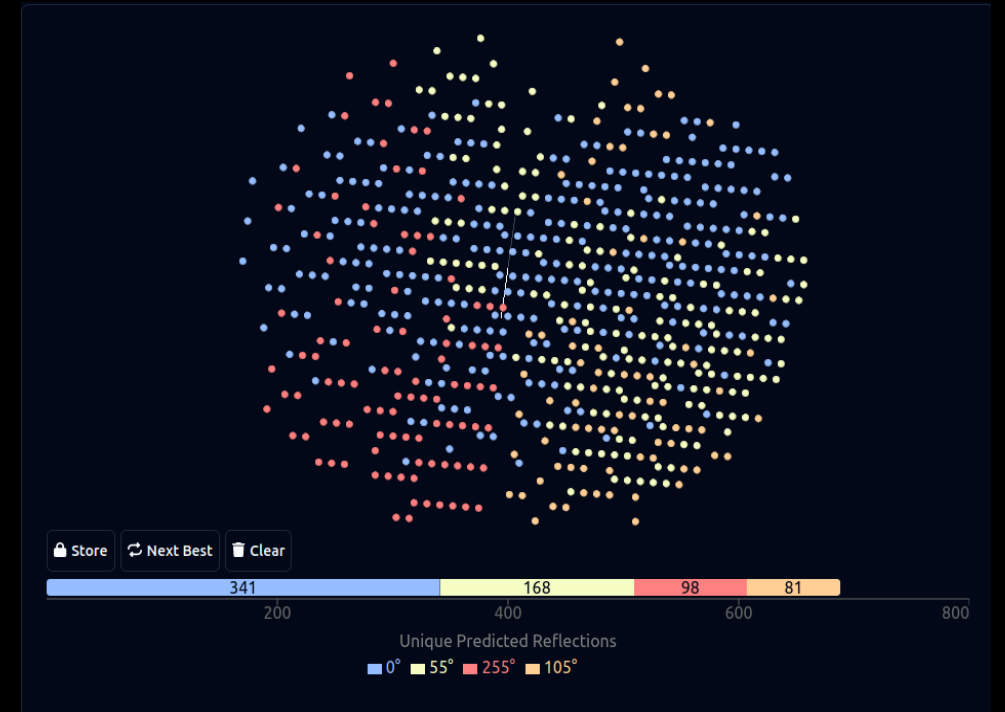
dials.rs\_mapper





# User Experience: Short-Term

- Users typically interact with DIALS via local installation
- Everything should be possible in the cloud
  - No installation friction
  - Inclusive to researchers with inadequate hardware
  - Concepts like shared workspaces more natural in this context
  - Far easier to measure and optimise energy efficiency
- Recent ALC work in providing data links between synchrotrons and the cloud removes key barriers



Jools Wills

Linking XRD  
facilities and CCP4  
Cloud



# Machine Learning: From Static to Dynamic Data Processing

- Machine learning is starting to be introduced to different parts of crystallography
- This needs to be turned into a strategy
- Models can be trained to approximate parts of the pipeline, or to potentially improve them
- These can be trained on old data, but could be learnt on the fly

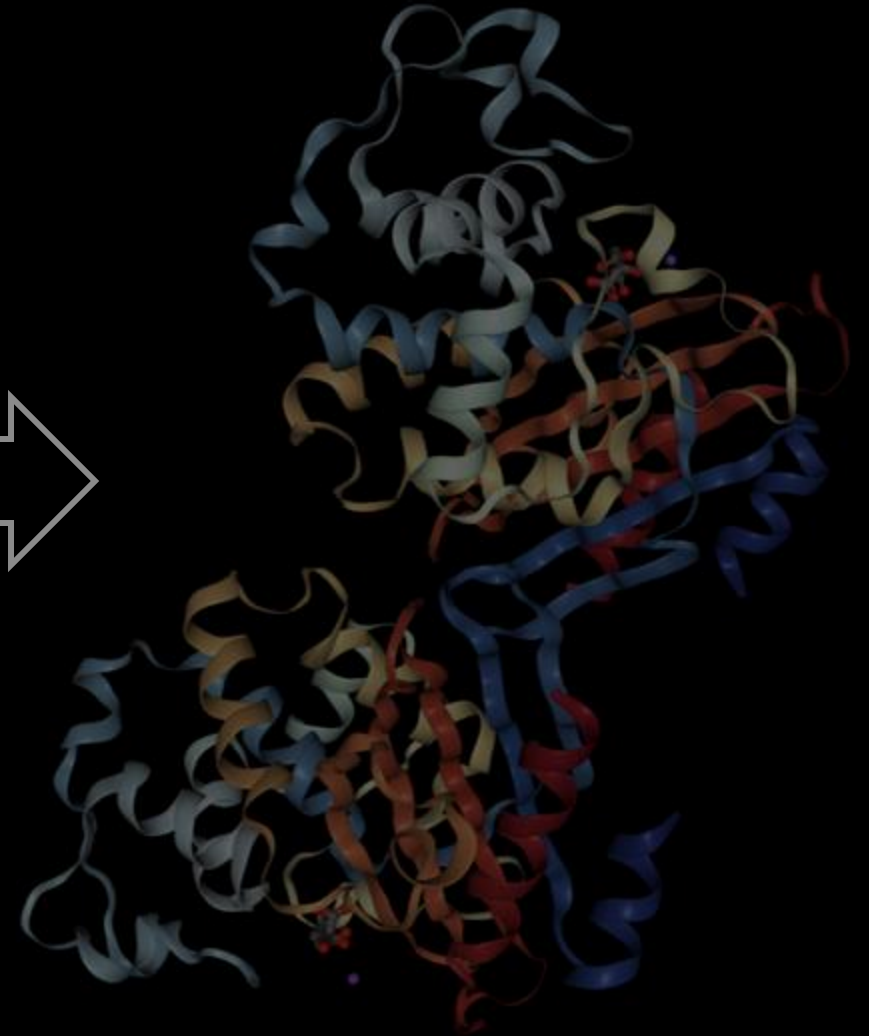
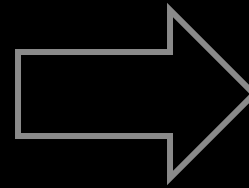


Marko Petrovic

Electron Diffraction  
Data Collection  
Accelerated via  
Machine Learning

# User Experience: Long-Term

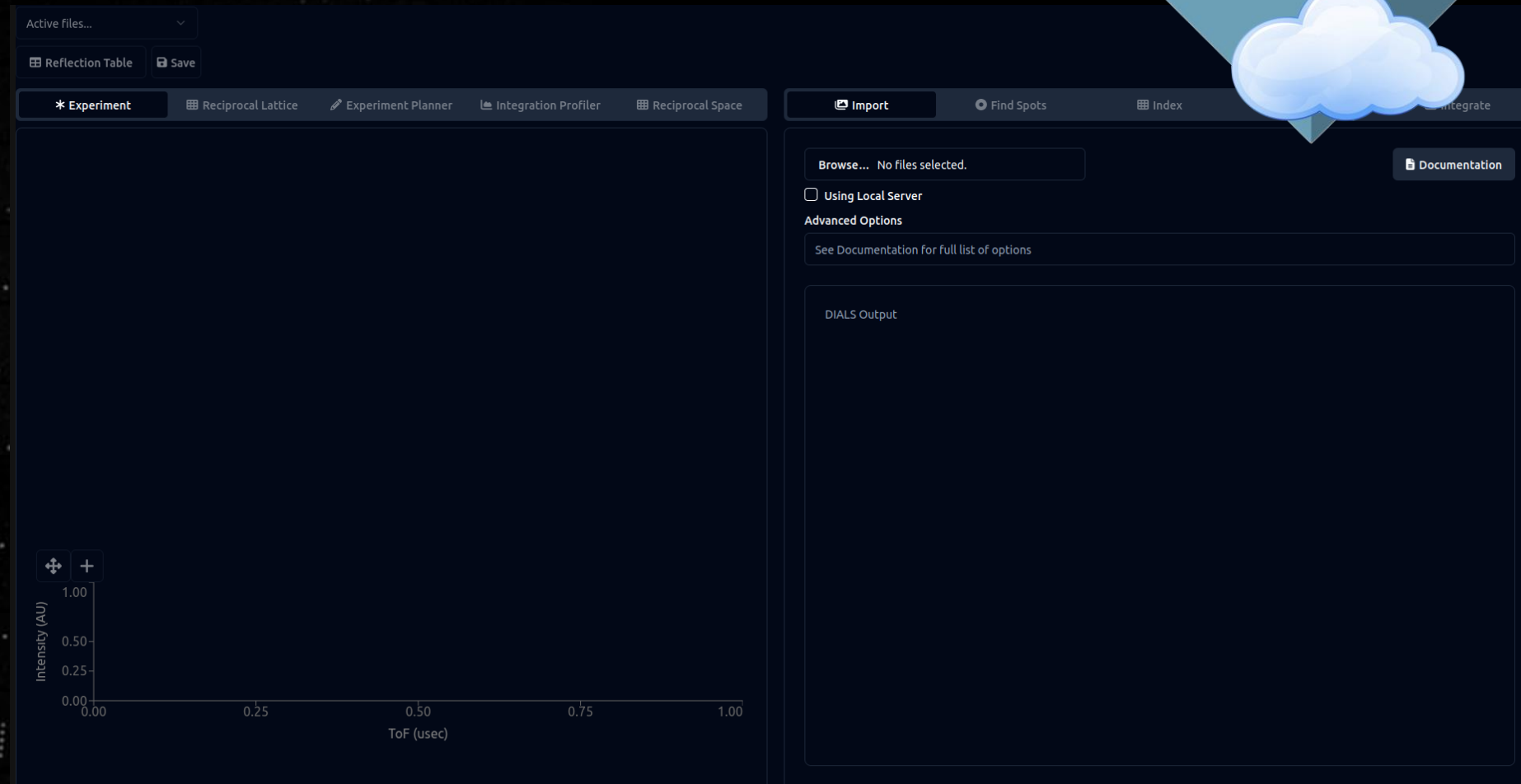
- Bespoke, instrument-specific software has largely been replaced by generic software
- Researchers now typically have data from multiple sources
- Should they have to learn multiple software packages?





# User Experience: Long-Term

- Bespoke, instrument-specific software has largely been replaced by generic software
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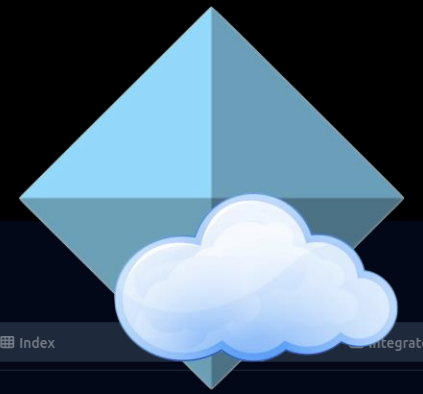


# User Experience: Long-Term

- Bespoke, instrument-specific software has largely been replaced by generic software
- Researchers now typically have data from multiple sources
- Should they have to learn multiple software packages?



The image shows a screenshot of a software interface, likely a diffraction data processing tool. The interface has a dark theme and a top menu bar with options like 'Reflection Table', 'Save', 'Experiment', 'Reciprocal Lattice', 'Experiment Planner', 'Integration Profiler', 'Reciprocal Space', 'Import', 'Find Spots', 'Index', and 'Integrate'. Below the menu bar, there are several panels. On the left, there is a plot area showing 'Intensity (AU)' on the y-axis (ranging from 0.00 to 1.00) and a scale on the x-axis (ranging from 0.00 to 1.00). The plot area contains the DIALS logo, which is a blue sphere with a grid pattern and the text 'DIALS' in yellow, with the subtitle 'Diffraction Integration for Advanced Light Sources' below it. On the right, there is a panel with a 'Browse...' button, a 'Documentation' button, and a 'DIALS Output' section. The MANTiD logo, which is a green stylized figure with the text 'MANTiD' in black, is overlaid on the right side of the interface. A large white double-headed arrow points between the DIALS and MANTiD logos, indicating a relationship or integration between the two software packages.



# Acknowledgements

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