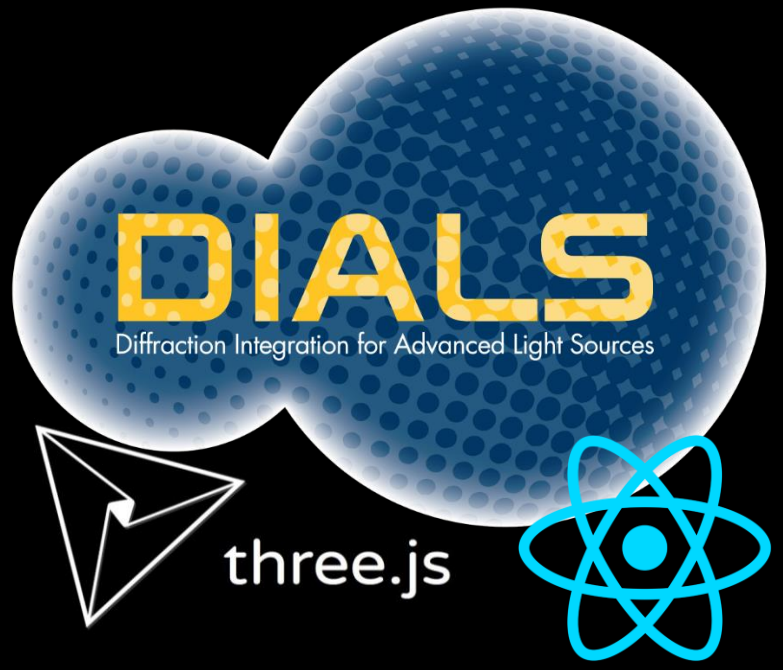
DIALS for Neutron and Laue Diffraction

Early Science on the NMX Macromolecular Diffractometer, 26 August 2024

David McDonagh



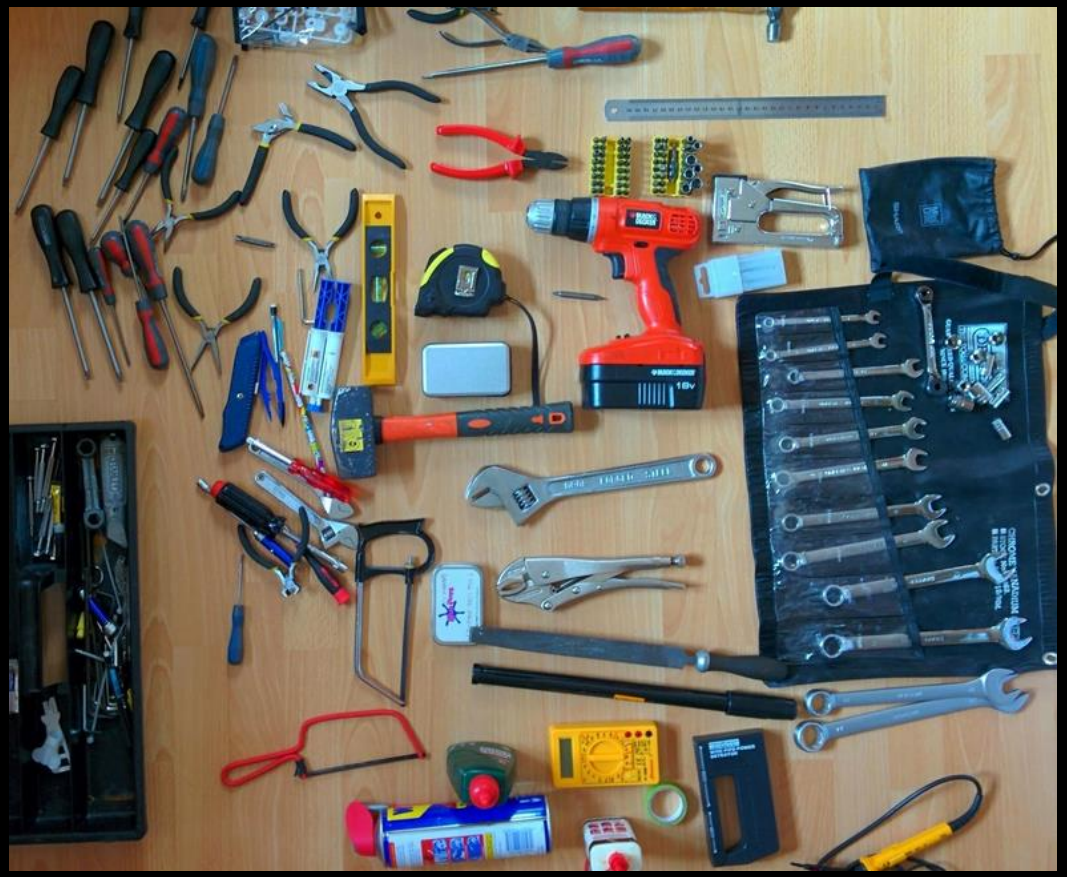
DIALS

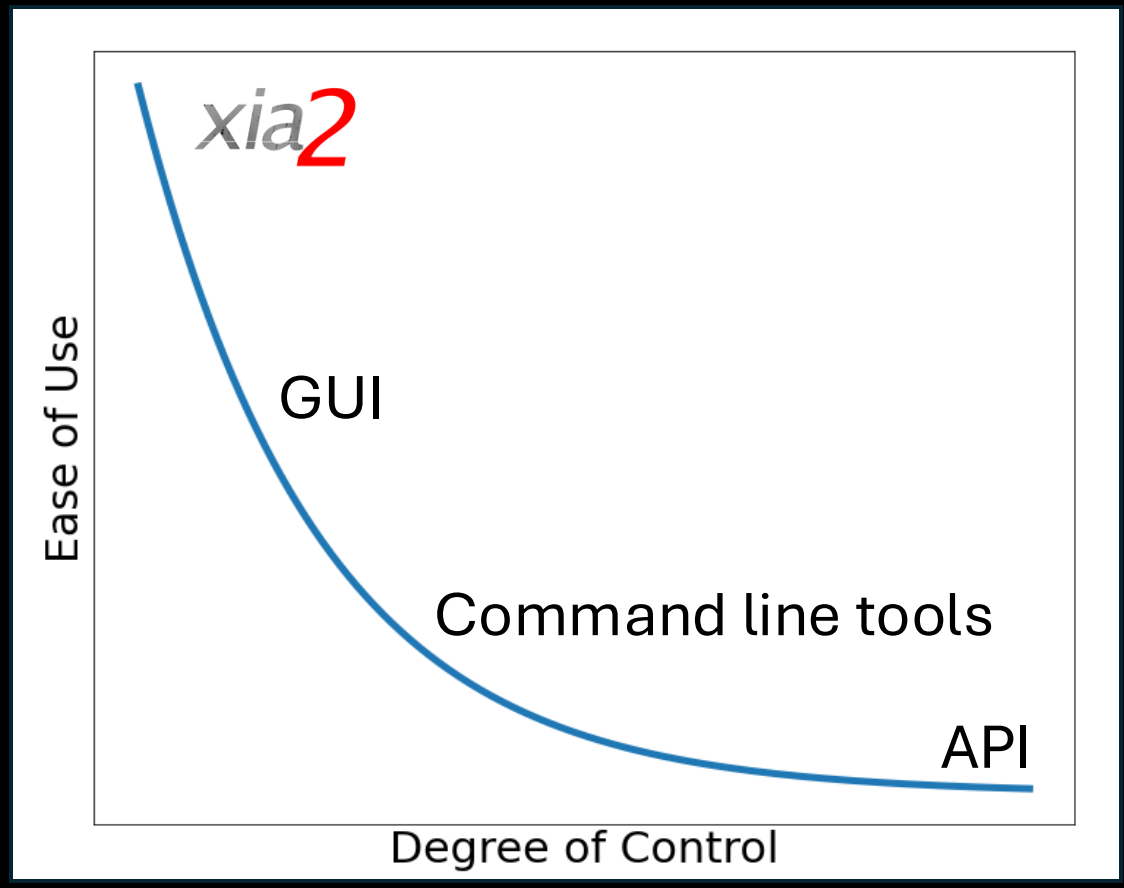
Diffraction Integration for Advanced Light Sources

Spot Finding → Indexing → Model Refinement → Scaling → Integration

Philosophy

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





History

Funding

2011 → 2024

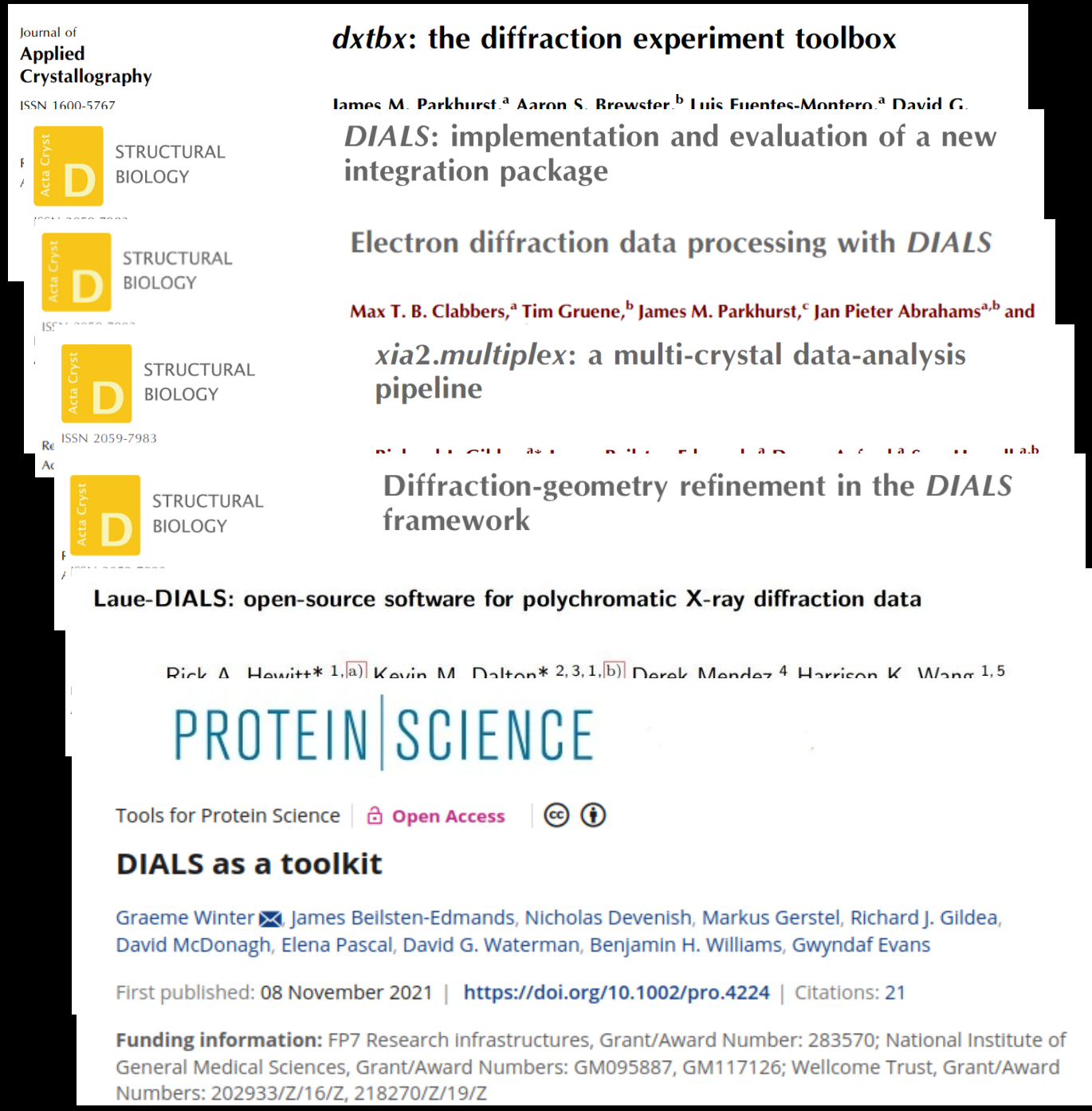
Developers

Developers

- Over 50 contributors worldwide

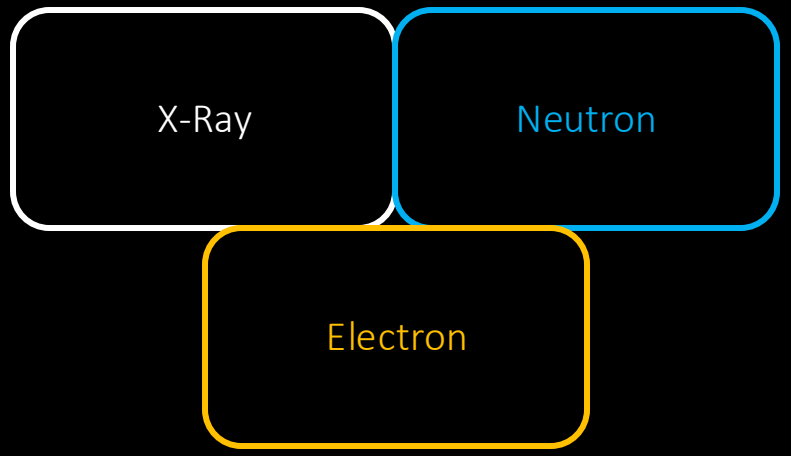
DIALS Today

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

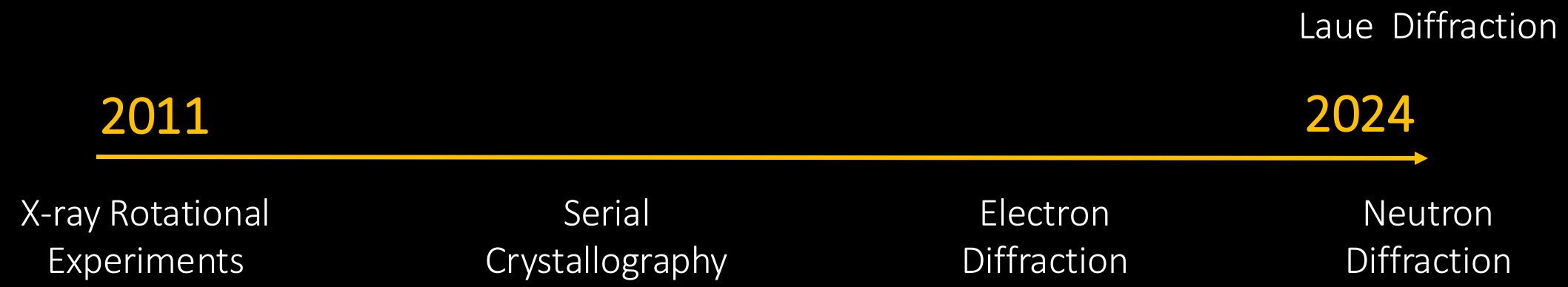


Beyond X-rays

- 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



Motivation

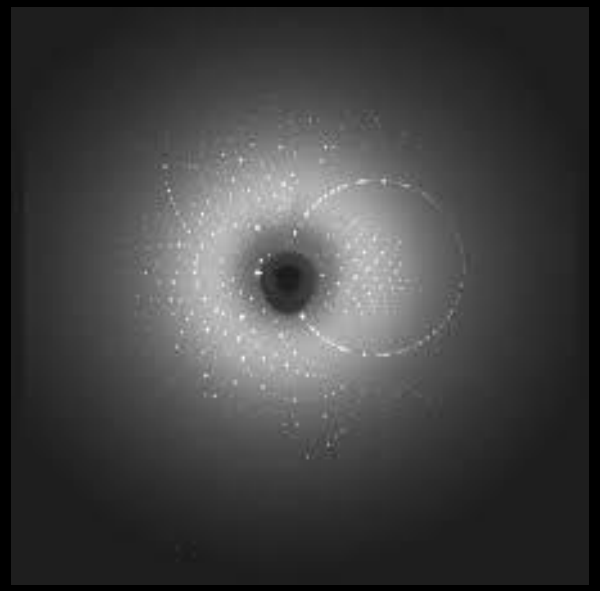
- Increasing demand for neutron macromolecular crystallography data

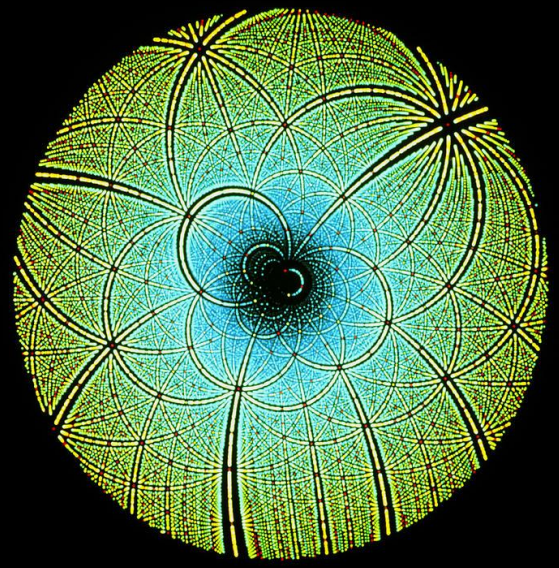
NEUTRONS FOR SOCIETY

Science & Technology Facilities Council
ISIS

EUROPEAN SPALLATION SOURCE

- 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

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Neutron time-of-flight Laue

X-ray Laue

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Neutron time-of-flight Laue

X-ray Laue

README MIT license

Build passing Documentation passing pypi v0.4 codecov 73% License MIT

laue-dials

Data analysis package for Laue crystallography.

`laue-dials` is an extension to the DIALS code for analyzing polychromatic crystallographic data. Building off the `DIALS` framework, and including modern tools like `numpy`, `scipy`, and `reciprocalspaceship`, this package allows for analysis of X-ray crystallographic data using wide-bandwidth light sources. This package is intended to be used in conjunction with DIALS, careless, and Phenix in order to generate molecular models from raw data. For documentation, see https://rs-station.github.io/laue-dials/index.html.

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

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

[1)] *Department of Molecular and Cellular Biology, Harvard University, Cambridge, MA 02138*

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R.A Hewitt, K.M Dalton, D. Mendez, H.K Wang, M.A Klureza, D.E Brookner, J.B Greisman, D. McDonagh, V. Srajer, N.K Sauter, A.S. Brewster, D.R Hekstra, Laue-DIALS: open-source software for polychromatic X-ray diffraction data, Structual Dynamics, *Submitted*.

The Work

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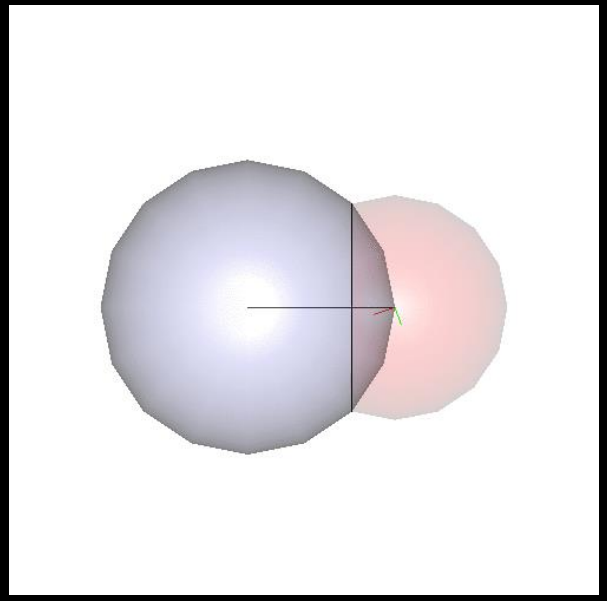
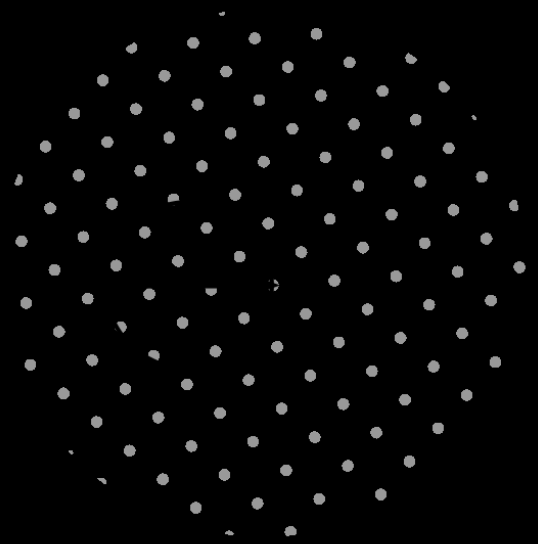


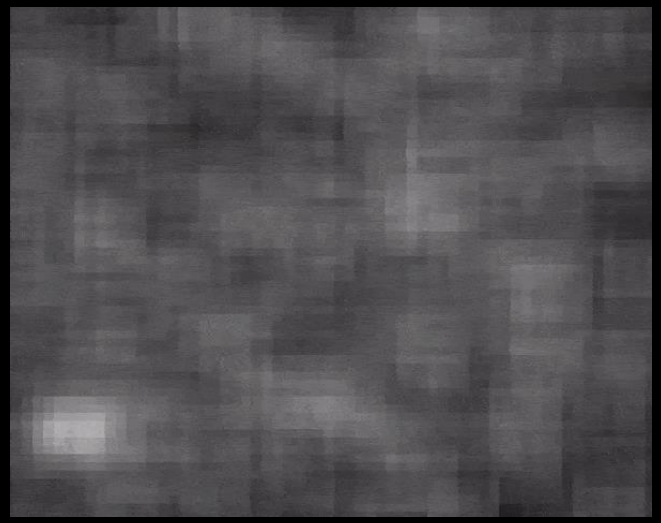
- Rotation scan

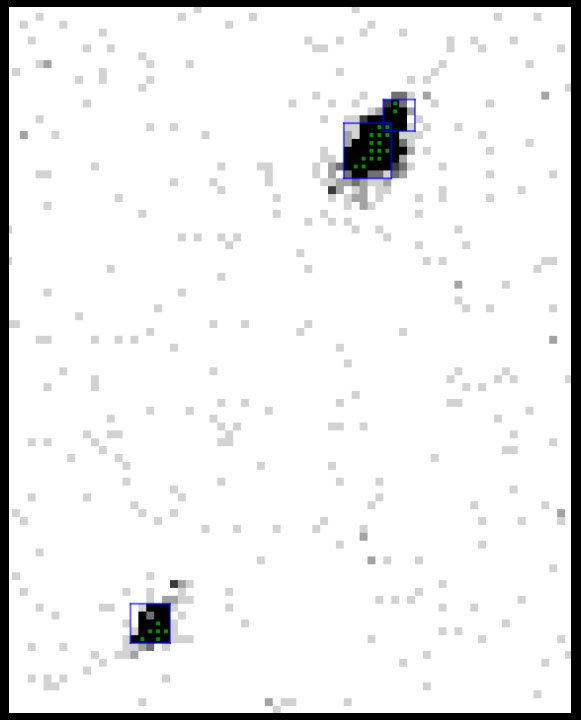


- Wavelength scan

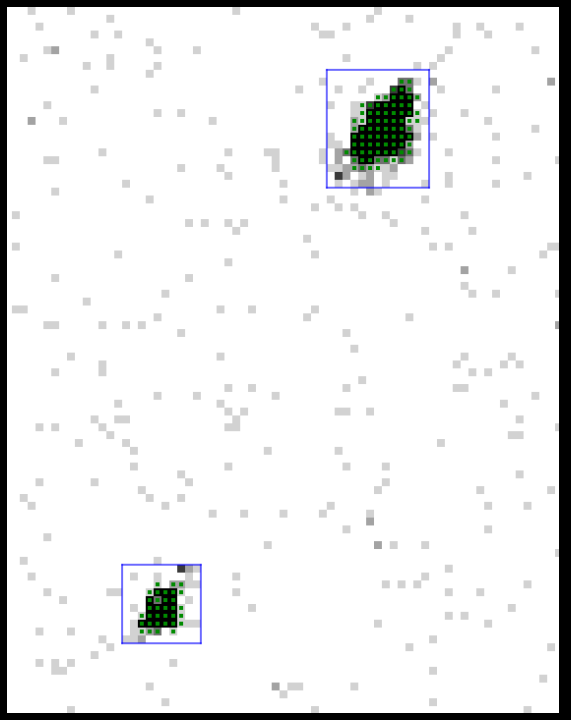
Spot Finding

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

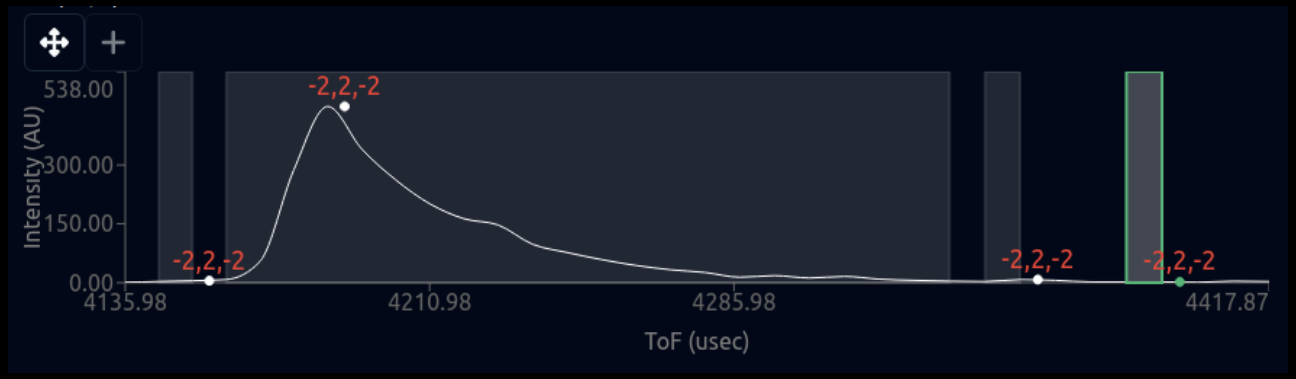




dispersion



dispersion-extended



- ToF profiles require specific post processing

Indexing

Spot Finding → **Indexing** → Model Refinement → Scaling → Integration

- 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

research papers

Acta Cryst A FOUNDATIONS ADVANCES

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

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

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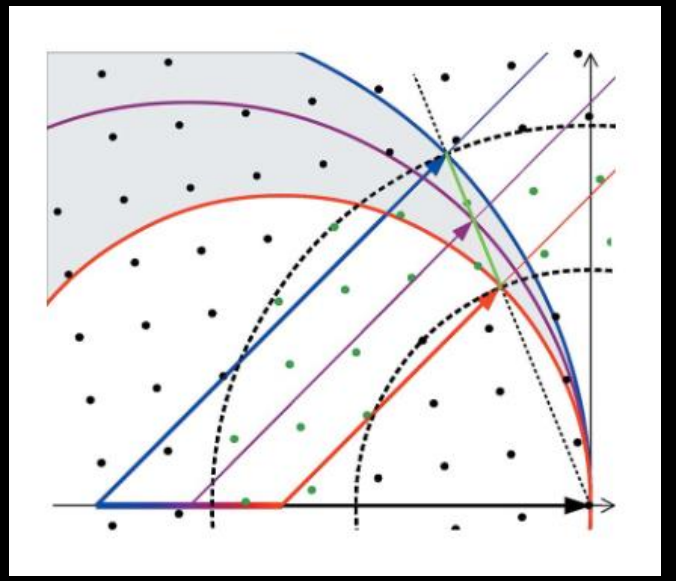
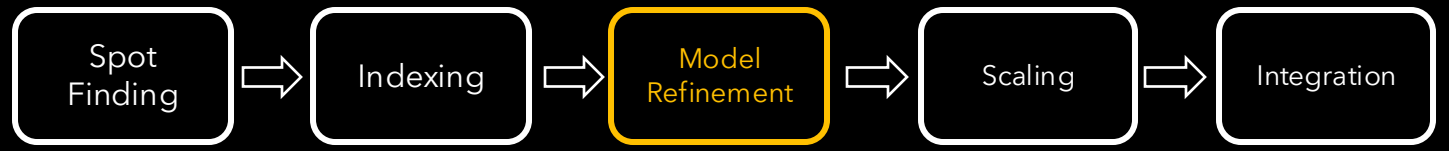
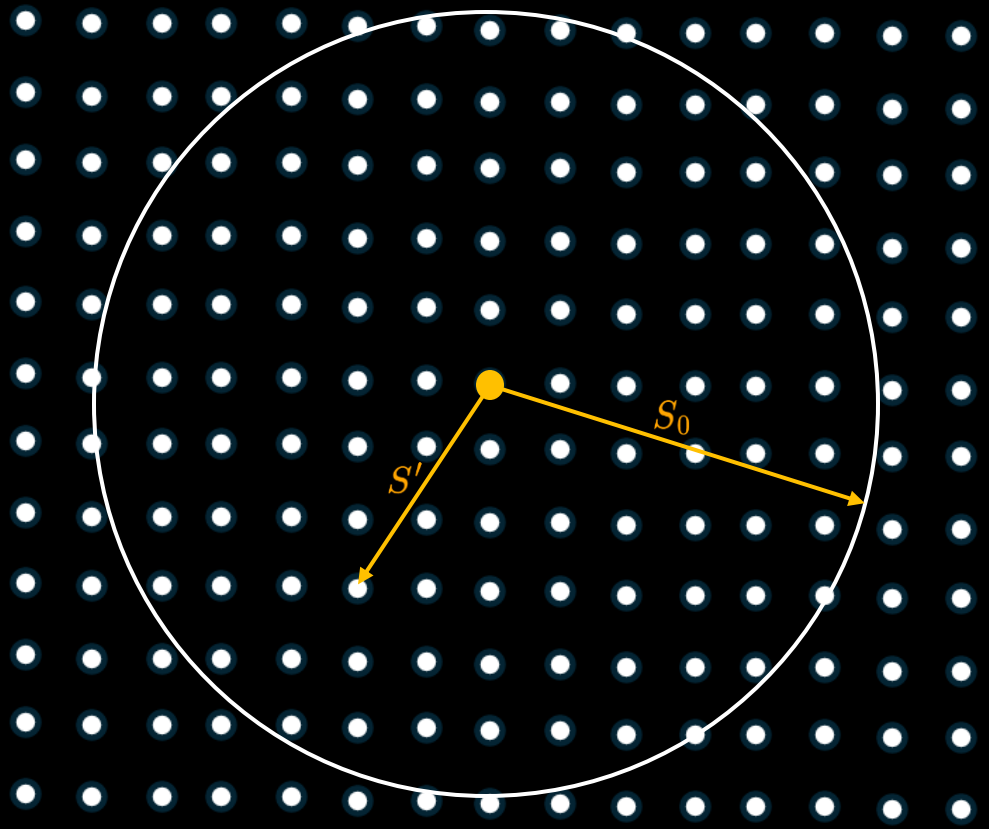


Laue Refinement





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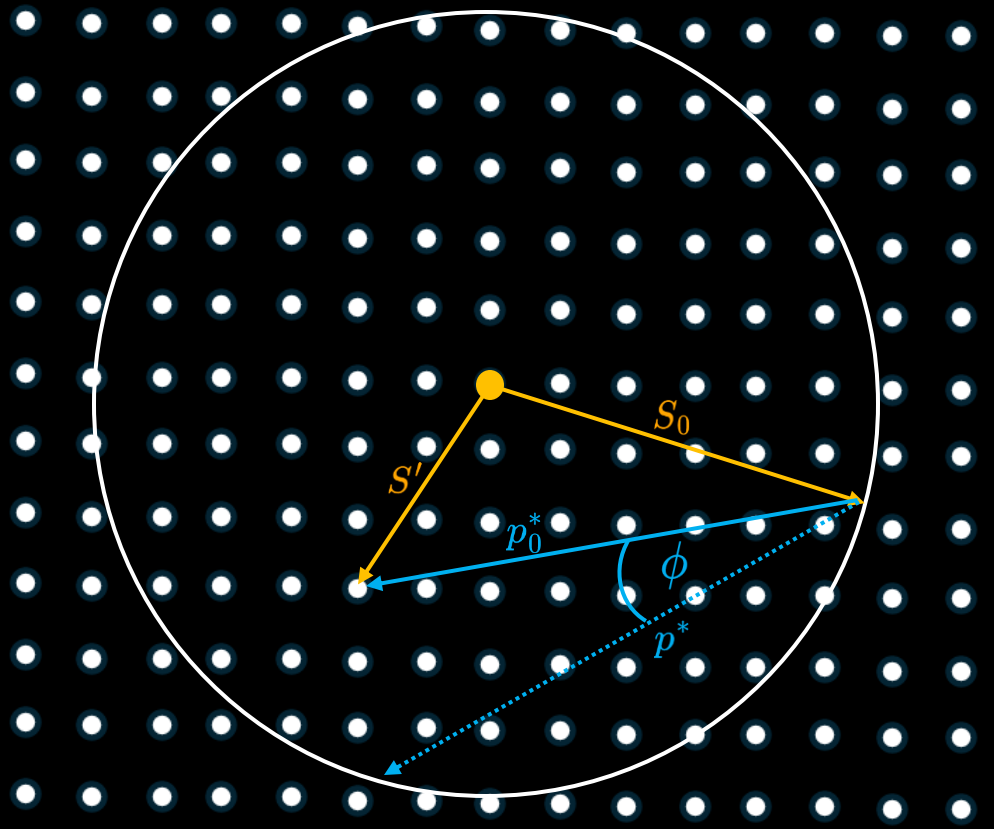
Laue Refinement

Spot Finding → Indexing → Model Refinement → Scaling → Integration



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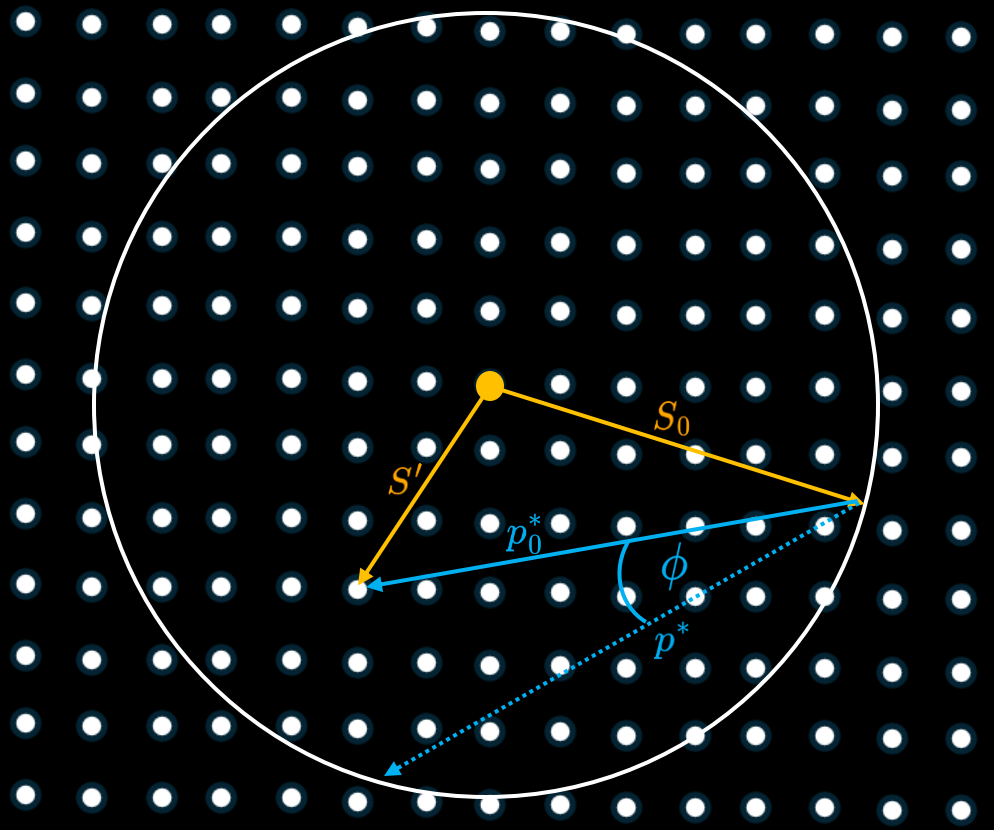
Laue Refinement

Spot Finding → Indexing → Model Refinement → Scaling → Integration

- Diffraction condition

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



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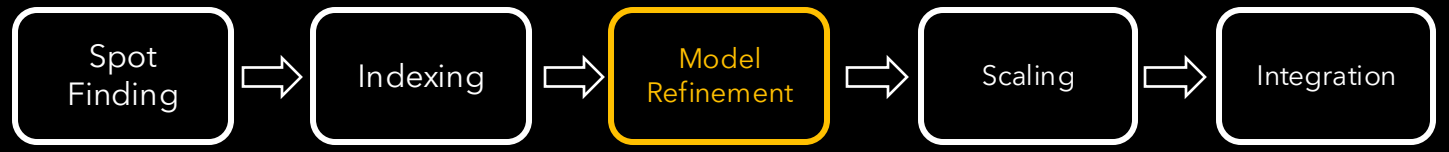
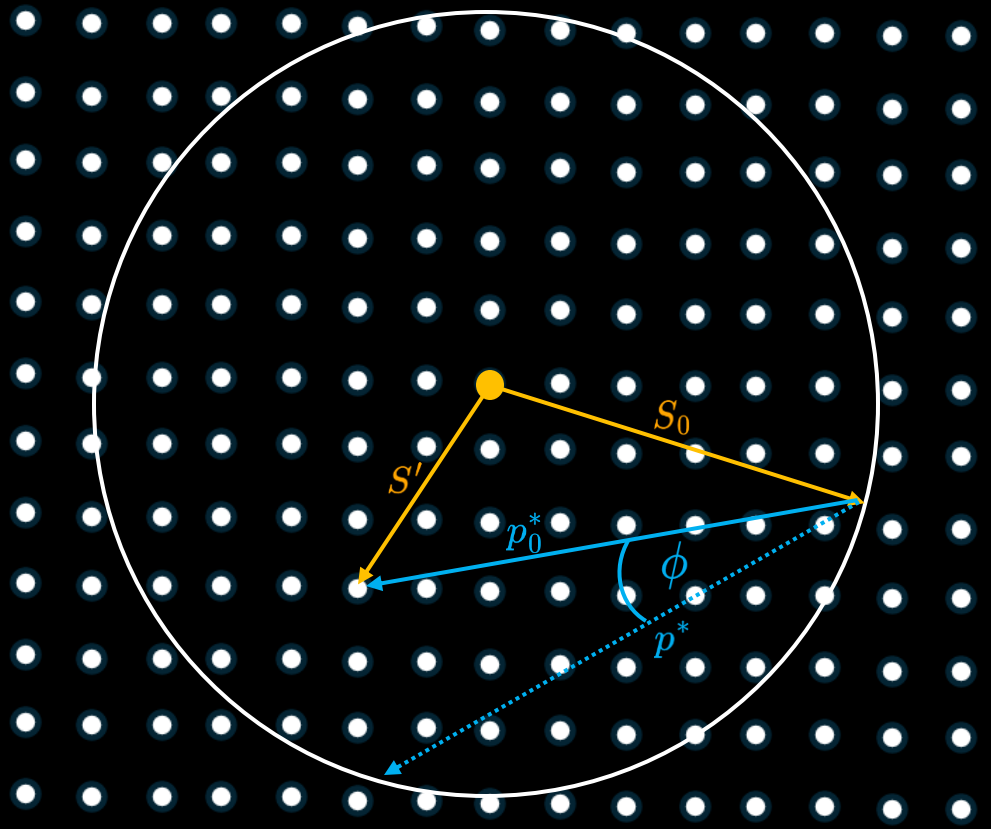


- Diffraction condition

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

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



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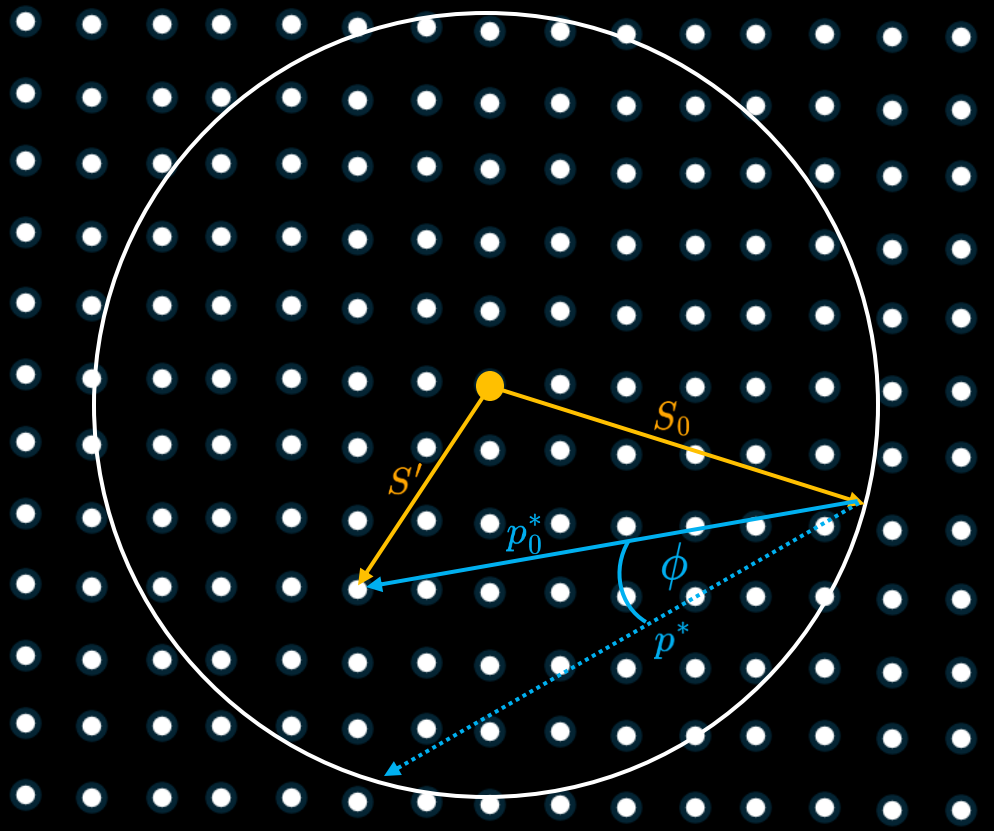
- Cost function

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

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



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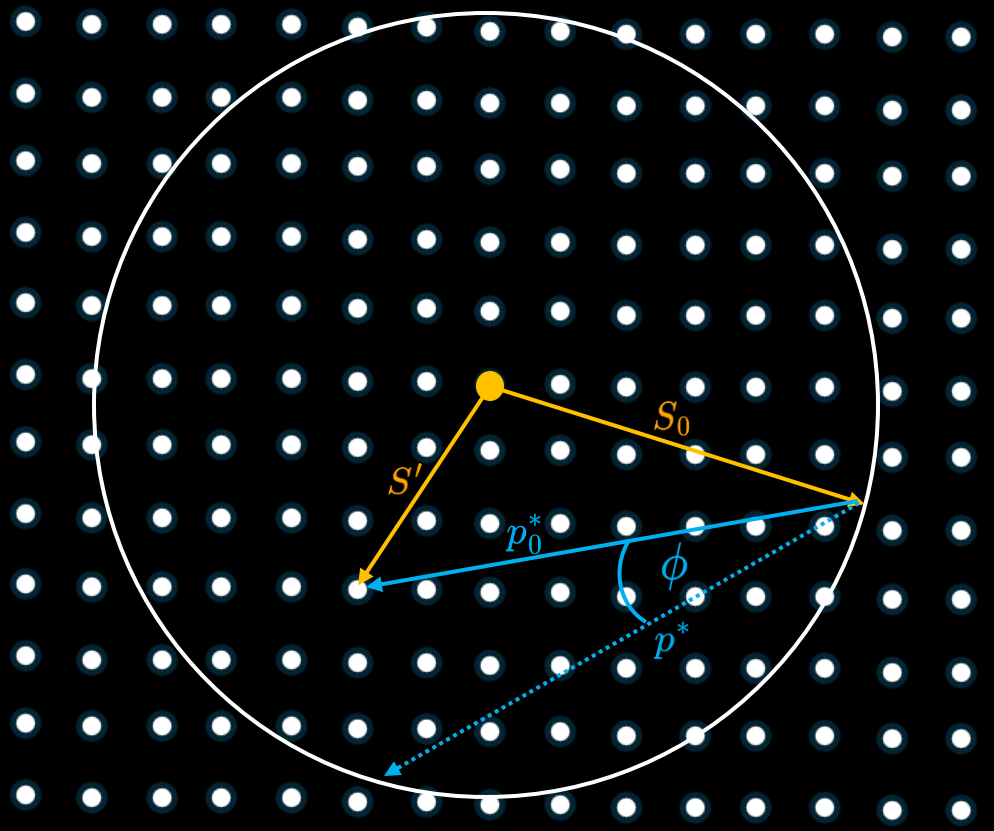
$$\frac{\partial \lambda}{\partial p} = -2\hat{S}_0 \left(\frac{\frac{\partial p_0^*}{\partial p}|p_0^*|^2 - 2p_0^*\frac{\partial p_0^*}{\partial p} \cdot p_0^*}{|p_0^*|^4} \right)$$



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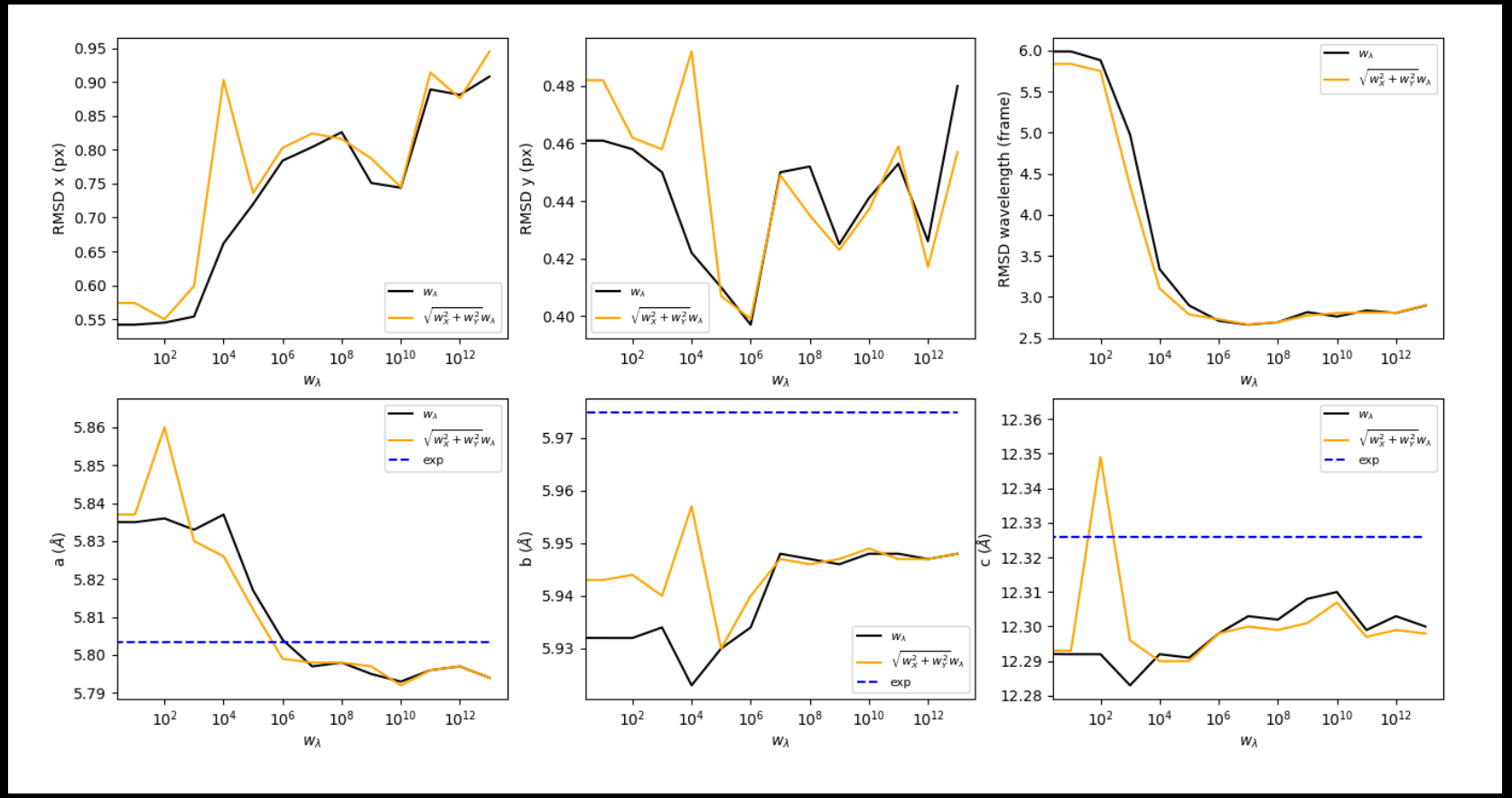
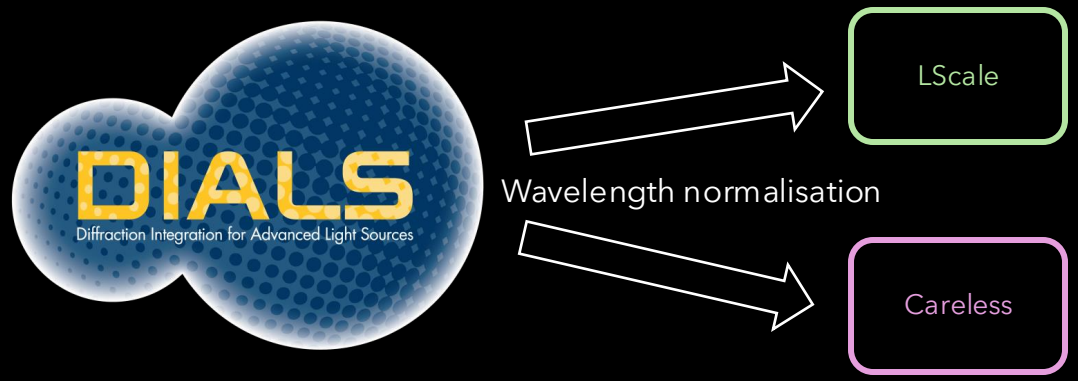


Scaling Pipeline



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Scaling Pipeline

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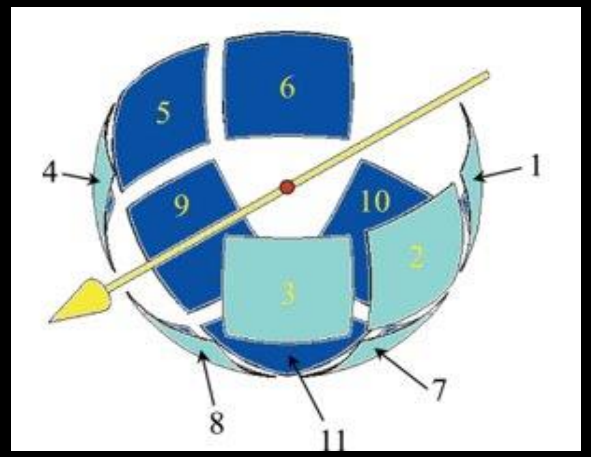
SXD



DIALS
Diffraction Integration for Advanced Light Sources

Wavelength normalisation → LScale

Wavelength normalisation → Careless

- Wavelength range: 0.2 - 10 Angstroms

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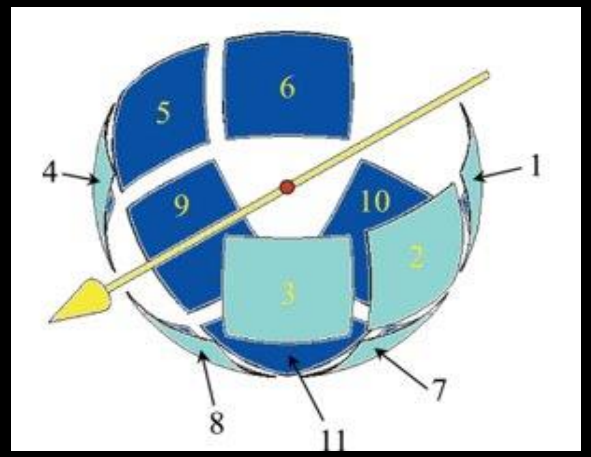

Wavelength normalisation

LScale

Careless

- 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

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

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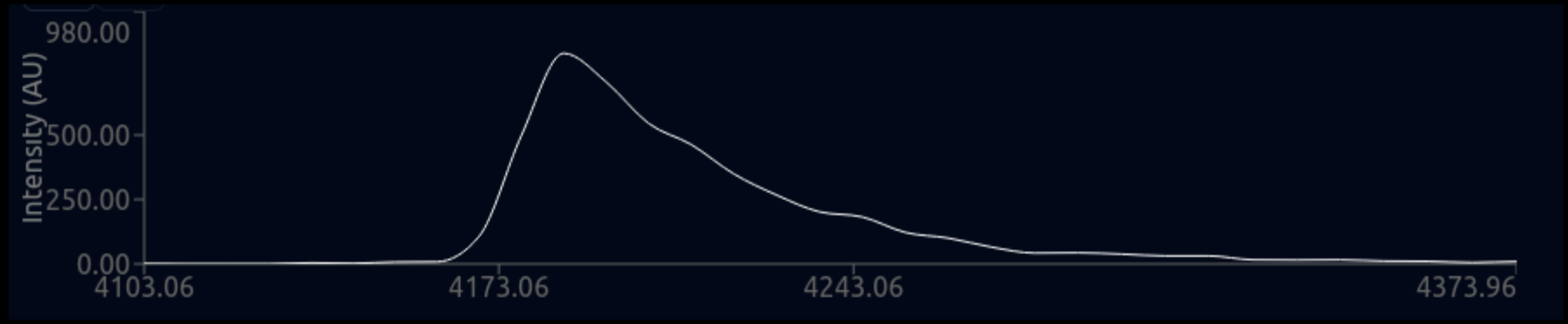
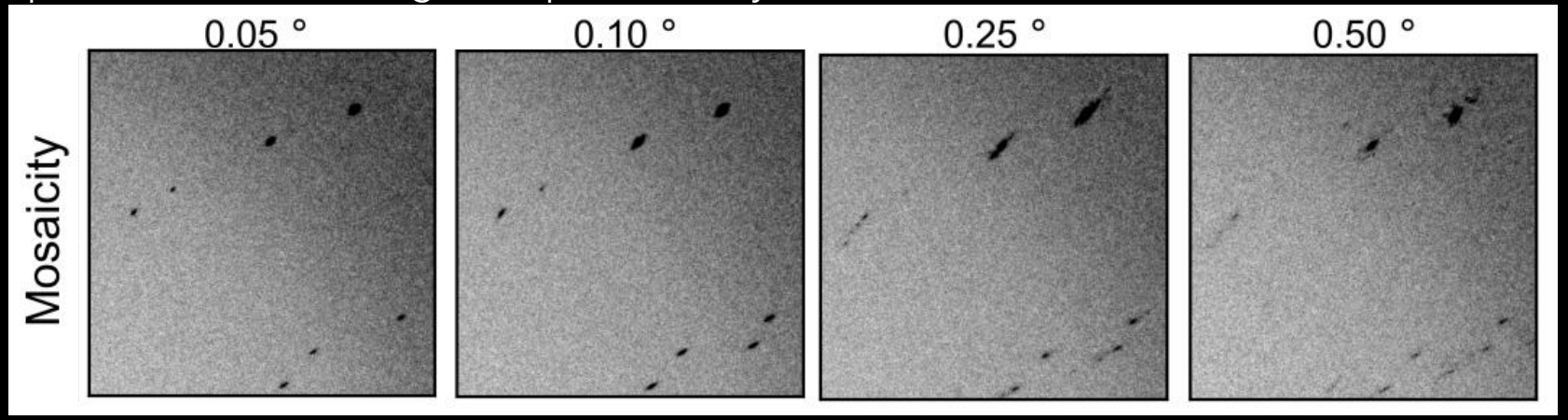
Laue Integration

Spot Finding ⇨ Indexing ⇨ Model Refinement ⇨ Scaling ⇨ Integration

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

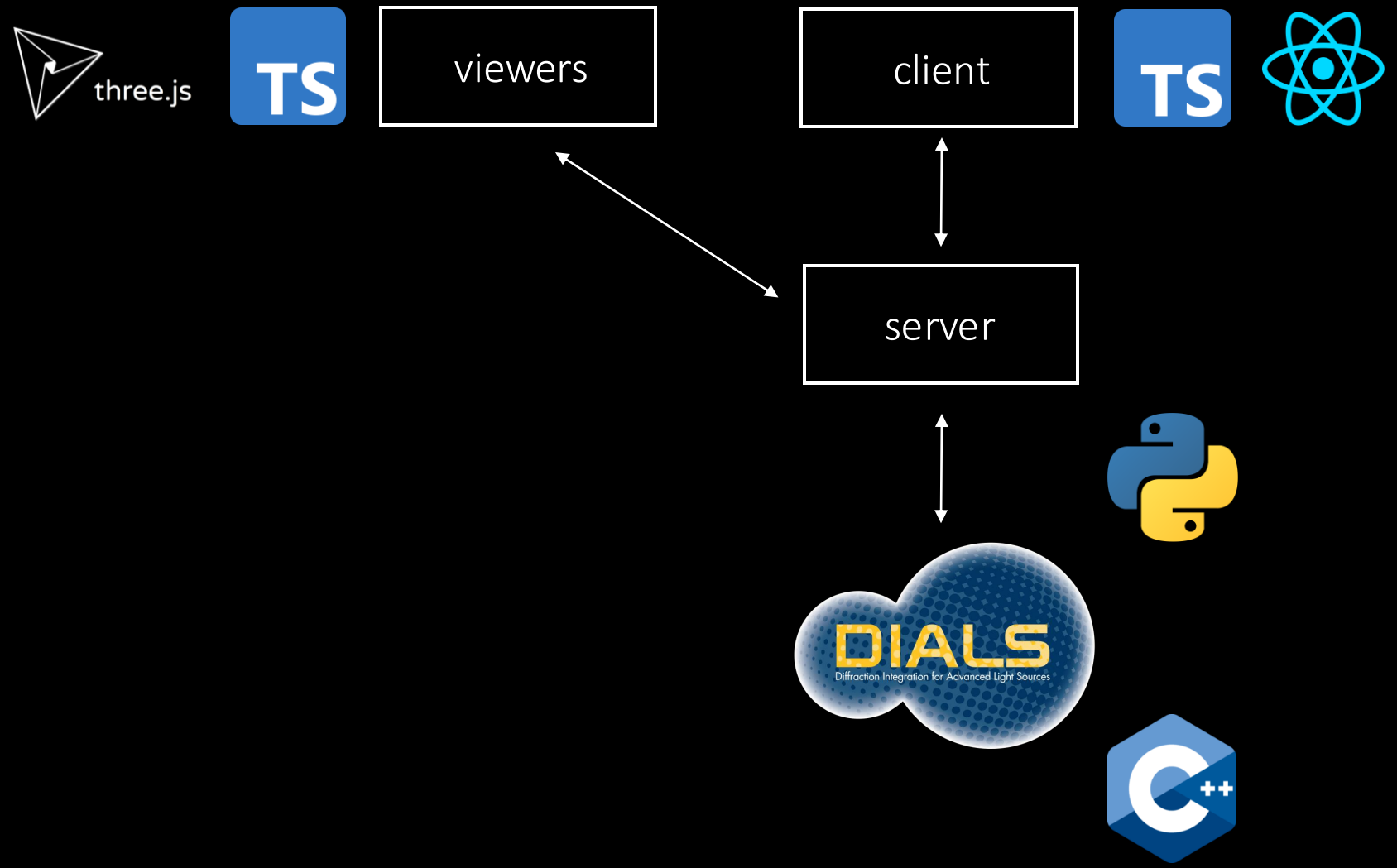


- Elliptical profiles used for elongated spots in X-ray Laue data



N. Yano, T. Yamada, T. Hosoya, T. Ohhara, I. Tanaka, K. Kusaka, Application of profile fitting method to neutron time-of-flight protein single crystal diffraction data collected at iBIX. Scientific Reports, 6, 2016.

Interface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viewers
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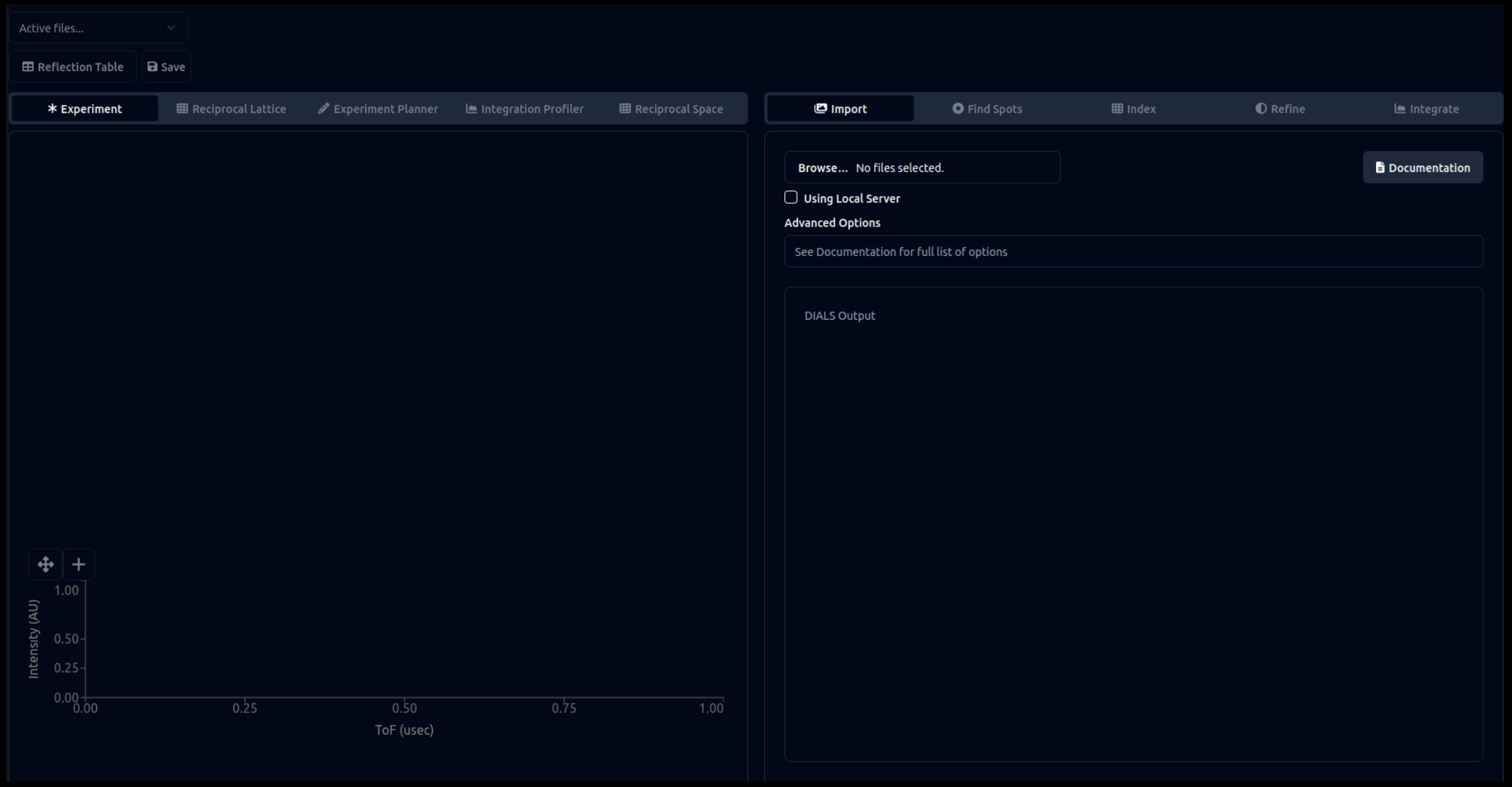
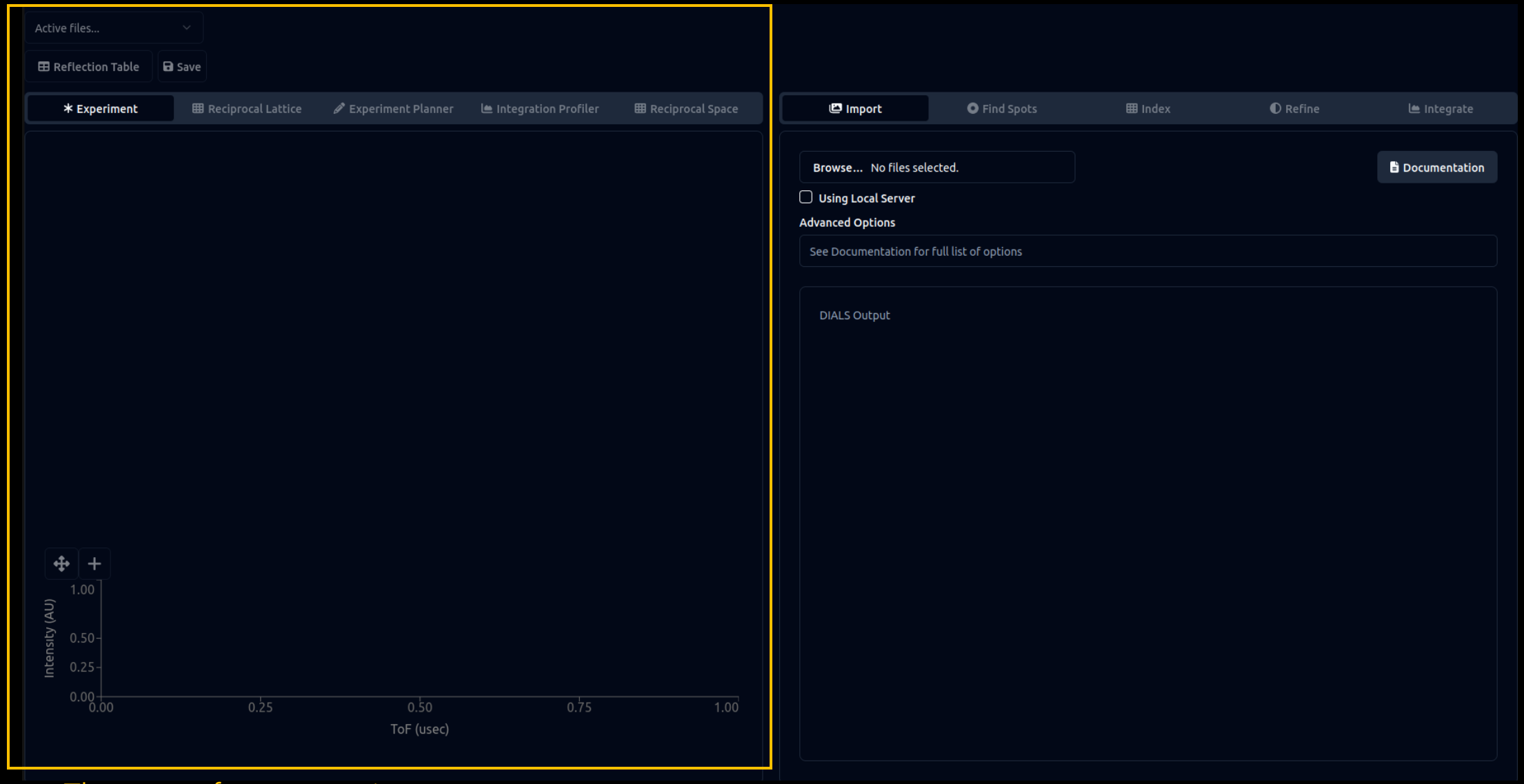
DIALS
Diffraction Integration for Advanced Light Sources
C++

Interface

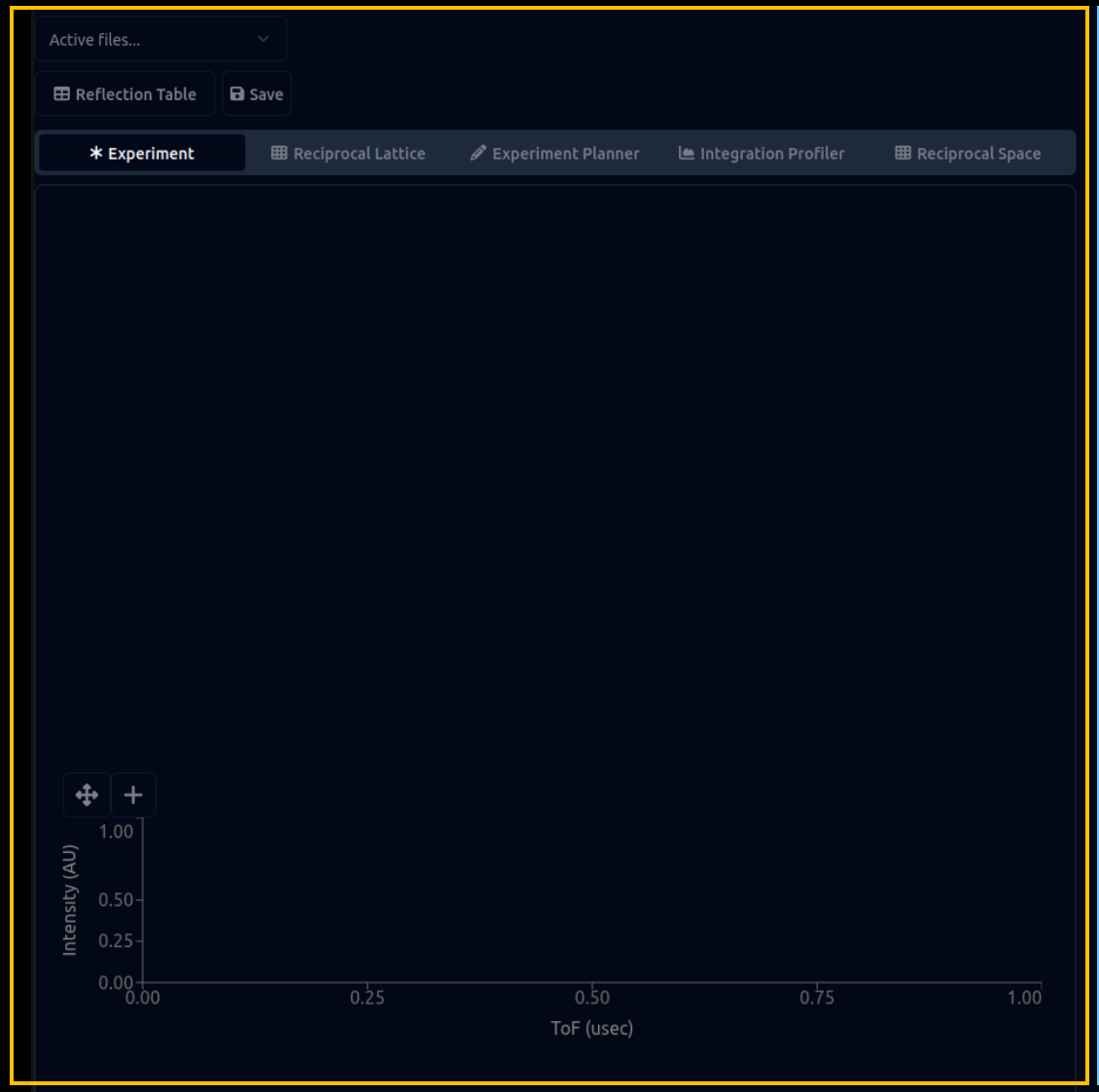

Active files...
Reflection Table
Save
Experiment
Reciprocal Lattice
Experiment Planner
Integration Profiler
Reciprocal Space
Import
Find Spots
Index
Refine
Integrate
Browse... No files selected.
Documentation
Using Local Server
Advanced Options
See Documentation for full list of options
DIALS Output
Intensity (AU)
1.00
0.50
0.25
0.00
0.00
0.25
0.50
0.75
1.00
ToF (usec)

Interface



- The state of your experiment

Interface



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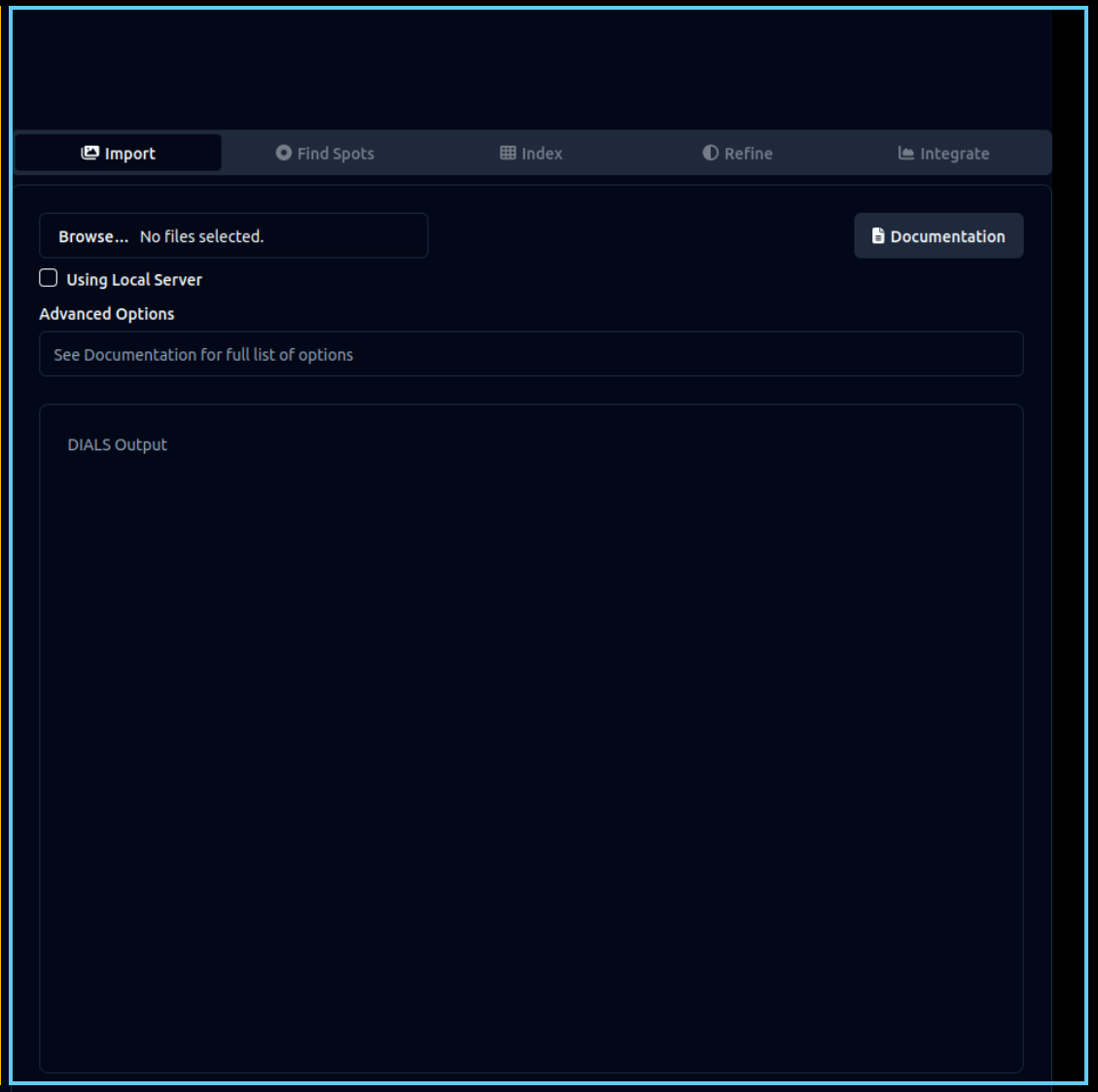
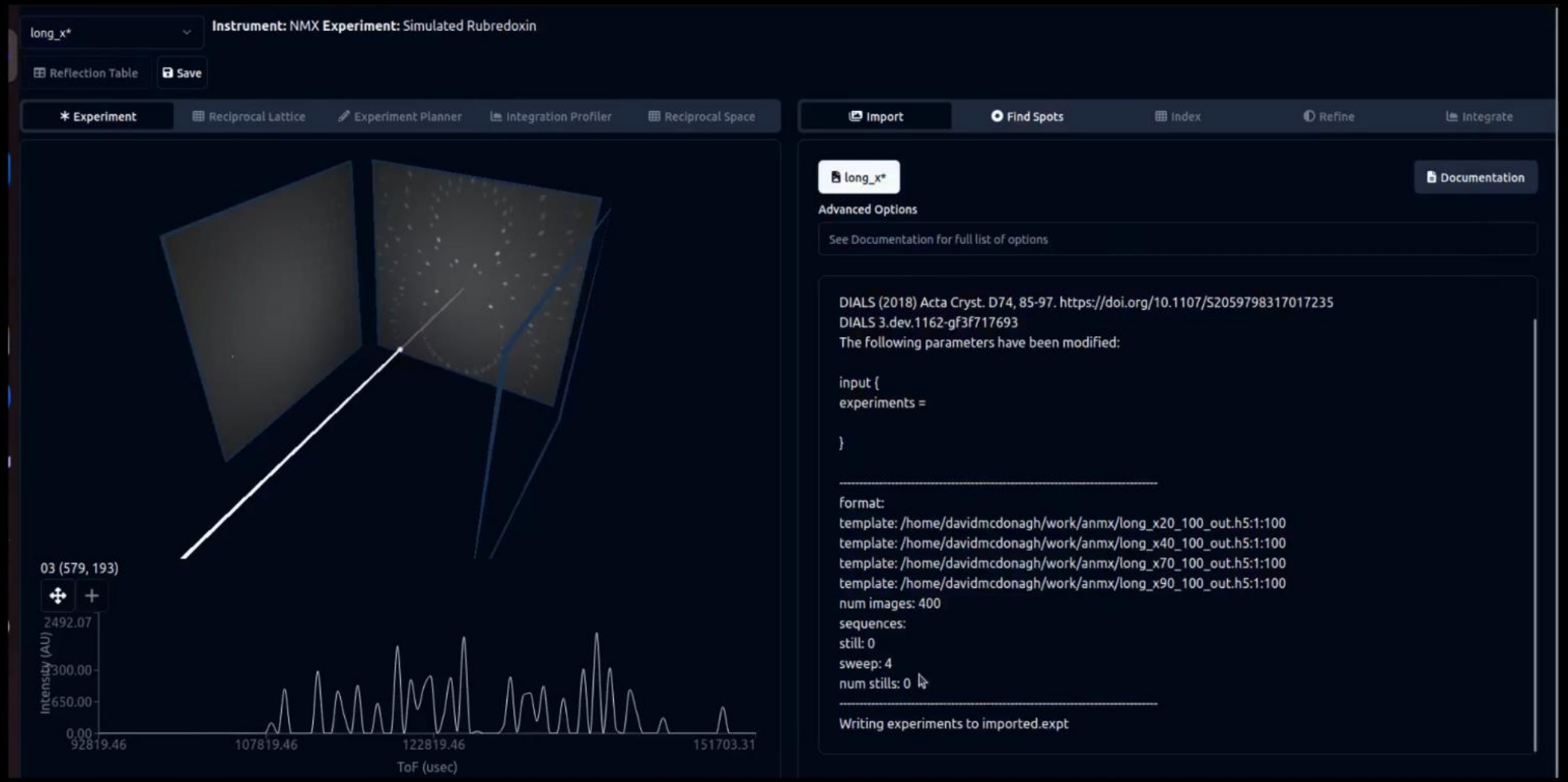


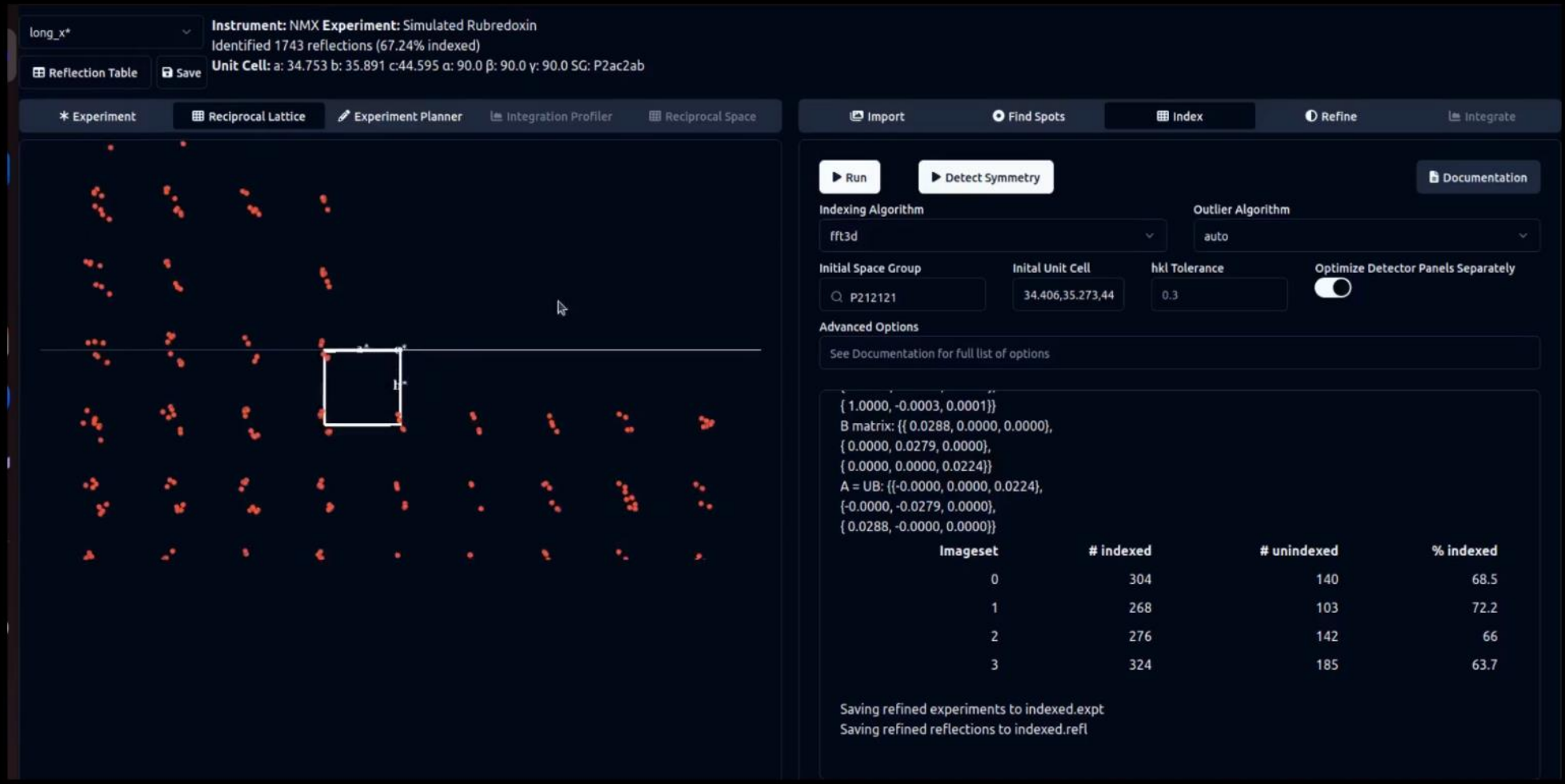
- Actions applied to your experiment

Interface: Importing Data

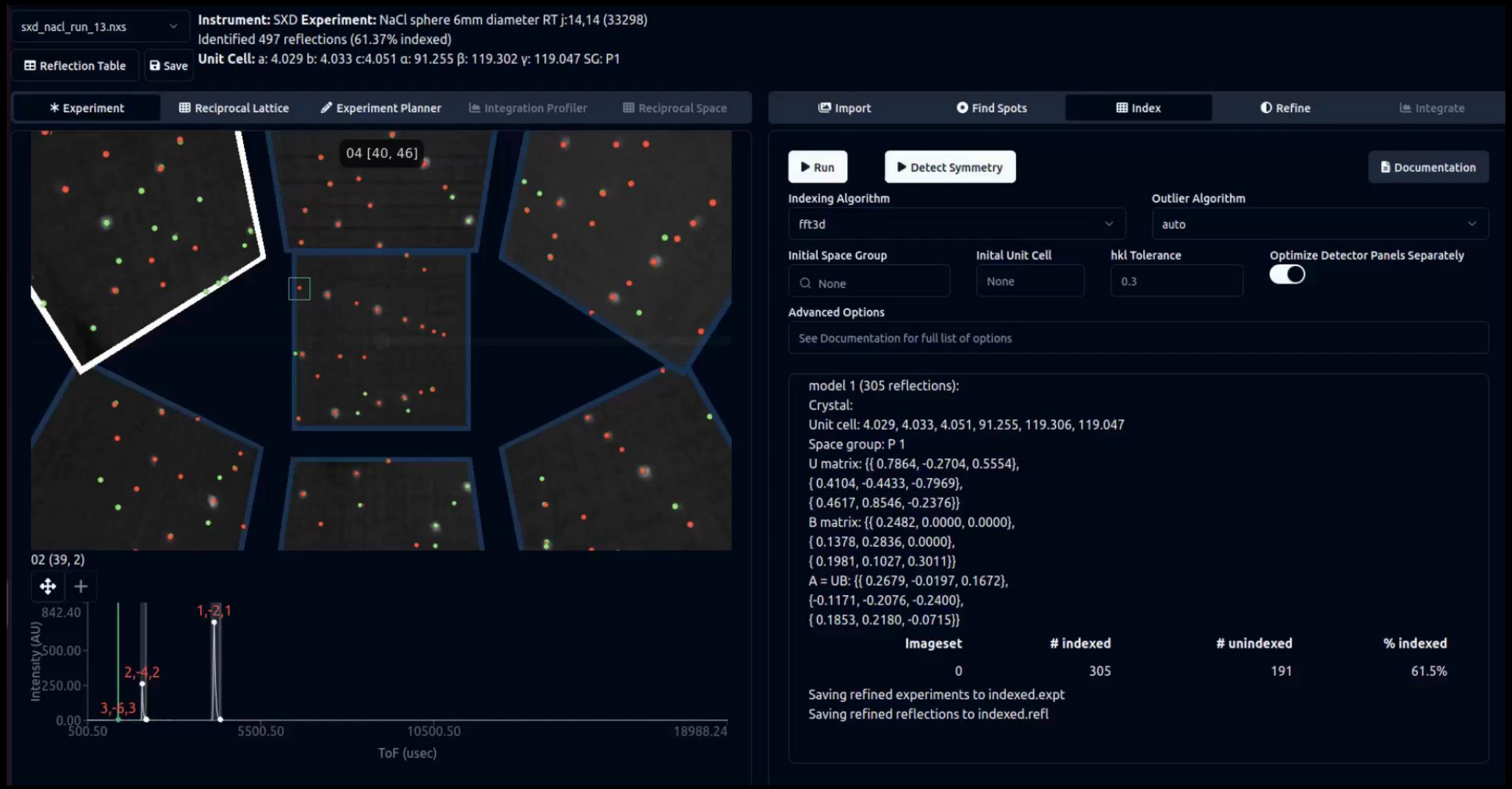


Interface: Spot Finding

Interface: Indexing



Interface: Planning and Applying Symmetry



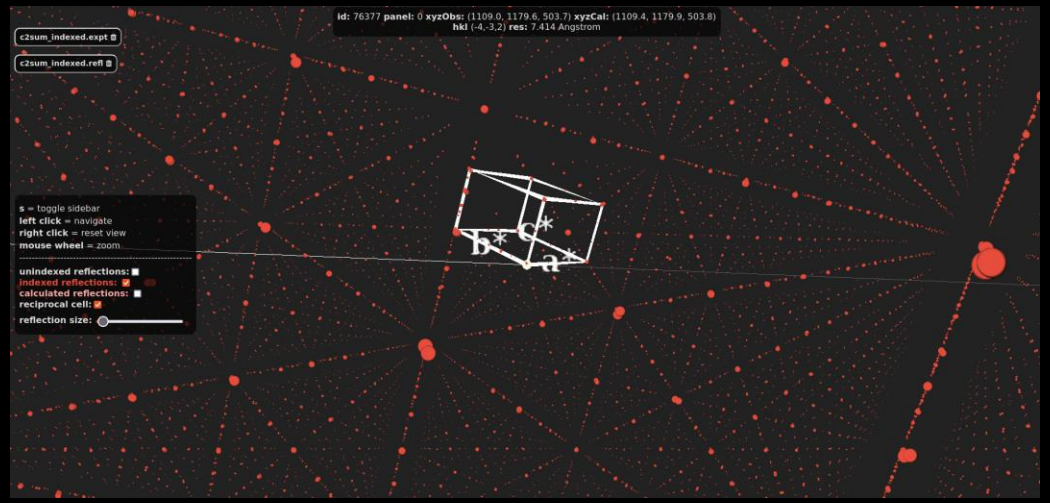
Interface: Integration Profiling

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)		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!



DIALS
Diffraction Integration for Advanced Light Sources

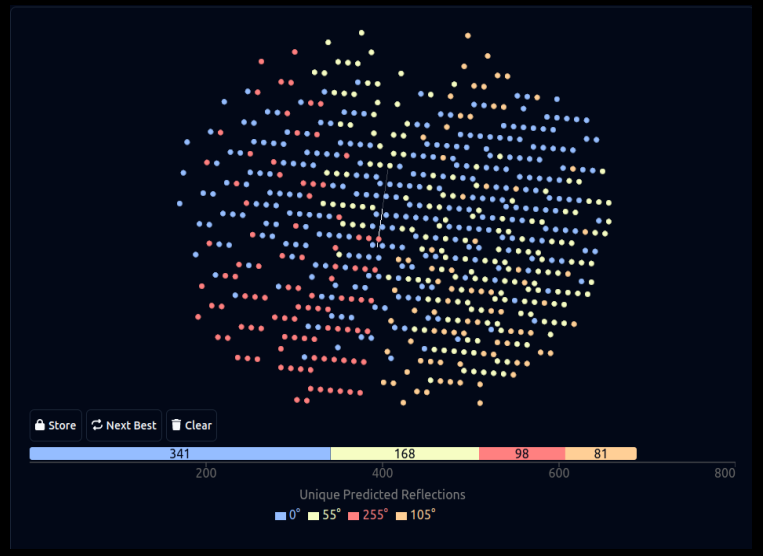
three.js

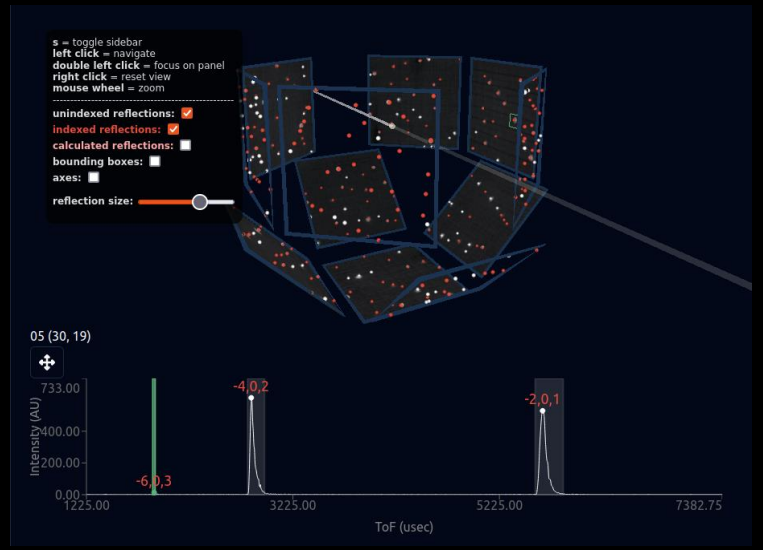
Science and Technology Facilities Council
ISIS Neutron and Muon Source
SXD
LMX

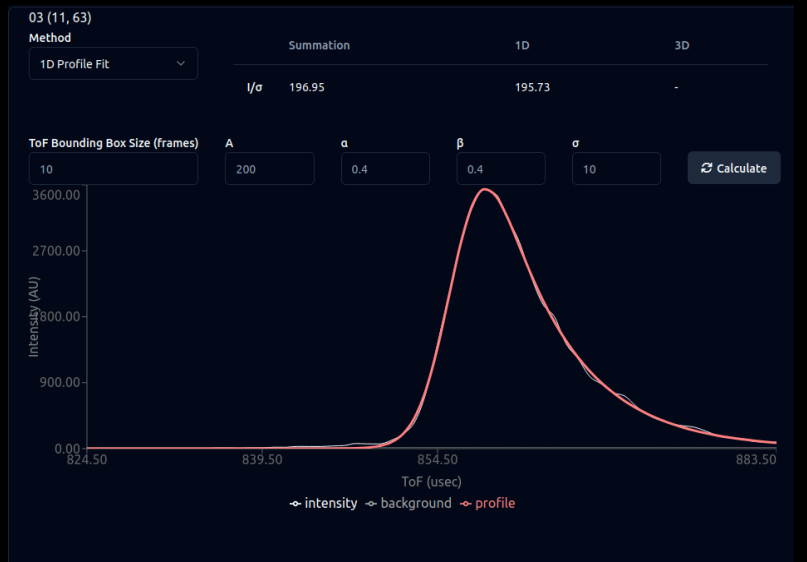
OAK RIDGE National Laboratory
MANDI

ess EUROPEAN SPALLATION SOURCE
NMX

VE RI TAS HARVARD
X-ray Laue

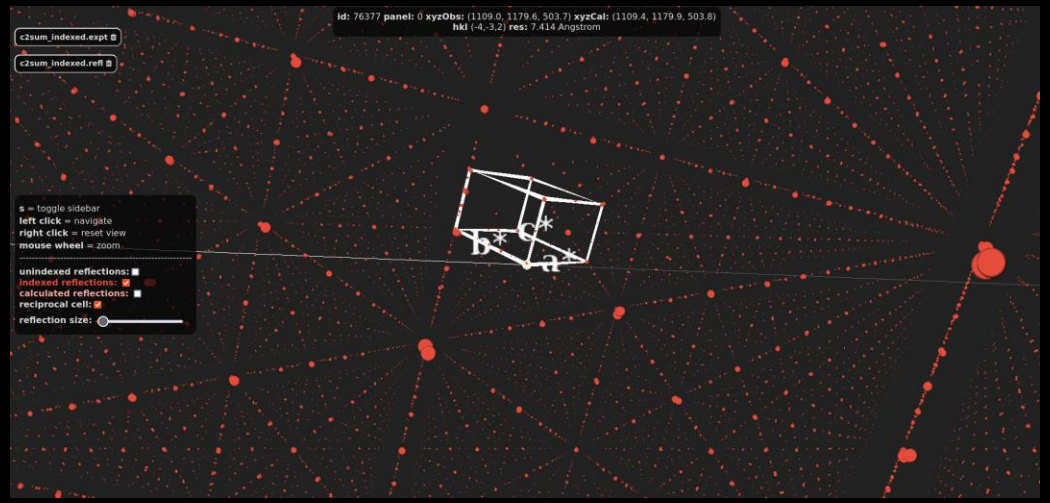




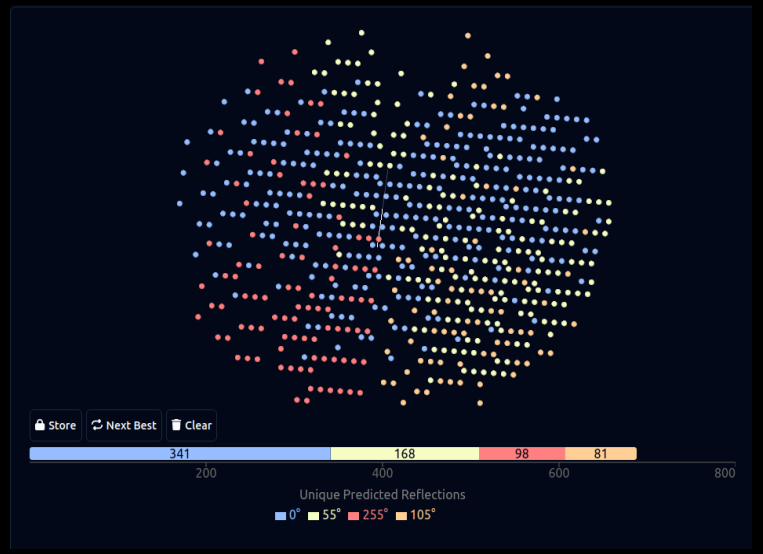


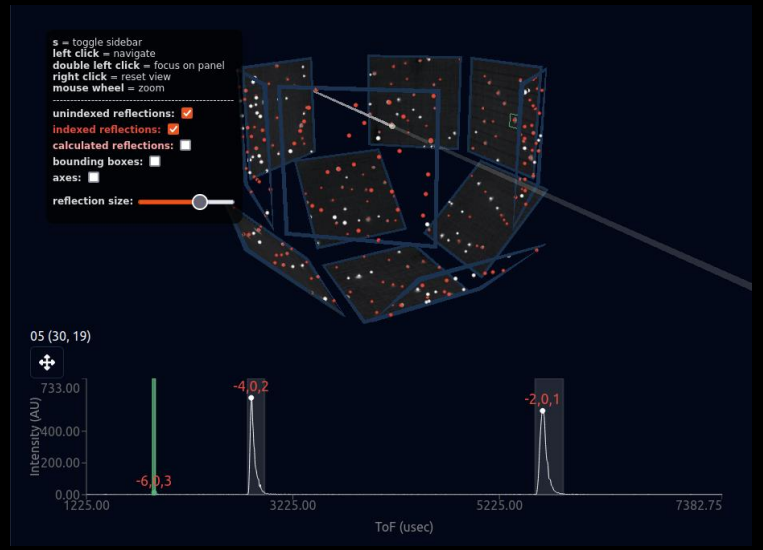
Status: Beta testing

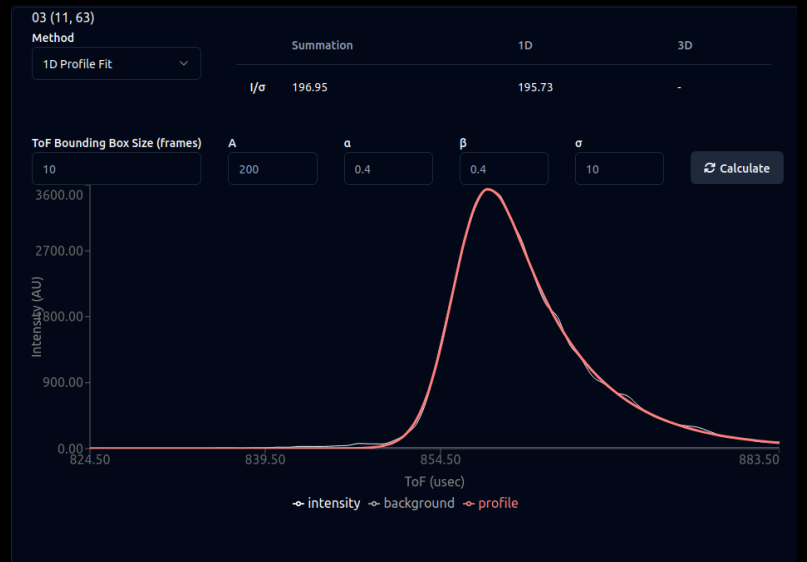
- Send me data! david.mcdonagh@stfc.ac.uk



dials.rs_mapper





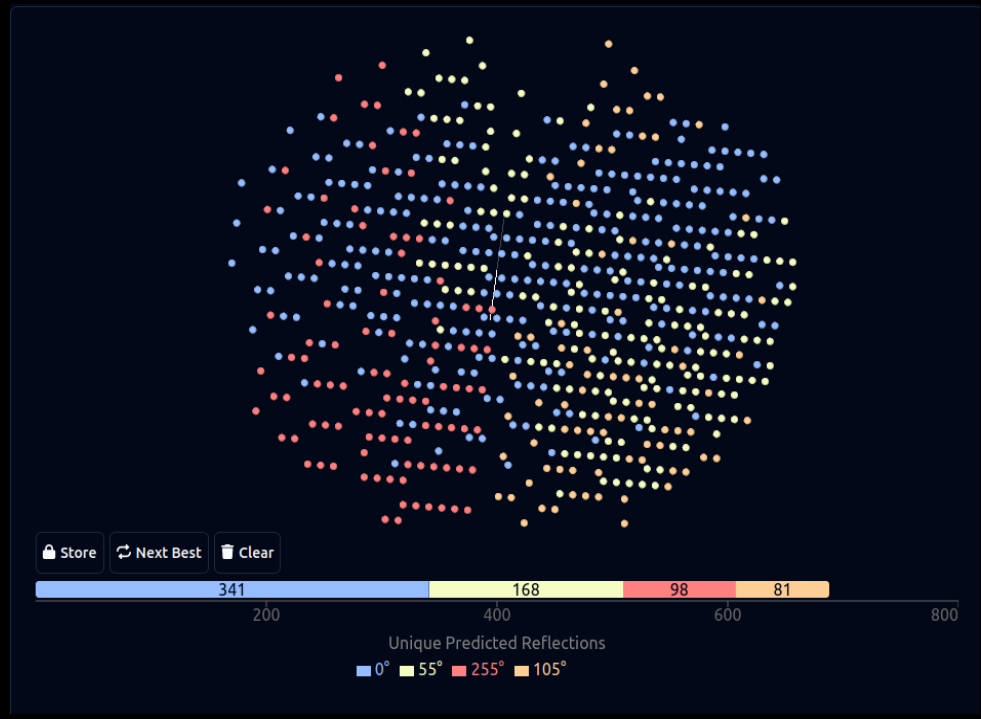


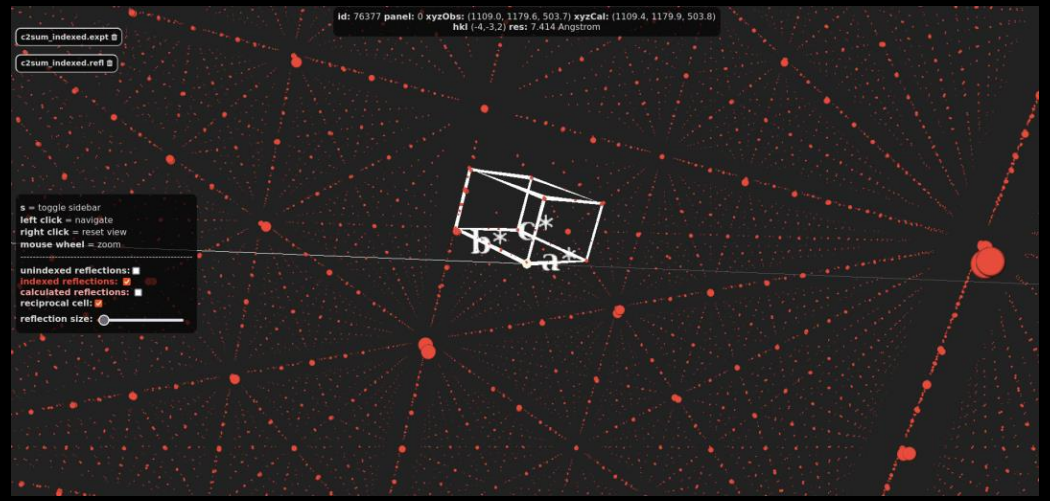
User Experience: Short-Term

- 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





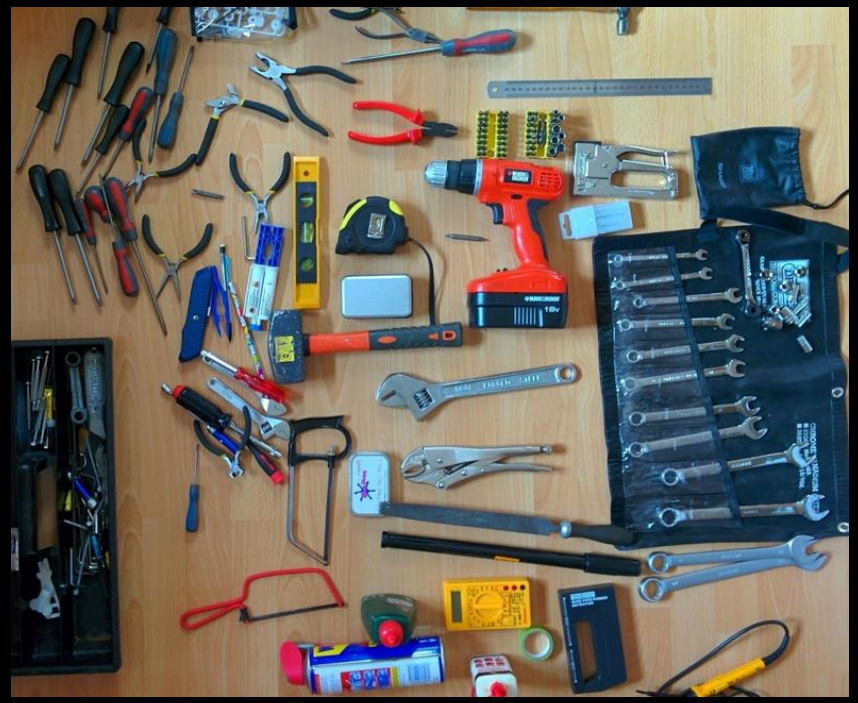
Jools Wills

Linking XRD facilities and CCP4 Cloud

CCP4

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



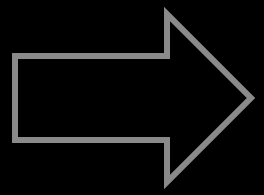
xia2

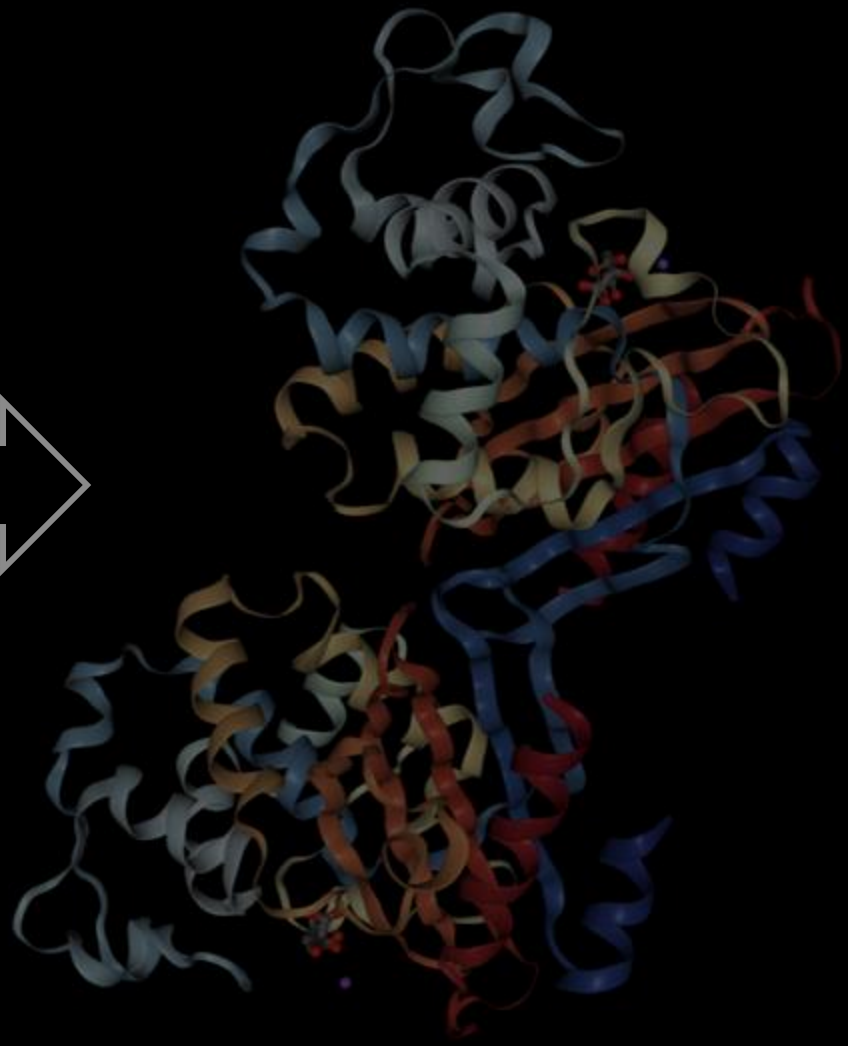
Marko Petrovic

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?





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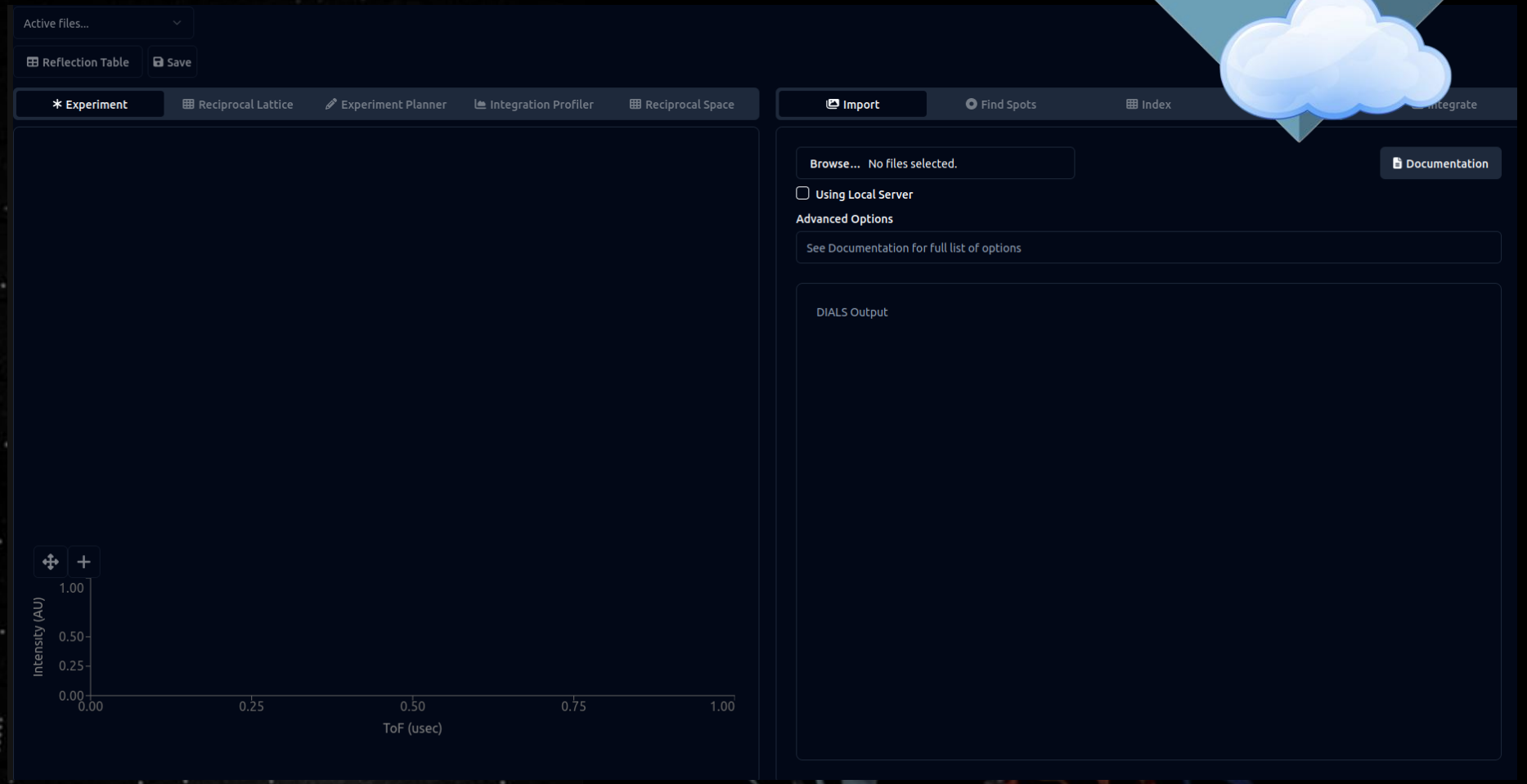

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Acknowledgements

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