Mantid at MLZ for powder and single crystal diffraction

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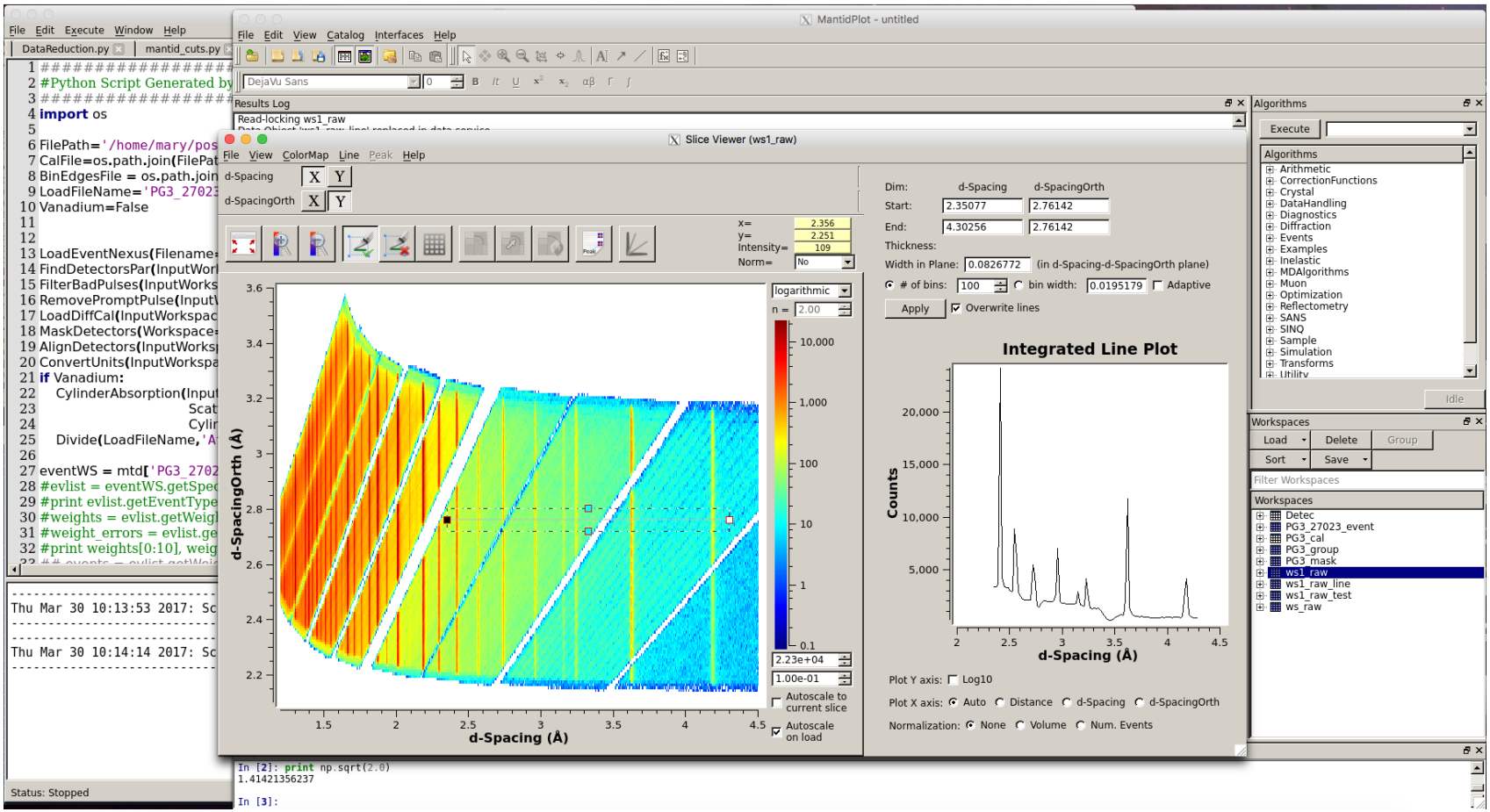
MLZ is a cooperation between

JÜLICH FORSCHUNGSZENTRUM

Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technische Universität München

Mantid



www.mantidproject.org

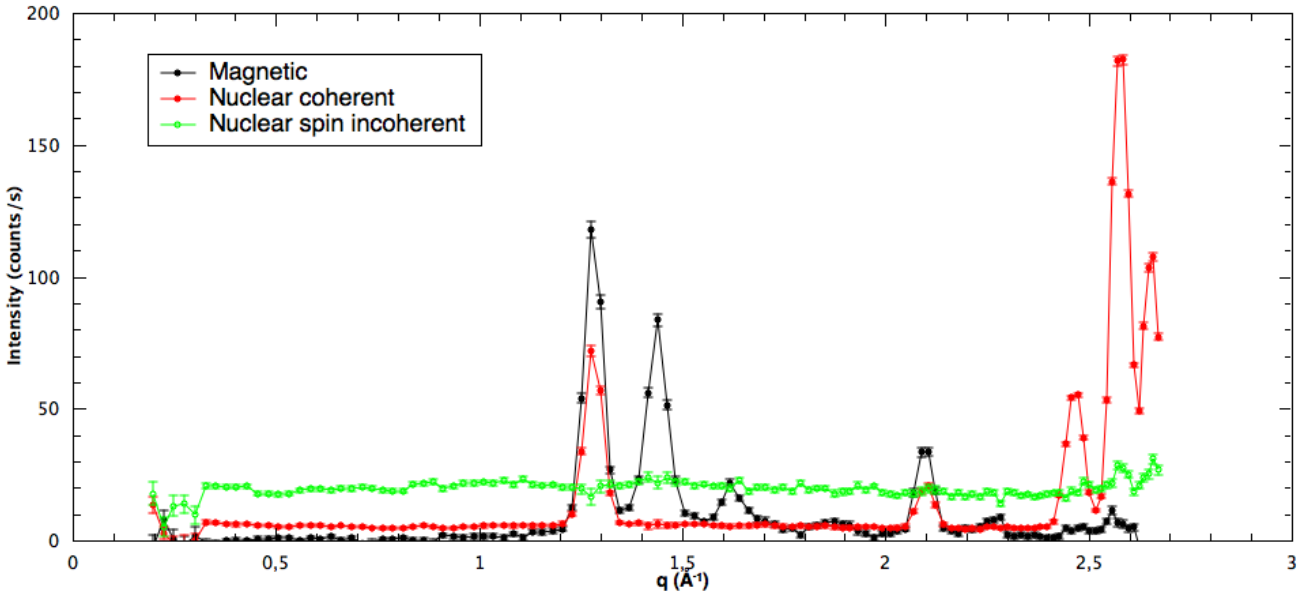
Mantid status at MLZ

- **TOFTOF:** in production, maintenance.
- **DNS diffraction mode:** commissioning in May, 2017;
- **DNS TOF/TOPAS:** in development.
- **POWTEX:** in development.

Diffraction data reduction: DNS

- Normalization by time or monitor
- Subtraction of instrument background
- Correction for detector efficiency (using Vanadium)
- Flipping ratio correction (using $Ni_{0.89}Cr_{0.11}$)
- Merge runs measured at different detector bank positions
- Multiple scattering correction (optional)
- Self-shielding correction (optional)

DNS: magnetic powder



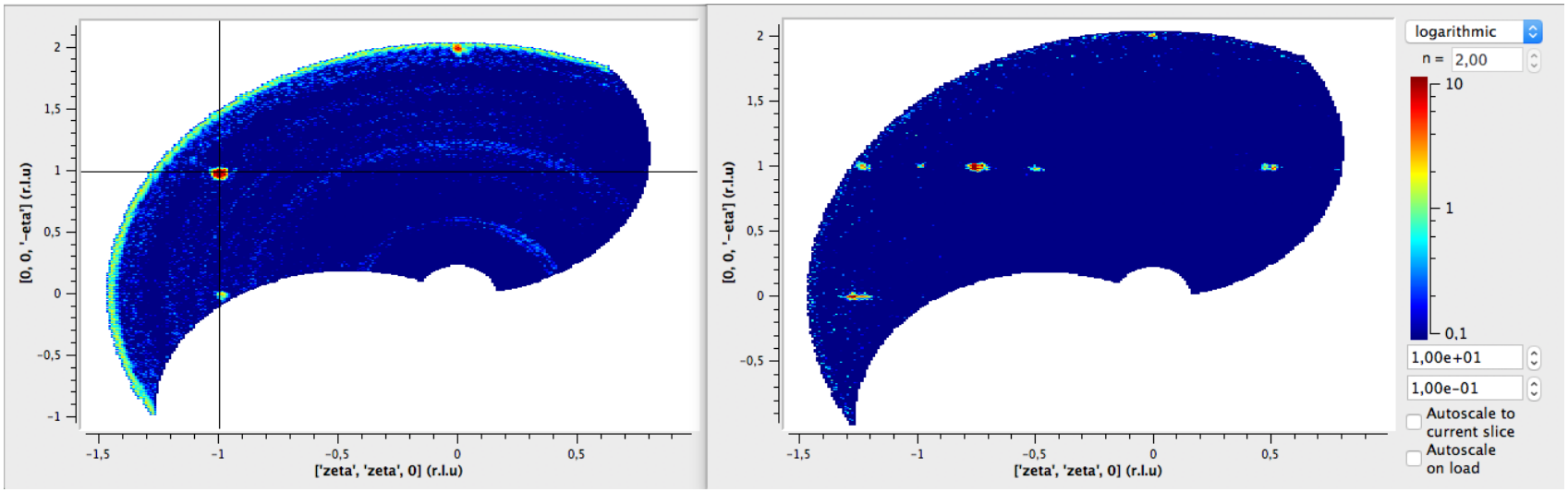
Data: courtesy K. Nemkovski

$$I_{mag} = I_{x,SF} + I_{y,SF} - 2 \cdot I_{z,SF}; \quad I_{incoh} = \frac{1}{3} \cdot (3 \cdot I_{z,SF} - I_{x,SF} - I_{y,SF})$$

$$I_{coh} = I_{z,NSF} - \frac{1}{2} \cdot I_{mag} - \frac{1}{3} \cdot I_{incoh}$$

DNS: magnetic single crystal

Data are accumulated into a multidimensional Mantid workspace.



Data: courtesy K. Nemkovski

$$I_{x,\,NSF} = \frac{1}{3}\cdot I^{spin}_{incoh} + I^{isot}_{incoh} + I_{coh} + 0; \quad I_{x,\,SF} = \frac{2}{3}\cdot I^{spin}_{incoh} + 0 + 0 + I^{y}_{mag} + I^{z}_{mag}$$

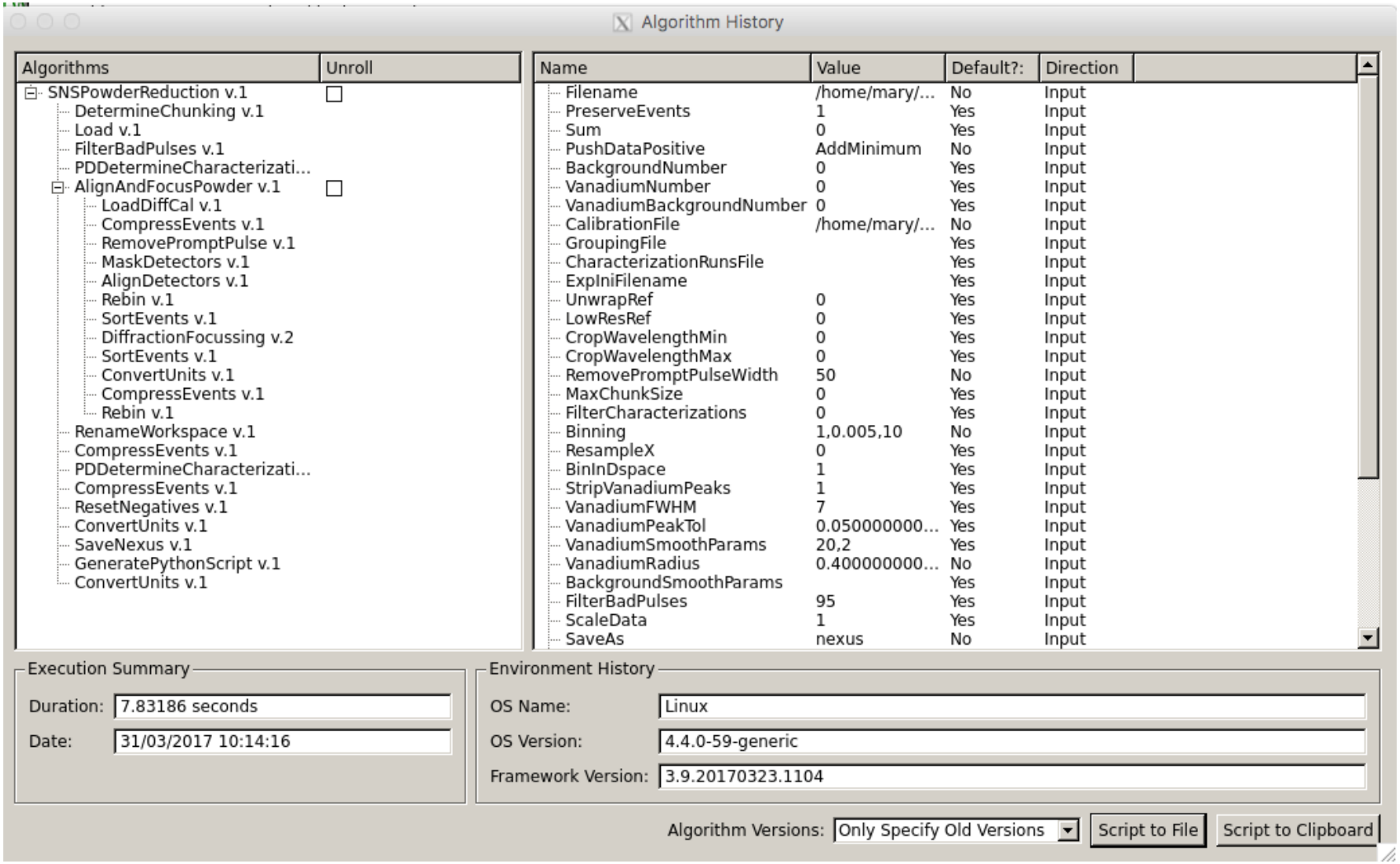
DNS: presently in development

- Multiple spin-flip scattering correction based on the approach of R. Zorn (NIM A **479** (2002), 568–584).

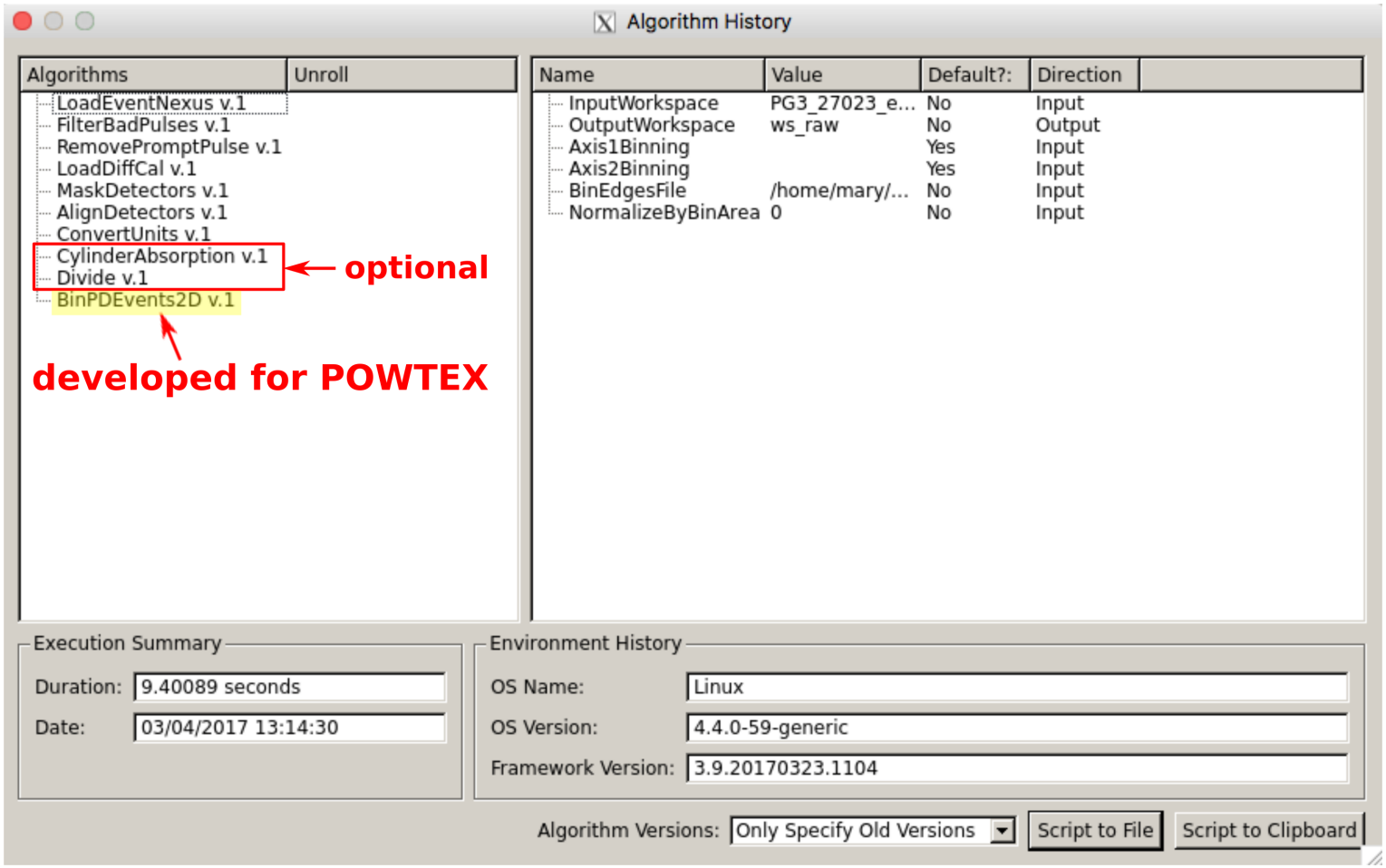
- Normalization: order of operations is important to correctly account for the statistical weight of the data (J. Appl. Cryst. (2016) **49**, 497–506):

$$\left.\frac{d\sigma}{d\Omega}\right|_{\text{old}} = \frac{1}{n}\sum_i \frac{N_i}{V_i} \quad \text{vs.} \quad \left.\frac{d\sigma}{d\Omega}\right|_{\text{new}} = \frac{\sum_i N_i}{\sum_i V_i}$$

SNS Powder diffraction reduction



POWTEX data reduction



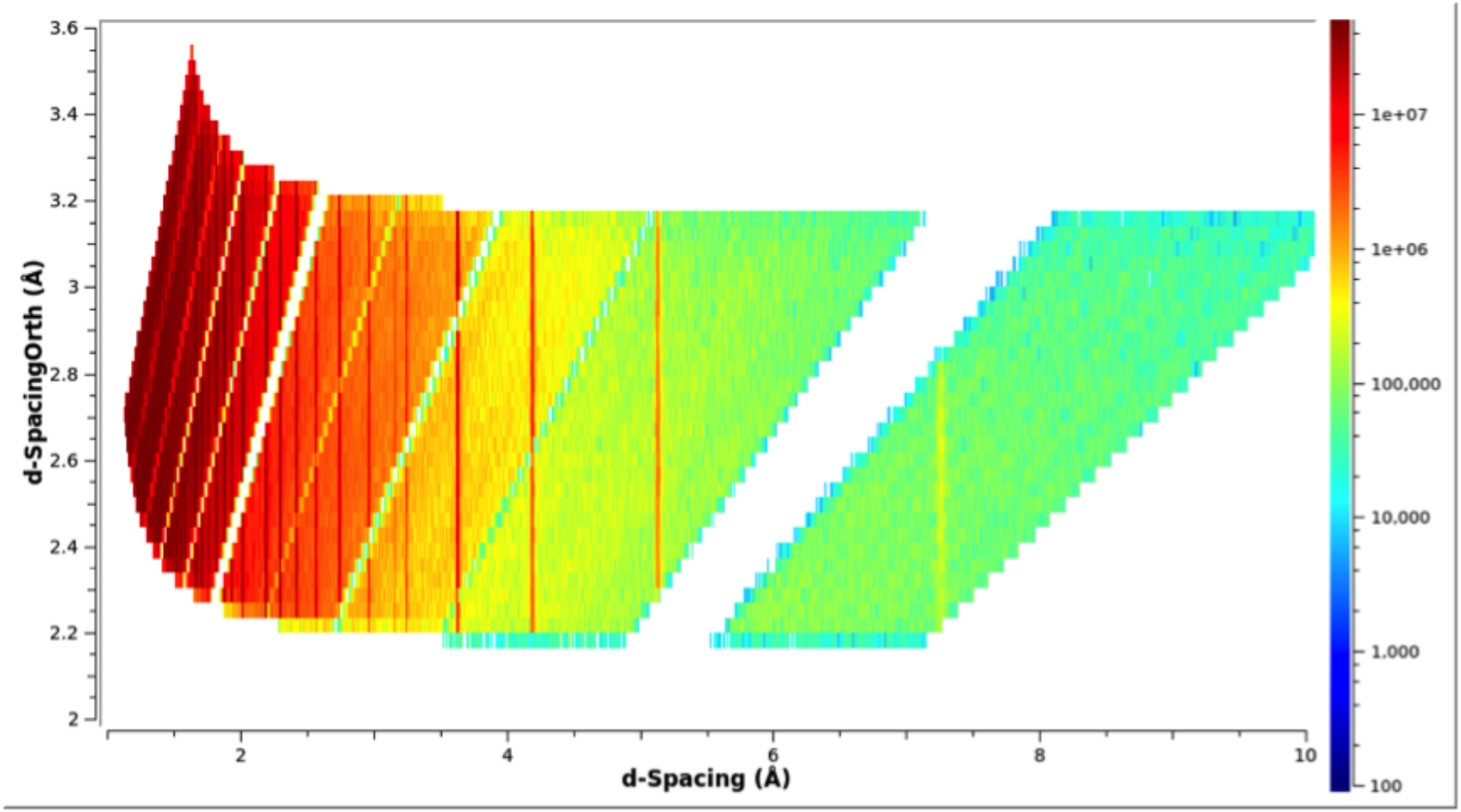
POWTEX data reduction: 2D binning

Algorithm `BinPDEvents2D` takes the event workspace in $(\lambda, 2\vartheta)$ axes and produces the matrix workspace with $(d, d_\perp)$ axes, where

$$d = \frac{\lambda}{2 \sin \vartheta}$$
$$d_\perp = \sqrt{\lambda^2 - 2 \log \cos \vartheta}$$

J. Appl. Cryst. (2015) **48**, 1627–1636

2D binning: preliminary result



Data: courtesy P. Jacobs, A. Houben

Diffraction data analysis: single crystal

A

- AddPeak
- AddPeakHKL

C

- CalculatePeaksHKL
- CentroidPeaks
- CombinePeaksWorkspaces
- CreatePeaksWorkspace

D

- DiffPeaksWorkspaces

F

- FilterPeaks

F

- FindSXPeaks

G

- GeneratePeaks

I

- IndexPeaks
- IndexSXPeaks

M

- MaskPeaksWorkspace

P

- PeaksInRegion
- PeaksOnSurface

P

- PredictFractionalPeaks
- PredictPeaks

S

- ShowPeakHKLOffsets
- SortHKL
- SortPeaksWorkspace
- StatisticsOfPeaksWorkspace

T

- TransformHKL

Category: Crystal

docs.mantidproject.org/nightly/algorithms/categories/Crystal/Peaks.html

Diffraction data analysis: fitting

C

- CreateLeBailFitInput

E

- EnggFitDIFCFromPeaks
- EnggFitPeaks

F

- FitPowderDiffPeaks

G

- GSASIIRefineFitPeaks

L

- LeBailFit

P

- PawleyFit

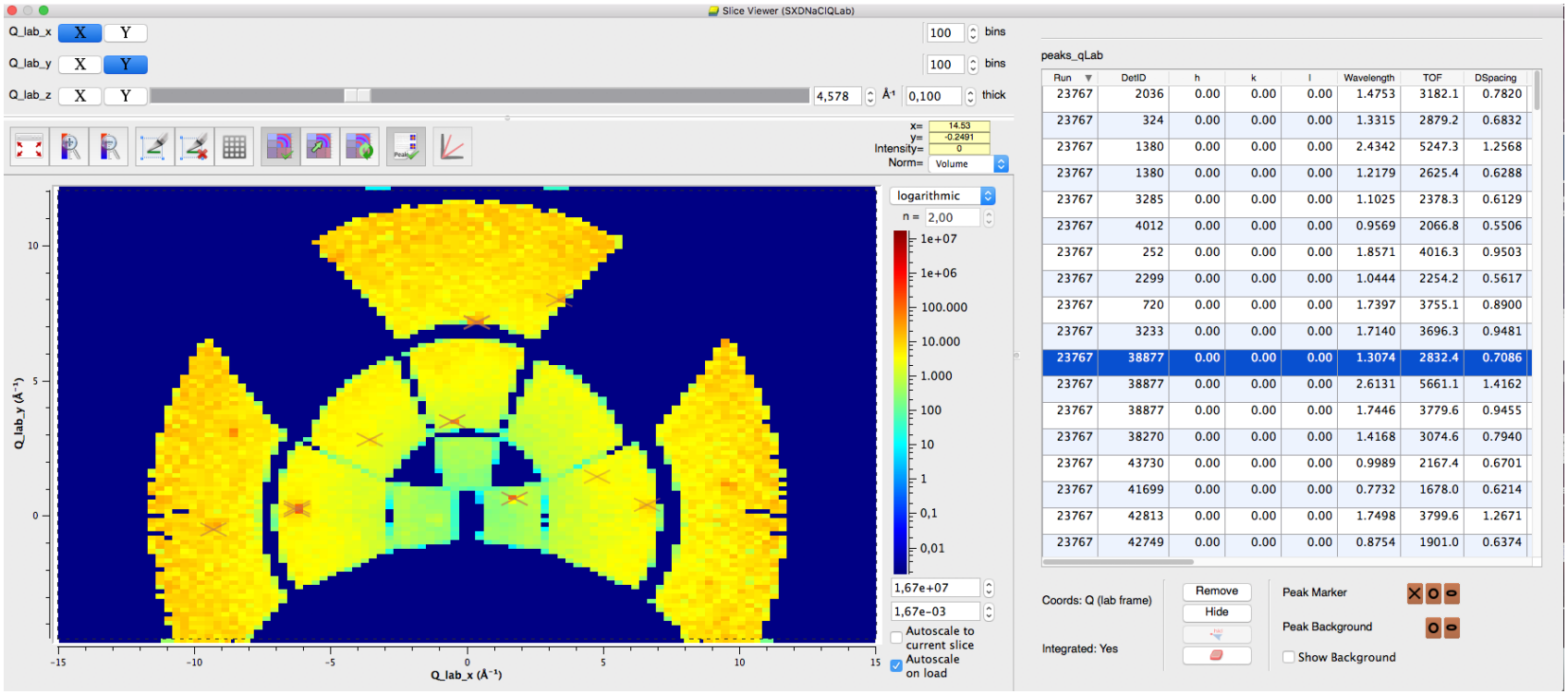
R

- RefinePowderDiffProfileSeq
- RefinePowderInstrumentParameters

Category: Diffraction

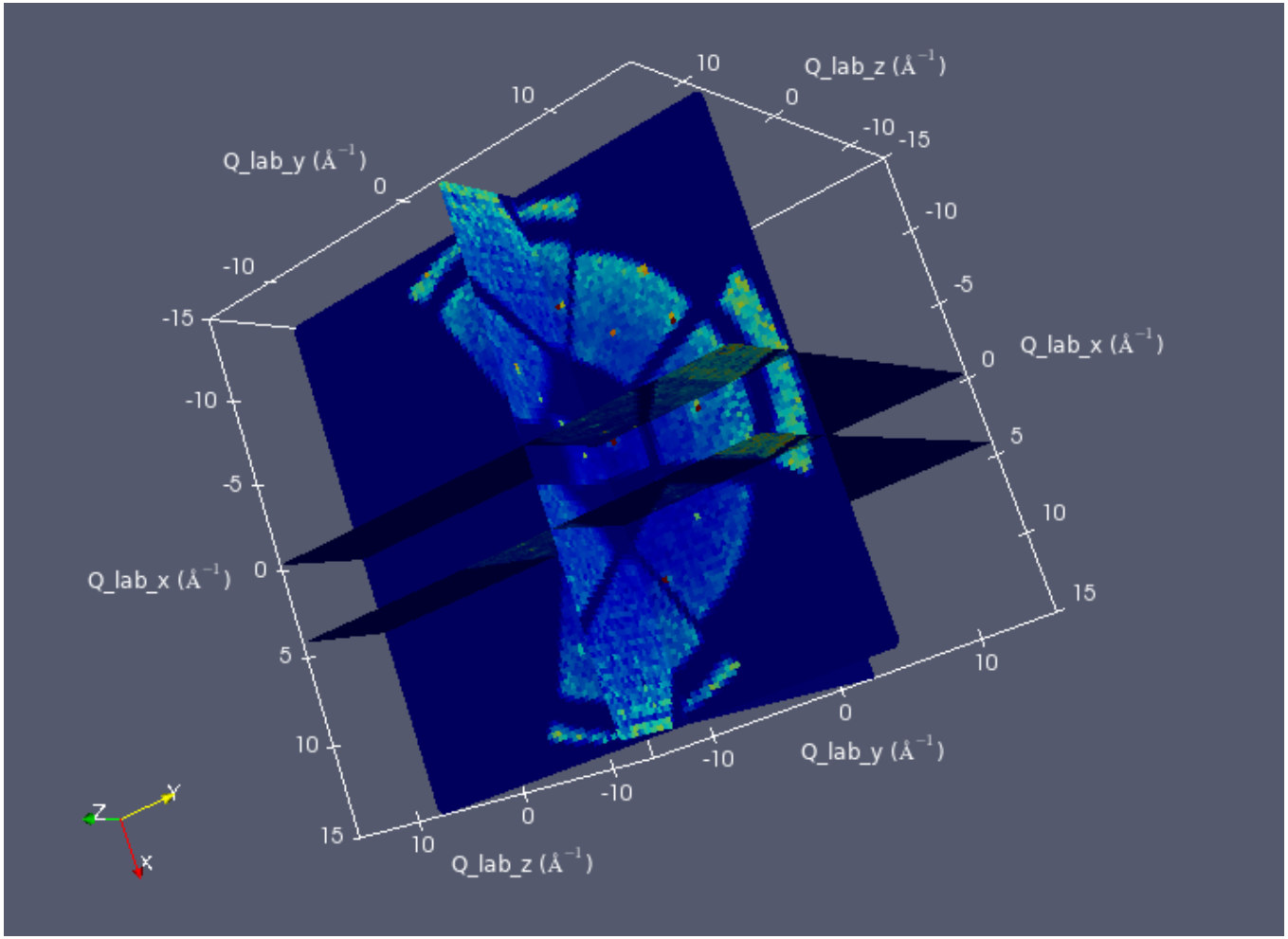
docs.mantidproject.org/nightly/algorithms/categories/Diffraction/Fitting.html

Data visualization: Mantid Slice Viewer



Data: Mantid training course

Data visualization: Mantid VATES



Issues to address

Support of ragged workspaces:

X bins $x_0, x_1, \ldots x_{n_j}$ for each j-th spectrum can vary, but the number n_j must stay constant. Many Mantid algorithms do not operate on ragged workspaces.

docs.mantidproject.org/nightly/concepts/Ragged_Workspace.html

Support of 2D data:

- Unit conversion in 2D
- Normalization by the bin area
- 2D fitting/refinement

Thank you for your attention!