

# Mantid at MLZ for powder and single crystal diffraction

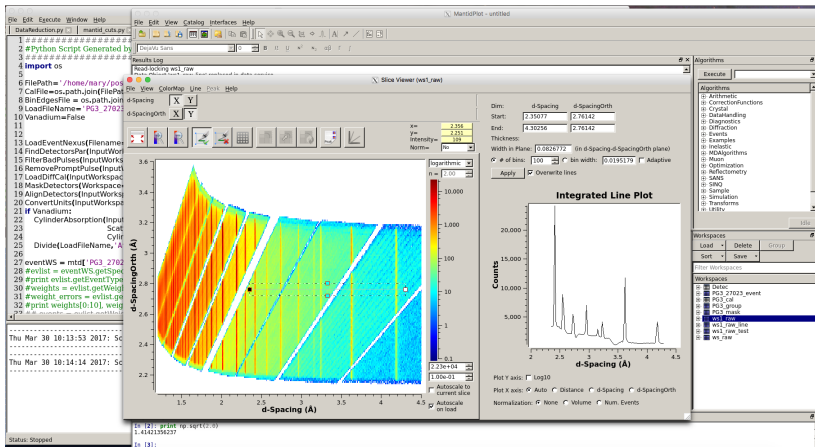
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JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

7th April 2017

MLZ is a cooperation between

# Mantid



The screenshot displays the Mantid software interface with the following components:

- Python Script (Left Panel):** A script titled 'mantid\_cuts.py' containing the following code:
 

```

1 #####
2 #Python Script Generated by Mantid
3 #####
4 Import os
5
6 FilePath = "/home/nary/po3"
7 CalFile = os.path.join(FilePath,
8 BinEdgesFile = os.path.join(
9 LoadFileName = "PG3_27023"
10 Vanadium = False
11
12
13 LoadEventNexus(FileName=
14 FindDetectorsPart(InputWorksp
15 FilterBadPulses(InputWorksp
16 RemovePromptPulse(Input
17 LoadDiffCal(InputWorkspac
18 MaskDetectors(Workspac
19 AlignDetectors(InputWorksp
20 ConvertUnits(InputWorksp
21 if Vanadium:
22 CylinderAbsorption(Input
23 Scale
24 Cylind
25 Divide(LoadFileName, A
26
27 eventWS = mtd["PG3_27023"]
28 #evlist = eventWS.getSp
29 #print evlist.getEventTyp
30 #weights = evlist.getEvent
31 #weight_error = evlist.g
32 #print weights[0:10], weig
33 # # #
34 # # #

```
- Slice Viewer (Center Panel):** A 2D heatmap plot showing intensity as a function of d-spacing (x-axis, 1.5 to 4.5 Å) and d-spacingOrth (y-axis, 2.2 to 3.6 Å). The plot features a color scale from 0.1 to 10,000 and several white diagonal lines representing Bragg reflections.
- Integrated Line Plot (Right Panel):** A line plot showing 'Counts' (y-axis, 0 to 20,000) versus 'd-spacing (Å)' (x-axis, 2 to 4.5). The plot displays a series of sharp peaks corresponding to the reflections in the slice viewer.
- Algorithms Panel (Far Right):** A list of available algorithms such as 'Arithmetic', 'Crystal', 'DataHandling', 'Diagnosics', 'Diffraction', 'Events', 'Examples', 'Inelastic', 'MDAlgorithms', 'Mean', 'Optimization', 'Reflectometry', 'SANS', 'SNO', 'Strip', 'Simulation', 'Transforms', and 'UnitV'.
- Workspaces Panel (Bottom Right):** A list of loaded workspaces including 'PG3\_27023\_event', 'PG3\_cal', 'PG3\_group', 'PG3\_mask', 'wsl\_raw\_bin', 'wsl\_raw\_bin\_test', and 'wsl\_raw'.

[www.mantidproject.org](http://www.mantidproject.org)

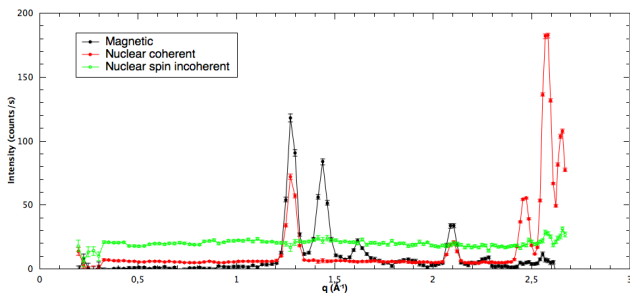
## Mantid status at MLZ

- **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  $\text{Ni}_{0.89}\text{Cr}_{0.11}$ )
- Merge runs measured at different detector bank positions
- Multiple scattering correction (optional)
- Self-shielding correction (optional)

# DNS: magnetic powder



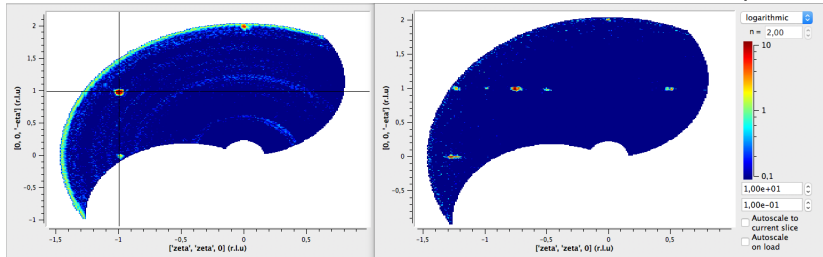
Data: courtesy K. Nemkovski

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

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

# DNS: magnetic single crystal

Data are accumulated into a multidimensional Mantid workspace.



Data: courtesy K. Nemkovski

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

## 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

Algorithm History

Algorithms	Unroll	Name	Value	Default?:	Direction
[-] SNSPowderReduction v.1	<input type="checkbox"/>	-- Filename	/home/mary/...	No	Input
[-] DetermineChunking v.1	<input type="checkbox"/>	-- PreserveEvents	1	Yes	Input
[-] Load v.1		-- Sum	0	Yes	Input
[-] FilterBadPulses v.1		-- PushDataPositive	AddMinimum	No	Input
[-] PPDetermineCharacterizati...		-- BackgroundNumber	0	Yes	Input
[-] AlignAndFocusPowder v.1	<input type="checkbox"/>	-- VanadiumNumber	0	Yes	Input
[-] LoadDiffCal v.1		-- VanadiumBackgroundNumber	0	Yes	Input
[-] CompressEvents v.1		-- CalibrationFile	/home/mary/...	No	Input
[-] RemovePromptPulse v.1		-- GroupingFile		Yes	Input
[-] MaskDetectors v.1		-- CharacterizationRunsFile		Yes	Input
[-] AlignDetectors v.1		-- ExplIniFilename		Yes	Input
[-] Rebin v.1		-- UnwrapRef	0	Yes	Input
[-] SortEvents v.1		-- LowResRef	0	Yes	Input
[-] DiffractionFocussing v.2		-- CropWavelengthMin	0	Yes	Input
[-] SortEvents v.1		-- CropWavelengthMax	0	Yes	Input
[-] ConvertUnits v.1		-- RemovePromptPulseWidth	50	No	Input
[-] CompressEvents v.1		-- MaxChunkSize	0	Yes	Input
[-] Rebin v.1		-- FilterCharacterizations	0	Yes	Input
[-] RenameWorkspace v.1		-- Binning	1,0.005,10	No	Input
[-] CompressEvents v.1		-- ResampleX	0	Yes	Input
[-] PPDetermineCharacterizati...		-- BinInDspace	1	Yes	Input
[-] CompressEvents v.1		-- StripVanadiumPeaks	1	Yes	Input
[-] ResetNegatives v.1		-- VanadiumFWHM	7	Yes	Input
[-] ConvertUnits v.1		-- VanadiumPeakTol	0.050000000...	Yes	Input
[-] SaveNexus v.1		-- VanadiumSmoothParams	20.2	Yes	Input
[-] GeneratePythonScript v.1		-- VanadiumRadius	0.400000000...	No	Input
[-] ConvertUnits v.1		-- BackgroundSmoothParams		Yes	Input
		-- FilterBadPulses	95	Yes	Input
		-- ScaleData	1	Yes	Input
		-- SaveAs	nexus	No	Input

Execution Summary		Environment History	
Duration:	7.83186 seconds	OS Name:	Linux
Date:	31/03/2017 10:14:16	OS Version:	4.4.0-59-generic
		Framework Version:	3.9.20170323.1104

Algorithm Versions:



# POWTEX data reduction

Algorithm History

Algorithms	Unroll	Name	Value	Default?:	Direction
- LoadEventNexus v.1		- InputWorkspace	PG3_27023_e...	No	Input
- FilterBadPulses v.1		- OutputWorkspace	ws_raw	No	Output
- RemovePromptPulse v.1		- Axis1Binning		Yes	Input
- LoadDiffCal v.1		- Axis2Binning		Yes	Input
- MaskDetectors v.1		- BinEdgesFile	/home/mary/...	No	Input
- AlignDetectors v.1		- NormalizeByBinArea	0	No	Input
- ConvertUnits v.1					
- CylinderAbsorption v.1					
- Divide v.1					
- BinPDEvents2D v.1					

**optional** (points to CylinderAbsorption v.1)

**developed for POWTEX** (points to BinPDEvents2D v.1)

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Execution Summary

Duration: 9.40089 seconds

Date: 03/04/2017 13:14:30

Environment History

OS Name: Linux

OS Version: 4.4.0-59-generic

Framework Version: 3.9.20170323.1104

Algorithm Versions: Only Specify Old Versions [v] Script to File Script to Clipboard

## POWTEX data reduction: 2D binning

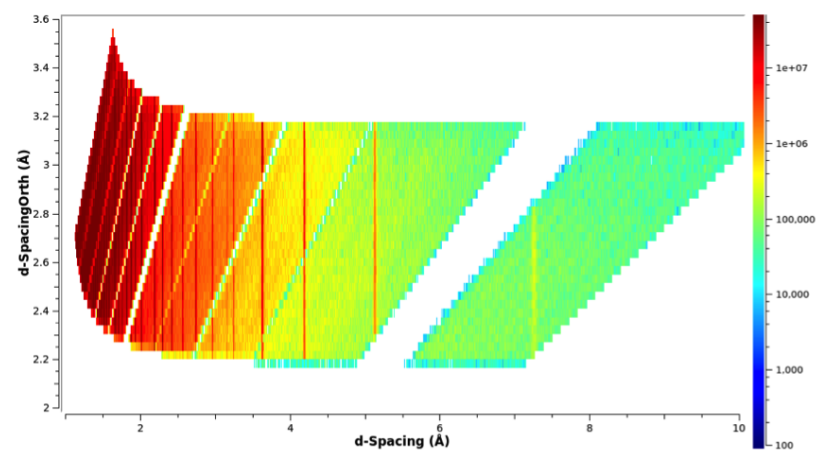
Algorithm BinPDEvents2D takes the event workspace in  $(\lambda, 2\vartheta)$  axes and produces the matrix workspace with  $(d, d_{\perp})$  axes, where

$$d = \frac{\lambda}{2 \sin \vartheta}$$

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

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

Category: Crystal

## F

- FindSXPeaks

## G

- GeneratePeaks

## I

- IndexPeaks
- IndexSXPeaks

## M

- MaskPeaksWorkspace

## P

- PeaksInRegion
- PeaksOnSurface

## P

- PredictFractionalPeaks
- PredictPeaks

## S

- ShowPeakHKLOffsets
- SortHKL
- SortPeaksWorkspace
- StatisticsOfPeaksWorkspace

## T

- TransformHKL

[docs.mantidproject.org/nightly/algorithms/categories/Crystal/Peaks.html](https://docs.mantidproject.org/nightly/algorithms/categories/Crystal/Peaks.html)

# Diffraction data analysis: fitting

## C

- CreateLeBailFitInput

## E

- EnggFitDIFCFromPeaks
- EnggFitPeaks

Category: Diffraction

## F

- FitPowderDiffPeaks

## G

- GSASIIRefineFitPeaks

## L

- LeBailFit

## P

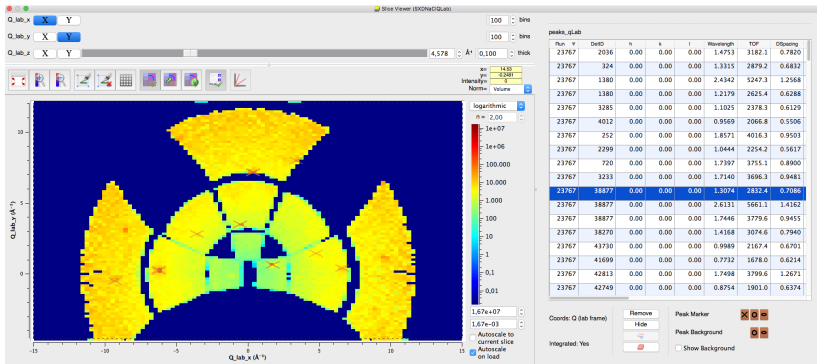
- PawleyFit

## R

- RefinePowderDiffProfileSeq
- RefinePowderInstrumentParameters

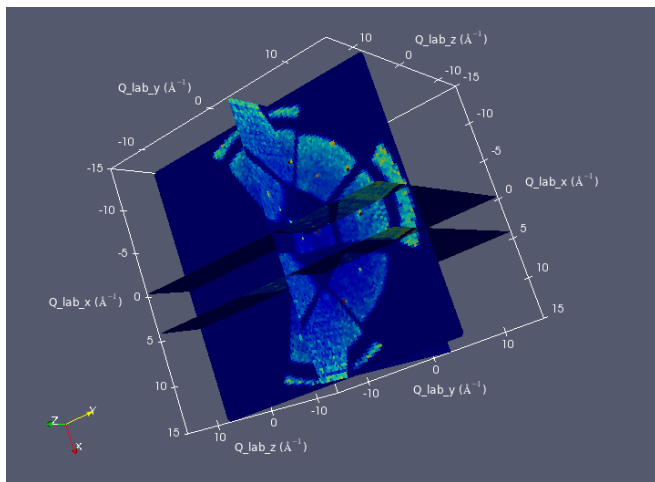
[docs.mantidproject.org/nightly/algorithms/categories/Diffraction/Fitting.html](https://docs.mantidproject.org/nightly/algorithms/categories/Diffraction/Fitting.html)

# Data visualization: Mantid Slice Viewer



Data: Mantid training course

# Data visualization: Mantid VATES



## Issues to address

### Support of ragged workspaces:

$X$  bins  $x_0, x_1, \dots, x_{n_j}$  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](https://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!