

Mantid for MLZ instruments

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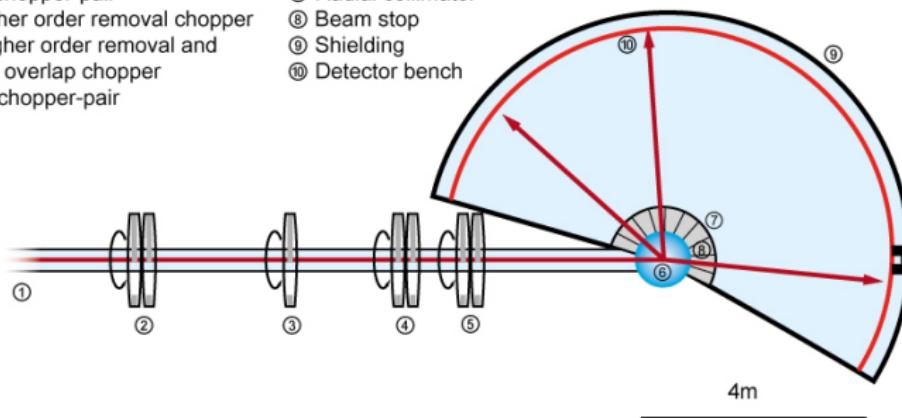
January 29th 2018

MLZ is a cooperation between

The time-of-flight spectrometer TOFTOF

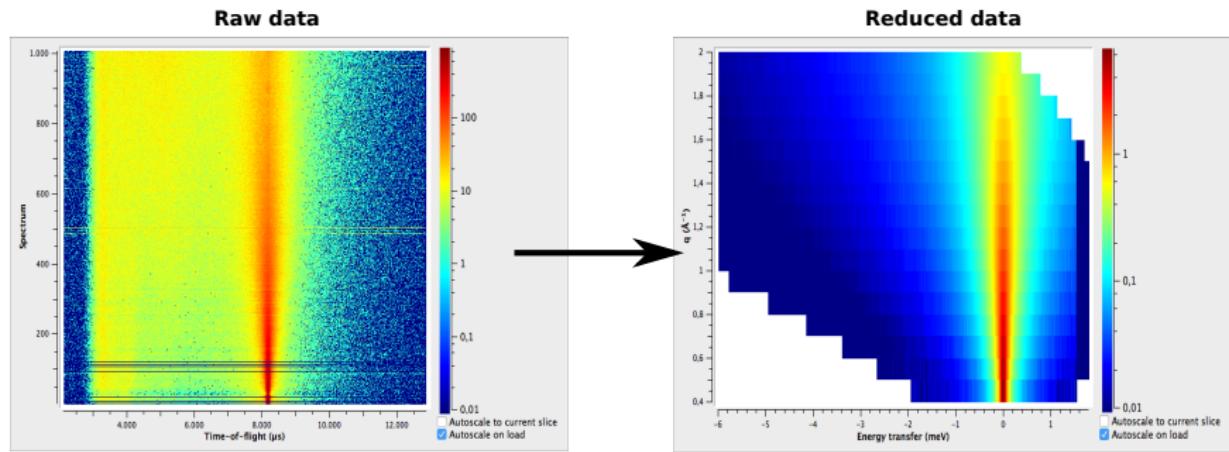
- ① Neutron guide NL2a-u
- ② PCR chopper-pair
- ③ 1st higher order removal chopper
- ④ 2nd higher order removal and frame overlap chopper
- ⑤ MCR chopper-pair

- ⑥ Sample position
- ⑦ Radial collimator
- ⑧ Beam stop
- ⑨ Shielding
- ⑩ Detector bench



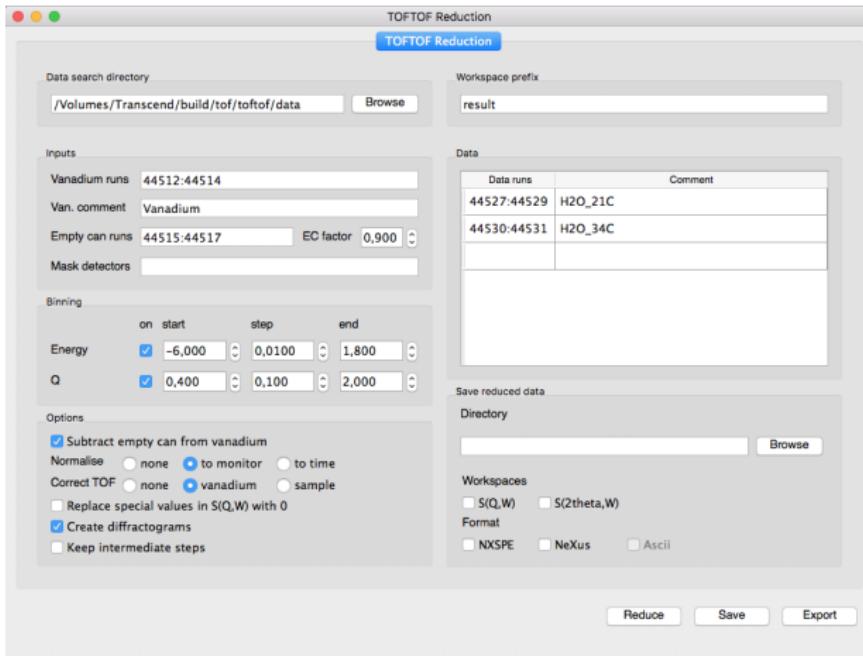
TOFTOF data reduction

Implementation in Mantid started by C. Durniak in 2014



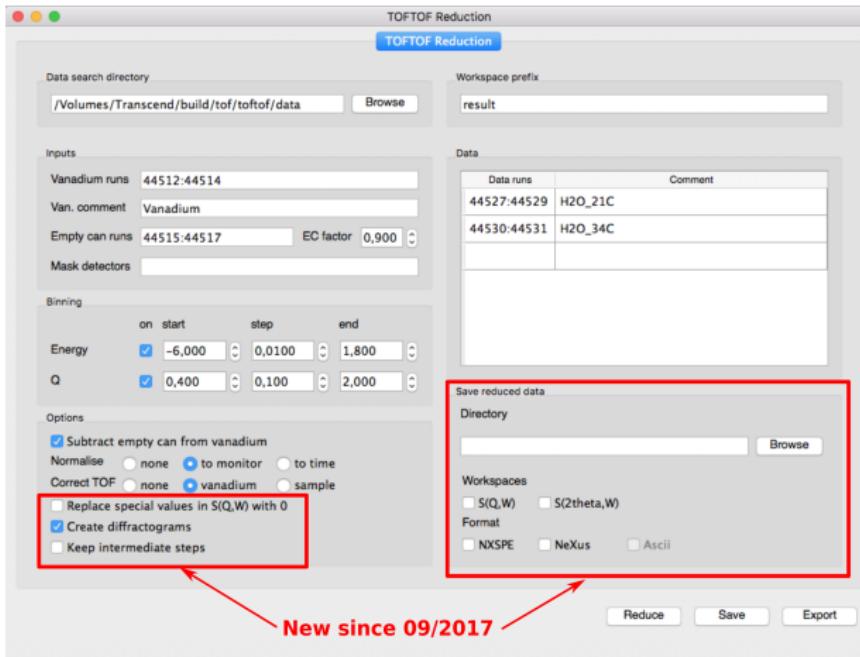
$$\frac{d^2\sigma}{d\Omega dE_f} \propto \frac{k_f}{k_i} \cdot S(Q, \omega)$$

TOFTOF data reduction GUI: view



Developed by Jan Burle, September 2016

TOFTOF data reduction GUI: view



TOFTOF data reduction GUI: Python script

```
72 # convert units
73 gresultDataDeltaE = ConvertUnits(gresultDataToCorr, Target='DeltaE', EMode='Direct', EFixed=Ei)
74 ConvertToDistribution(gresultDataDeltaE)
75
76 # correct for energy dependent detector efficiency
77 gresultDataCorrDeltaE = DetectorEfficiencyCorUser(gresultDataDeltaE)
78
79 # calculate S (Ki/kF correction)
80 gresultDataS = CorrectKiKf(gresultDataCorrDeltaE)
81
82 # energy binning
83 rebinEnergy = '-6.000, 0.010, 1.800'
84 gresultDataBinE = Rebin(gresultDataS, Params=rebinEnergy, IgnoreBinErrors=True)
85
86 # calculate momentum transfer Q for sample data
87 rebinQ = '0.400, 0.100, 2.000'
88 gresultDataSQW = SofQW3(gresultDataBinE, QAxisBinning=rebinQ, EMode='Direct', EFixed=Ei)
```

TOFTOF next step: QENS data analysis

Incoherent scattering function

$$S_{\text{inc}}(Q, \omega) = S_{\text{diff}}(Q, \omega) \otimes S_{\text{rot}}(Q, \omega) \otimes S_{\text{vib}}(Q, \omega)$$

Fit function

$$S_{\text{meas}} = \text{DWF} * [A_0 L(\dots)_{\text{diff}} + A_1 L(\dots)_{\text{rot}} + \dots] \otimes \text{Res}$$

Used Mantid interfaces

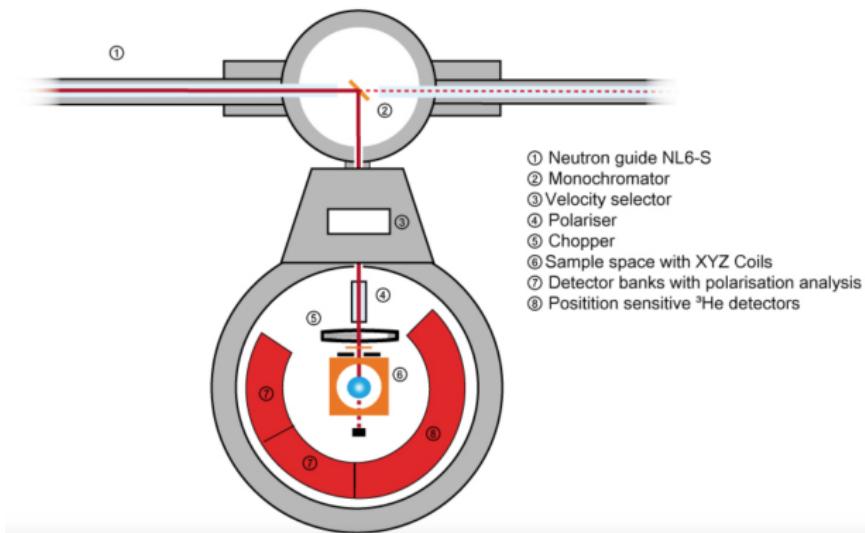
- Multi dataset fitting
- Indirect data analysis

ISIS plans new QENS fitting GUI

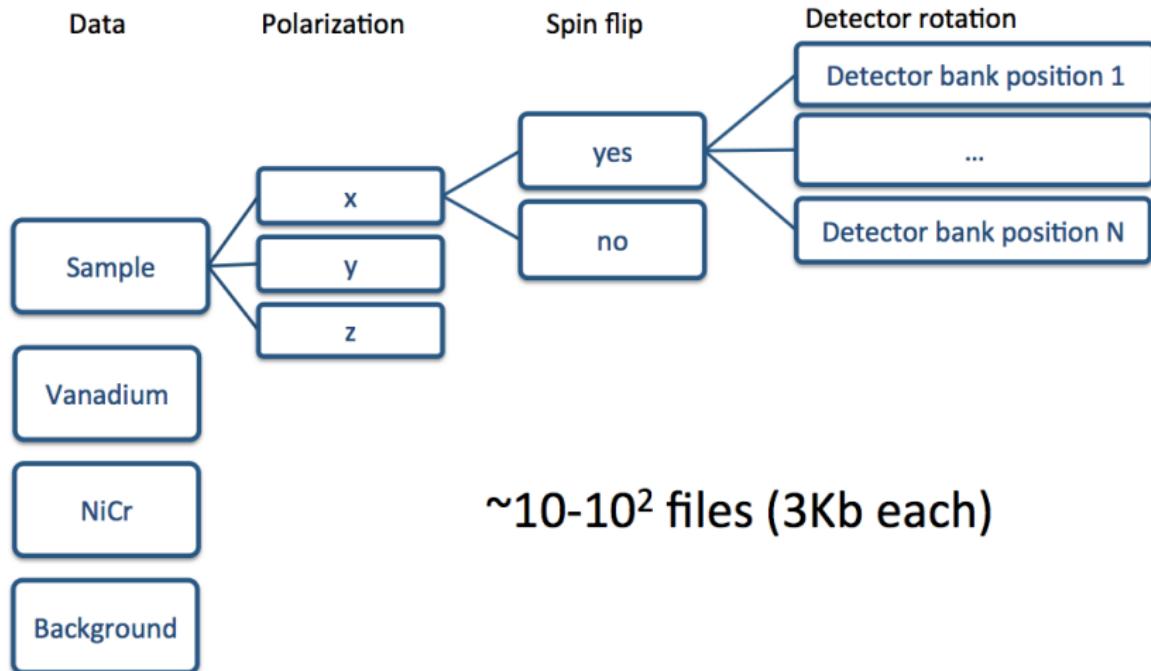
Diffuse neutron scattering spectrometer with polarization analysis DNS.

Two operation modes:

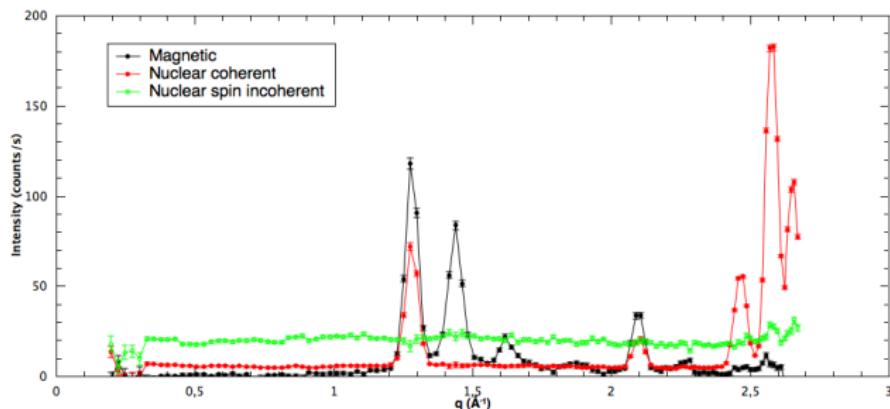
- **diffraction mode**
(user operation)
- **TOF mode**
(commissioning)



DNS: soft matter or magnetic powder data



DNS: magnetic powder

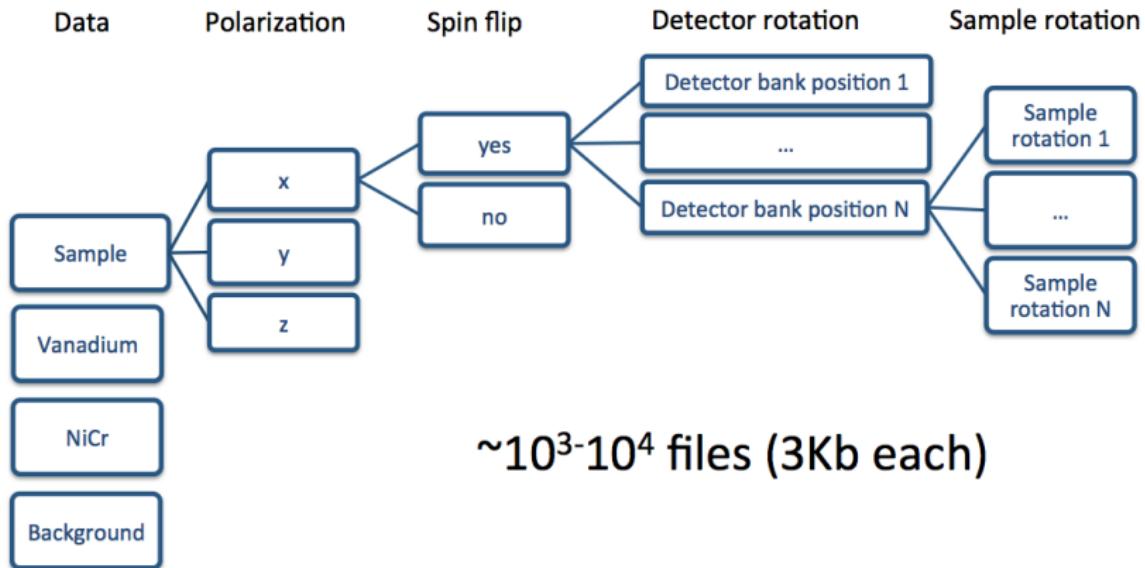


Data: courtesy K. Nemkovski

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

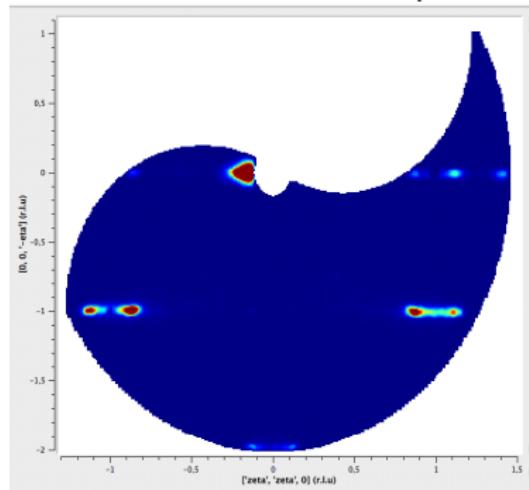
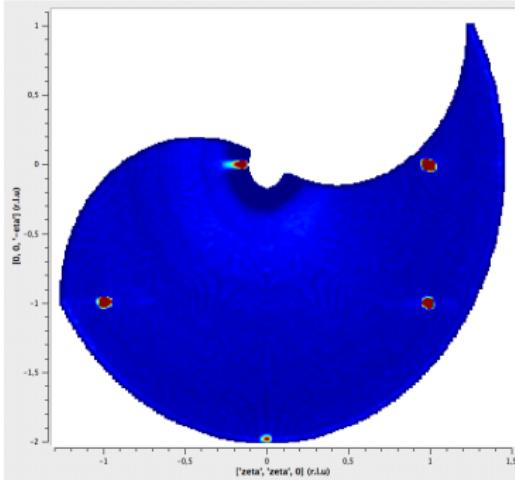
$$I_{coh} = I_{z,NSF} - \frac{1}{2} \cdot I_{mag} - \frac{1}{3} \cdot I_{incoh}$$

DNS: single crystal data



DNS: magnetic single crystal

Data are accumulated into a multidimensional Mantid workspace.



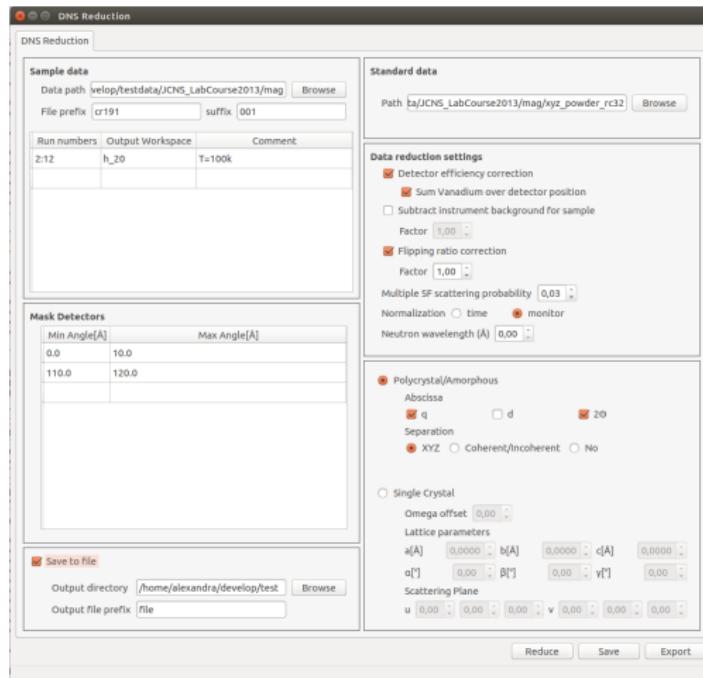
Data: courtesy K. Nemkovski

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

DNS: presently in development

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

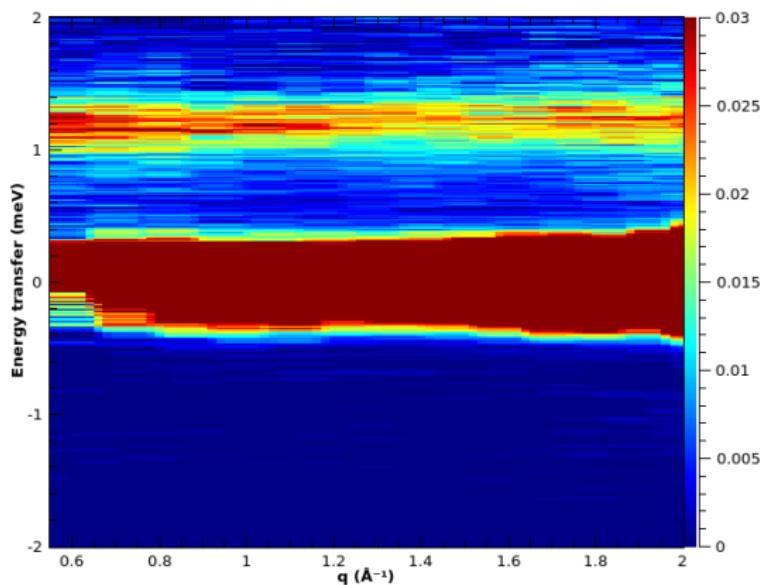
DNS data reduction GUI: view



Implementation: Alexandra Mayer, Jan Burle

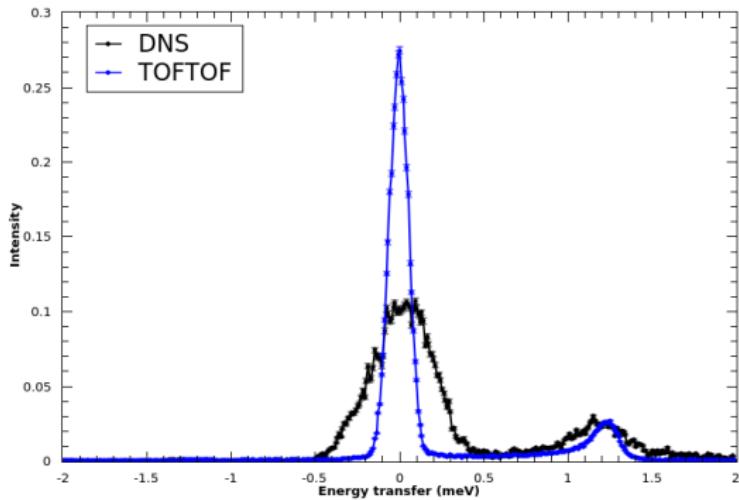
DNS TOF mode: first data

Data: Courtesy Y. Su, E. Feng



TOFTOF data reduction workflow can be applied to DNS data

DNS TOF mode: presently in development



Data: Courtesy Y. Su, E. Feng

Calibration:

- Zero time channel (data acquisition)
- Instrument geometry (flight paths)

Detector rotation:

- Merge datasets measured at different detector positions

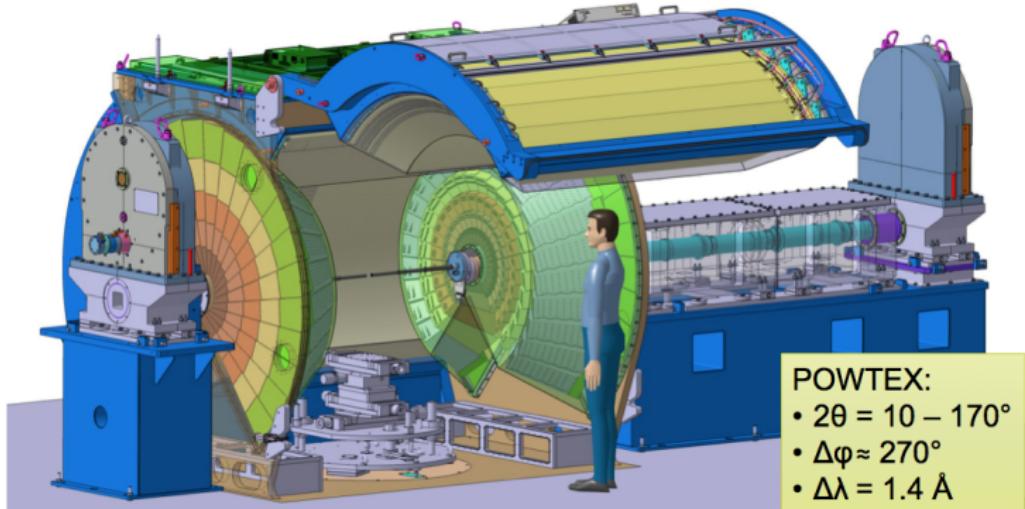
DNS TOF objectives

- DNS TOF data reduction for powder samples:
 - commissioning in January – March 2018
- DNS TOF data reduction for single crystal samples:
 - design the data reduction workflow (2017–2018, in cooperation with DNS team)
 - implementation in 2018, as soon as test data will be available
- DNS PSD bank event mode powder and single crystal data:
 - DAQ software is still be to finalised (data acquisition team)
 - design and implementation of the data reduction workflow as soon as data will be available

A number of algorithms for processing and visualisation of PSD event data are available in Mantid

POWTEX: High-intensity time-of-flight diffractometer

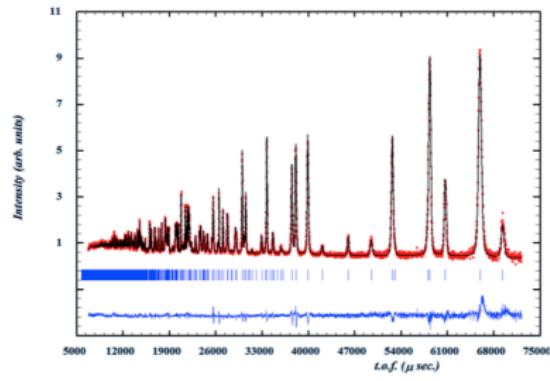
A. Houben, P. Jacobs, W. Schweika et. al.



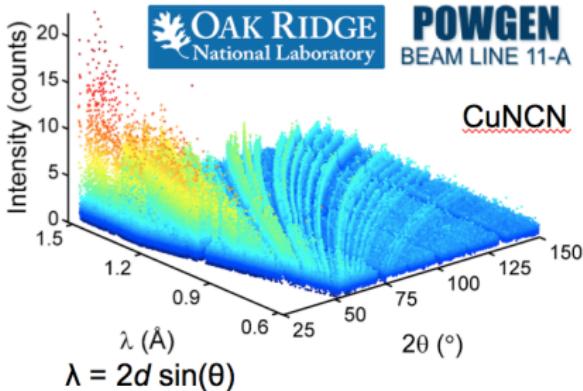
<http://mlz-garching.de/powtex>

TOF powder diffraction data reduction

A. Houben, P. Jacobs, W. Schweika et. al.



1D pattern



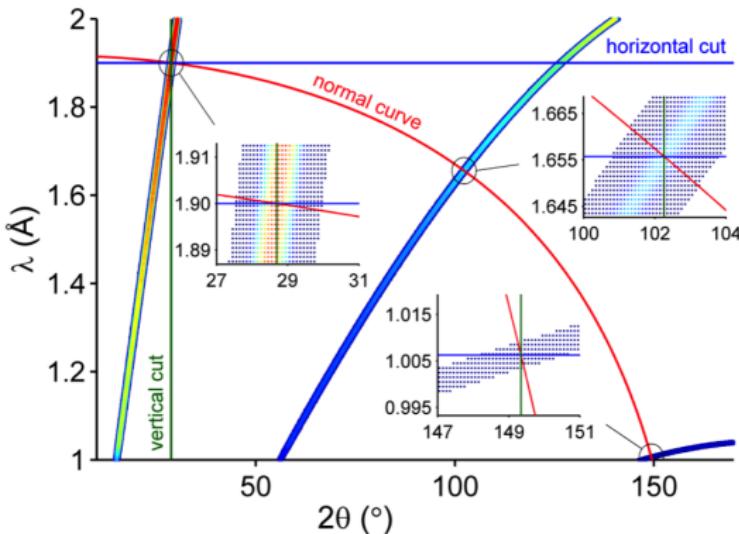
2D pattern

Motivation for multidimensional data treatment

- mixing of resolutions (peak width) and peak shapes
- background treatment (e.g., Hydrogen)

Proposed solution

A. Houben, P. Jacobs, W. Schweika et. al.



New coordinate system

$$(d, d_{\perp})$$

where

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

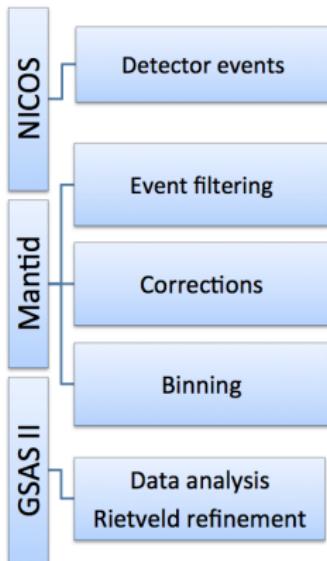
$$d_{\perp} = \sqrt{\lambda^2 - 2\lambda_K^2 \log \cos \theta}$$

$$\lambda_K = 1 \text{ \AA}$$

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

J. Appl. Cryst. (2017) **50**, 866–875

Planned procedure for POWTEX

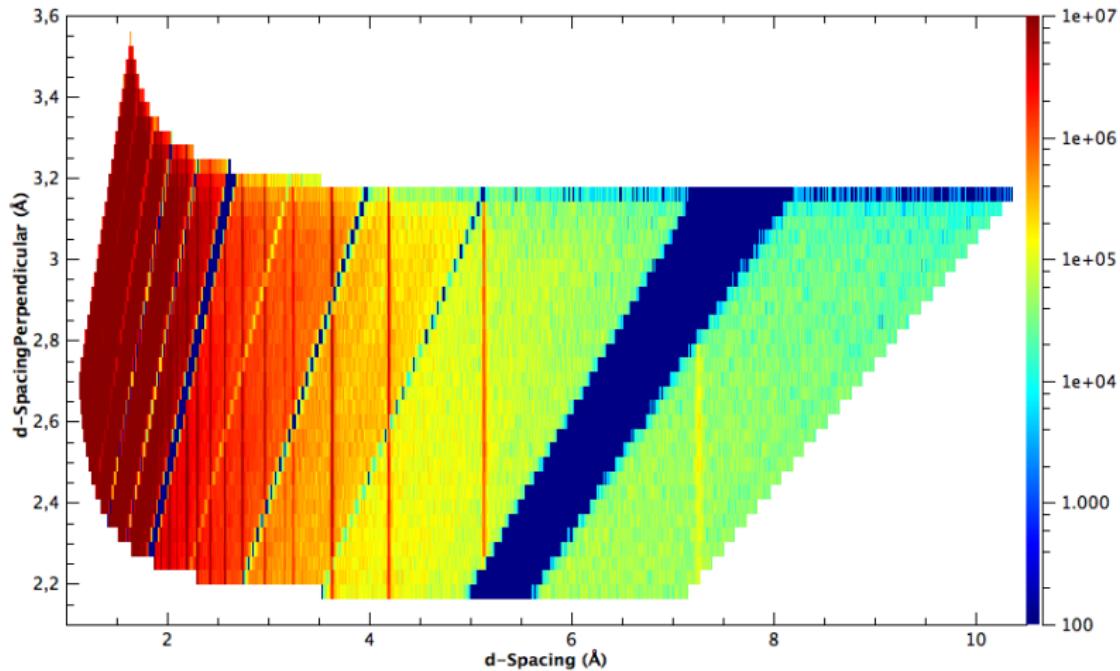


- Export detector events as raw data + meta data
- Use Mantid for data reduction
→ supported by SCG
- Multidimensional data treatment, e.g., Rietveld refinement

Test with POWTEX detector module at POWGEN, 11/2017

(d, d_{\perp}) -binning in Mantid

Data: NAC measured at POWGEN, courtesy A. Houben, P. Jacobs



Summary: Mantid status at MLZ

- **TOFTOF:** since 2016 in user operation, maintenance.
- **DNS diffraction mode:** commissioning, GUI coming soon
- **DNS TOF powder:** commissioning (01–03/2018)
- **DNS TOF SCD/PSD/TOPAS:** in development.
- **POWTEX:**
 - New unit d_{\perp} (d-SpacingPerpendicular) is added to Mantid
 - New algorithm for binning in (d, d_{\perp}) implemented in Mantid
- **SPHERES:** requested.
- **SANS-1:** development will start in spring 2018

Thank you for your attention!