

Facility news and updates from MLZ

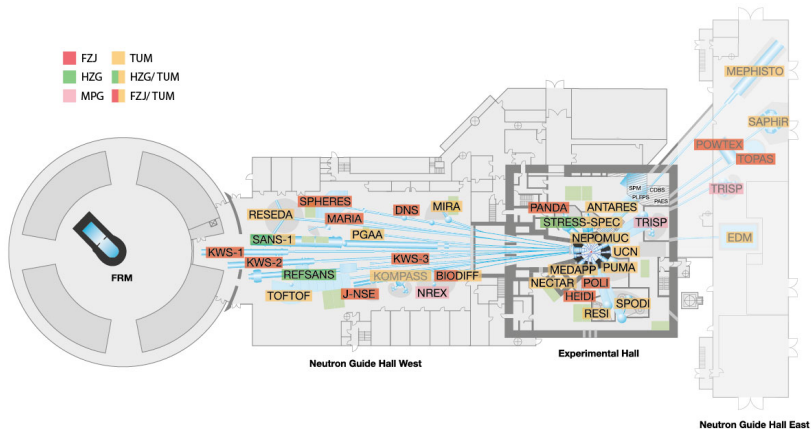
Marina Ganeva

JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

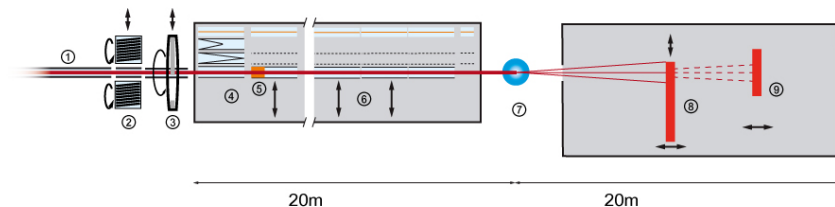
April 3rd 2019

MLZ is a cooperation between

Heinz-Maier Leibnitz Center



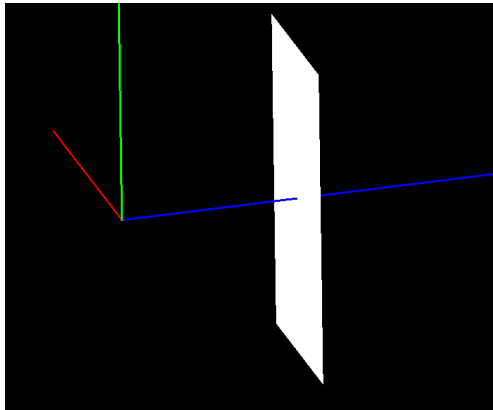
SANS-1: Small angle neutron scattering



- ① Neutron guide NL4a
- ② Velocity selector 1+2
- ③ TISANE Chopper
- ④ Changeable polarisers
- ⑤ Spin flipper
- ⑥ 4 collimation sections 19 m
(neutron guide, collimation slits)

- ⑦ Sample position
- ⑧ Position sensitive area detector, $1 \times 1 \text{ m}^2$
- ⑨ High resolution position-sensitive area detector, $0.5 \times 0.5 \text{ m}^2$
(installation 2016)

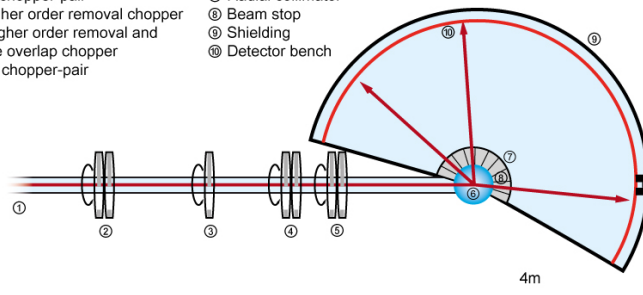
Development just starts

[illegible]

Data reduction workflow is very similar to ILL SANS

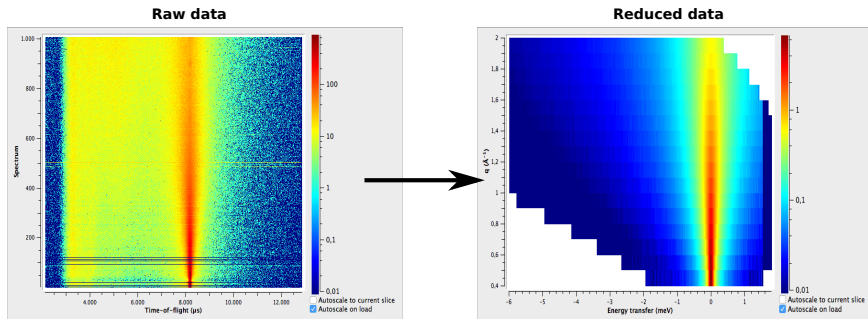
The time-of-flight spectrometer TOFTOF

- | | |
|--|---------------------|
| ① Neutron guide NL2a-u | ⑥ Sample position |
| ② PCR chopper-pair | ⑦ Radial collimator |
| ③ 1 st higher order removal chopper | ⑧ Beam stop |
| ④ 2 nd higher order removal and frame overlap chopper | ⑨ Shielding |
| ⑤ MCR chopper-pair | ⑩ Detector bench |



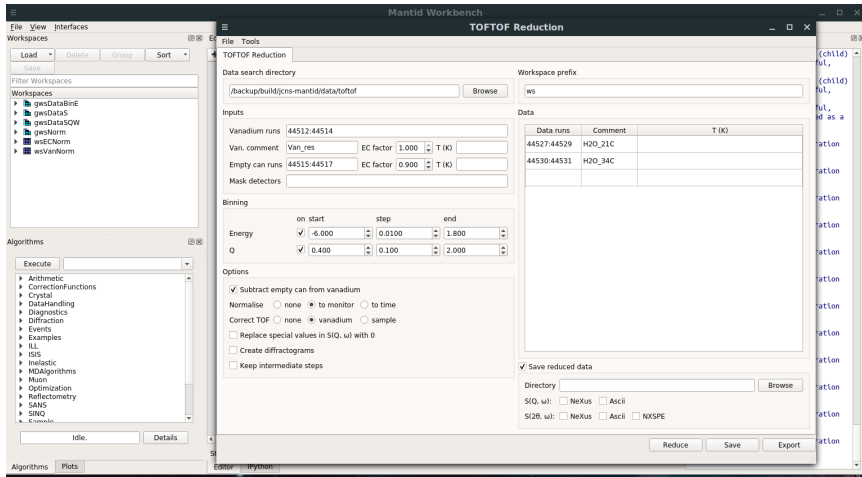
TOFTOF data reduction

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



The screenshot shows the MANTID Workbench interface with the TOFTOF Reduction GUI open. The GUI is divided into several sections:

- File Tools:** Includes buttons for Load, Delete, Group, Sort, and Save.
- Workspaces:** A list of workspaces on the left, including gwsDataBinE, gwsDataS, gwsDataSQW, gwsNorm, wsECNorm, and wsVanNorm.
- Algorithms:** A list of algorithms on the left, including Arithmetic, CorrectionFunctions, Crystal, DataHandling, Diagnostics, Diffraction, Events, Examples, ILL, ISIS, Inelastic, MDAAlgorithms, Muon, Optimization, Reflectometry, SANS, and SINO.
- TOFTOF Reduction Section:**
 - Data search directory:** /backup/build/jcns-mantid/data/toftof
 - Workspace prefix:** ws
 - Inputs:**
 - Vanadium runs: 44512:44514
 - Van. comment: Van_res, EC factor: 1.000, T (K):
 - Empty can runs: 44515:44517, EC factor: 0.900, T (K):
 - Mask detectors:
 - Binning:**
 - on start: -6.000, step: 0.0100, end: 1.800
 - Q: 0.400, step: 0.100, end: 2.000
 - Options:**
 - ☒ Subtract empty can from vanadium
 - Normalise: ☐ none, ☒ to monitor, ☐ to time
 - Correct TOF: ☐ none, ☒ vanadium, ☐ sample
 - ☐ Replace special values in S(Q, u) with 0
 - ☐ Create diffractograms
 - ☐ Keep intermediate steps
 - Data Table:**

Data runs	Comment	T (K)
44527:44529	H2O_21C	
44530:44531	H2O_34C	
 - Save reduced data:**
 - ☒ Save reduced data
 - Directory: , Browse
 - S(Q, u): ☐ NeXus, ☐ Ascii
 - S(2θ, u): ☐ NeXus, ☐ Ascii, ☐ NXSPe
 - Buttons:** Reduce, Save, Export

TOFTOF data reduction GUI: Python script

```

72 # convert units
73 gresultDataDeltaE = ConvertUnits(gresultDataTofCorr, 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: QENS data analysis

Incoherent scattering function

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

The fit function has the general form:

$$S_{\text{meas}} = [L_1(\dots) + L_2(\dots) + D(\dots)] \otimes \text{Res} + \text{bg}$$

Where

- D — δ -function modeled by a small Lorentzian
- L_1, L_2 — Lorentzian functions
- $\text{bg} = A_0 + A_1 \cdot dE$ — linear background

The Lorentzian take into account the detailed balance factor, the temperature is read from the data file.

TOFTOF: QENS data analysis

Requirements

- fit multiple datasets simultaneously
- fix particular fit parameters for the all functions (fwhm or peak center for all Lorenzians, for example)
- custom fit metric

Used Mantid interfaces

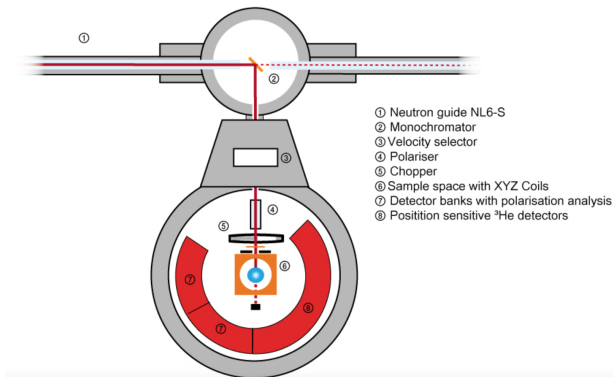
- Multi dataset fitting
- Indirect data analysis

The best option for the moment: jupyter notebook

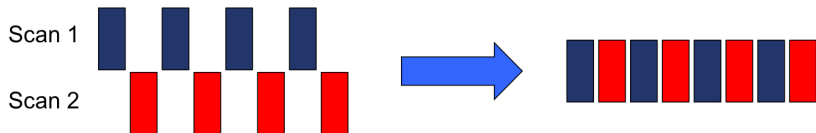
Diffuse neutron scattering spectrometer with polarization analysis DNS.

Two operation modes:

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

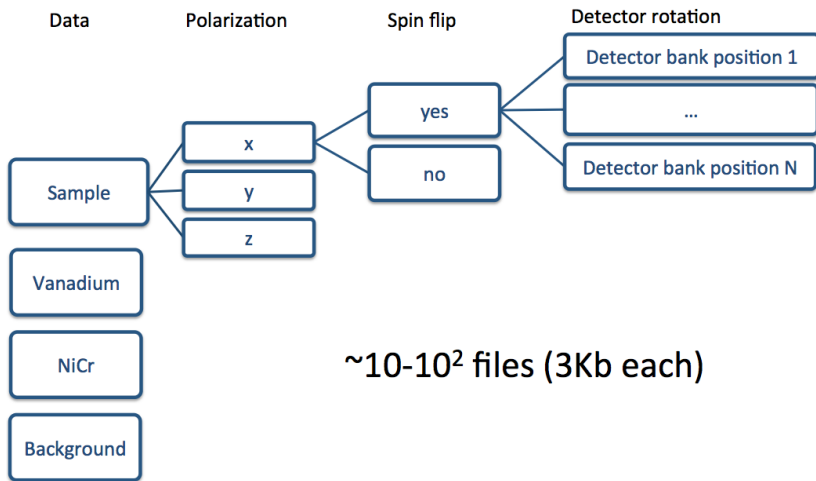


Detector rotation

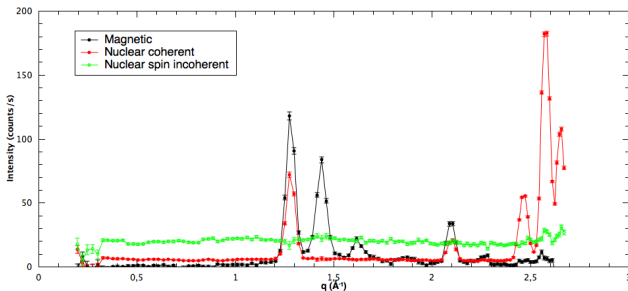


- Each scan is saved as a separate file \Rightarrow loaded to a separate workspace
- Required output of the data reduction is a merged workspace

DNS: soft matter or magnetic powder data



DNS: magnetic powder

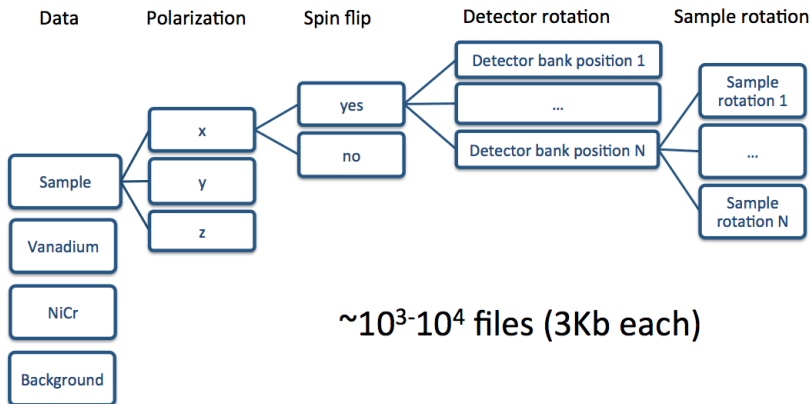


Data: courtesy K. Nemkovski

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

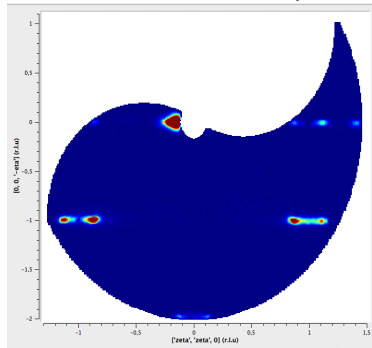
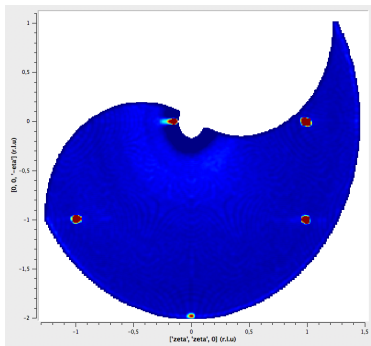
$$I_{coh} = I_{z,NSF} - \frac{1}{2} \cdot I_{mag} - \frac{1}{3} \cdot I_{incoh}$$

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 data reduction GUI prototype: view

DNS Reduction

Sample data

Data path:

File prefix: suffix:

Run numbers	Output Workspace	Comment
2:12	h_20	T=100k

Mask Detectors

Min Angle[A]	Max Angle[A]
0.0	10.0
110.0	120.0

☒ Save to file

Output directory:

Output file prefix:

Standard data

Path:

Data reduction settings

☒ Detector efficiency correction

☒ Sum Vanadium over detector position

☐ Subtract instrument background for sample

Factor:

☒ Flipping ratio correction

Factor:

Multiple SF scattering probability:

Normalization: ☐ time ☒ monitor

Neutron wavelength (Å):

☒ Polycrystal/Amorphous

Abscissa: ☒ q ☐ d ☒ 2θ

Separation: ☒ XYZ ☐ Coherent/Incoherent ☐ No

☐ Single Crystal

Omega offset:

Lattice parameters

a[Å]: b[Å]: c[Å]:

α[°]: β[°]: γ[°]:

Scattering Plane

u: v: w:

Implementation: Alexandra Mayer, Jan Burle

MD Workspaces for DNS

New data reduction workflow

Pro

- 😊 Less workspaces
- 😊 Fast, robust data reduction
- 😊 More transparent data reduction Python code
- 😊 Masking is possible
- 😊 Universal: works for all DNS operation modes

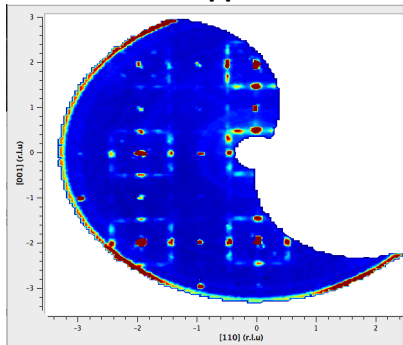
Contra

- 😞 ConvertUnits is applicable only to matrix workspaces
- 😞 Only uniform binning
- 😞 Raw data stored in MDEventWorkspaces \Rightarrow additional binning step

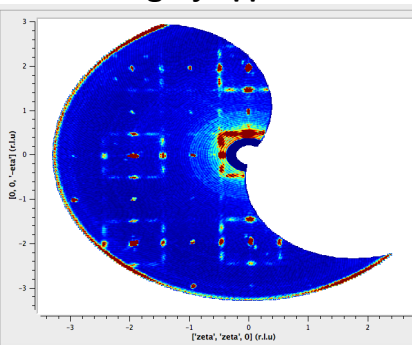
Diffraction mode: single crystal data

Data: K. Nemkovski

MD approach



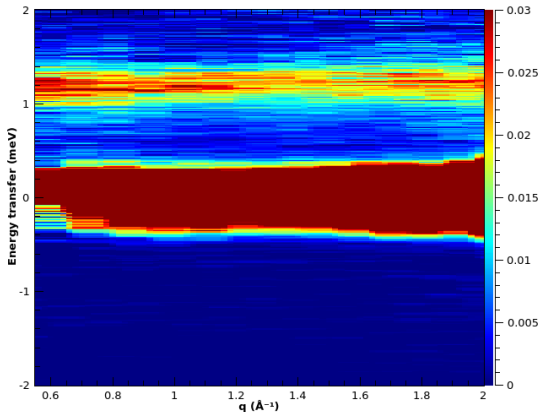
Legacy approach



Speed-up about 1000 times for data reduction

DNS TOF mode: first data

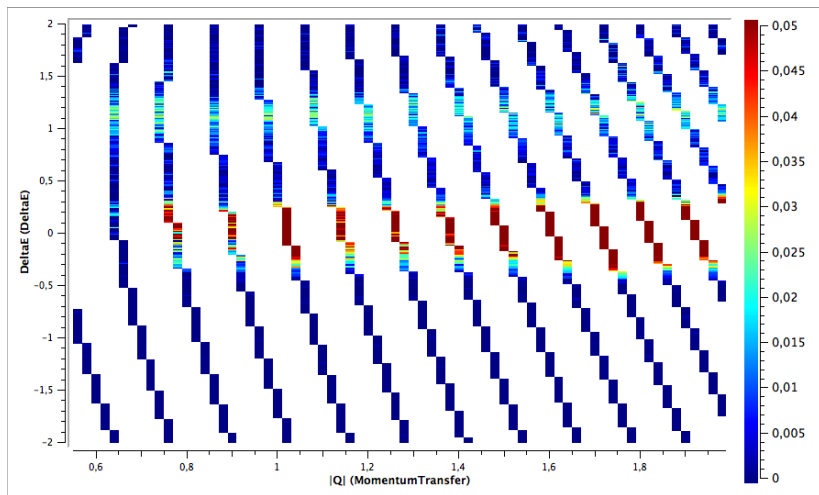
Data: Courtesy Y. Su, E. Feng



TOFTOF data reduction workflow can be applied to DNS data

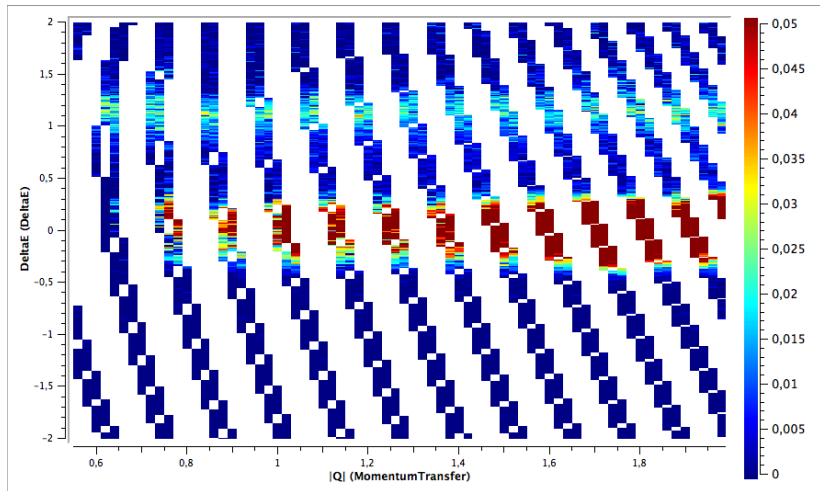
TOF mode data: one detector position

Data: Y. Su



TOF mode data: two detector positions

Data: Y. Su



Summary: Mantid status at MLZ

- **TOFTOF:** in user operation, maintenance. Development of data analysis workflow.
- **DNS diffraction mode:** refactoring data reduction workflow to use MD workspaces.
- **DNS TOF powder/SCD:** commissioning, first users
- **DNS TOF PSD/TOPAS:** in development.
- **POWTEX:** no new requests
 - New unit d_{\perp} (d-SpacingPerpendicular) is added to Mantid
 - New algorithm for binning in (d, d_{\perp}) implemented in Mantid
- **SANS-1:** development just started

$S(Q, \omega)$ for non-PSD detectors

Available algorithms

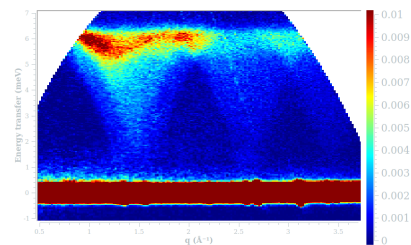
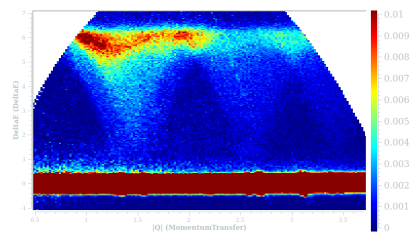
- **SofQWCentre, ConvertToMD:** The momentum transfer Q for each detector is calculated for the **detector center**.
- **SofQWPolygon:** The polygon in $Q - \Delta E$ space is calculated from the energy bin boundaries and the detector scattering angle 2θ . **The detectors (pixels) are assumed to be uniform, and characterized by a single angular width $\Delta 2\theta$.**
- **SofQWNormalisedPolygon:** Scattering angle 2θ range covered by a detector is calculated for each detector individually. Signal and error are normalized by a fractional weight of the bin. **Accounts for shaded detectors.**

$S(Q, \omega)$ for non-PSD detectors

TOFTOF. Data: M. Feygenson

ConvertToMD
(SofQWCentre)

SofQWNormalizedPolygon



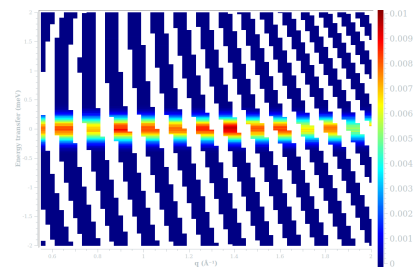
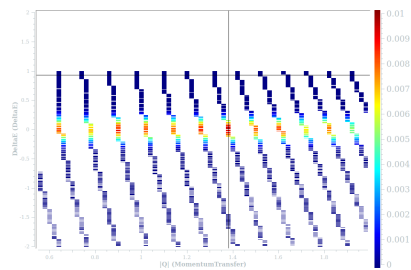
For TOFTOF difference is negligible

$S(Q, \omega)$ for non-PSD detectors

DNS 1 detector position. Data: Y. Su

ConvertToMD
(SofQWCentre)

SofQWNormalizedPolygon



For DNS difference is significant

$S(Q, \omega)$ for non-PSD detectors

Discussion

- Can finite-size detectors be considered as points?
- Is assumption that detector is uniform correct?

Thank you for your attention!