Facility news and updates from MLZ

Marina Ganeva

JCNS at MLZ, Forschungszentrum Jülich GmbH, Germany

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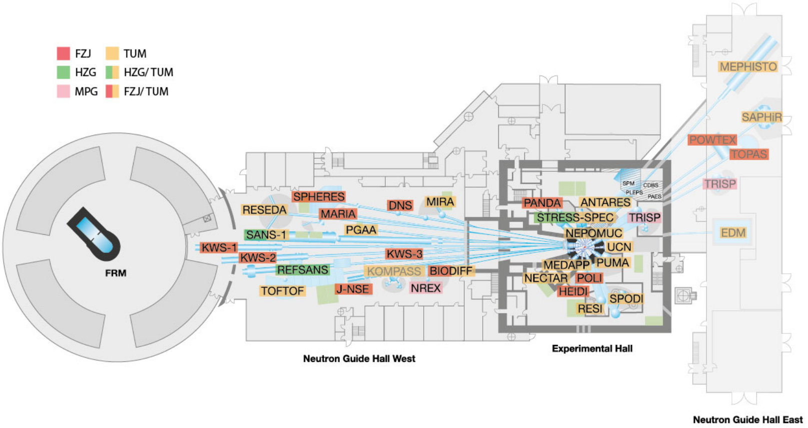
MLZ is a cooperation between

JÜLICH FORSCHUNGSZENTRUM

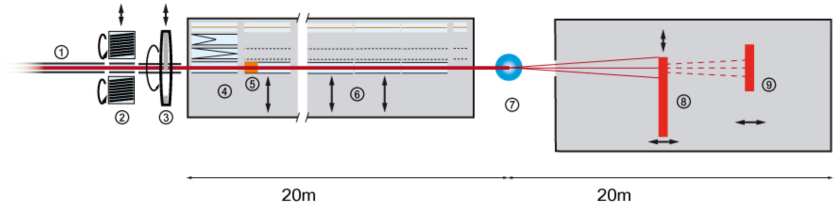
Helmholtz-Zentrum Geesthacht
Zentrum für Material- und Küstenforschung

Technische Universität München

Heinz-Maier Leibnitz Center



SANS-1: Small angle neutron scattering

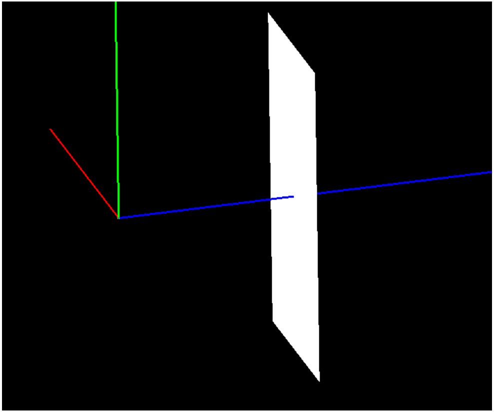


① Neutron guide NL4a
② Velocity selector 1+2
③ TISANE Chopper
④ Changeable polarisers
⑤ Spin flipper
⑥ 4 collimation sections 19 m
(neutron guide, collimation slits)

⑦ Sample position
⑧ Position sensitive area detector, 1 x 1 m^2
⑨ High resolution position-sensitive
area detector, 0.5 x 0.5 m^2
(installation 2016)

SANS-1

Development just starts



```
st1_phi_userlimits=(-5.00, 5.00)
st1_phi_value=-0.00
st1_x_offset=0.00
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st1_x_userlimits=(-750.00, 150.00)
st1_x_value=-150.00
st1_y_offset=0.00
st1_y_precision=0.01
st1_y_status=ok: idle
st1_y_userlimits=(-99.00, 99.00)
st1_y_value=50.00
st1_z_offset=-0.30
st1_z_precision=0.01
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tisane_fc_precision=0.000000
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tisane_fc_value=96.771695
tisane_fg_multi_status=ok: indeterminate
tisane_fg_multi_value=off

%Counts
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,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
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0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
```
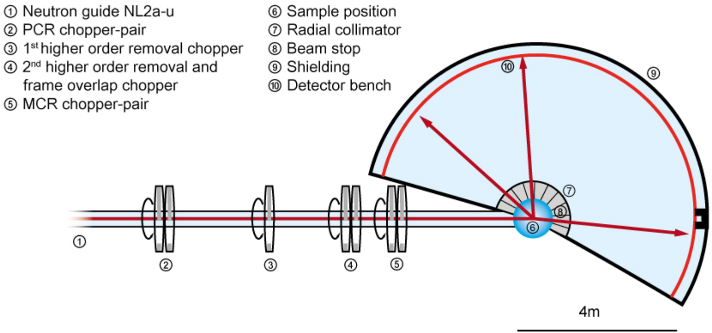

Data reduction workflow is very similar to ILL SANS

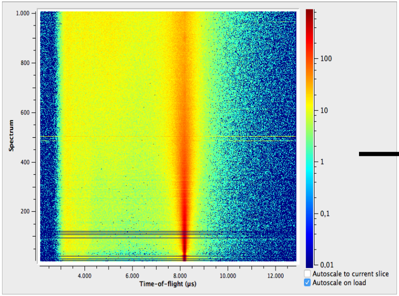
The time-of-flight spectrometer TOFTOF



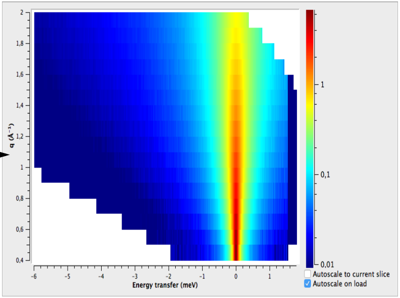
TOFTOF data reduction

Implementation in Mantid started by C. Durniak in 2014

Raw data

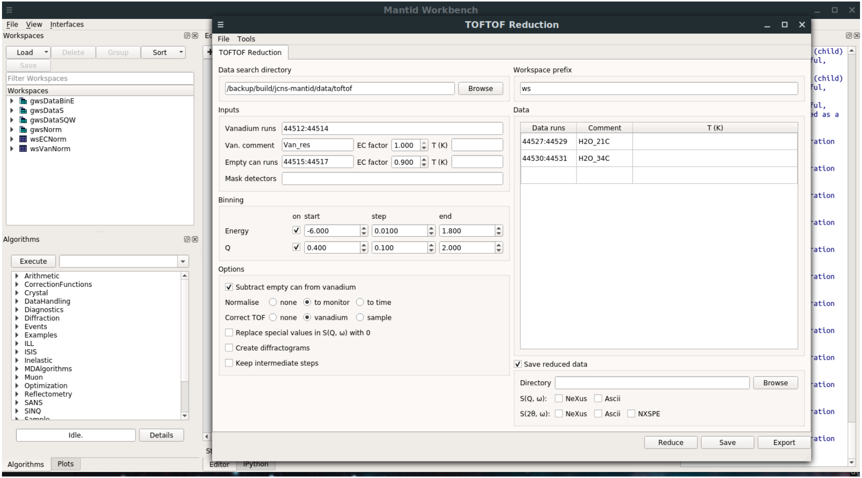


Reduced data



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

TOFTOF data reduction GUI: view



TOFTOF data reduction GUI: Python script

```python
# convert units
gresultDataDeltaE = ConvertUnits(gresultDataTofCorr, Target='DeltaE', EMode='Direct', EFixed=Ei)
ConvertToDistribution(gresultDataDeltaE)

# correct for energy dependent detector efficiency
gresultDataCorrDeltaE = DetectorEfficiencyCorUser(gresultDataDeltaE)

# calculate S (Ki/kF correction)
gresultDataS = CorrectKiKf(gresultDataCorrDeltaE)

# energy binning
rebinEnergy = '-6.000, 0.010, 1.800'
gresultDataBinE = Rebin(gresultDataS, Params=rebinEnergy, IgnoreBinErrors=True)

# calculate momentum transfer Q for sample data
rebinQ = '0.400, 0.100, 2.000'
gresultDataSQW = SofQW3(gresultDataBinE, QAxisBinning=rebinQ, EMode='Direct', EFixed=Ei)
```

TOFTOF: QENS data analysis

Incoherent scattering function

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

The fit function has the general form:

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

Where

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

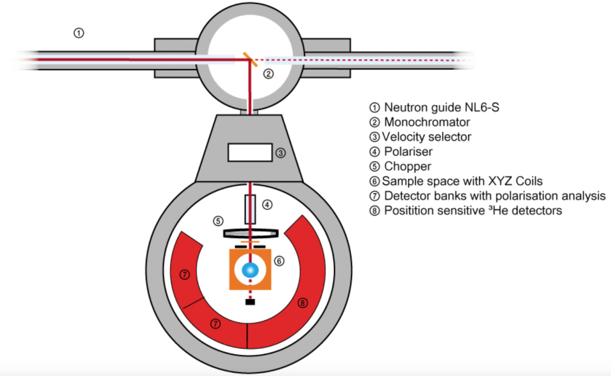
- Multi dataset fitting
- Indirect data analysis

The best option for the moment: jupyter notebook

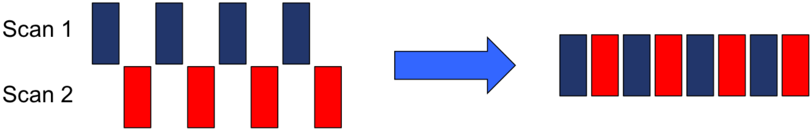
Diffuse neutron scattering spectrometer with polarization analysis DNS.

Two operation modes:

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

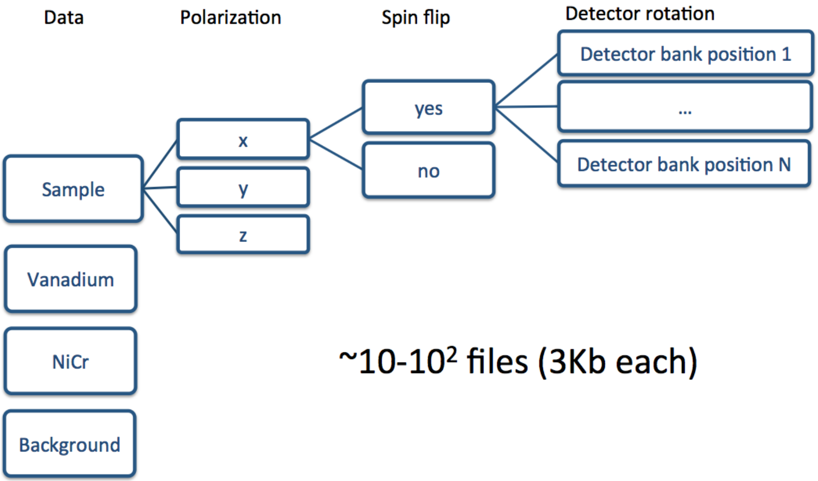


Detector rotation



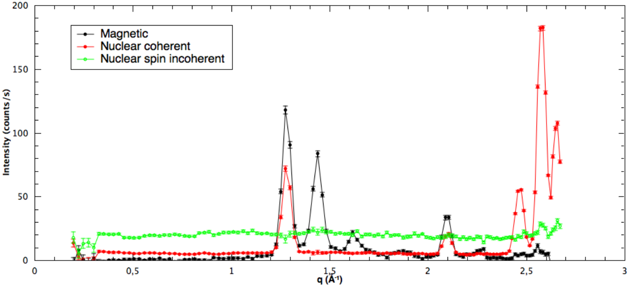
- Each scan is saved as a separate file ⇒ loaded to a separate workspace
- Required output of the data reduction is a merged workspace

DNS: soft matter or magnetic powder data



~10-10^2 files (3Kb each)

DNS: magnetic powder

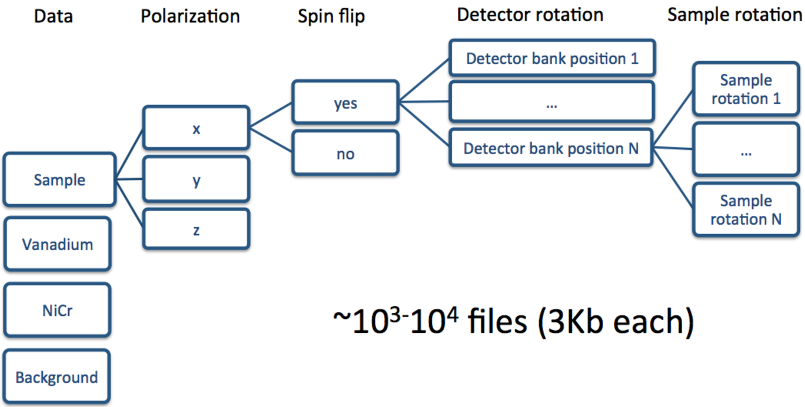


Data: courtesy K. Nemkovski

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

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

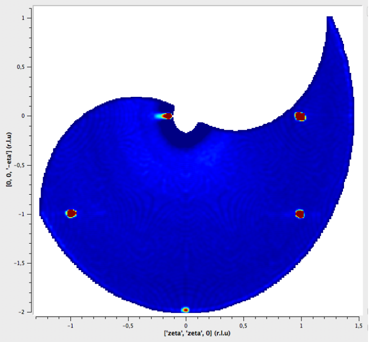
DNS: single crystal data

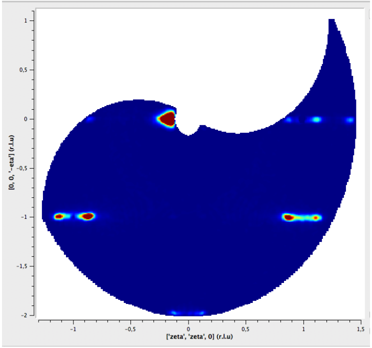


~10^3-10^4 files (3Kb each)

DNS: magnetic single crystal

Data are accumulated into a multidimensional Mantid workspace.

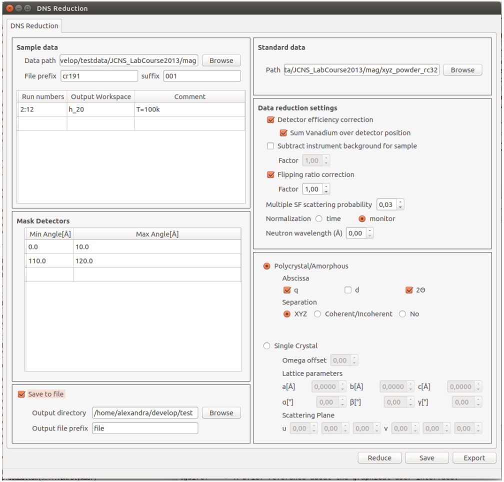




Data: courtesy K. Nemkovski

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

DNS data reduction GUI prototype: view



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

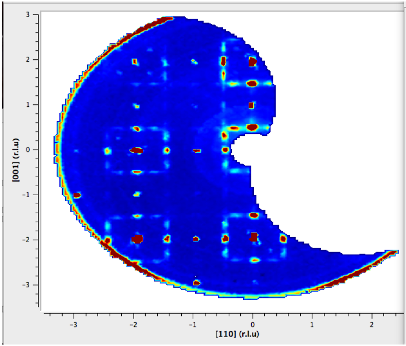
Contra

- ☹ ConvertUnits is applicable only to matrix workspaces
- ☹ Only uniform binning
- ☹ Raw data stored in MDEventWorkspaces ⇒ additional binning step

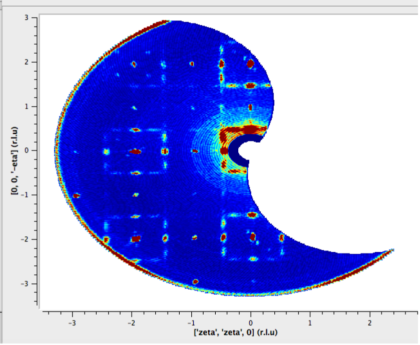
Diffraction mode: single crystal data

Data: K. Nemkovski

MD approach



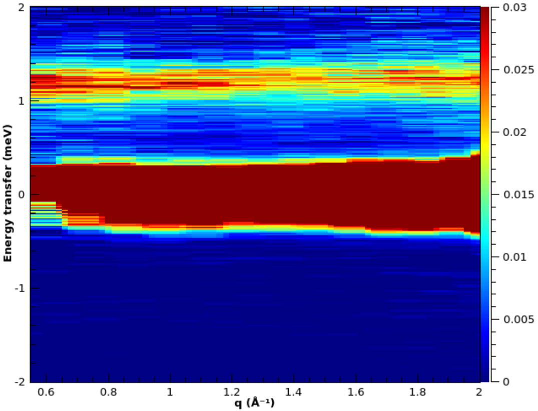
Legacy approach



Speed-up about 1000 times for data reduction

DNS TOF mode: first data

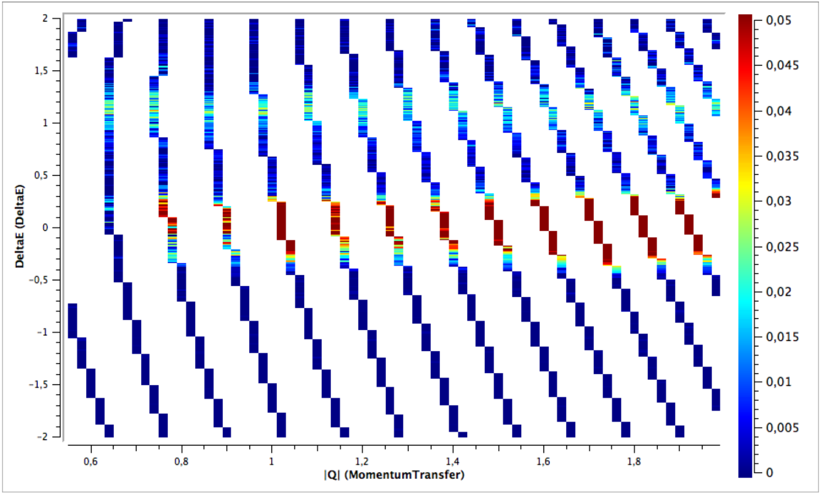
Data: Courtesy Y. Su, E. Feng



TOFTOF data reduction workflow can be applied to DNS data

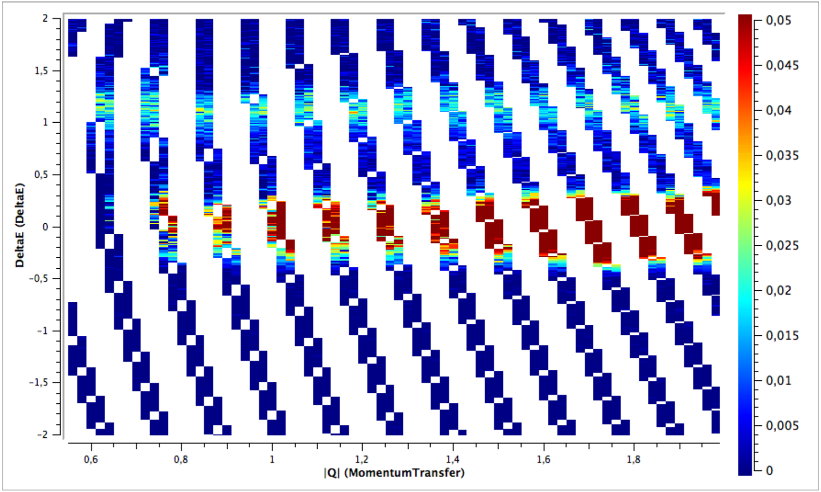
TOF mode data: one detector position

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

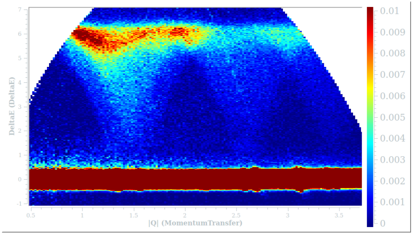
Available algorithms

- **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.

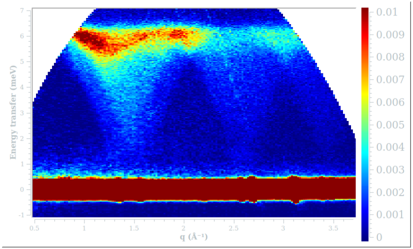
$S(Q, \omega)$ for non-PSD detectors

TOFTOF. Data: M. Feygenson

ConvertToMD (SofQWCentre)



SofQWNormalizedPolygon

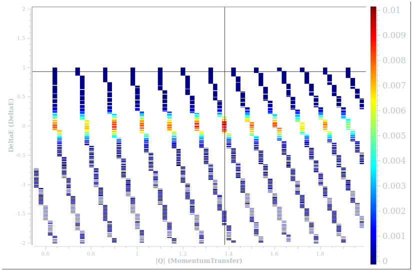


For TOFTOF difference is negligible

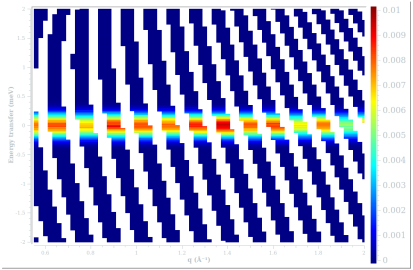
$S(Q, \omega)$ for non-PSD detectors

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!