OAK RIDGE National Laboratory

Data reduction and visualization using SHIVER

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U.S. DEPARTMENT of ENERGY

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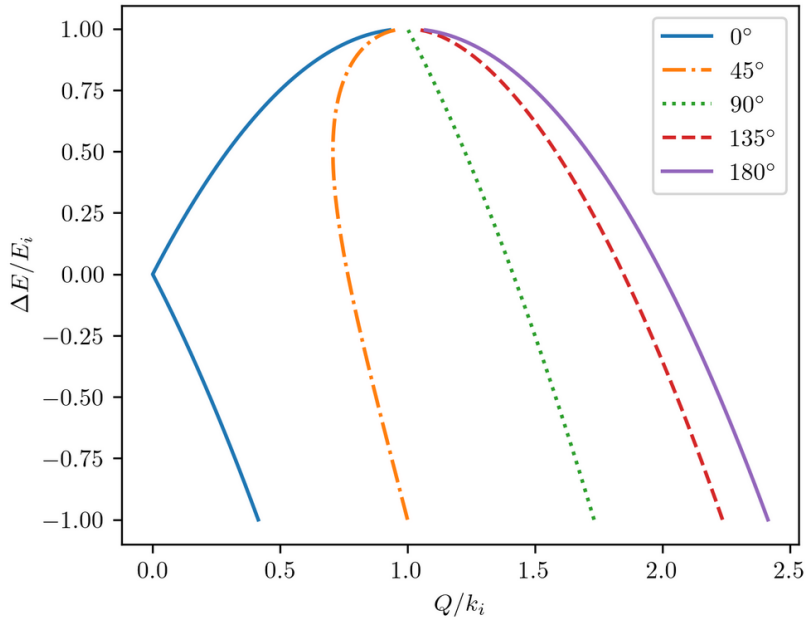
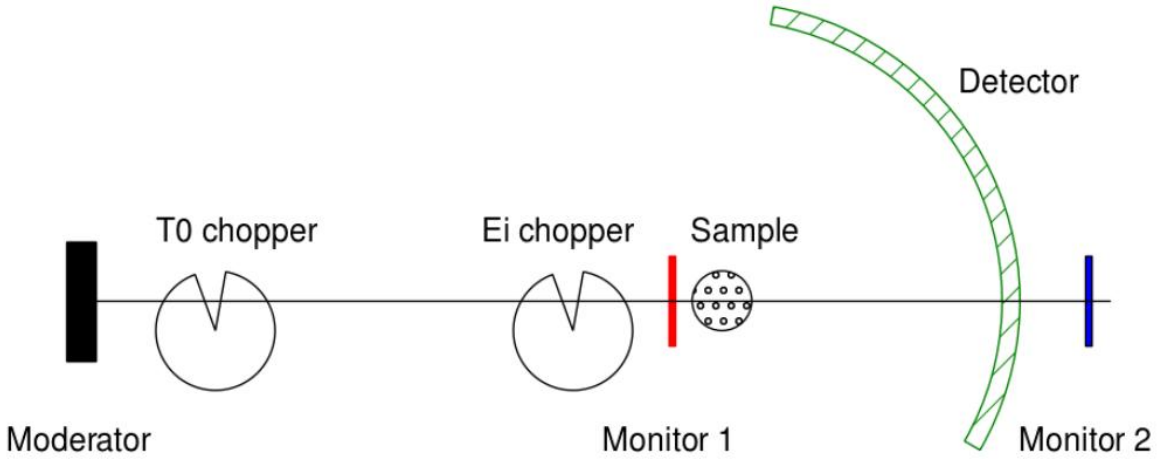
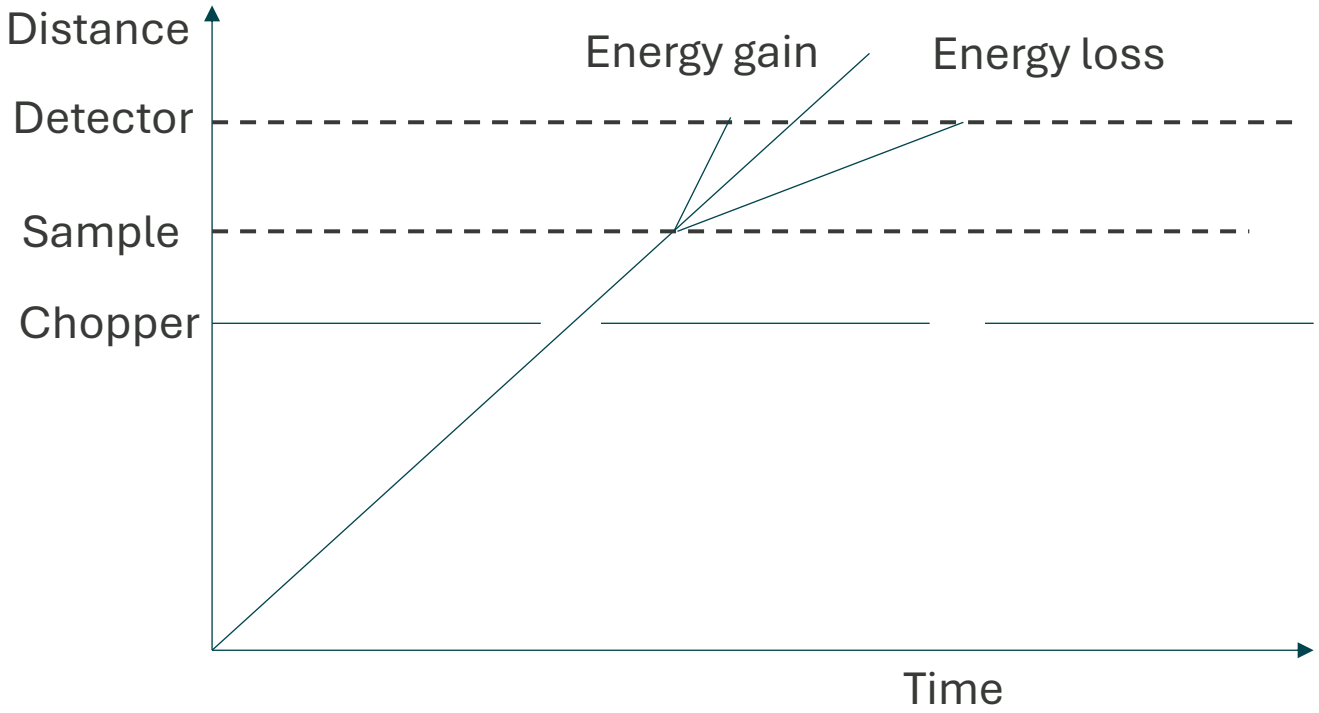
TOF DGS spectrometers

- Incident energy is set by the chopper system
- Final energy is calculated from time of flight
- Momentum transfer also depends on the detector position

$$\frac{\Delta E}{E_i} = 1 - \left(\frac{k_f}{k_i}\right)^2 \qquad \frac{Q^2}{k_i^2} = 1 + \left(\frac{k_f}{k_i}\right)^2 - 2\frac{k_i}{k_f}\cos\theta$$

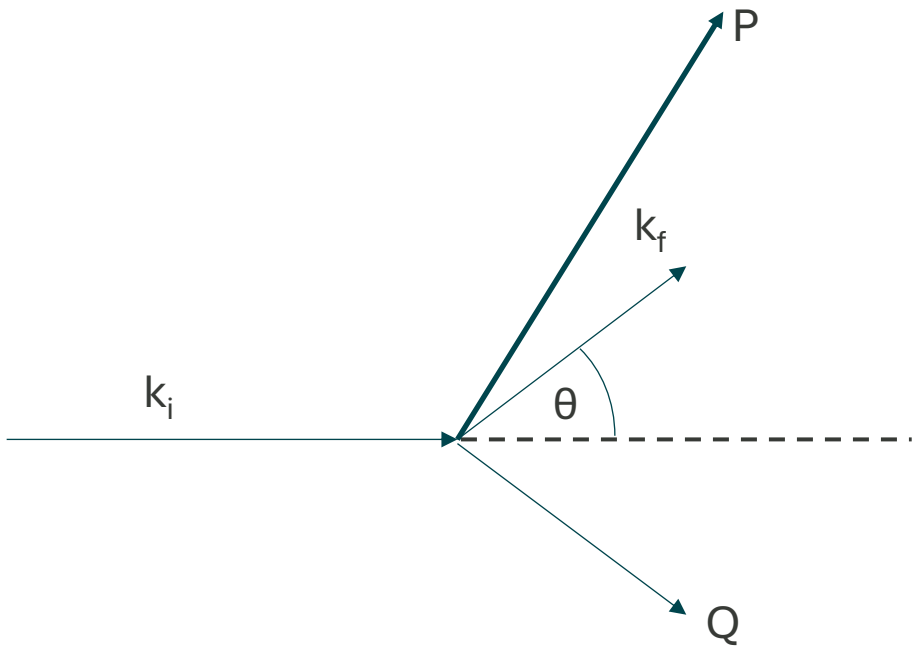


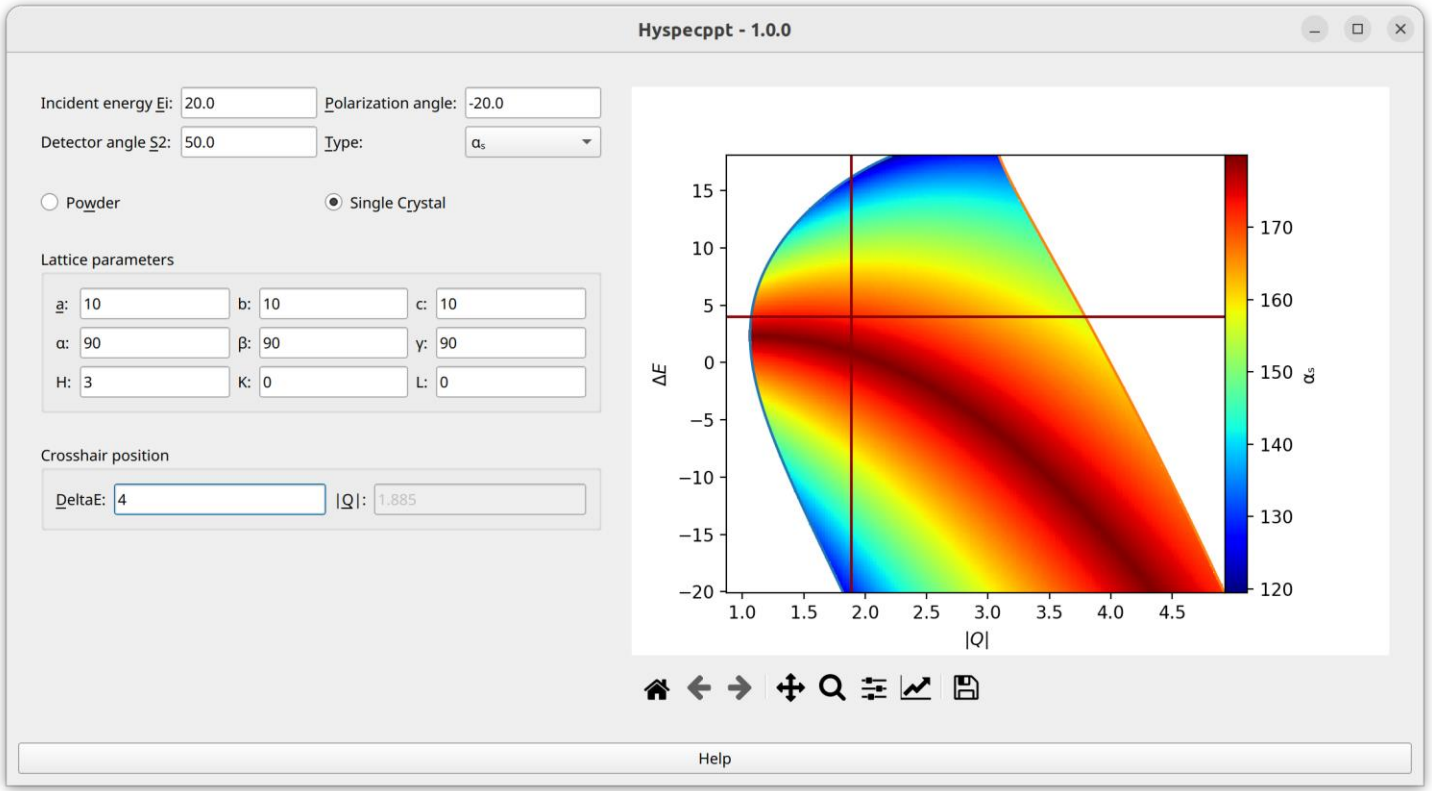




HYSPECPPT – polarization planning tool

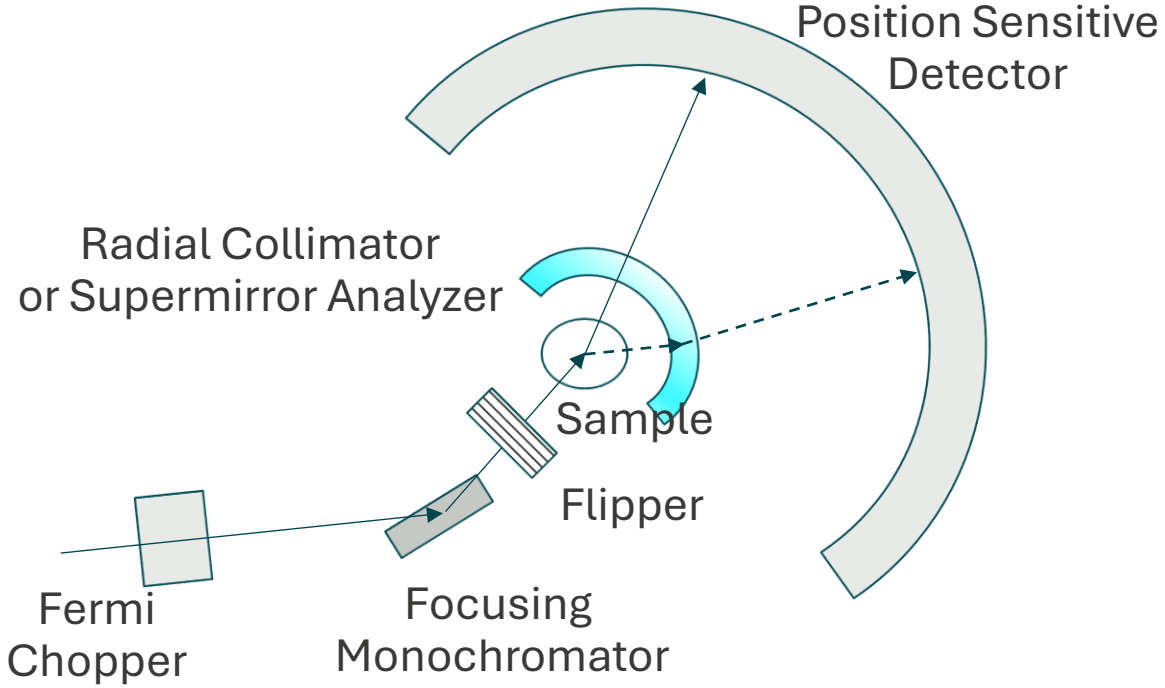
Calculate angle between polarization and momentum transfer

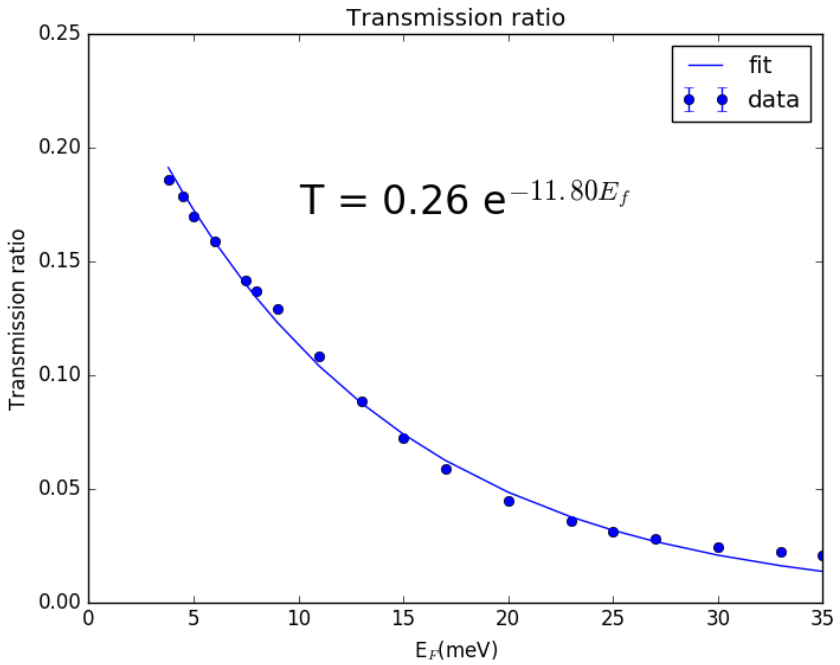




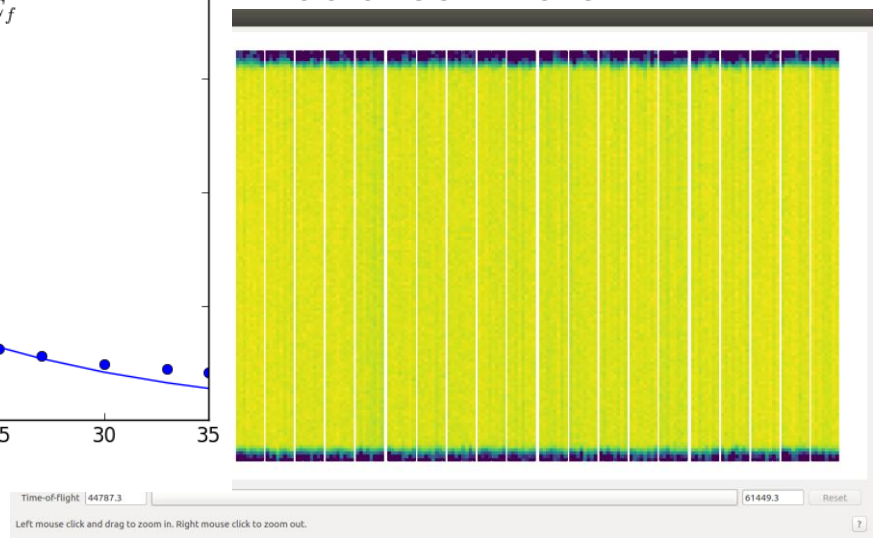
HYSPEC instrument corrections

- Geometry – deflection in the analyzer
- Transmission through the analyzer
  - Overall efficiency
  - Energy dependent efficiency
- Spin flip corrections

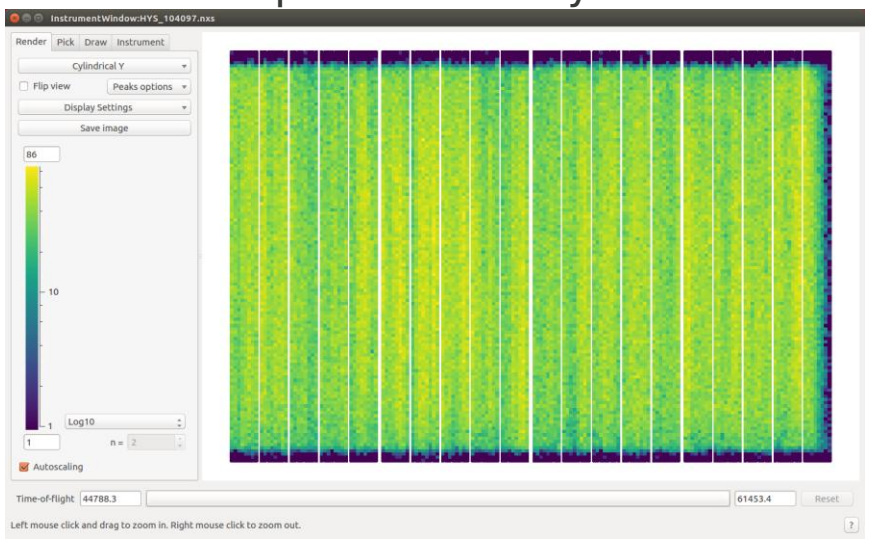




Radial collimator



Supermirror analyzer



What do we measure?

- Neutron events – TOF and detector position
- What we want is the differential scattering cross section

$$\frac{d^2\sigma}{d\Omega dE} = \frac{Number\ of\ scattered\ neutrons}{Incident\ flux\ \times d\Omega \times dE}$$

- For multiple detectors/sample orientations

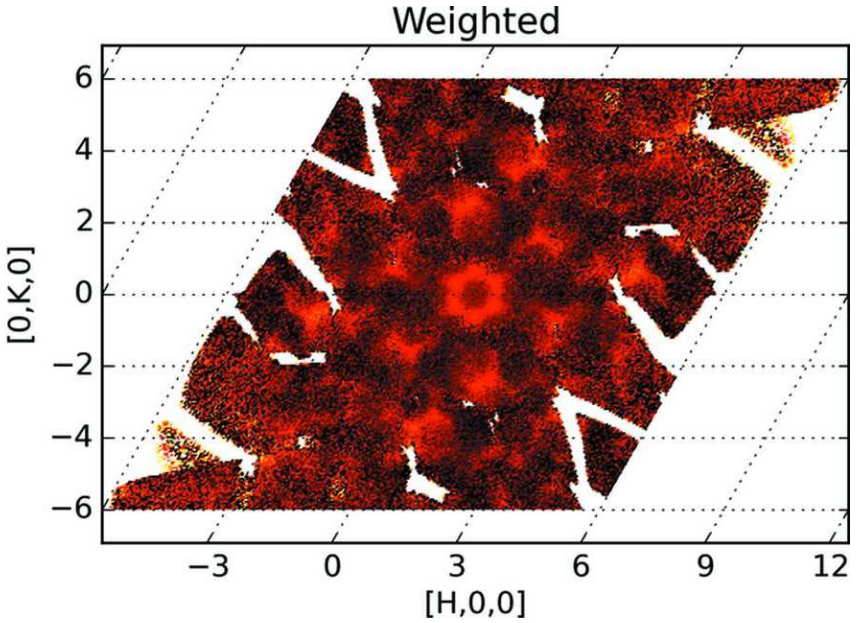
$$\frac{d^2\sigma}{d\Omega dE} = \frac{\Sigma Number\ of\ scattered\ neutrons}{\Sigma Incident\ flux\ \times d\Omega \times dE}$$

MDNorm algorithm

Theoretical description

JOURNAL OF APPLIED CRYSTALLOGRAPHY

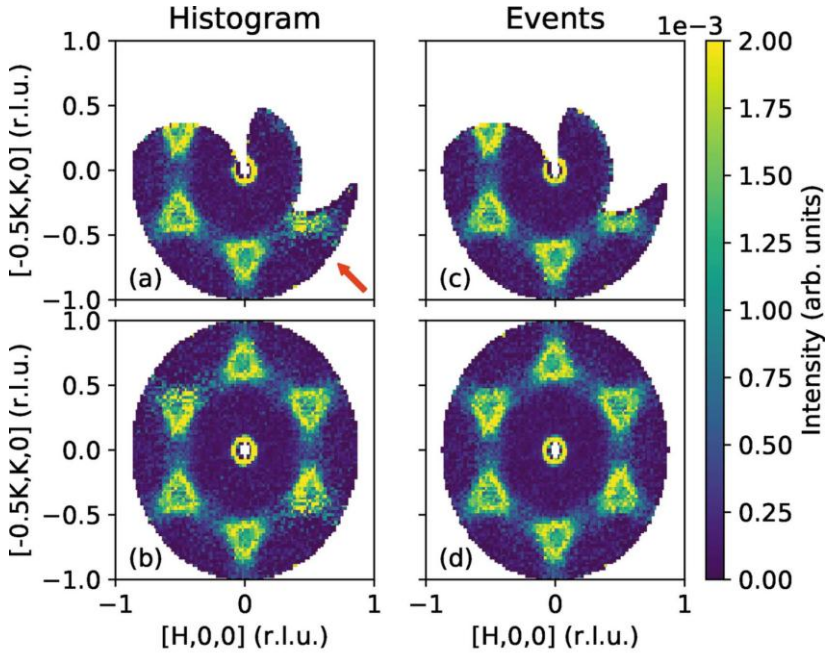
- **Michels-Clark *et al.***
- **Volume 49** | **Part 2** | April 2016 | Pages 497–506 | 10.11107/S1600576716001369



Implementation details

JOURNAL OF APPLIED CRYSTALLOGRAPHY

- **Savici *et al.***
- **Volume 55** | **Part 6** | December 2022 | Pages 1514–1527 | 10.11107/S1600576722009645



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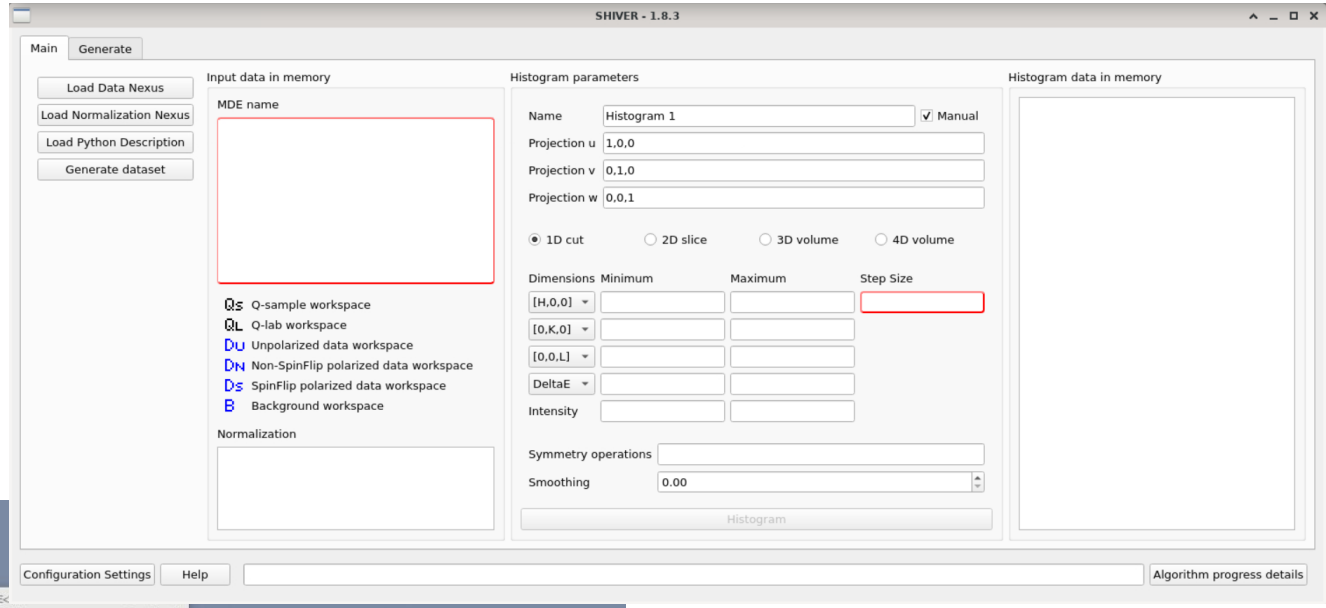
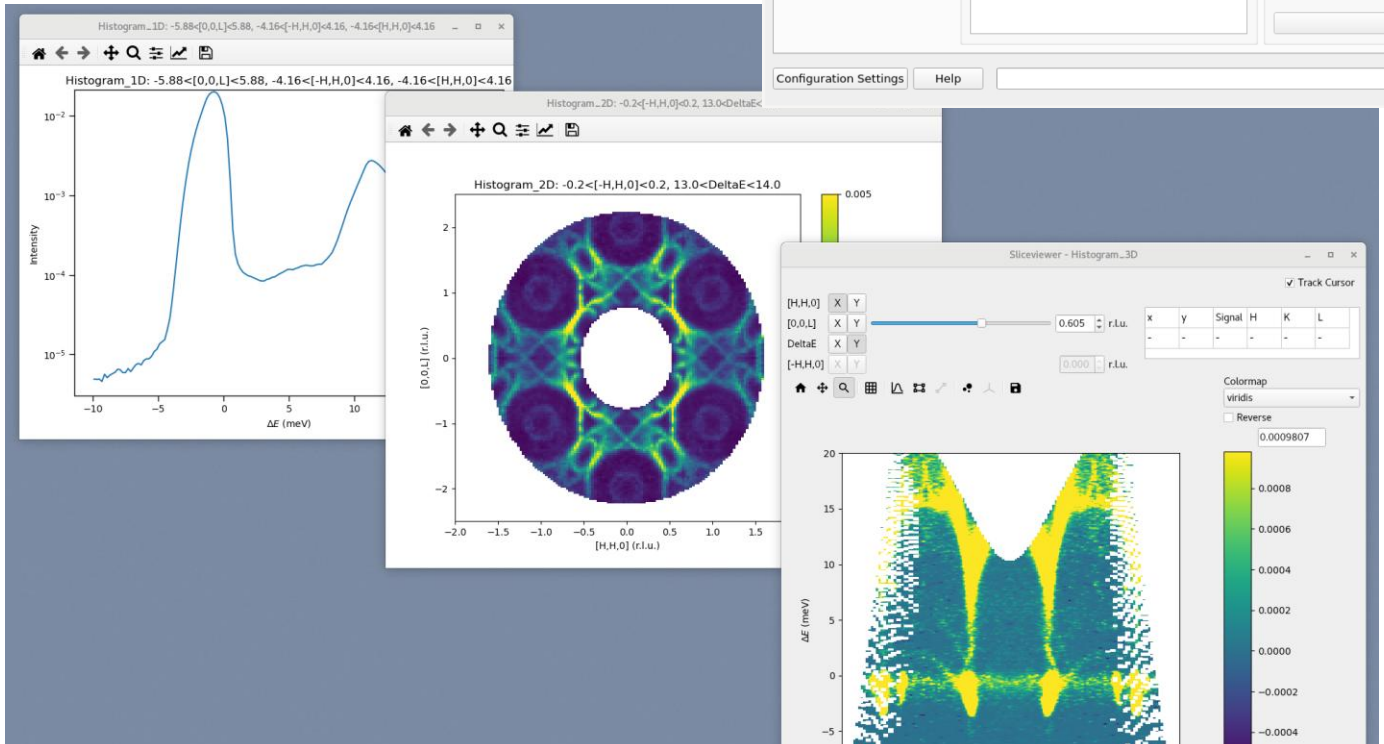
SHIVER – spectroscopy histogram visualization for event reduction

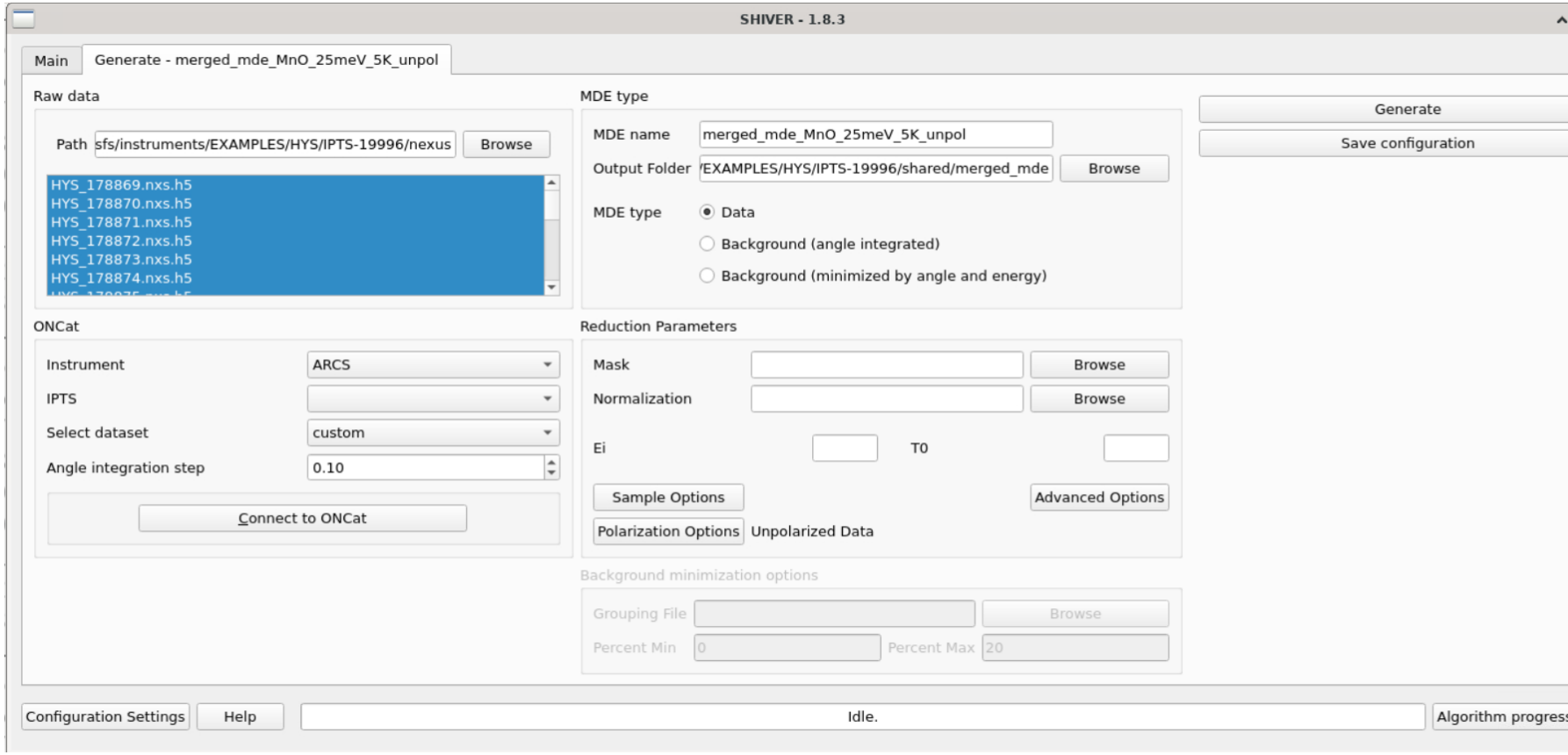
- Make histograms/plots
- Intermediate data storage as multi-dimensional events
- Corrections
- Polarization options
- Scripting



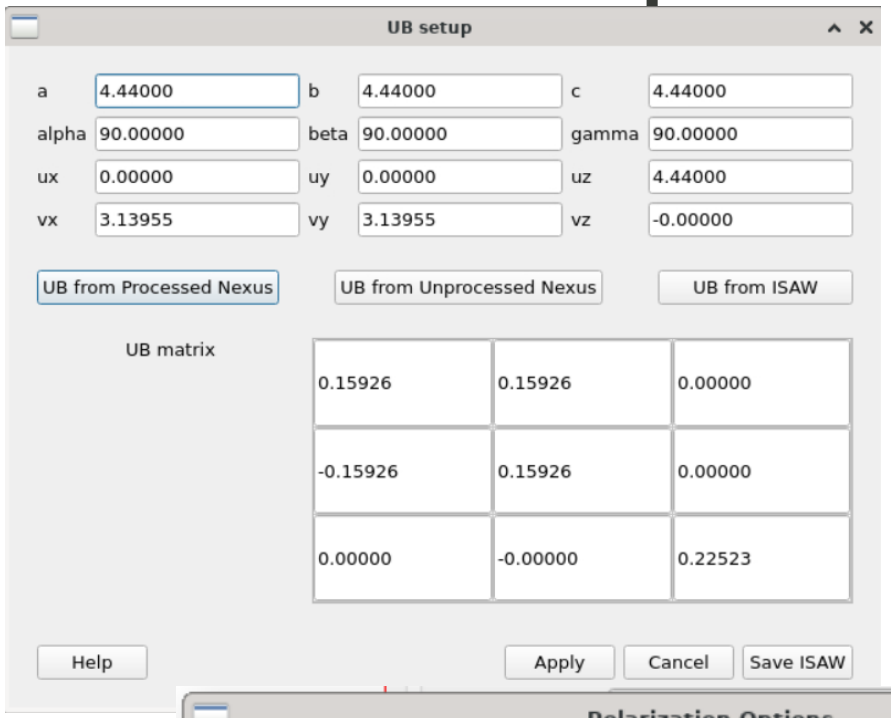


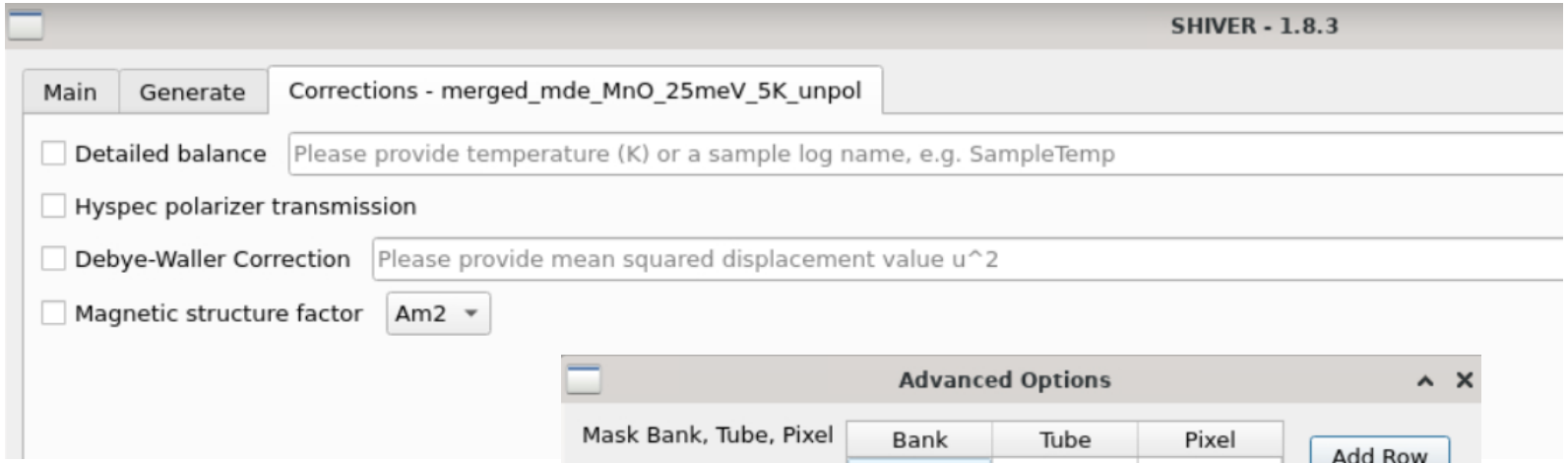
SHIVER – generating intermediate data

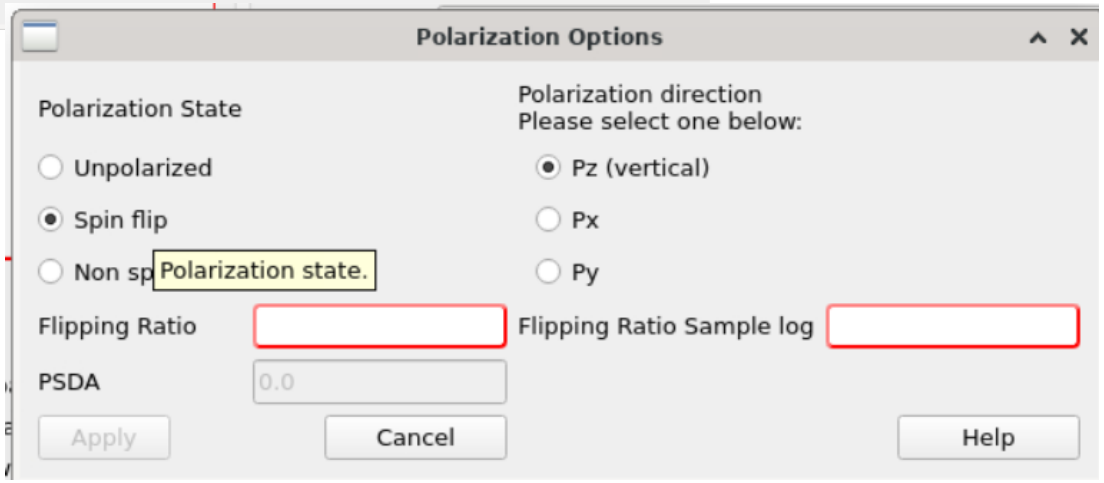
- Select data
- Set name and output folder
- Set parameters
- Save configuration
- Generate

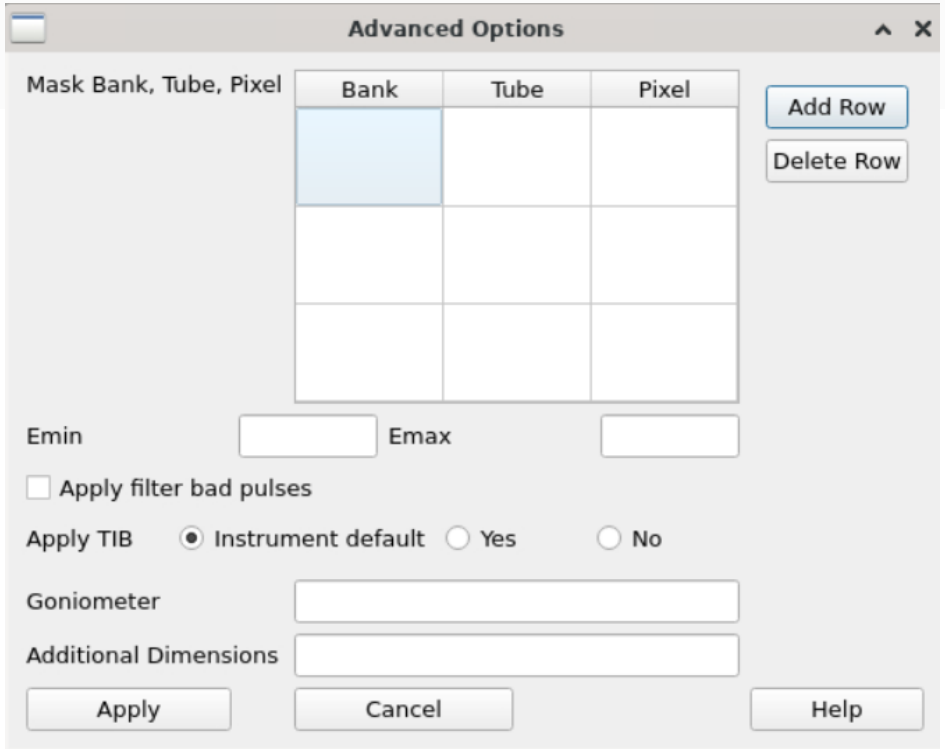


Shiver – lattice parameters, corrections and advanced options









Integration with Mantid

- Allow scripting
- Additional corrections
- Integrate data