



Data reduction and visualization using **SHIVER**

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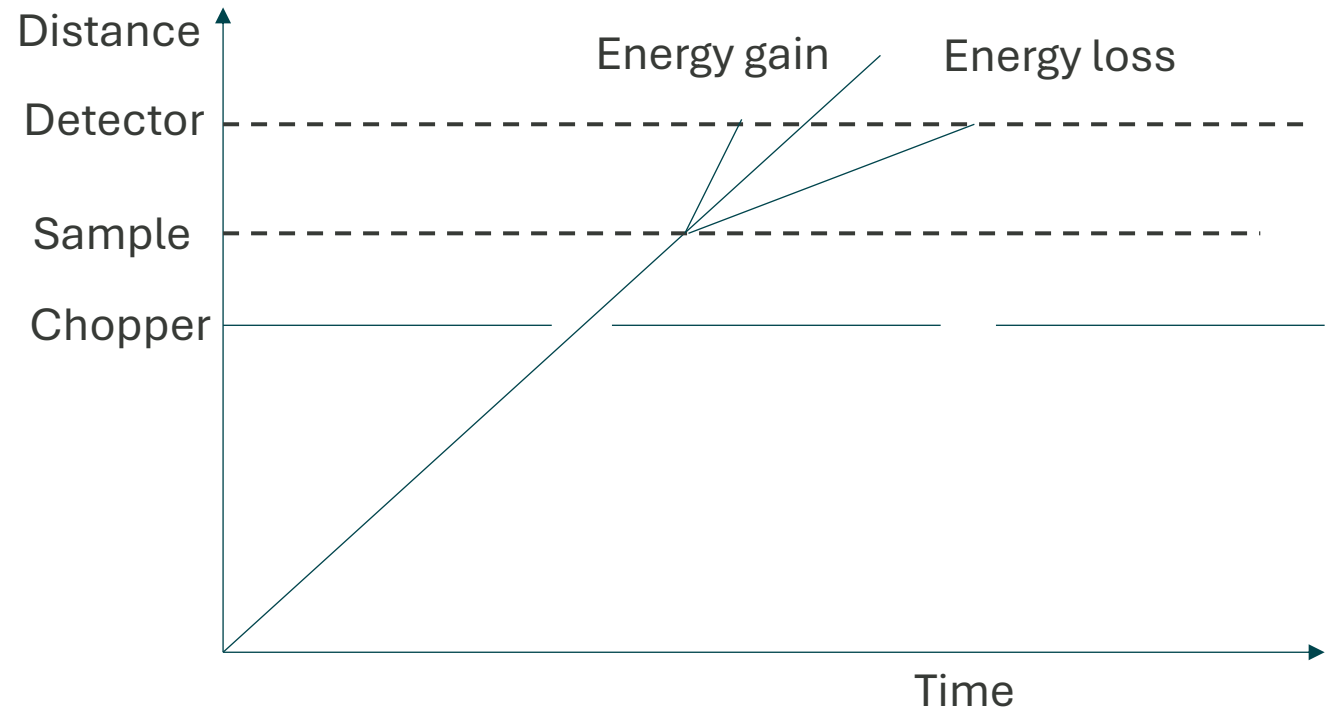
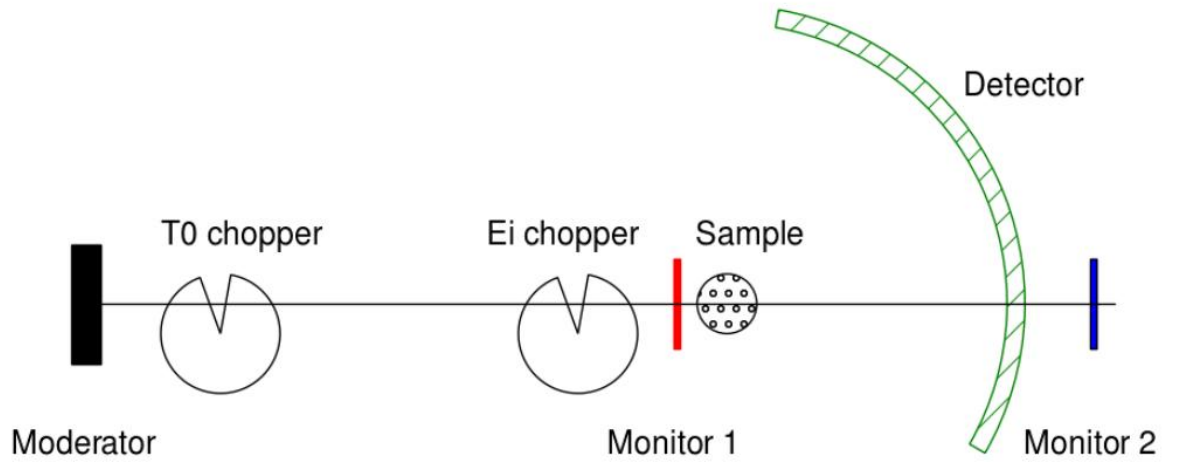
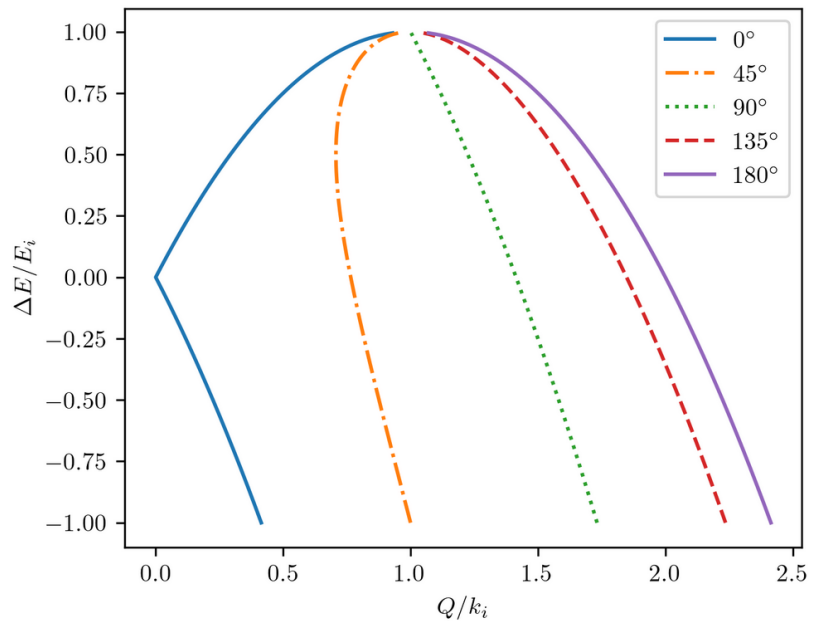
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TOF DGS spectrometers

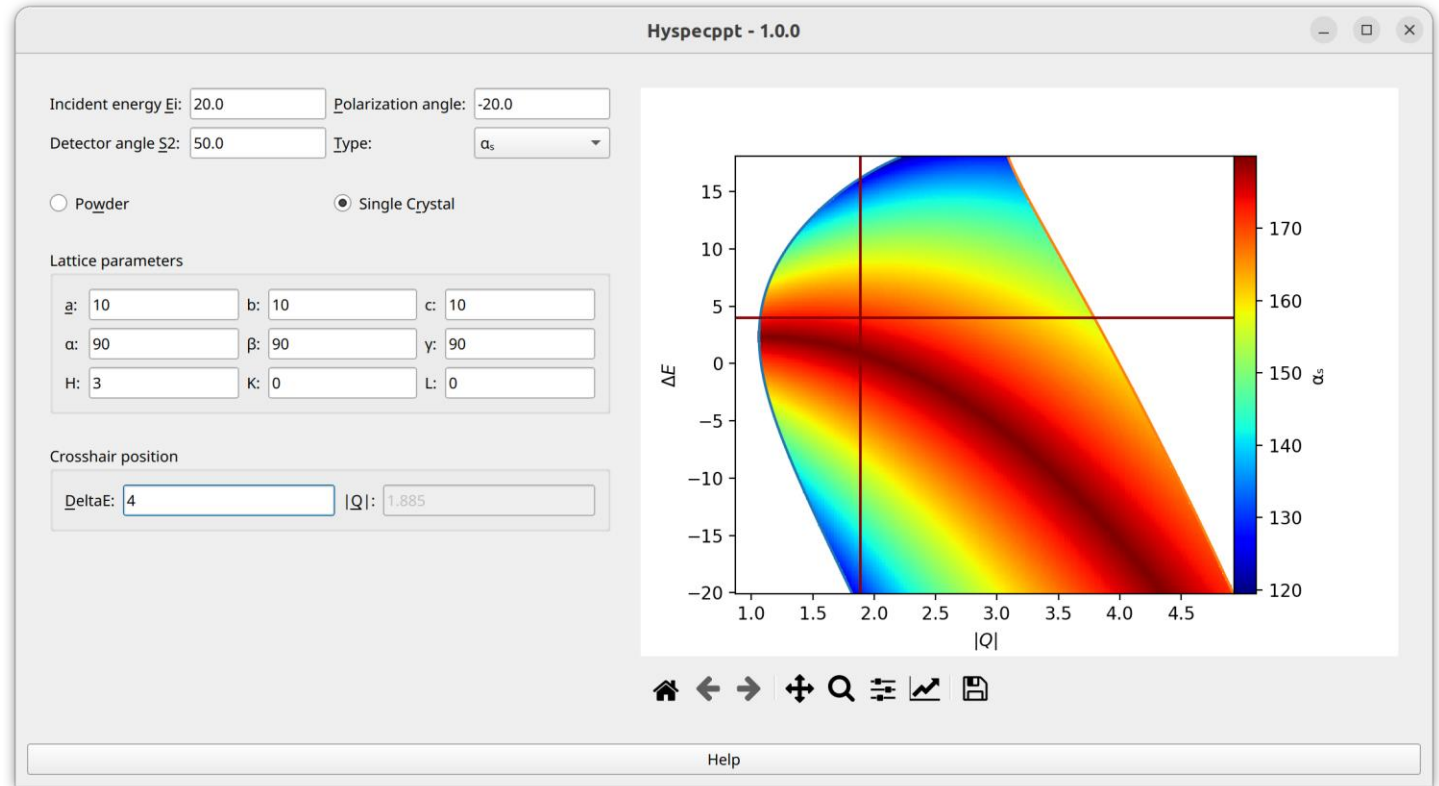
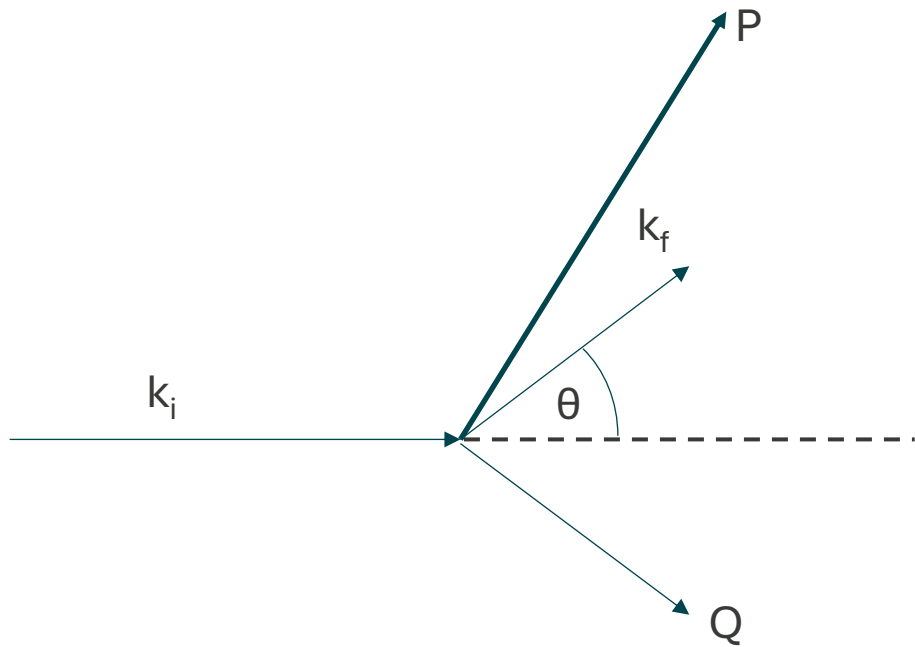
- Incident energy is set by the chopper system
- Final energy is calculated from time of flight
- Momentum transfer also depends on the detector position

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



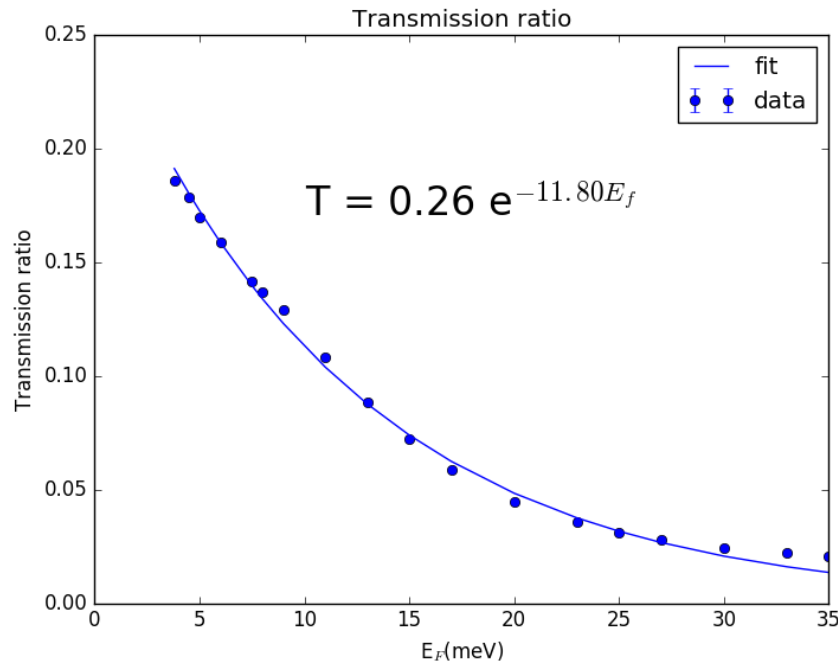
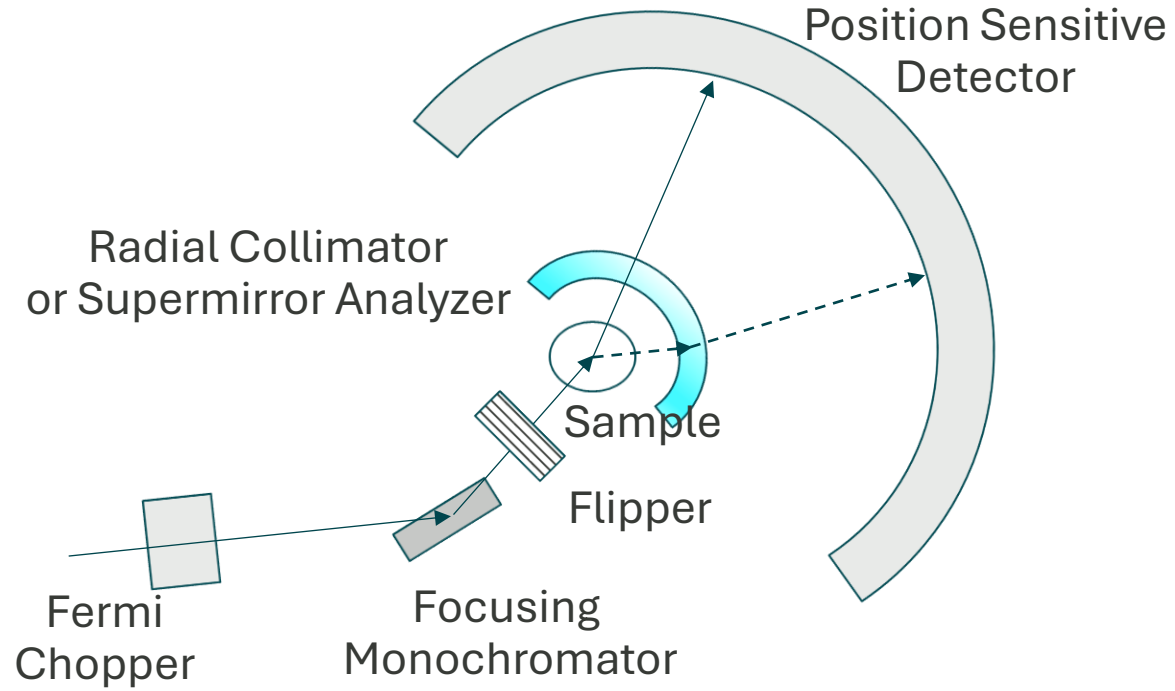
HYSPECPPT – polarization planning tool

Calculate angle between polarization and momentum transfer

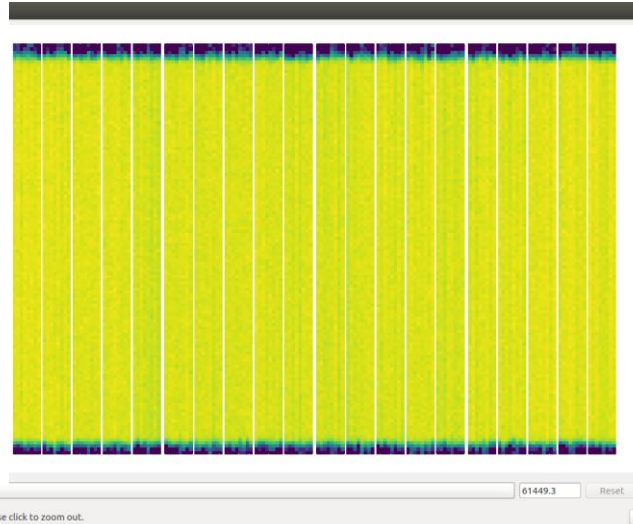


HYSPEC instrument corrections

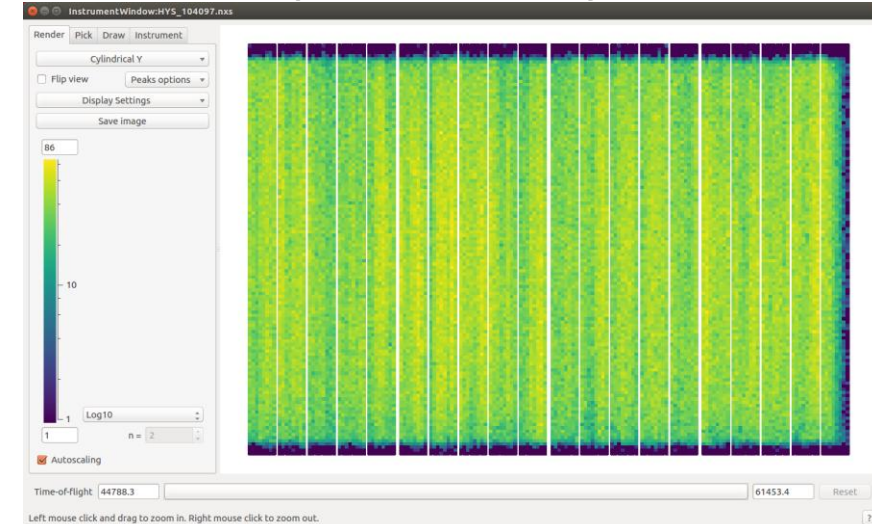
- Geometry – deflection in the analyzer
- Transmission through the analyzer
 - Overall efficiency
 - Energy dependent efficiency
- Spin flip corrections



Radial collimator



Supermirror analyzer



What do we measure?

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

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

- For multiple detectors/sample orientations

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

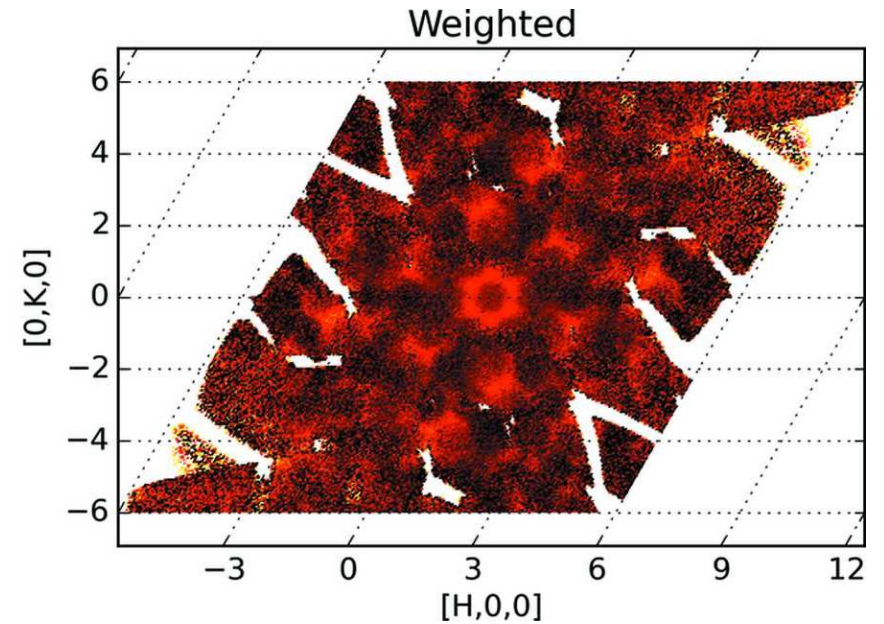
MDNorm algorithm

Theoretical description



• **Michels-Clark *et al.***

• **Volume 49 | Part 2** | April 2016 | Pages 497–506 | [10.11107/S1600576716001369](https://doi.org/10.11107/S1600576716001369)

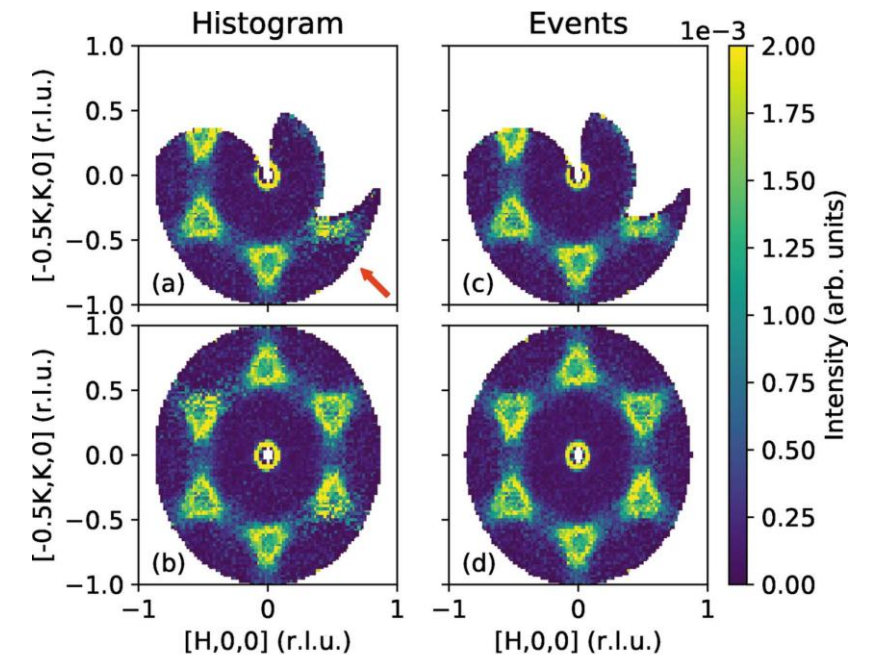


Implementation details



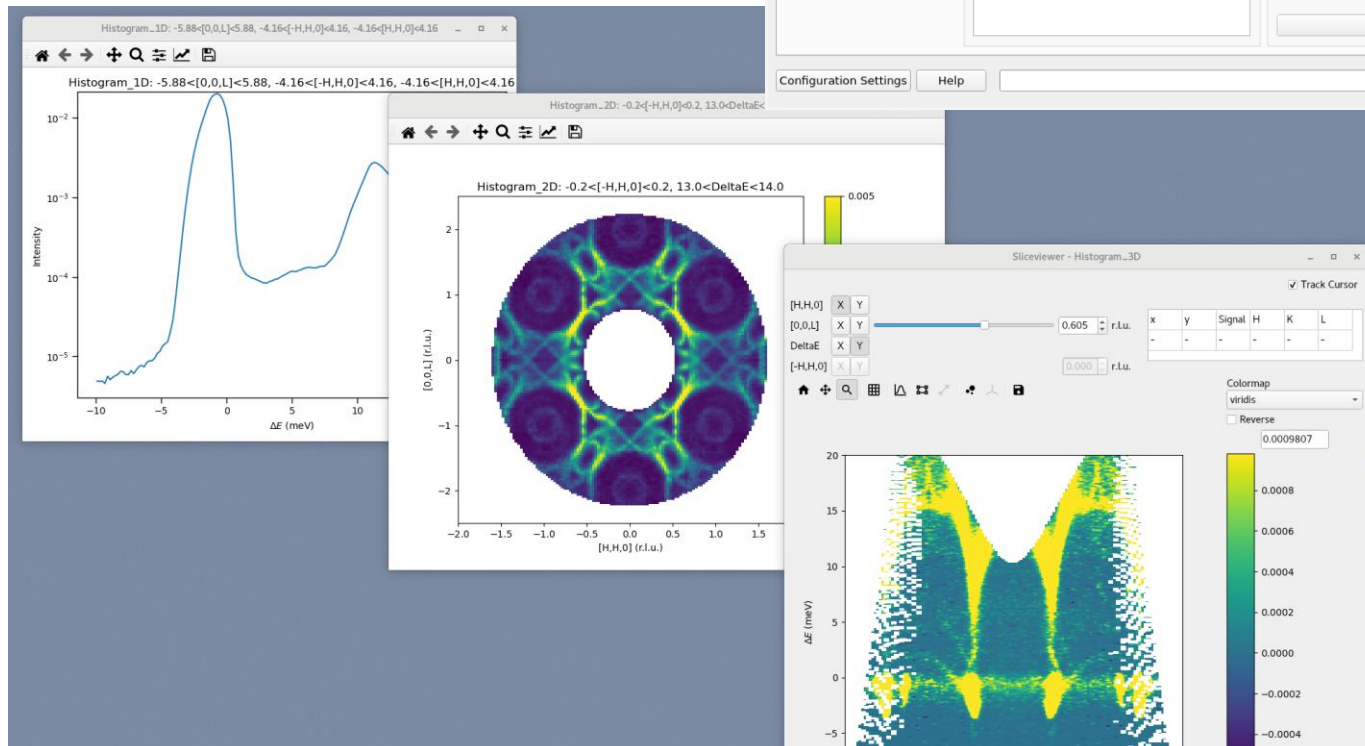
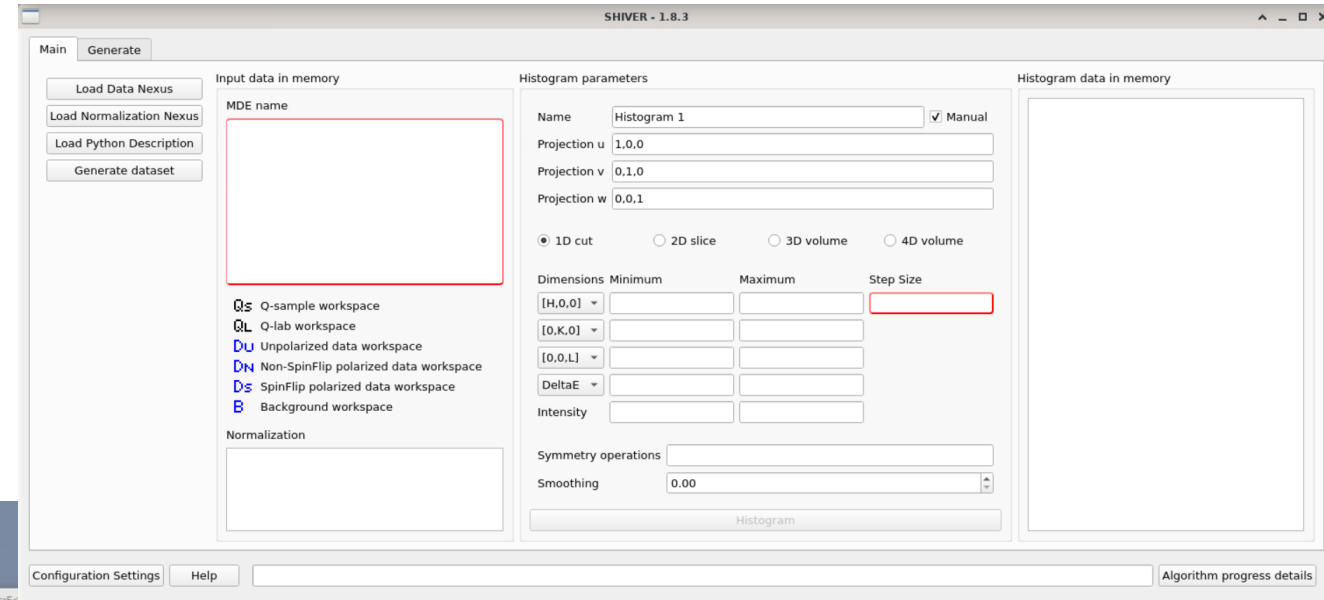
• **Savici *et al.***

• **Volume 55 | Part 6** | December 2022 | Pages 1514–1527 | [10.11107/S1600576722009645](https://doi.org/10.11107/S1600576722009645)



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

The screenshot displays the SHIVER 1.8.3 software interface, specifically the 'Generate' configuration window. The window title is 'SHIVER - 1.8.3' and the main tab is 'Main Generate - merged_mde_MnO_25meV_5K_unpol'. The interface is divided into several sections:

- Raw data:** A text box shows the path 'sfs/instruments/EXAMPLES/HYS/IPTS-19996/nexus' with a 'Browse' button. Below it is a list of files: HYS_178869.nxs.h5, HYS_178870.nxs.h5, HYS_178871.nxs.h5, HYS_178872.nxs.h5, HYS_178873.nxs.h5, HYS_178874.nxs.h5, and HYS_178875.nxs.h5.
- MDE type:** A text box for 'MDE name' contains 'merged_mde_MnO_25meV_5K_unpol'. Below it, 'Output Folder' is 'EXAMPLES/HYS/IPTS-19996/shared/merged_mde' with a 'Browse' button. The 'MDE type' section has three radio buttons: 'Data' (selected), 'Background (angle integrated)', and 'Background (minimized by angle and energy)'.
- ONCat:** A section with dropdown menus for 'Instrument' (ARCS), 'IPTS', and 'Select dataset' (custom). The 'Angle integration step' is set to 0.10. A 'Connect to ONCat' button is at the bottom.
- Reduction Parameters:** Includes 'Mask' and 'Normalization' text boxes with 'Browse' buttons. Below are 'Ei' and 'TO' input fields. There are buttons for 'Sample Options', 'Advanced Options', and 'Polarization Options' (Unpolarized Data).
- Background minimization options:** Includes 'Grouping File' with a 'Browse' button, and 'Percent Min' (0) and 'Percent Max' (20) input fields.

At the bottom right, there are 'Generate' and 'Save configuration' buttons. The status bar at the bottom shows 'Configuration Settings', 'Help', 'Idle.', and 'Algorithm progress'.

Shiver – lattice parameters, corrections and advanced options

UB setup

a b c
alpha beta gamma
ux uy uz
vx vy vz

UB matrix

0.15926	0.15926	0.00000
-0.15926	0.15926	0.00000
0.00000	-0.00000	0.22523

SHIVER - 1.8.3

Main Generate Corrections - merged_mde_MnO_25meV_5K_unpol

Detailed balance

Hyspec polarizer transmission

Debye-Waller Correction

Magnetic structure factor

Advanced Options

Mask Bank, Tube, Pixel

Bank	Tube	Pixel

Emin Emax

Apply filter bad pulses

Apply TIB Instrument default Yes No

Goniometer

Additional Dimensions

Polarization Options

Polarization State

Unpolarized Spin flip Non spin

Polarization direction
Please select one below:

Pz (vertical) Px Py

Flipping Ratio Flipping Ratio Sample log

PSDA

Integration with Mantid

- Allow scripting
- Additional corrections
- Integrate data

The screenshot displays the Mantid Workbench interface. At the top, the menu bar includes 'File', 'View', 'Interfaces', and 'Help'. The 'Workspaces' panel on the left shows a list of workspaces, with 'HH_L5_cut_E-0.5to0.5_5K' selected. The 'Algorithms' panel on the left lists various processing steps, with 'ApplyDetailedBalanceMD' selected. The central 'Editor' window shows a Python script named 'make_slices_unpolarized.py' with the following code:

```
108 'Dimension3Name': 'QDimension1',
109 'Dimension3Binning': '{},{}'.format(hh-dhh, hh+dhh),
110 'SymmetryOperations': 'x,y,z;-x,-y,z;x,y,-z;-x,-y,-z;y,x,z;y,x,-z',
111 'Smoothing': 1,
112 'OutputWorkspace': 'LE_slice',
113 'Plot_parameters': {'vmin': 0}
114 }
115 dsl.append(description)
116
117 return dsl
118
119
120 mde_folder = "/SNS/EXAMPLES/HYS/IPTS-19996/shar
121 output_folder = "/SNS/EXAMPLES/HYS/IPTS-19996/s
122 mde_5K_unpolarized = "merged_mde_MnO_25meV_5K_u
123
124 # Load data if not in memory
125 if mde_5K_unpolarized not in mtd.getObjectNames
126     LoadMD(Filename=os.path.join(mde_folder, f
127         OutputWorkspace=mde_5K_unpolarized)
128 slices_unpolarized_5K = define_slices('5K')
129
130 # make pdf
131 pdf_filename = os.path.join(output_folder, f'slice
132 with PdfPages(pdf_filename) as pdf_handle:
133     for slice_description in slices_unpolarized_5
134         plot_parameters = slice_description.pop('
135         MakeSlice(InputWorkspace=mde_5K_unpolariz
136
137     fig, ax=plt.subplots(subplot_kw={'projecti
138     ws = mtd[slice_description['OutputWorkspa
139     num_dims=len(ws.getNonIntegratedDimension
140     if num_dims==1:
141         slice_plot=ax.errorbar(ws,**plot_para
142     elif num_dims==2:
143         slice_plot=ax.pcolormesh(ws,**plot_pa
144         cbar=ax.get_figure().colorbar(slice_p
145         cbar.set_label("Intensity")
146     pdf_handle.savefig(fig)
147     plt.close('all')
148
```

Two input dialog boxes are overlaid on the script. The 'SpectralMomentMD input dialog' has 'InputWorkspace' set to 'merged_mde_MnO_25meV_5K_unpol' and 'Moment' set to 1. The 'ApplyDetailedBalanceMD input dialog' has 'InputWorkspace' set to 'merged_mde_MnO_25meV_5K_unpol'. The 'System Memory Usage' panel in the top right shows 7.3/1511.1 GB (0%) used, with a green bar indicating 701.8/1511.1 GB (46%) available. The bottom status bar shows 'Status: Idle. Last job completed successfully at Tue Mar 31 16:36:39 2026 in 72.359s'. The 'Workspace Calculator' at the bottom shows '1.0 * [] + 1.0 * [] = [] Go'.