SHIVER - A graphical user interface for visualization of single crystal inelastic neutron experiments

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Abstract:

Historically, data workflows for single crystal inelastic neutron experiments were using a pre-histogramming step, storing data for each detector as a histogram in energy transfer. Therefore, each bin of these histograms is then a measurement of the dynamic structure factor (or double differential cross section). A useful representation of this data includes transformation into momentum transfer, and a final histogramming step in the desired momentum and energy transfer grid. The main deficiencies of such existing approach are (i) the large amount of memory resources needed to store the histogram bins with zero neutron counts, and (ii) the difficulty of error propagation in re-histogramming, which resulted in the absence of weighting of contributions with different statistical significance.

We have developed a different approach, where the histogramming to energy-momentum space is based on neutron detection events and accounts for their statistical significance. The algorithm [1] is implemented in the Mantid software.

The script based interface was made available a few years ago. Here will focus on showing the newly implemented graphical interface [2], and will emphasize lessons learned for improvement of the software code and the user experience.

GUI:

Fig 1. Since histogramming and plotting are the most usual tasks, they are the basis of the main window. Missing information is highlighted in red.

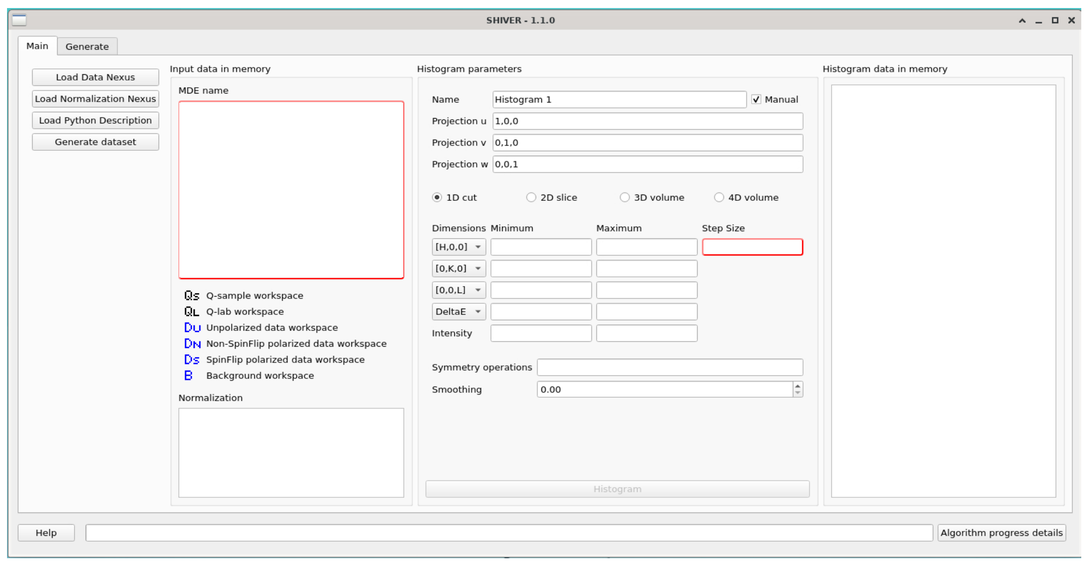


Fig 2. Intermediate data sets are selected to generate 1, 2, 3, or 4 dimensional histograms

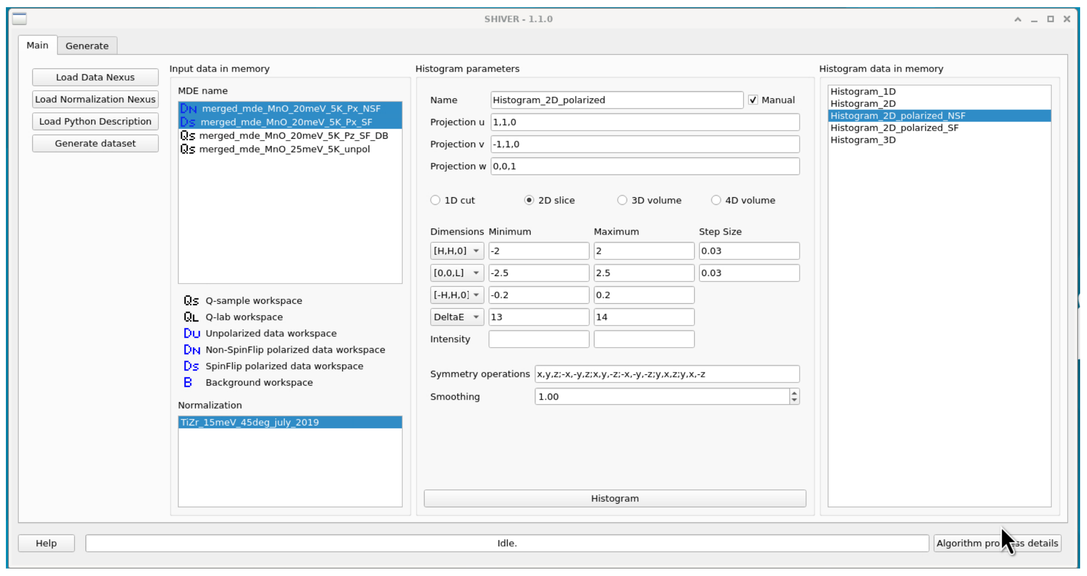


Fig 3. Various histograms are plotted using the matplotlib library or Mantid

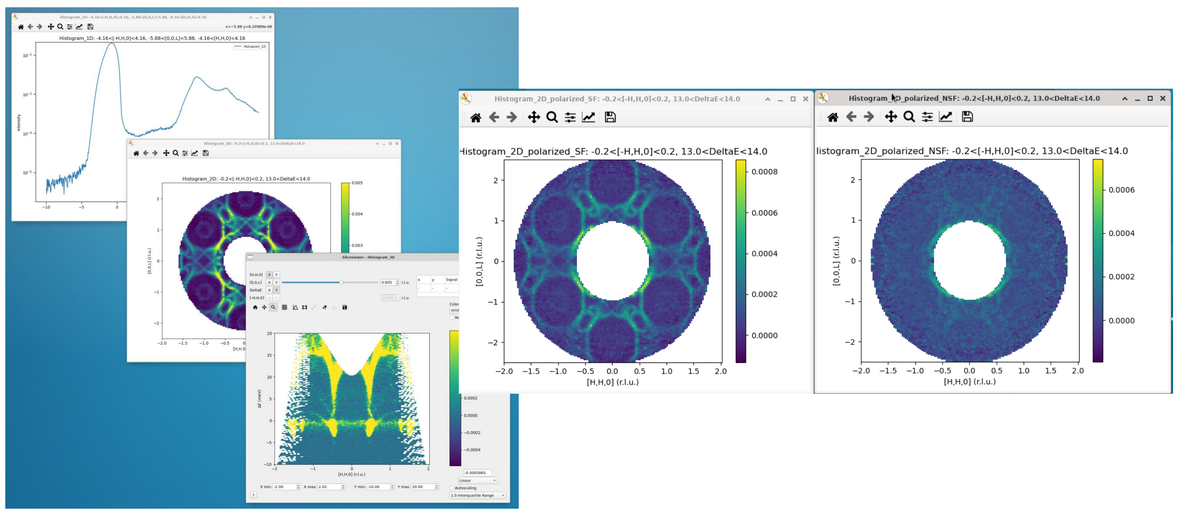


Fig 4. Generating intermediate datasets from raw event files is required only once. It helps keeping data organized and it improves speed.

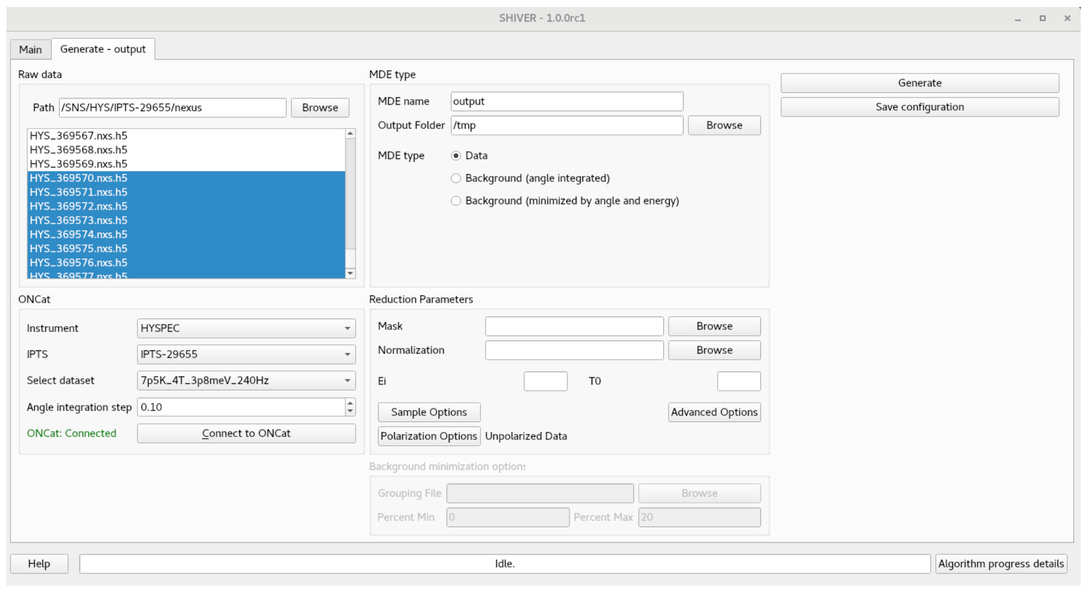


Fig 5. Additional interfaces control reduction parameters and corrections.

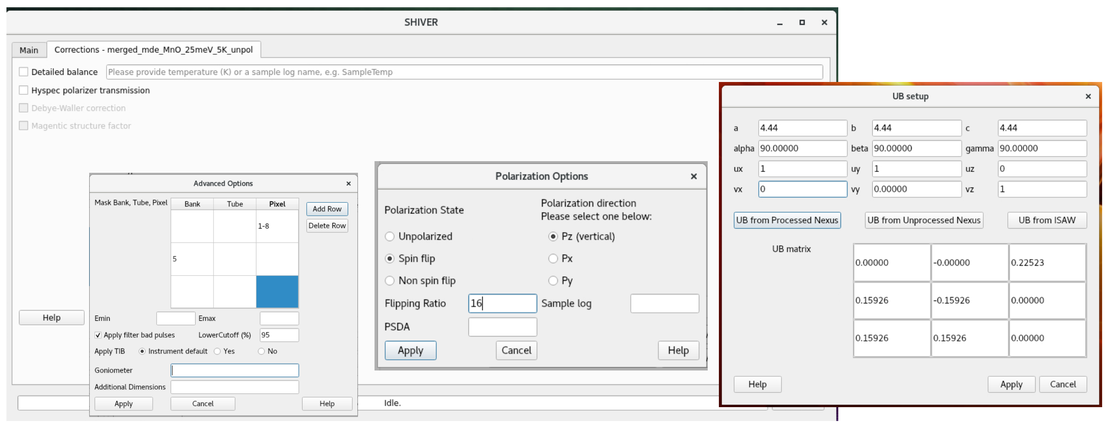
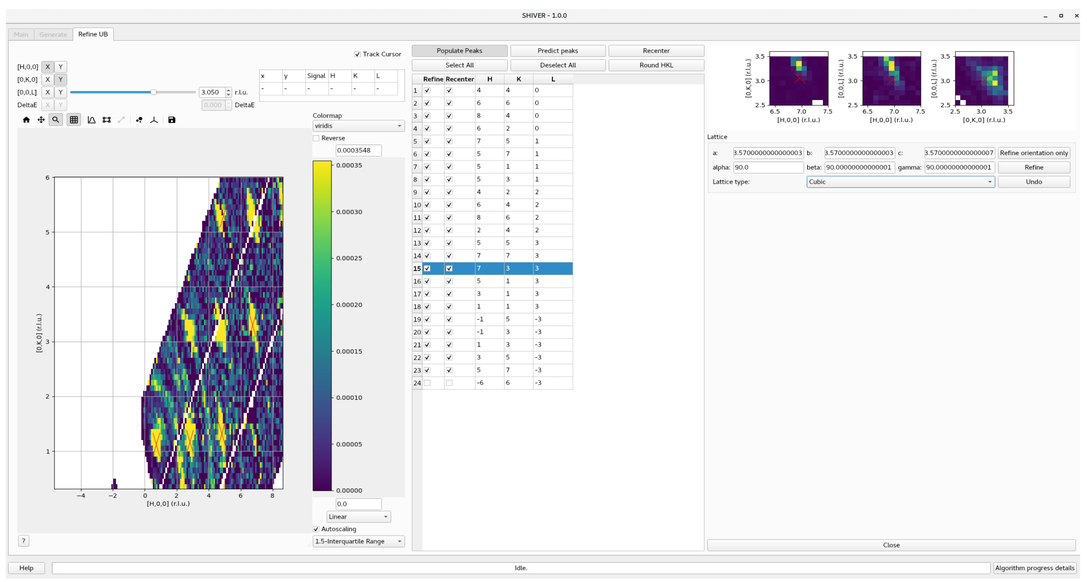
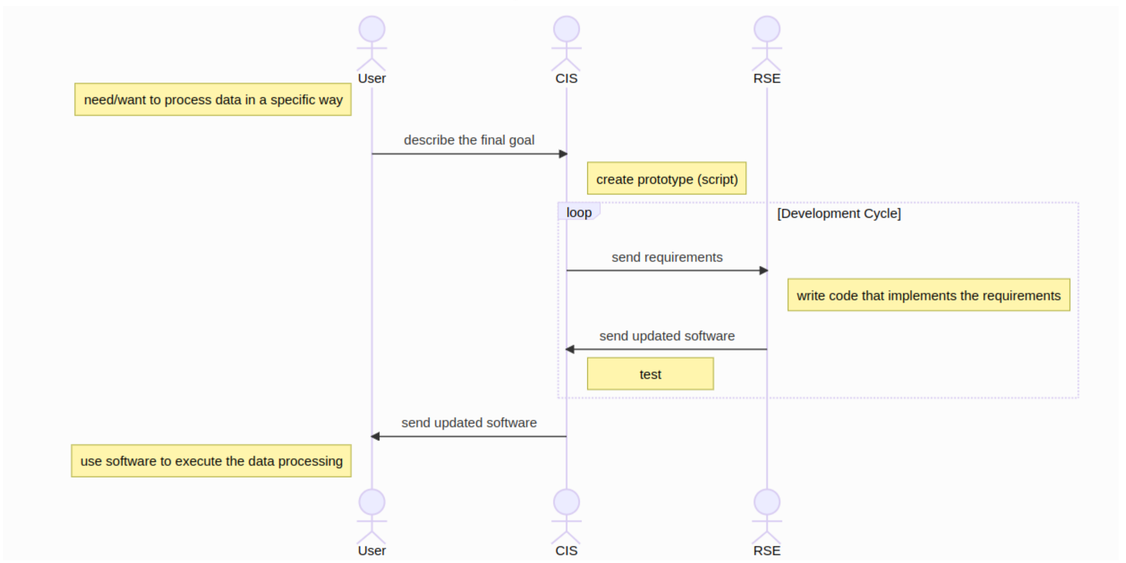


Fig 6. An interface to refine lattice parameters and orientation is also available.



Lessons learned:

- Fully develop scripting before starting work on the graphical user interface.
- Get a lot of feedback on User Experience (UX). We performed UX testing at several points in the development cycle.
- Incremental demonstrations during various stages.
- Frequent communication between users, computational instrument scientist (product owner) and research software engineers.



[1] Savici, A. T., Gigg, M. A., Arnold, O., Tolchenov, R., Whitfield, R. E., Hahn, S. E., Zhou, W. & Zaliznyak, I. A. (2022). Efficient data reduction for time-of-flight neutron scattering experiments on single crystals. J. Appl. Cryst. 55, 1514-1527.
[2] https://github.com/neutrons/Shiver

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