

Software status for inelastic neutron scattering – DGS and TAS

Andrei T. Savici

Oak Ridge National Laboratory

ORNL is managed by UT-Battelle, LLC for the US Department of Energy

Overview

- Organizational changes
- Status of DGS reduction
- Status of TAS reduction
- Data analysis

Starting point: 2018 Triennial Review

Reviewers noted:

- Improvements in data acquisition
- Need for prioritization
- Successes where “embedding” worked; pointing out that it is insufficient
- Lack of uniformity across instruments
- Reduction: users experiencing delays or having to rely heavily on beam line scientists

DOE Recommendation:

BES notes the chronic concerns, over several triennial reviews, that the shortcomings in the **data reduction software** at SNS and HFIR have not been adequately addressed. BES requests a plan with specific milestones and timelines to implement strategic enhancements to properly support the users' needs. BES will conduct a subject matter expert review of the plan, prior to its implementation in FY 2019.

New roles

- Why?

- Not everyone is an expert in the entire software development chain
- Remove distractions
- Clearly communicate who does what
- Improve quality

- Roles:

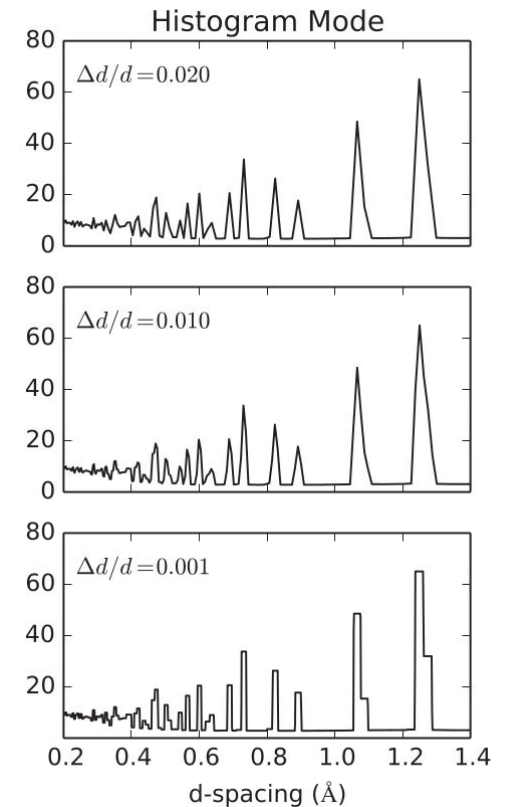
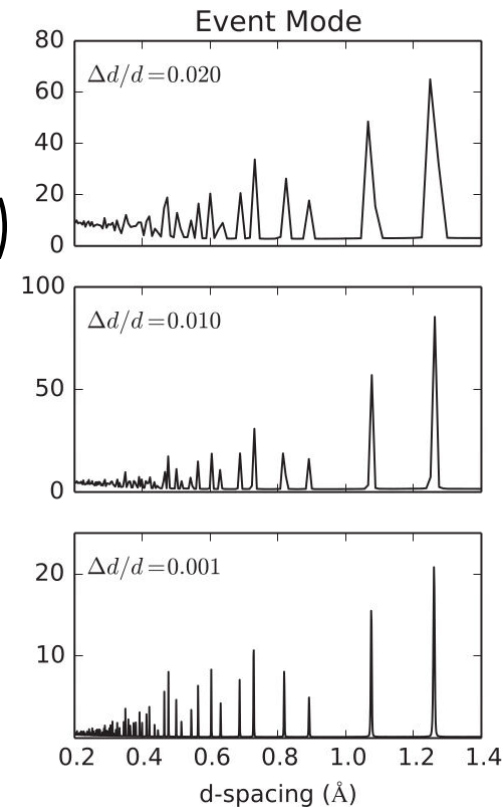
- Computational instrument scientist
- Computational scientist
- Research software engineer
- Software project manager
- Software quality assurance specialist
- Software release engineer
- Computational scientific associate
- Software user liaison

Overview

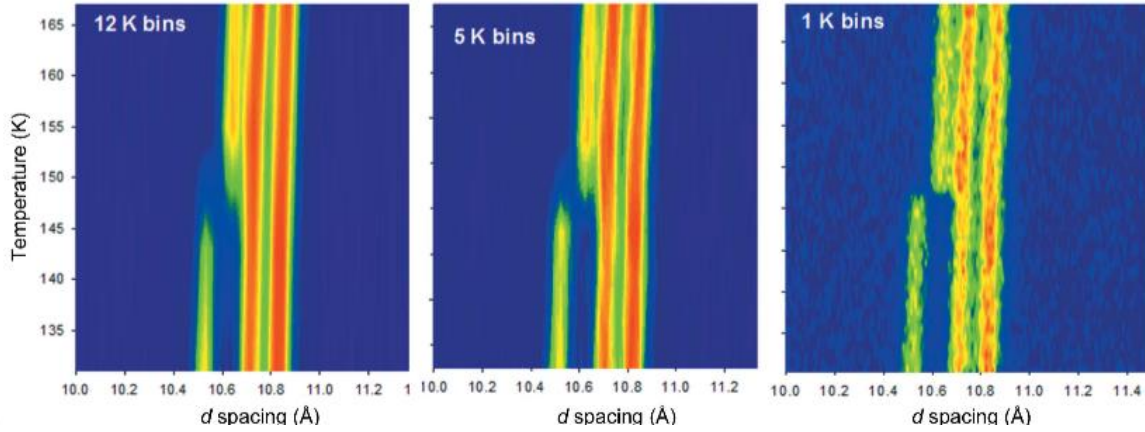
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Event based data

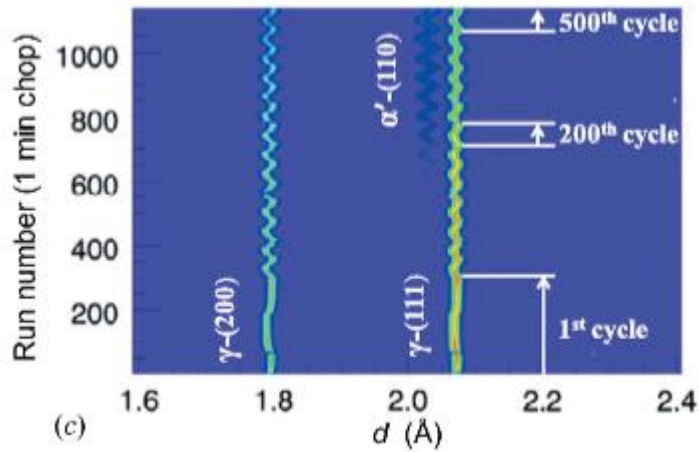
- Record detection time for each individual neutron
- Clean up spurious instrumentation mishaps
- Dynamic rebinning
- Time resolved data acquisition
 - Slow changes (temperature, goniometer)
 - Fast changes (pulse magnetic fields)



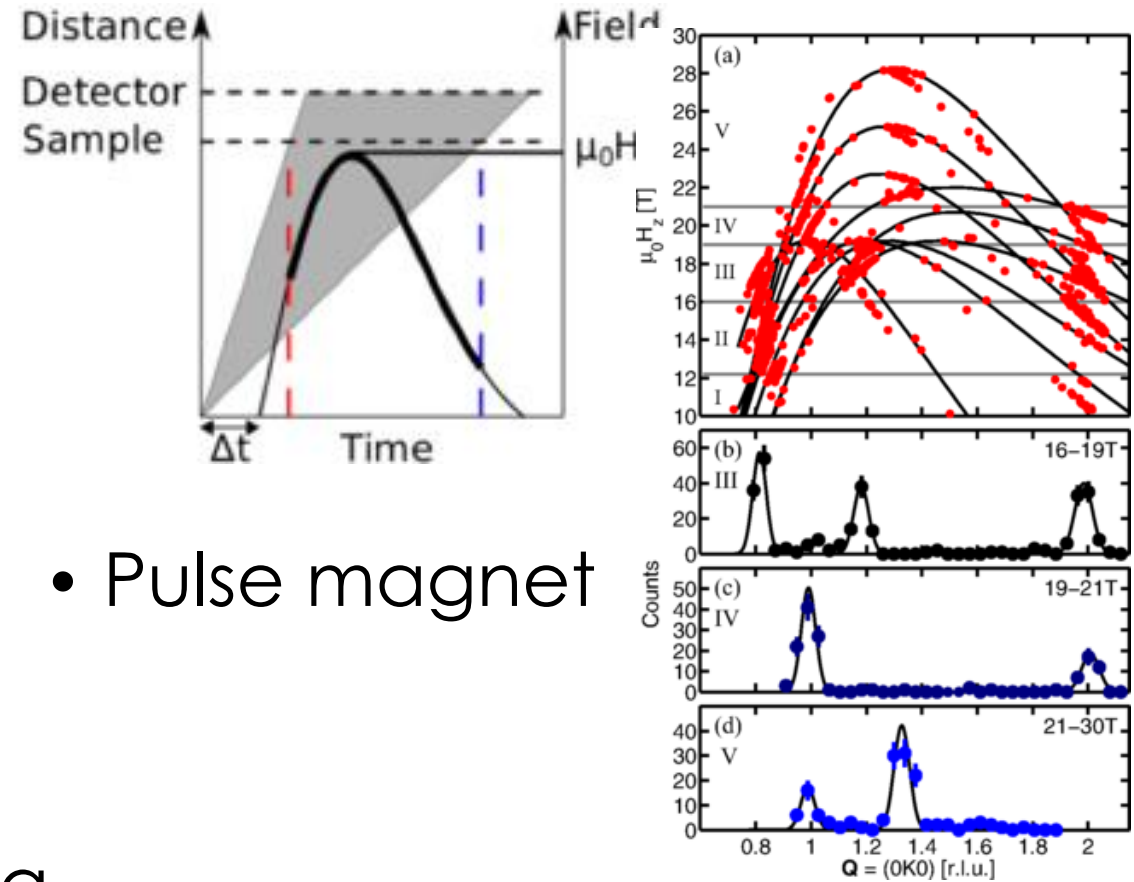
Examples of Event Filtering



- Continuous temperature ramping



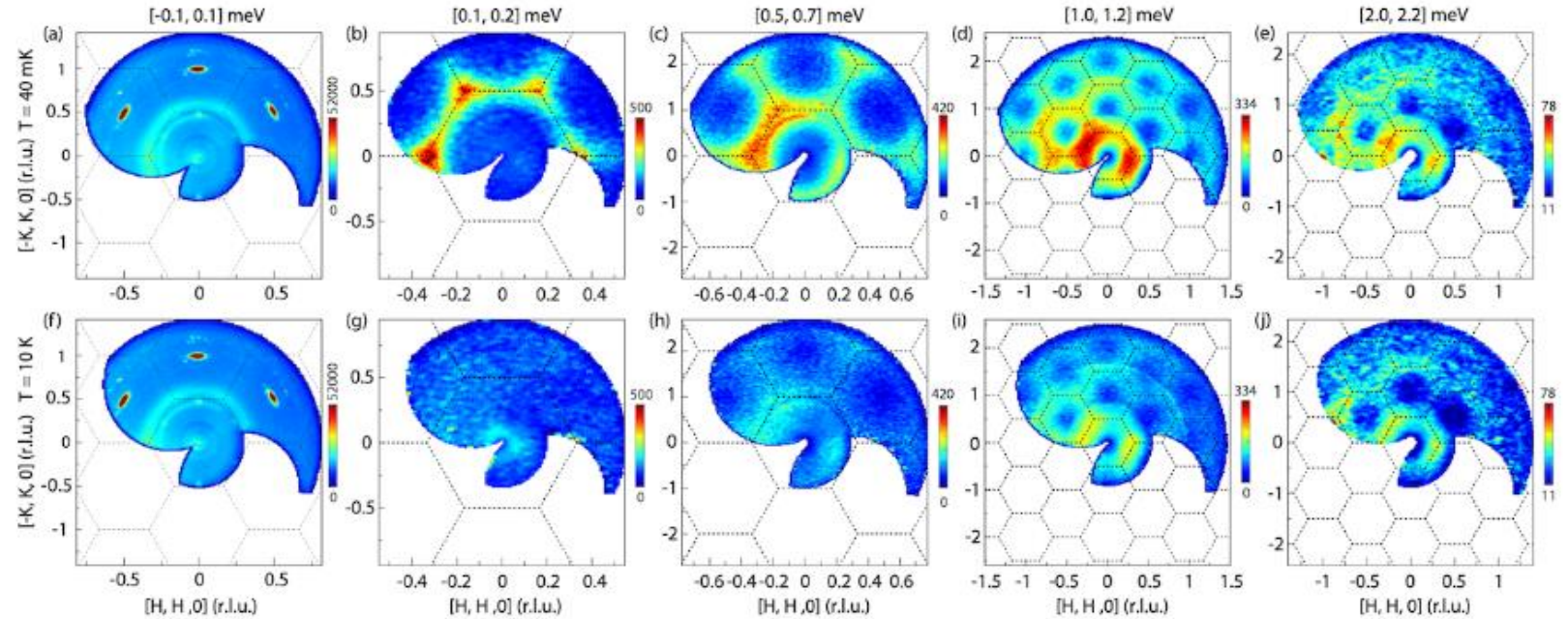
- Battery charging and discharging



- Pulse magnet

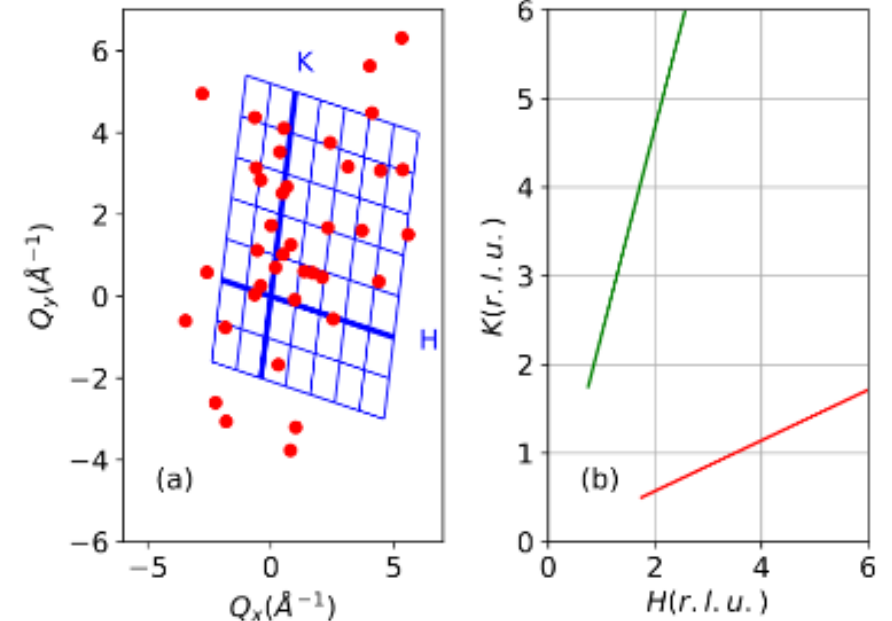
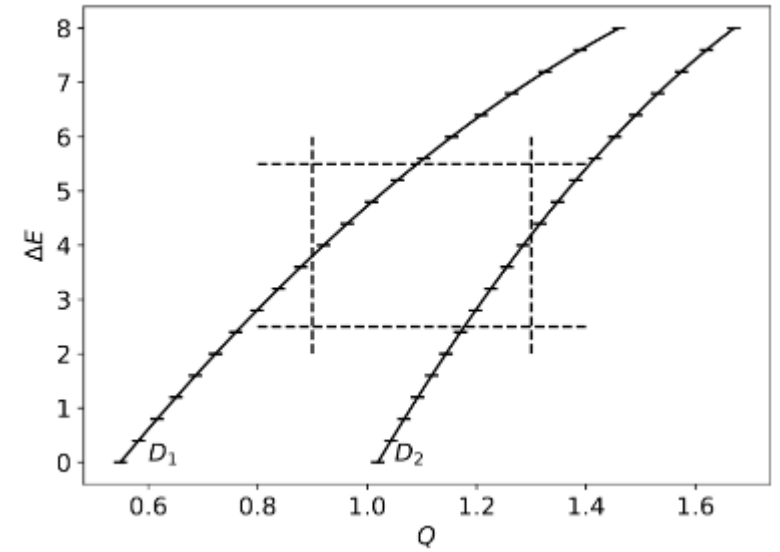
New normalization for multidimensional data

- We keep events (smaller files for inelastic)
- Procedure available for spectroscopy or diffraction measurements
- Correctly account for files with different statistics
- Keep data and normalization separately



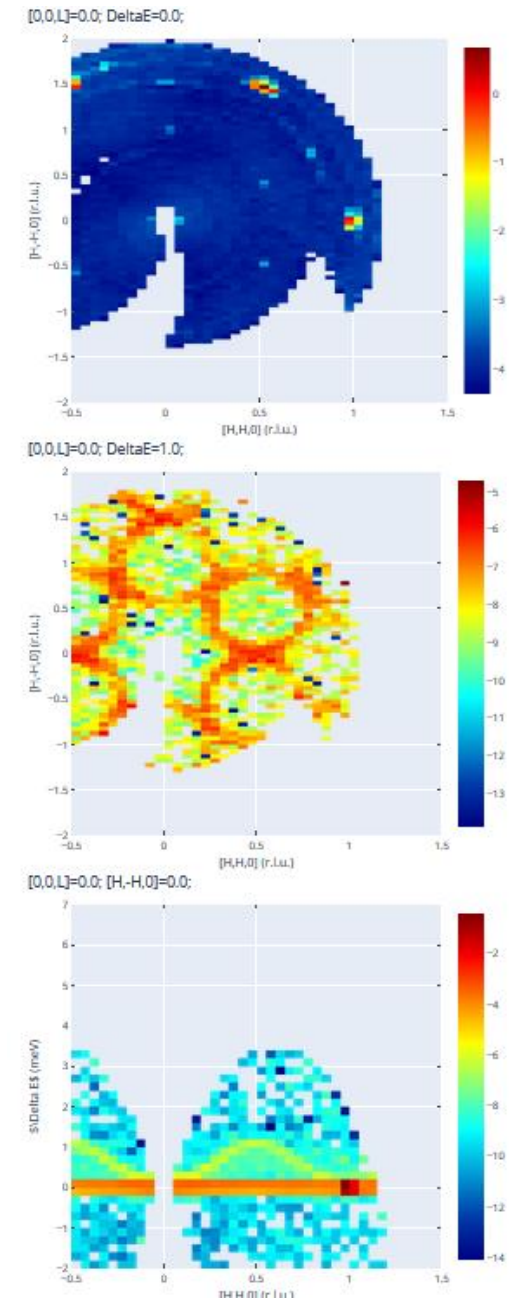
Comparison with mslice approach

- Mslice uses histograms in energy transfer where each bin is considered an independent measure of scattering cross section, then averages those numbers
- Better approach: bin counts and calculate separately the weighting factor from detector trajectories



Advantages of current approach

- Allows for correct accounting of multiple runs, with different proton charge, different geometry
- Much smaller memory footprint
- Non axis aligned cuts and symmetry operations
- Can correct UB matrix
- Implemented in MANTID, so the entire workflow can be implemented in a single script
- Can rely on autoreduction



Autoreduction update

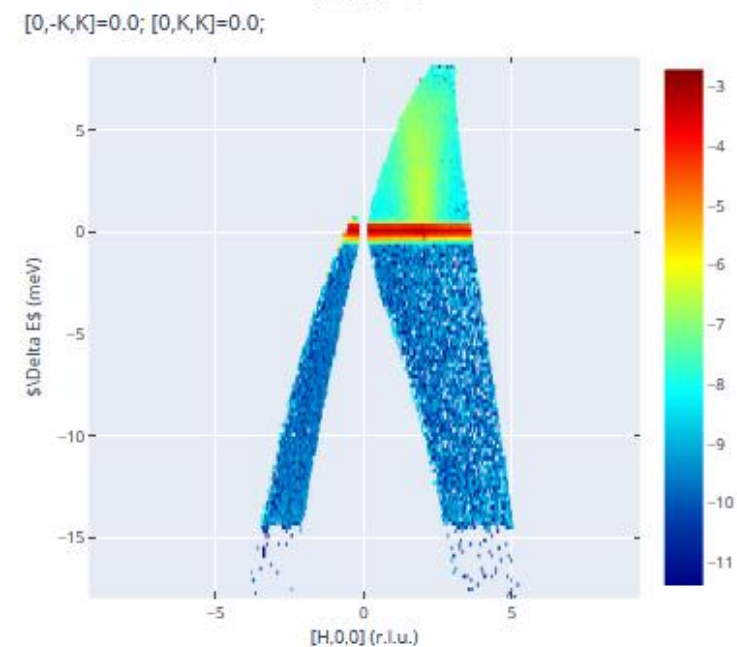
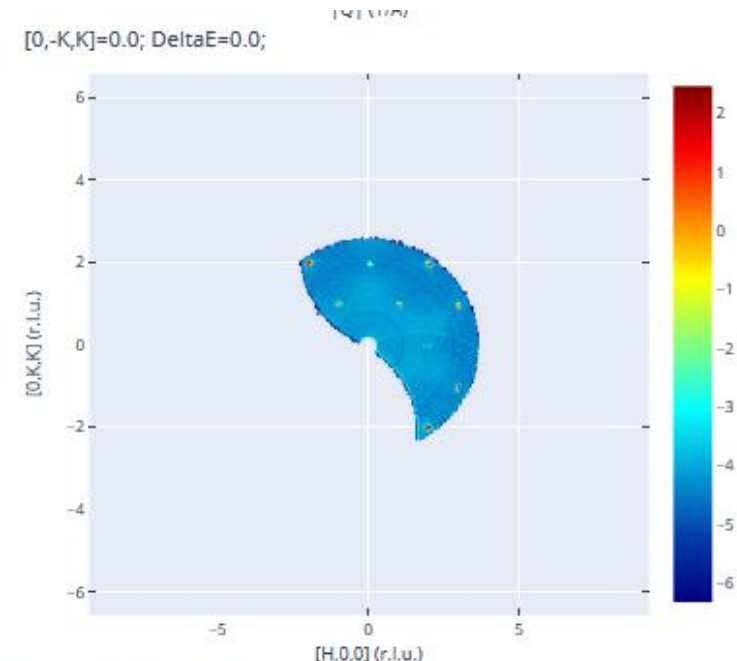
- Allow users to decide which plots they want to see on <https://monitor.sns.gov>

Autoreduction - plotting setup

Load configuration Save configuration Add 2D slice Add 1D cut

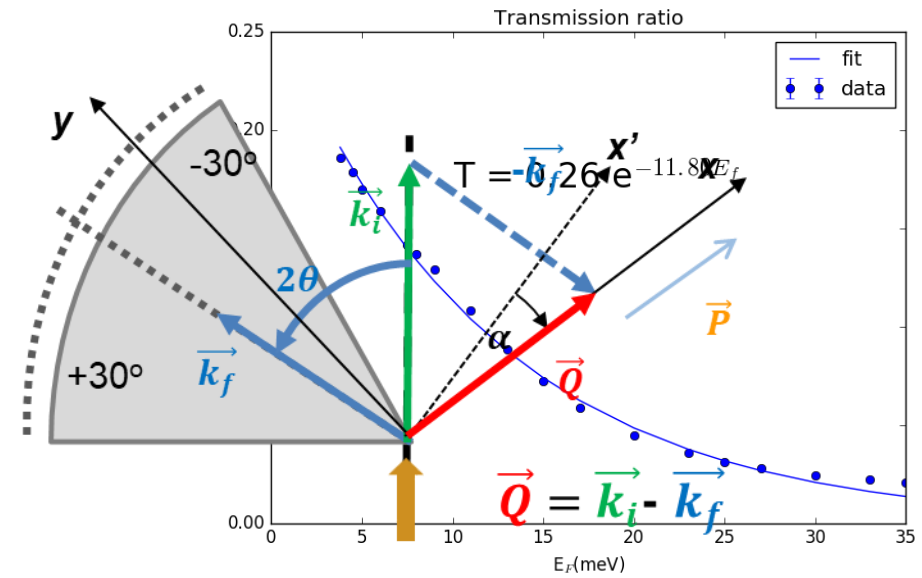
UB input Plot 1 ✕ Plot 2 ✕ Plot 3 ✕

	Min	Max	Step	Projection Basis
[H,0,0]			0.050	Projection u 1,0,0
[0,K,K]			0.050	Projection v 0,1,1
[0,-K,K]	-0.500	0.500		Projection w 0,-1,1
DeltaE	-0.500	0.500		



Polarization analysis

- Supermirror energy transmission
- Flipping ratio
- Wide angle detector and TOF - the direction of \mathbf{Q} with respect to the plane defined by the two vectors, \mathbf{k}_i and \mathbf{P} , varies significantly as a function of the energy transfer and the detector pixel position



α = Schärpf angle

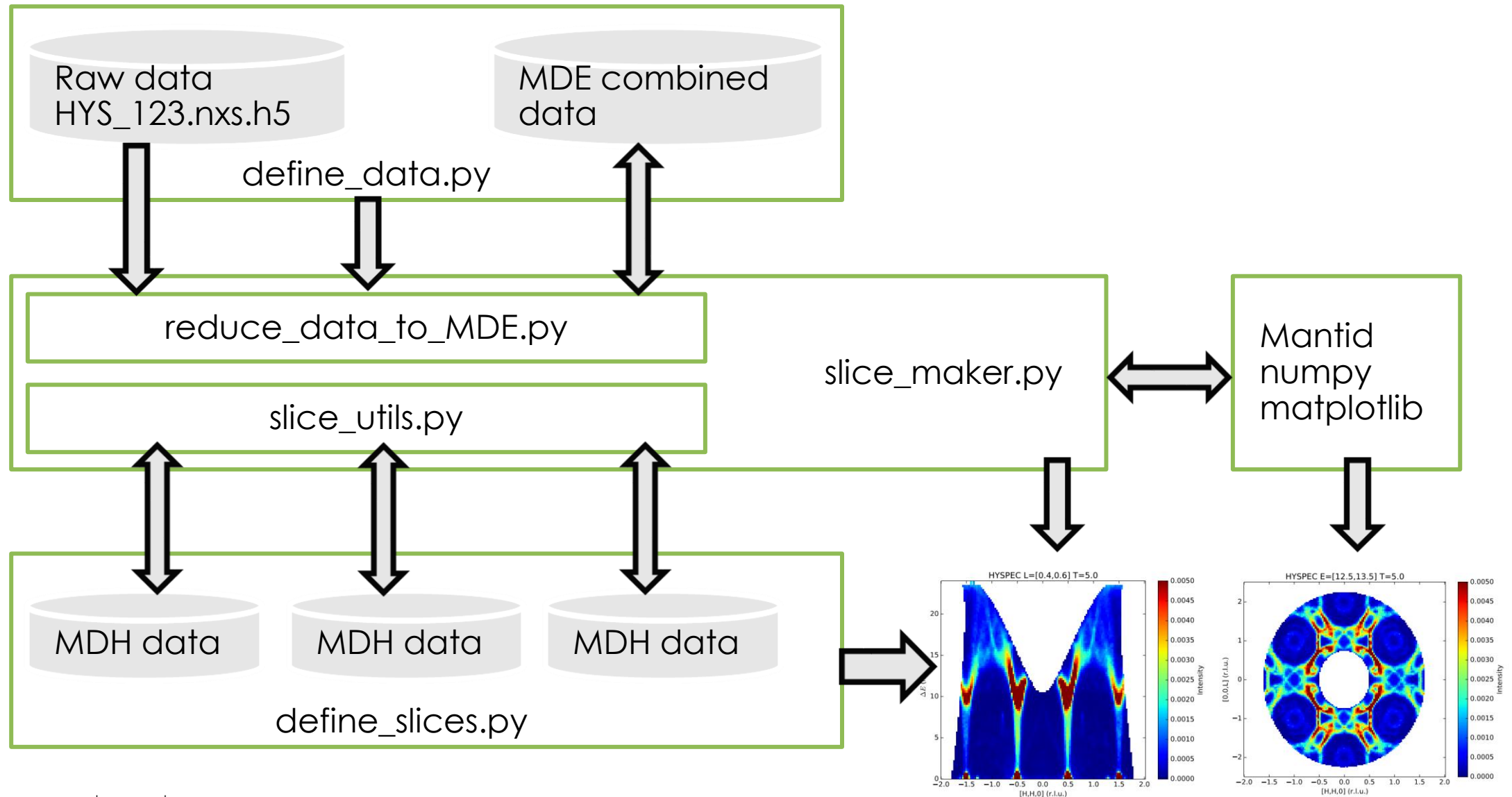
$$N^\dagger N = \frac{1}{2} (\Sigma_x^{nsf} + \Sigma_y^{nsf} - \Sigma_z^{sf}) = \frac{1}{2} (\Sigma_{x'}^{nsf} + \Sigma_{y'}^{nsf} - \Sigma_z^{sf})$$

$$I_{si} = \frac{3}{2} (\Sigma_x^{nsf} - \Sigma_y^{nsf} + \Sigma_z^{sf}) = \frac{3}{2} \frac{\Sigma_{x'}^{nsf} - \Sigma_{y'}^{nsf}}{\cos^2 \alpha - \sin^2 \alpha} + \frac{3}{2} \Sigma_z^{sf}$$

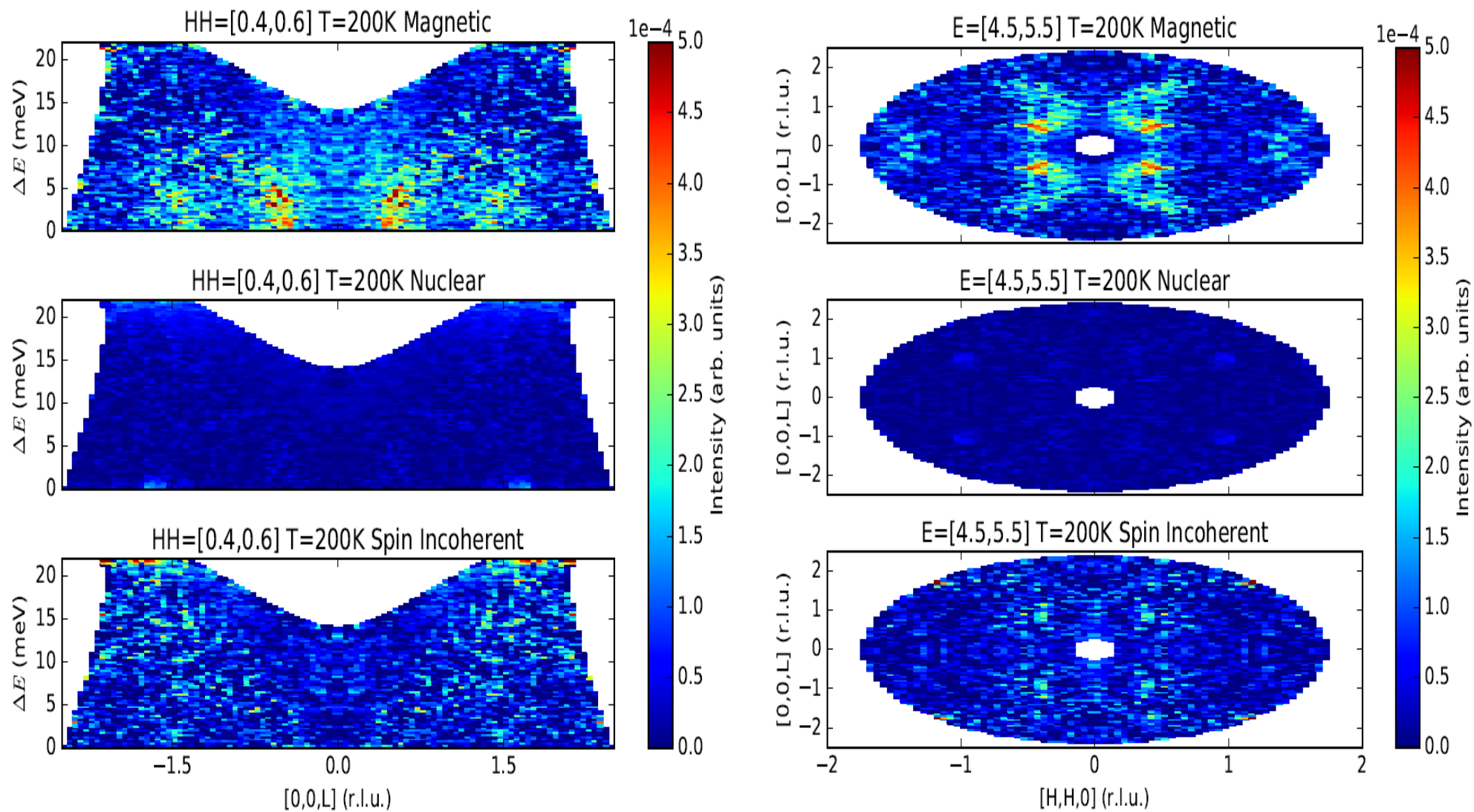
$$M_{\perp y}^\dagger M_{\perp y} = \Sigma_z^{sf} - \frac{2}{3} I_{si}$$

$$M_{\perp z}^\dagger M_{\perp z} = \Sigma_z^{nsf} - \frac{1}{3} I_{si} - N^\dagger N$$

Implemented workflow



Example: polarized measurements in MnO



Future plans for data reduction

- Finish MD algorithms for polarized SC
- MD algorithms for powder
- Mslice replacement for single crystal
- Efficient background subtraction
- Absolute scaling procedure
- UB matrix refinement
- Planning tools (polarized)

Issue tracking

The screenshot shows a GitLab issue board for the 'Spectroscopy' project. The board is organized into columns representing issue states: Open, High priority, Next, In progress, and Closed. Each issue card includes a title, a list of labels (e.g., ARCS, CNCS, HYSPEC, SEQUOIA), and an issue number. The 'High priority' column is highlighted with a red border.

Open	High priority	Next	In progress	Closed
<p>Polarization planning tool #2 HYSPEC</p>	<p>Complete the conversion of the prototype reduction scripts for polarization analysis to maintained code. #3 HYSPEC</p>	<p>Clean up CNCS autoreduction #14 CNCS</p>	<p>Interface for plots in autoreduction #1 2w ARCS CNCS HYSPEC SEQUOIA autoreduction</p>	<p>DGSplanner bug #26 Bug</p>
<p>Powder normalization #5 ARCS CNCS HYSPEC SEQUOIA</p>	<p>Scale the data to absolute units #4 ARCS CNCS Documentation/training HYSPEC SEQUOIA</p>	<p>Clean up single crystal scripts #19 ARCS CNCS Documentation/training HYSPEC SEQUOIA</p>	<p>Transition to Mantid workbench #25 High priority</p>	<p>Minor issues with dgsplanner and the sliceviewer #24 Bug</p>
<p>Pixel calibration #6 ARCS CNCS HYSPEC SEQUOIA</p>	<p>Transition to Mantid workbench #25 In progress</p>			
<p>Chop for all DGS instruments #7 ARCS CNCS HYSPEC SEQUOIA</p>				
<p>Resolution convolution for DGS #8 ARCS CNCS HYSPEC SEQUOIA</p>				
<p>Mantid Mslice for single crystal #9 ARCS CNCS HYSPEC SEQUOIA</p>				
<p>Simplify symmetry operations #10 ARCS CNCS HYSPEC SEQUOIA</p>				

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Data reduction

- Data already comes out in the correct units, one just needs to combine multiple measurements
- Done historically with Graffiti
- Can be done with DAVE (we have a new conversion tool to fix file format)
- Plan to have an ORNL standalone replacement
- Need planning tools for remote access
- Resolution calculator

Issue tracking

The screenshot shows a web browser displaying the GitLab issue tracking interface for the 'Spectroscopy' project. The browser's address bar shows the URL `https://code.ornl.gov/spectroscopy/tas/status/-/issues`. The GitLab navigation bar includes 'Projects', 'Groups', and 'More' options, along with a search bar and user profile icons. On the left sidebar, the 'Issues' section is active, showing a count of 5 issues. The main content area displays a list of issues with the following details:

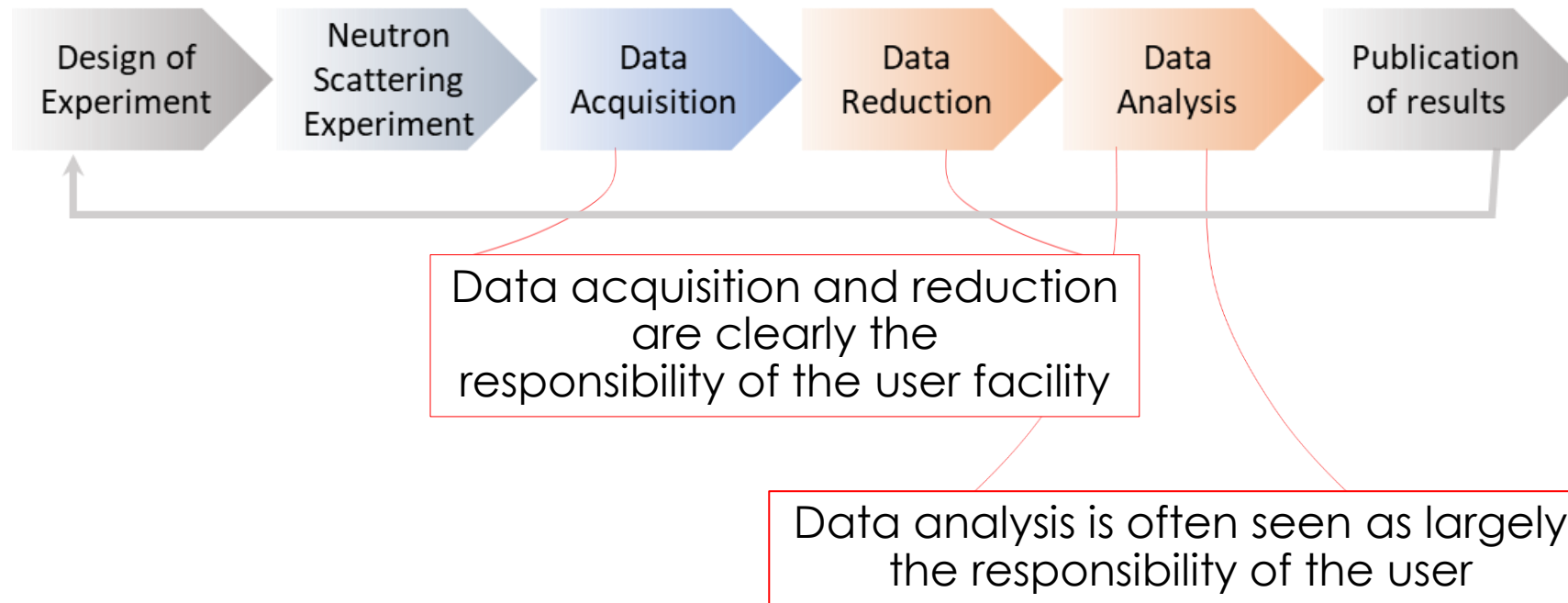
- Open 5**, Closed 0, All 5
- Search bar: 'Recent searches' and 'Search or filter results...'
- Sort: 'Created date' (descending)
- Issue #5: '2D visualization tools', opened 2 months ago by Savici, Andrei T. Labels: CTAX, HB1, HB1A, HB3. Updated 1 month ago.
- Issue #4: 'GUI tool for resolution calculation', opened 2 months ago by Savici, Andrei T. Labels: CTAX, Feature, HB1, HB1A, HB3. Updated 2 months ago.
- Issue #3: 'Correction for the resolution volume for inelastic scattering measurements with fixed Ei', opened 2 months ago by Savici, Andrei T. Labels: Feature, HB1A. Updated 2 months ago.
- Issue #2: 'Graffiti replacement', opened 2 months ago by Savici, Andrei T. Labels: CTAX, Feature, HB1, HB1A, HB3, High priority. Updated 1 month ago.
- Issue #1: 'Correction for lambda/n (n>1) contamination of beam monitor', opened 2 months ago by Savici, Andrei T. Labels: CTAX, Feature, HB1, HB1A, HB3. Updated 2 months ago.

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The data pipeline in the user experience

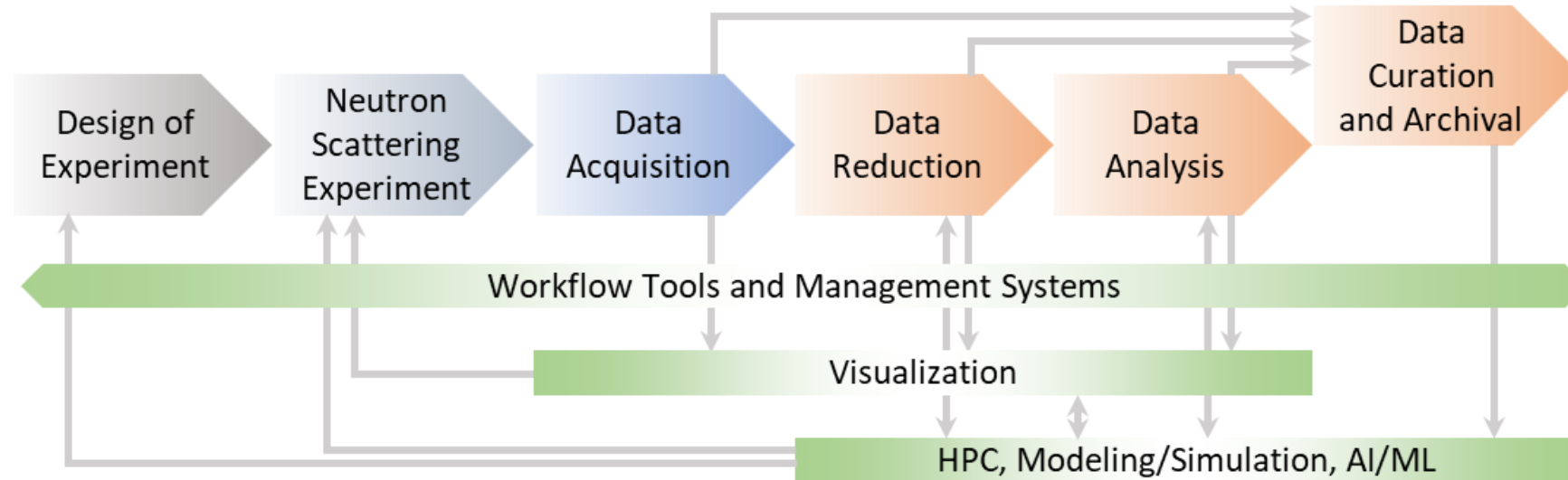
In a traditional linear workflow:



Raw data is instrument-specific (requires knowledge of detector geometry, motor positions, etc.)

Reduced data is proportional to the neutron scattering cross-section from the sample, expressed in terms of physically meaningful variables (e.g., momentum transfer, energy)

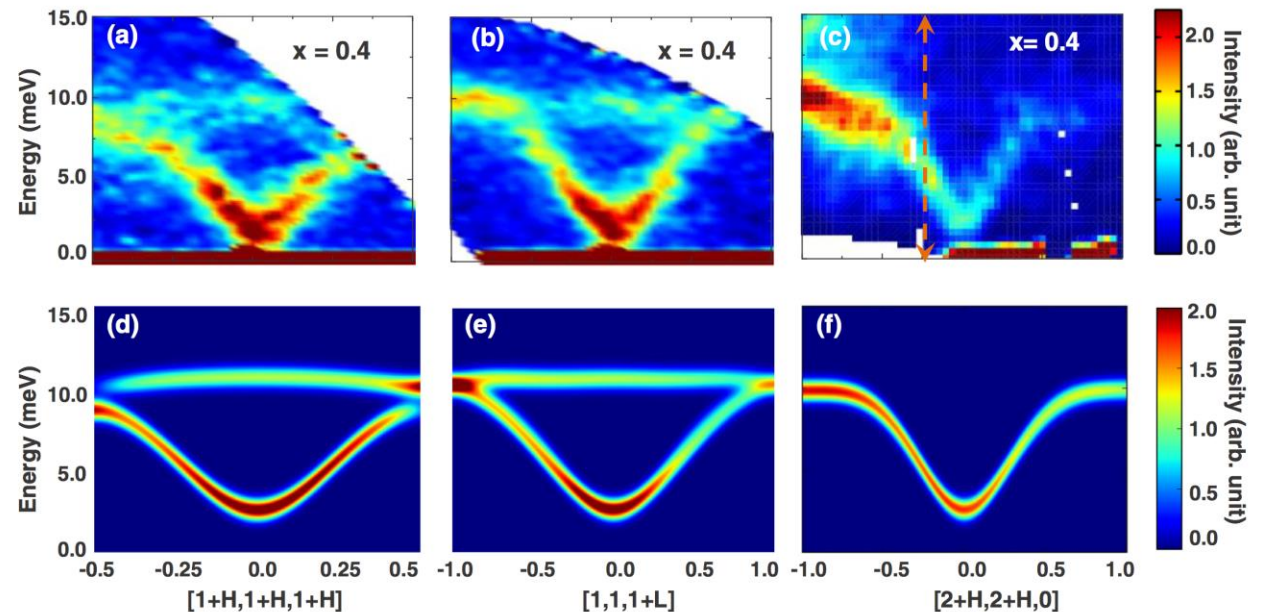
The data pipeline in the user experience



When data analysis, curation, and archival become integrated into the workflow, user facilities need to be enablers of these aspects

Spin Waves with SpinWaveGenie

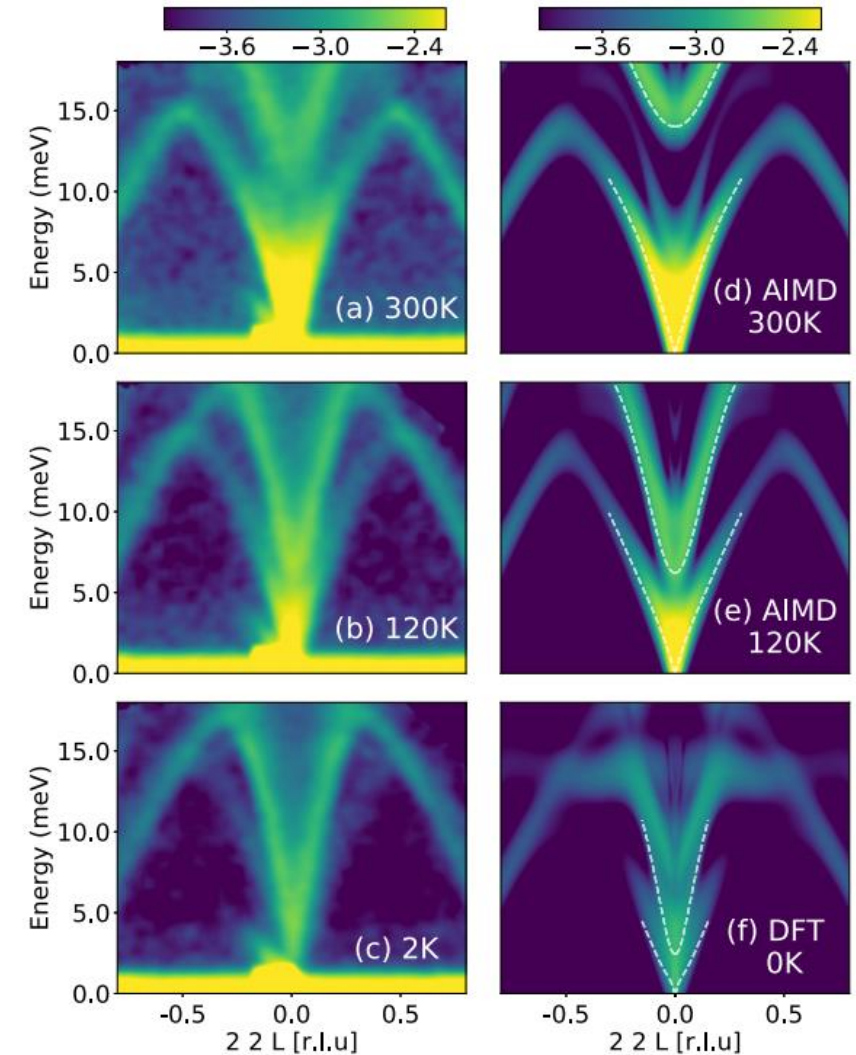
- Modeling Spin Waves in $\text{Mn}_{0.6}\text{Co}_{0.4}\text{V}_2\text{O}_4$
- Complex Hamiltonian
- Localized and itinerant component
- <https://github.com/spinwavegenie/spinwavegenie>



Phonon simulations with VASP and Phonopy

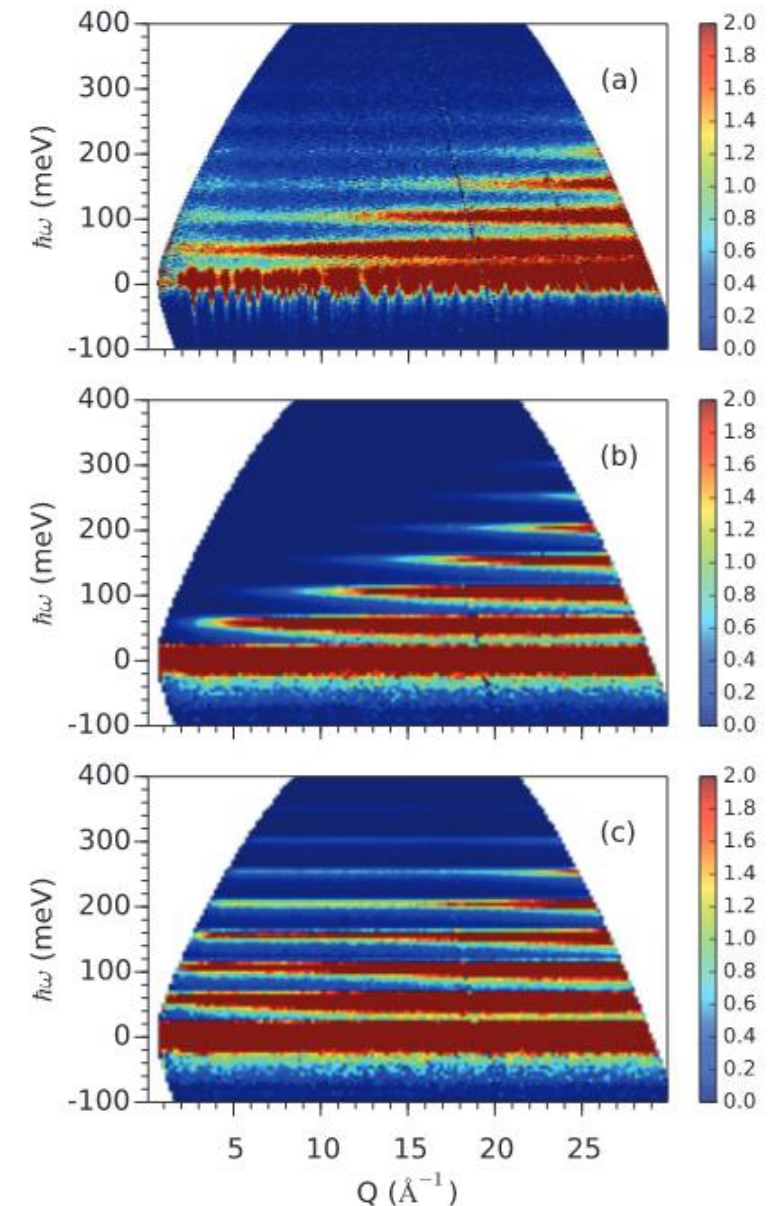
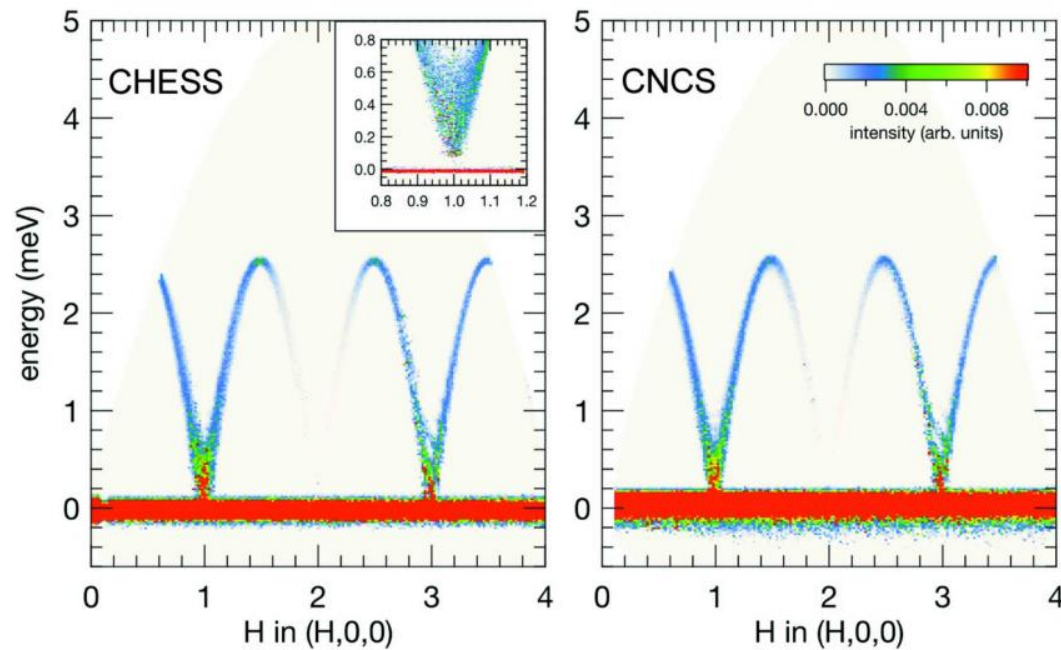
- Simulating phonons in SrTiO_3
- Ab initio molecular dynamic using VASP
<https://www.vasp.at/>
- DFT calculations using Phonopy
<https://phonopy.github.io/phonopy/index.html>
- Simulations can be done on NERSC or OLCF

Courtesy O. Delaire



MCViNE simulations of instrument effects

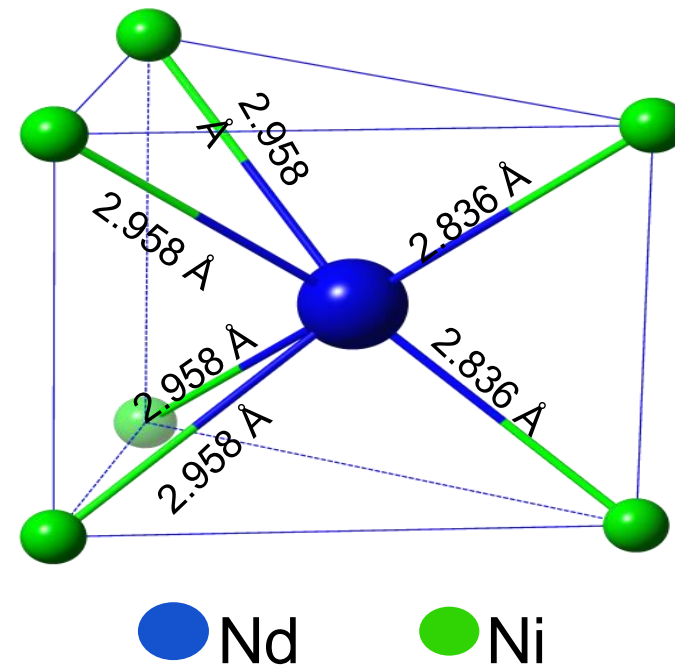
- Ray tracing Monte Carlo simulation of instrument and sample environment
- <https://mcvine.ornl.gov/>



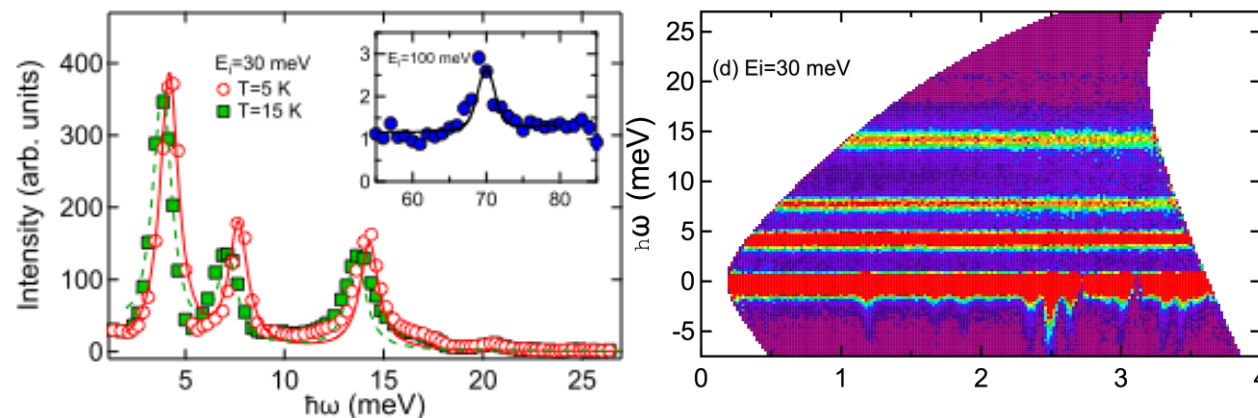
Crystal field calculations

- IDL functions based on the LS coupling approximation (M. Hutchings Solid State Physics, 1964), and intermediate coupling (B. G. Wybourne, 1965)
 - Can include bulk measurements (heat capacity and susceptibility) in the fit to constrain the wave functions
 - From G. Sala
- There is a Mantid alternative

Sala and Stone, Phys. Rev. Mat 1, 054404 (2017)



$$H = B_2^0 \hat{O}_2^0 + B_2^2 \hat{O}_2^2 + B_4^0 \hat{O}_4^0 + B_4^2 \hat{O}_4^2 + B_4^4 \hat{O}_4^4 + B_6^0 \hat{O}_6^0 + B_6^2 \hat{O}_6^2 + B_6^4 \hat{O}_6^4 + B_6^6 \hat{O}_6^6$$



Future data analysis

- Continue developing packages for spin wave, crystal field, and phonon calculations
- Continue development of MCViNE and provide analytical or simplified forms for resolution, absorption calculation
- Work on the interfacing between simulation and data reduction
- We can not do it all at ORNL – develop external collaborations