Software status for inelastic neutron scattering – DGS and TAS

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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.

Courtesy H. Christen

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

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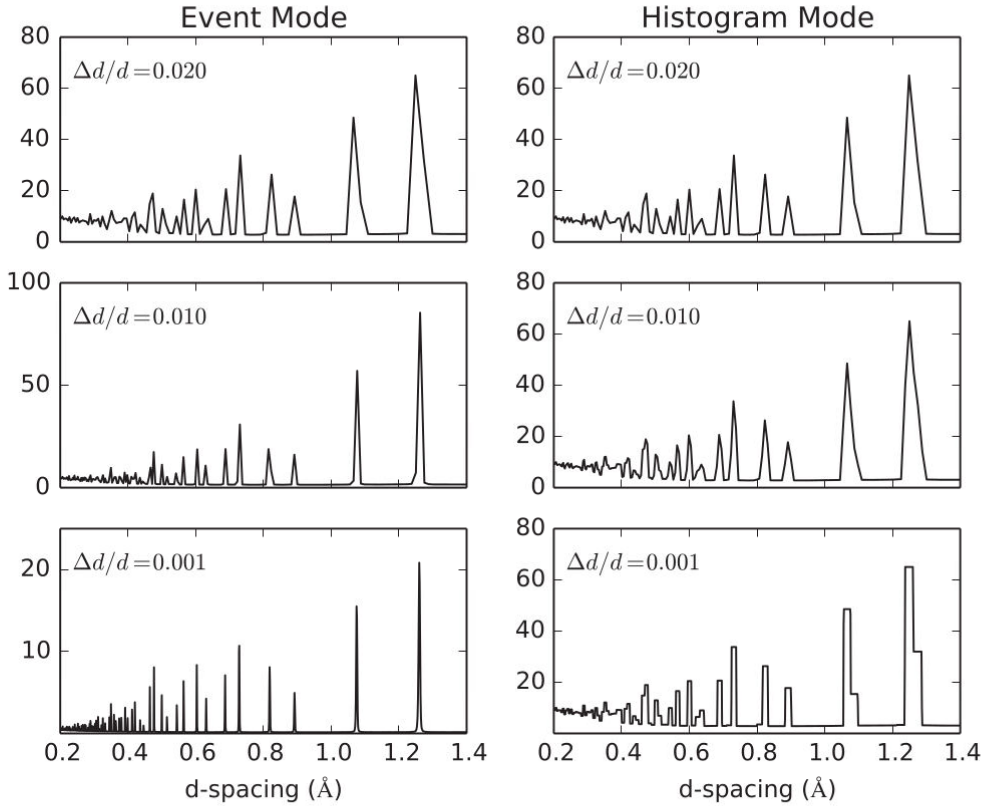
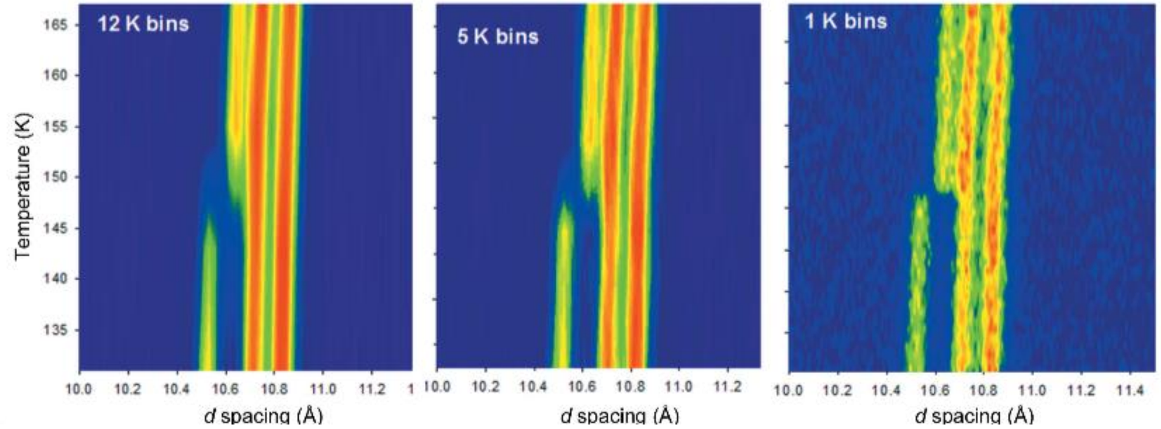
Event based data

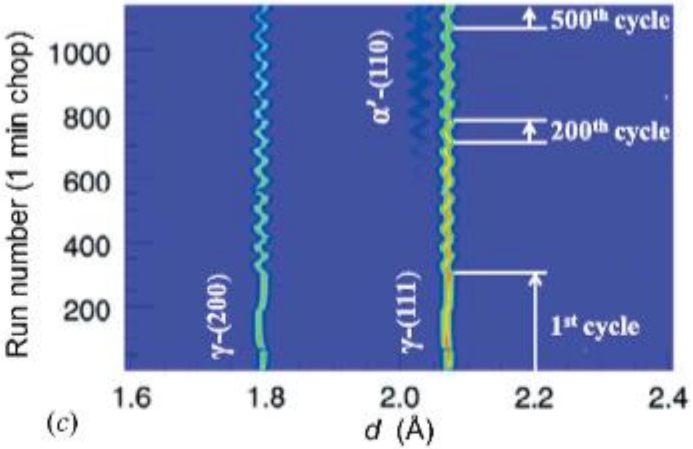
- Record detection time for each individual neutron
- Clean up spurious instrumentation mishaps
- Dynamic rebinning
- Time resolved data acquisition
  - Slow changes (temperature, goniometer)
  - Fast changes (pulse magnetic fields)



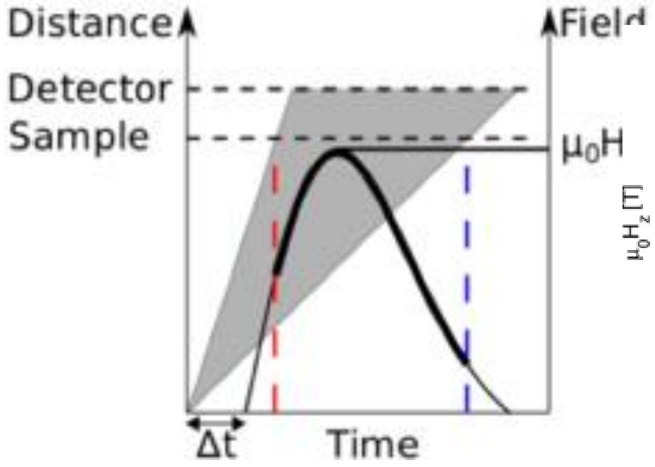
Examples of Event Filtering



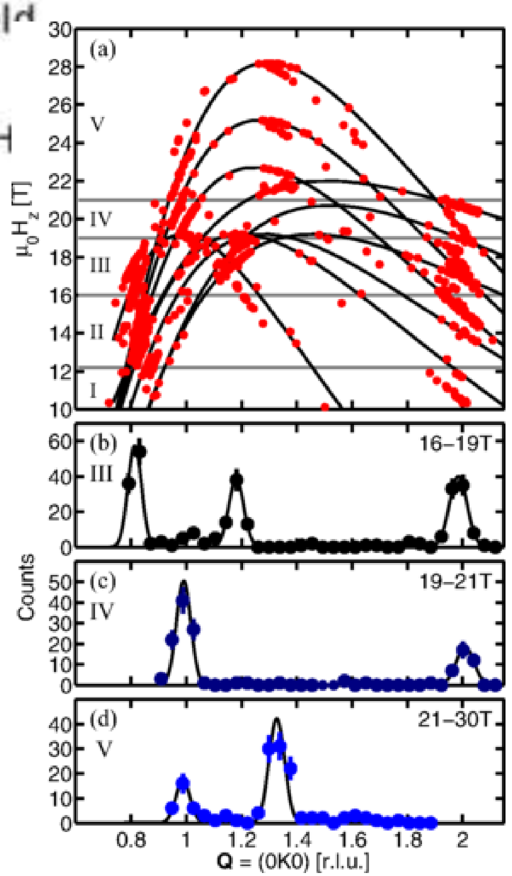
- Continuous temperature ramping



- Battery charging and discharging

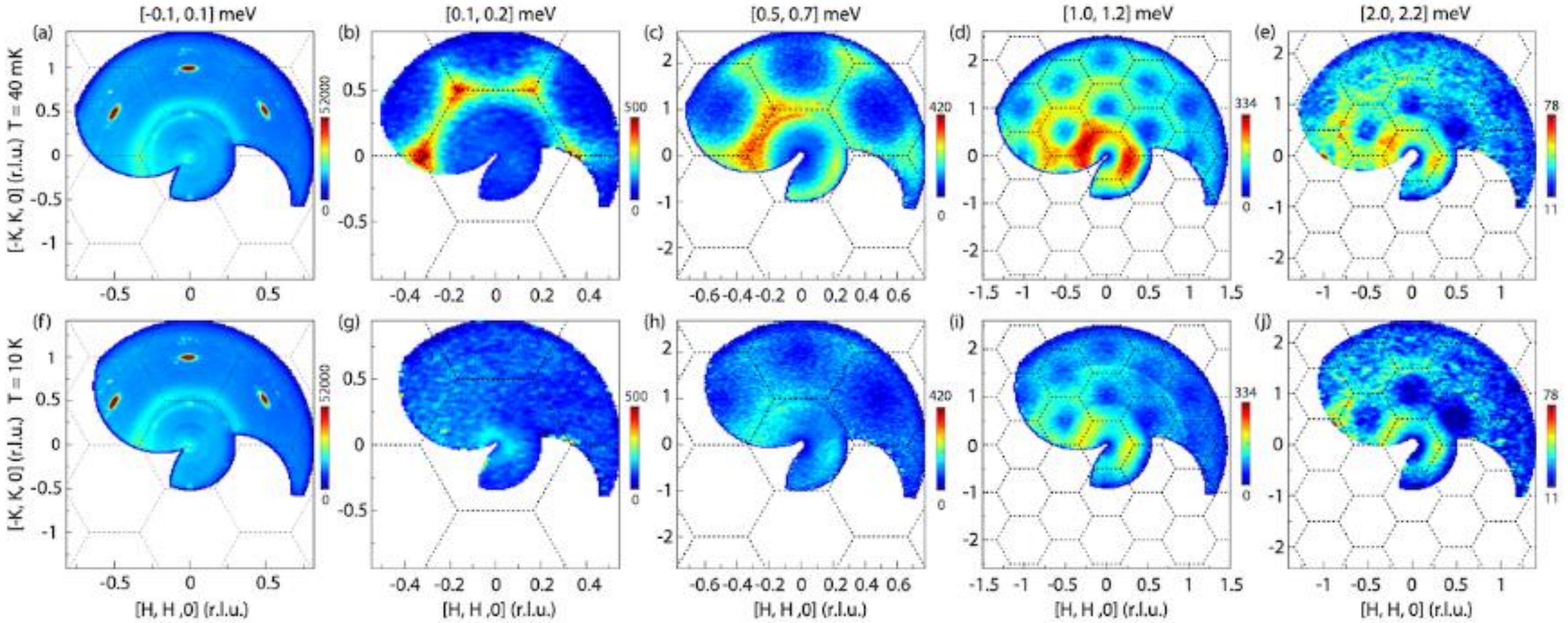


- Pulse magnet



New normalization for multidimensional data

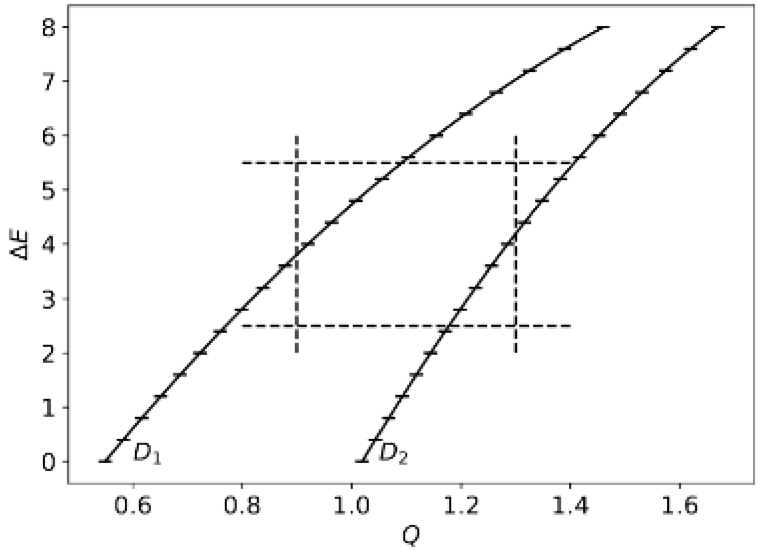
- We keep events (smaller files for inelastic)
- Procedure available for spectroscopy or diffraction measurements

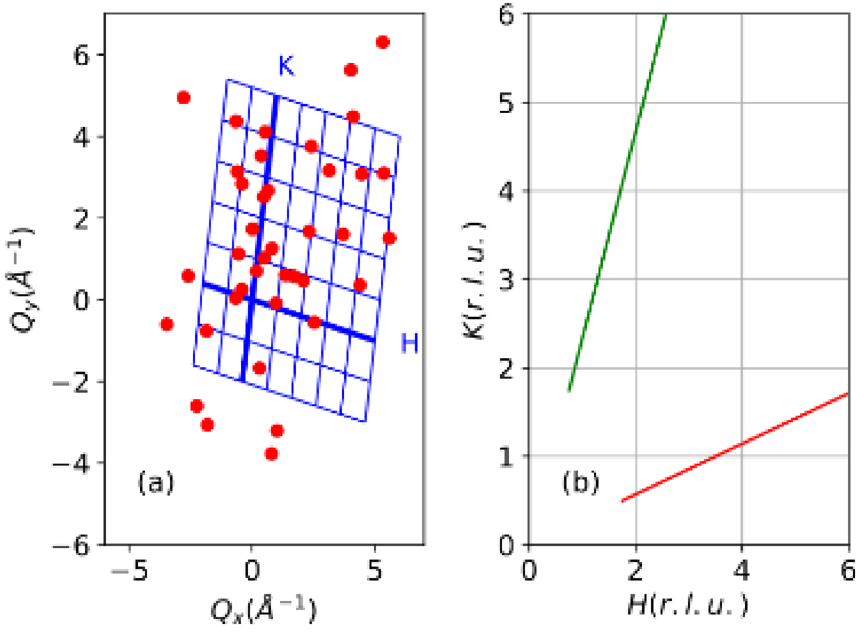


- Correctly account for files with different statistics
- Keep data and normalization separately

Comparison with mslice approach

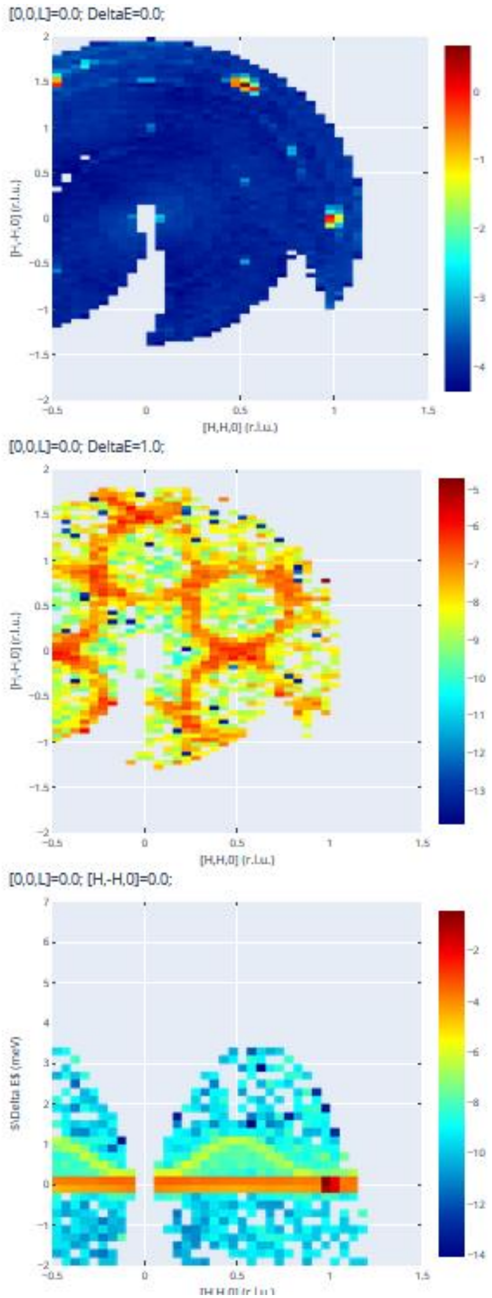
- Mslice uses histograms in energy transfer where each bin is considered an independent measure of scattering cross section, then averages those numbers
- Better approach: bin counts and calculate separately the weighting factor from detector trajectories





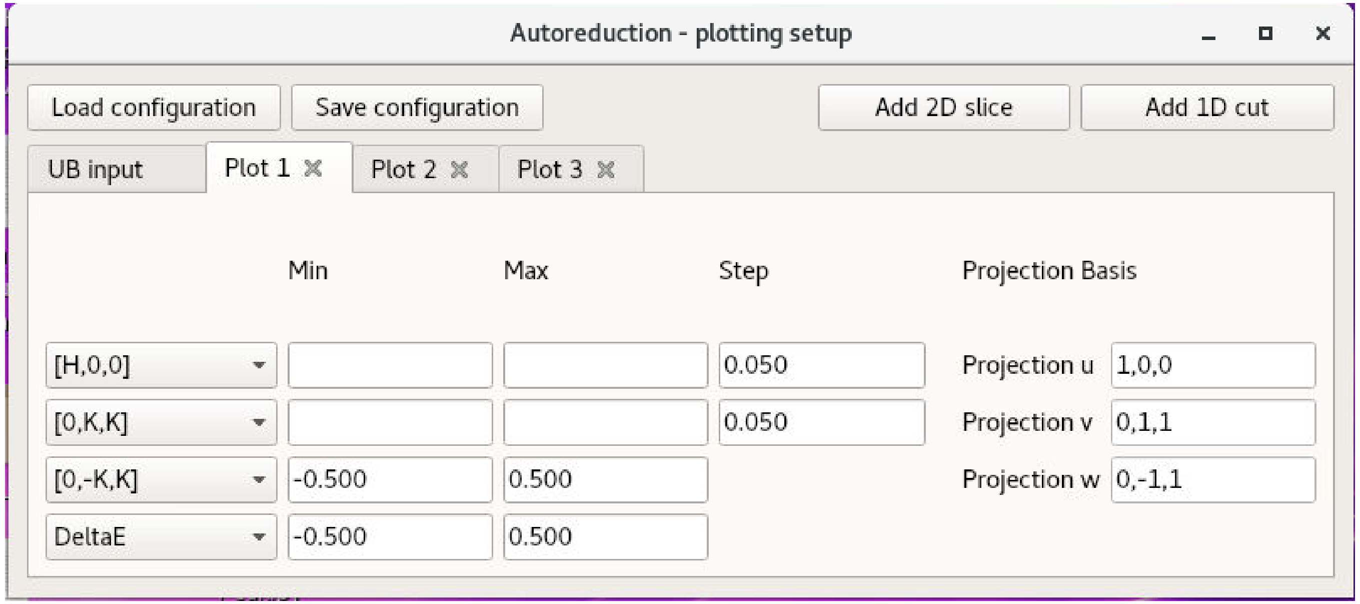
Advantages of current approach

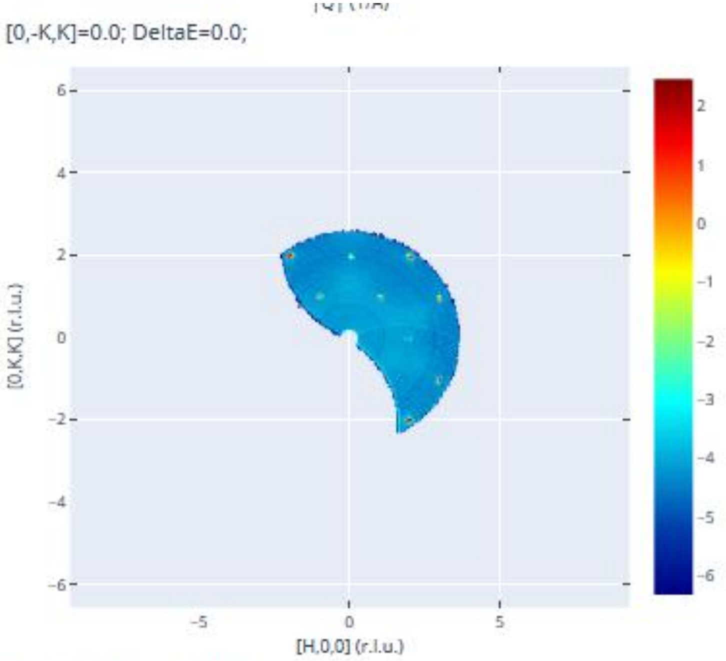
- Allows for correct accounting of multiple runs, with different proton charge, different geometry
- Much smaller memory footprint
- Non axis aligned cuts and symmetry operations
- Can correct UB matrix
- Implemented in MANTID, so the entire workflow can be implemented in a single script
- Can rely on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

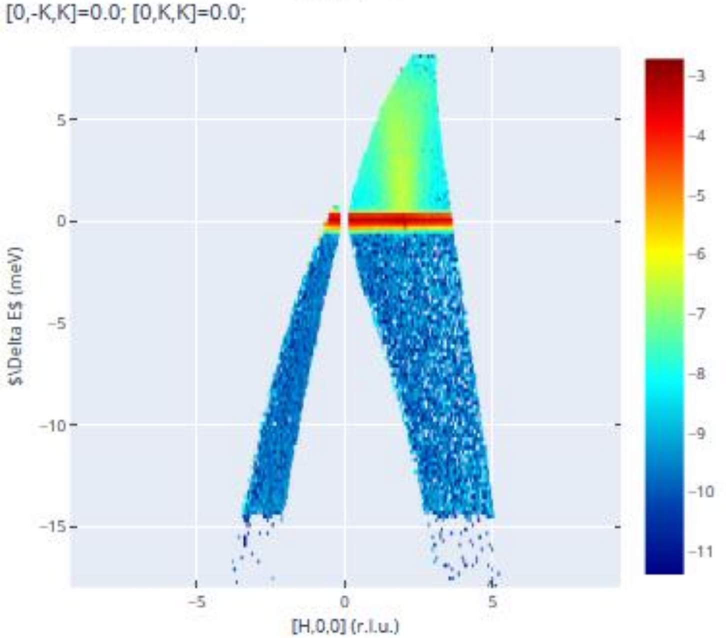


Autoreduction update

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

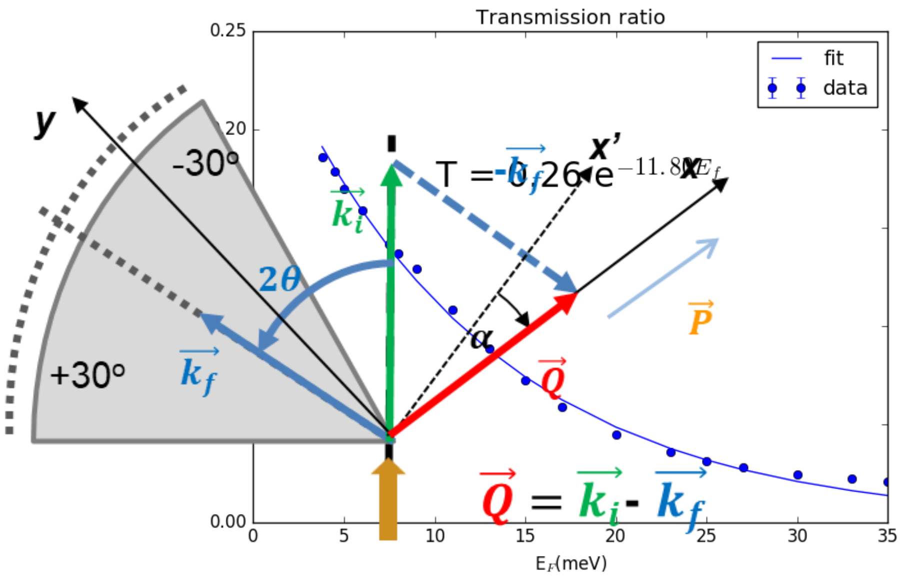






Polarization analysis

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



α = Schärpf angle

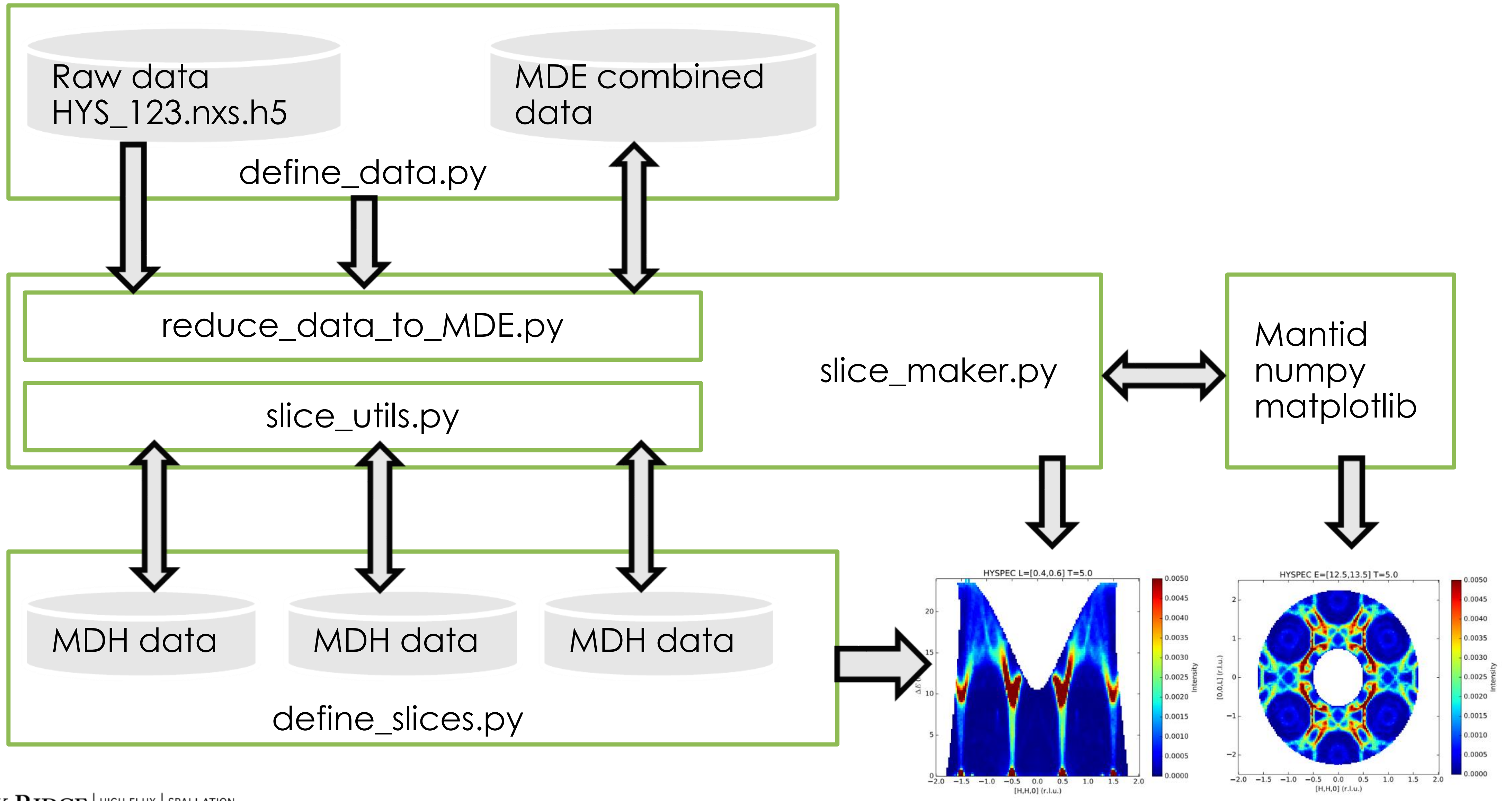
$$N^\dagger N = \frac{1}{2}\left(\Sigma_x^{nsf} + \Sigma_y^{nsf} - \Sigma_z^{sf}\right) = \frac{1}{2}(\Sigma_{x'}^{nsf} + \Sigma_{y'}^{nsf} - \Sigma_z^{sf})$$

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

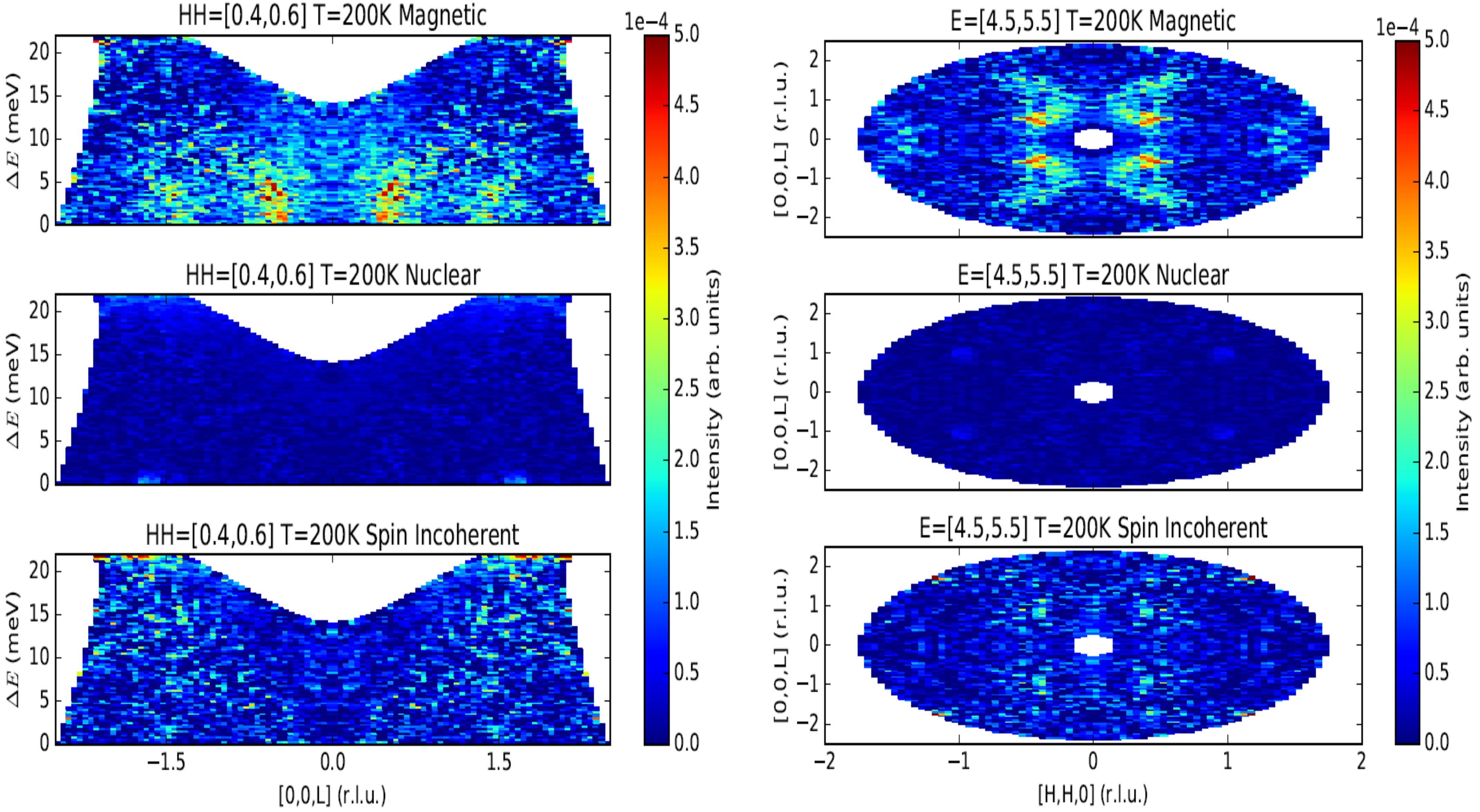
$$M_{\perp y}^\dagger M_{\perp y} = \Sigma_z^{sf} - \frac{2}{3} I_{si}$$

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

Implemented workflow



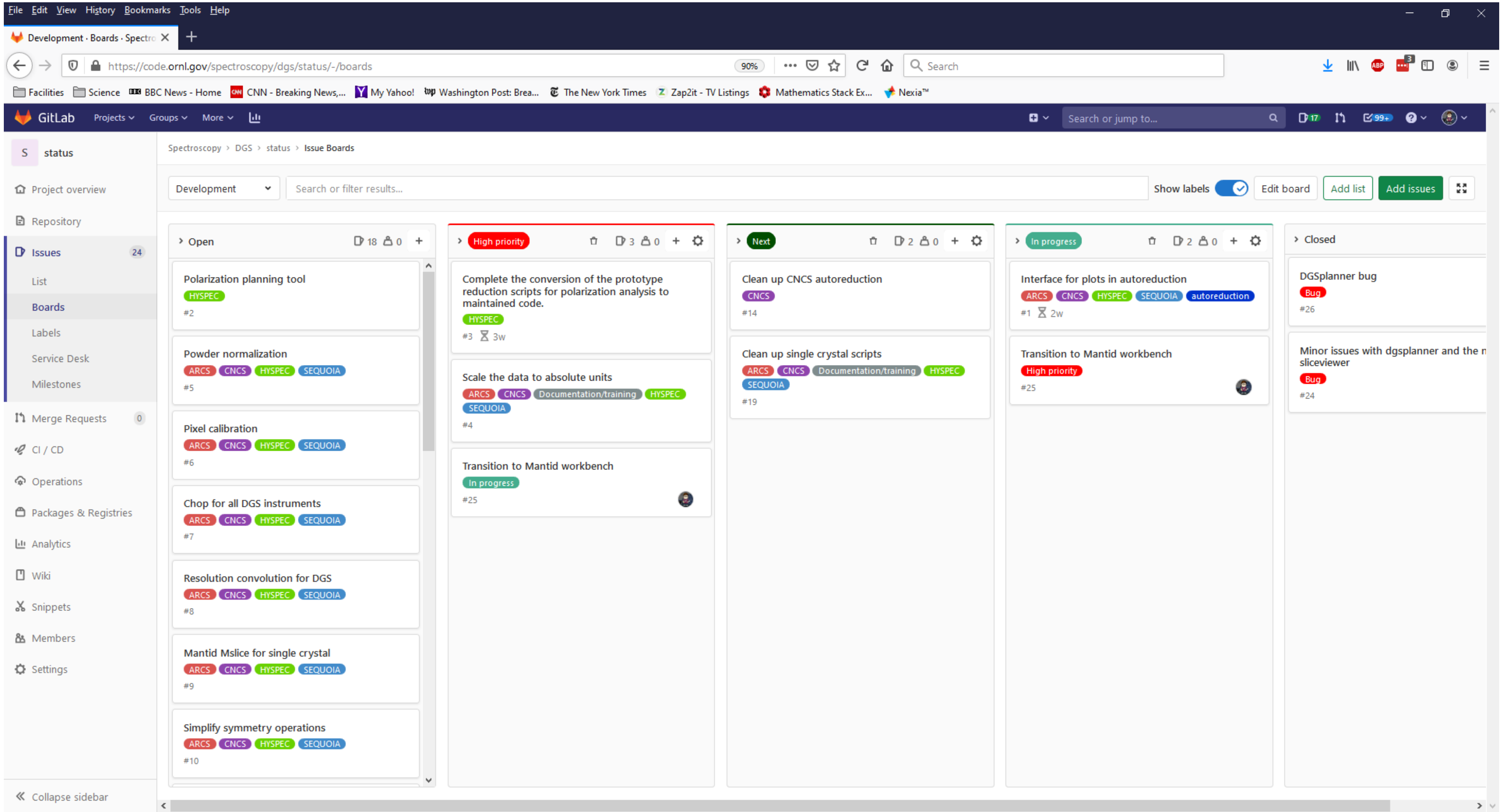
Example: polarized measurements in MnO



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



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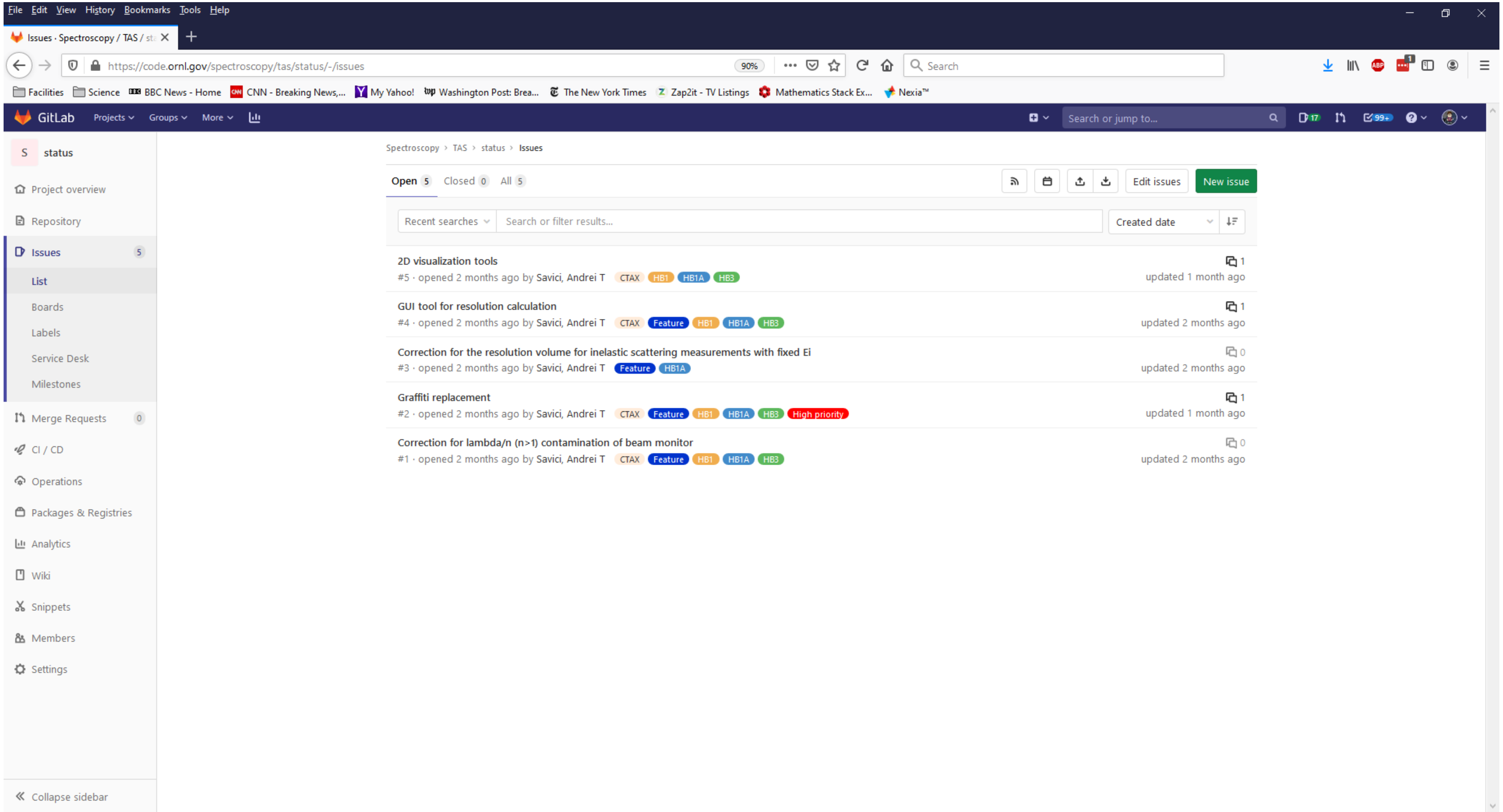
Data reduction

- 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



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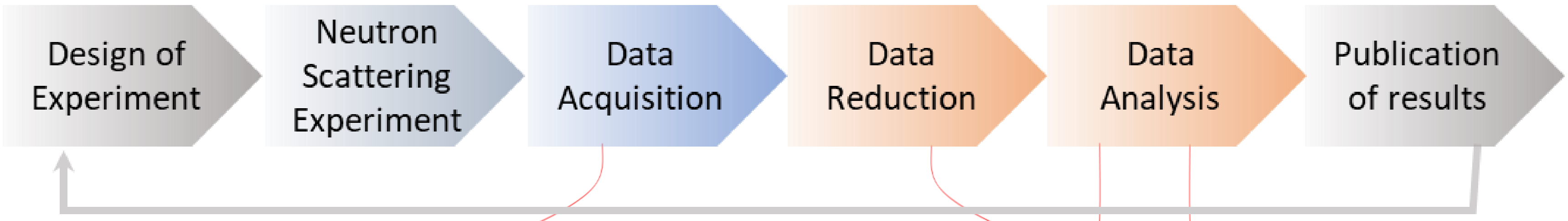
The data pipeline in the user experience

In a traditional linear workflow:



Data acquisition and reduction are clearly the responsibility of the user facility

Data analysis is often seen as largely the responsibility of the user

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)

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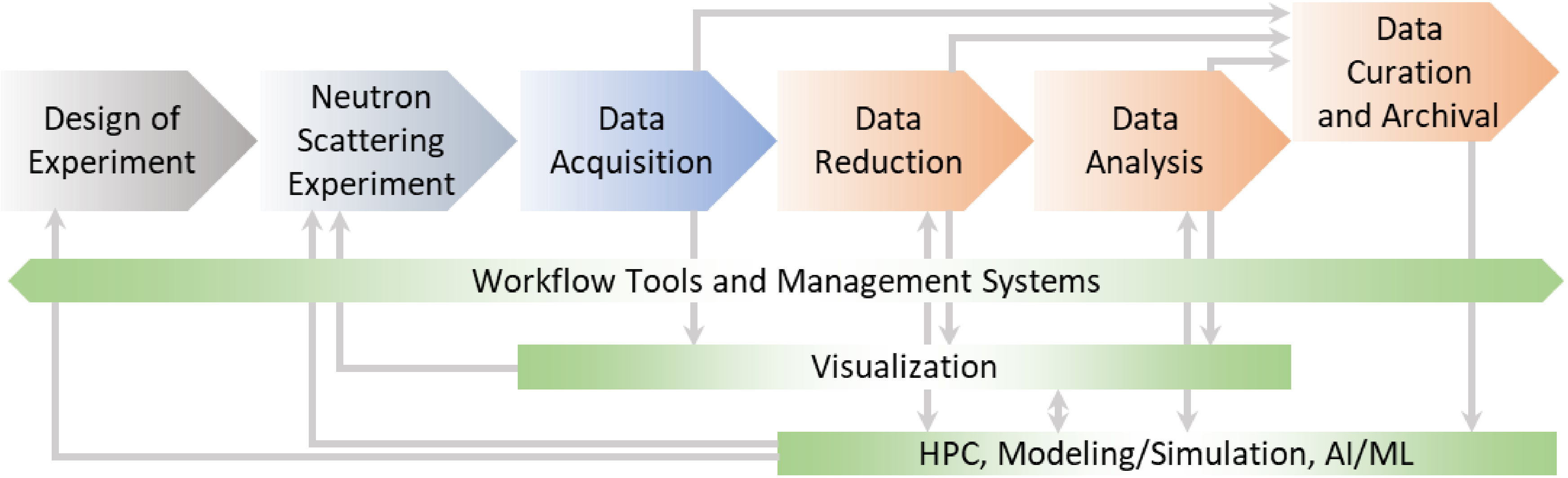
The data pipeline in the user experience



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

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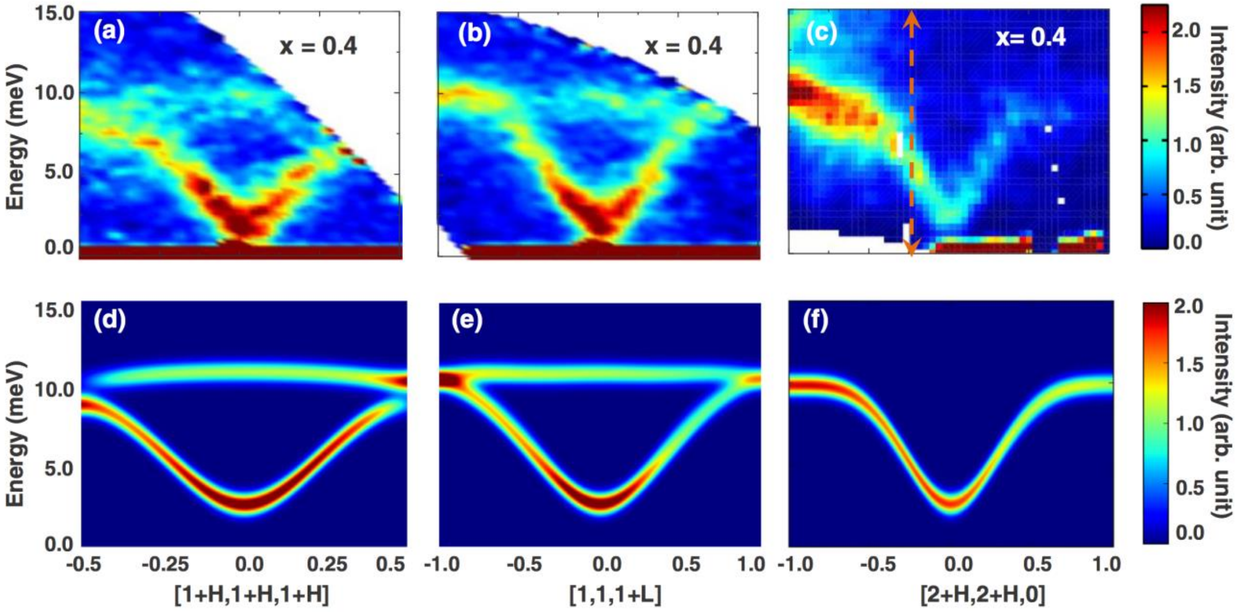
Spin Waves with SpinWaveGenie

- Modeling Spin Waves in $Mn_{0.6}Co_{0.4}V_2O_4$
- Complex Hamiltonian
- Localized and itinerant component
- https://github.com/spinwavegenie/spinwavegenie



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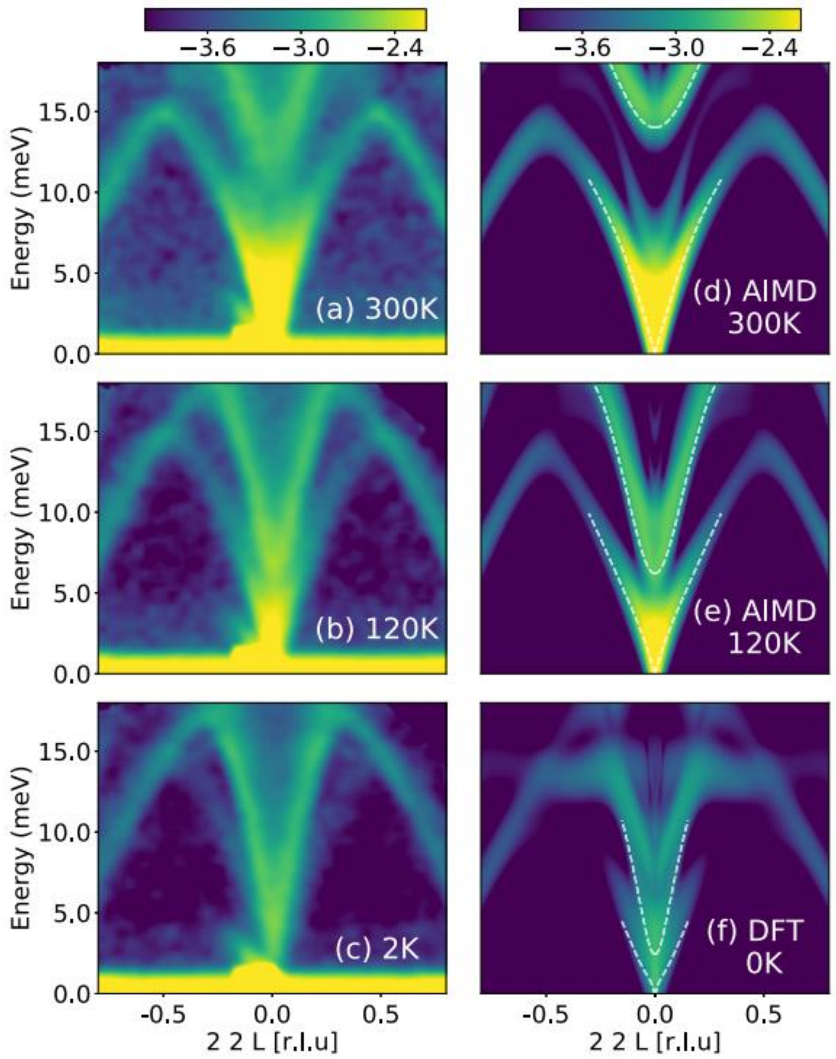
Phonon simulations with VASP and Phonopy

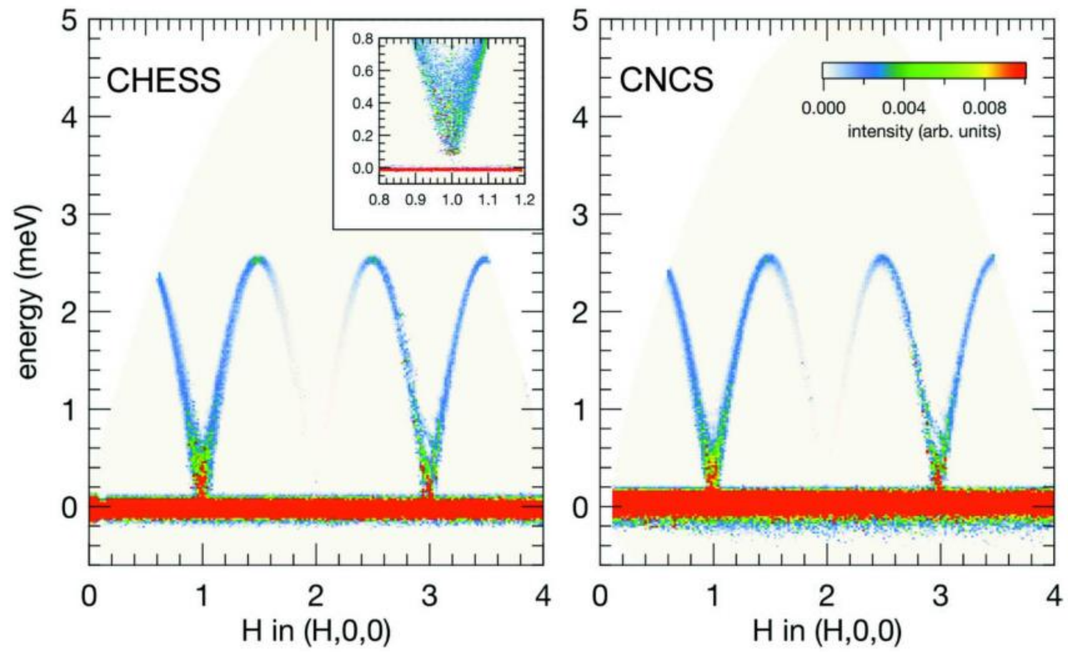
- Simulating phonons in $SrTiO_3$
- Ab initio molecular dynamic using VASP https://www.vasp.at/
- DFT calculations using Phonopy https://phonopy.github.io/phonopy/index.html
- Simulations can be done on NERSC or OLCF

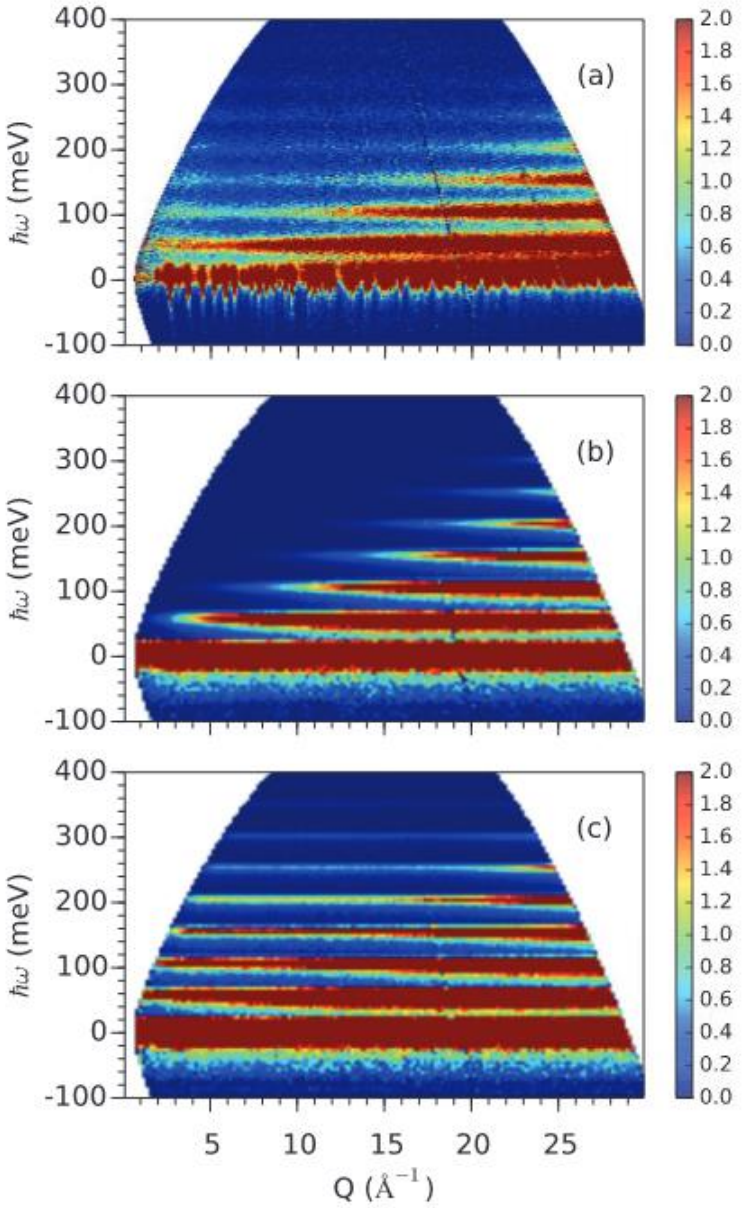
Courtesy O. Delaire



MCViNE simulations of instrument effects

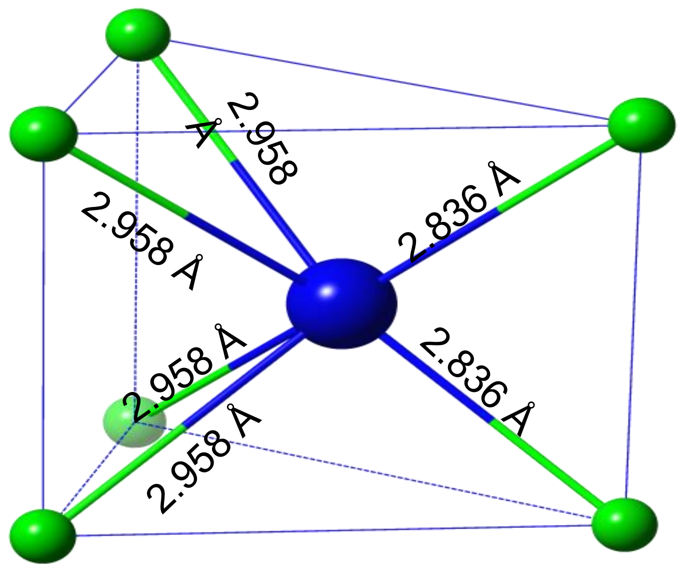
- Ray tracing Monte Carlo simulation of instrument and sample environment
- https://mcvine.ornl.gov/





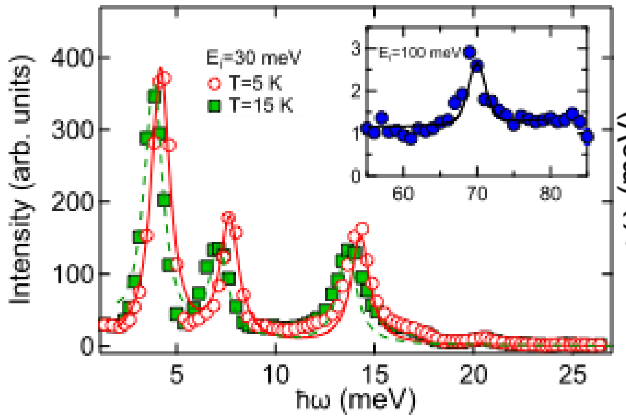
Crystal field calculations

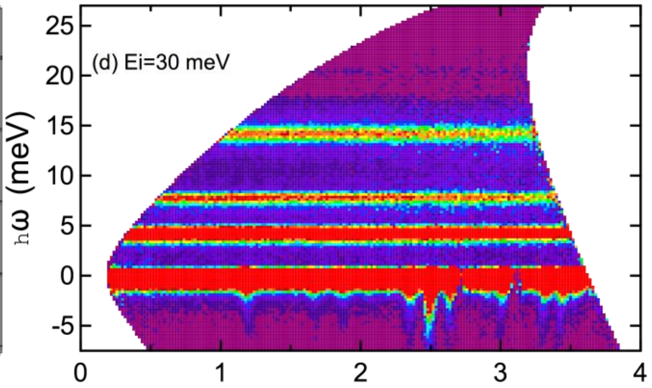
- IDL functions based on the LS coupling approximation (M. Hutchings Solid State Physics, 1964), and intermediate coupling (B. G. Wybourne, 1965)
  - Can include bulk measurements (heat capacity and susceptibility) in the fit to constrain the wave functions
  - From G. Sala
- There is a Mantid alternative



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

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





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