Dataflow: Web-based Triple-Axis Data Reduction

Alex Yee (SHIP, NCNR)
Mentor: Dr. William Ratcliff II

Neutron Diffractometry

Neutron diffraction is the process whereby neutrons are used to determine the atomic or magnetic properties of a material.

Neutrons penetrate the electron cloud and interact with an atom's nucleus, granting sensitivity to a range of elements, low-Z elements in particular. Furthermore, neutrons are sensitive to magnetism in a sample because they have a magnetic moment.

Web-based Data Reduction

Data reduction is the transformation of empirical or experimentally derived data into a corrected, ordered, and/or simplified form. Data gathered from a triple-axis spectrometer is raw and requires reducing now available online through Dataflow.

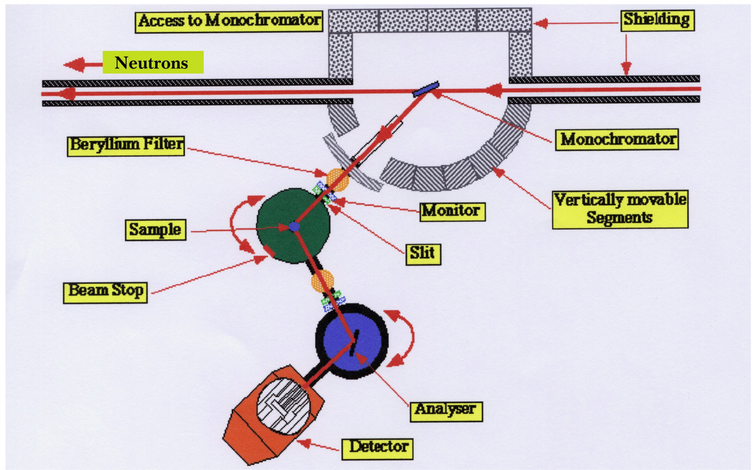
Web-apps have numerous advantages, including:

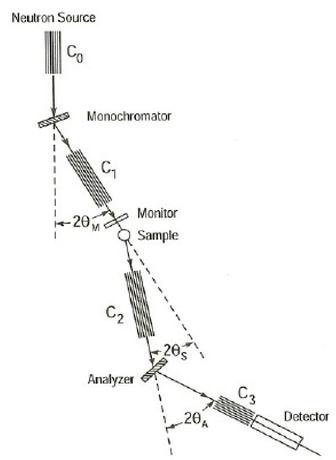
- Platform independence
- Browser independence
- Version unity
- Ease of access
- Potential for cluster computing
- Immediate data reception and use
- View and save intermediate steps in reduction

Triple-Axis Spectrometer

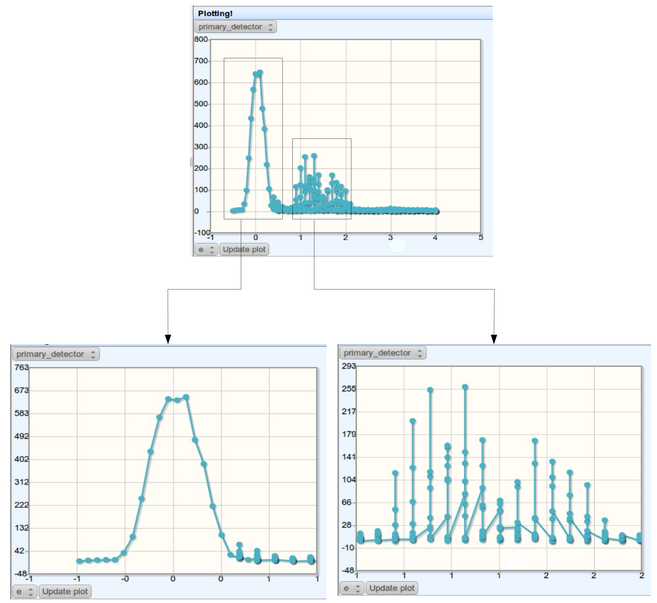
A triple-axis spectrometer is used to conduct neutron diffraction experiments. For this device, a neutron beam is produced in the Reactor and directed into a Monochromator, which sorts and admits neutrons of a specified wavelength and energy. These neutrons then pass through the Monitor for counting before hitting the sample being studied. The neutrons will scatter off the sample into the Analyzer, the change in energy can be analyzed. Finally the neutrons are directed into the Detector for counting, ultimately providing a quantitative and qualitative analysis of the neutrons and, by extension, the material itself.

During the neutron beam's journey, the beam is subjugated to multiple collimators (C_0 – C_3) which are an array of Cadmium walls that absorb incident neutrons. Thus, the only neutrons that pass through are those with momentum such that they do not collide with the walls. This defines the momentum for the neutrons.



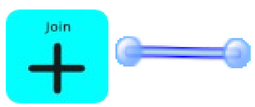


Dataflow Plots

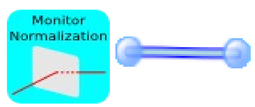


Above is a triple-axis data plot of multiple joined and reduced files. The various data peaks are zoomed in on, as indicated by the black boxes, and displayed in separate graphs.

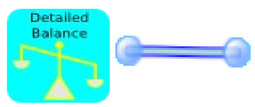
Reduction Modules



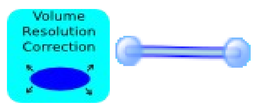
- Combines two data files by joining their rows of data
- Handles metadata appropriately
- Removes duplicate points by averaging their detector counts
- Efficiency



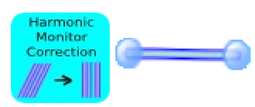
- For multiple data scans with unequal monitor counts
- Normalizes all detector counts to the same monitor count
- Defaults to normalizing the detector counts to the first data scan's monitor count



- Incident neutrons can create or destroy excitations in the sample
- Population of excitations depends on temperature
- Different strength of intensity depending on whether excitations are created or destroyed

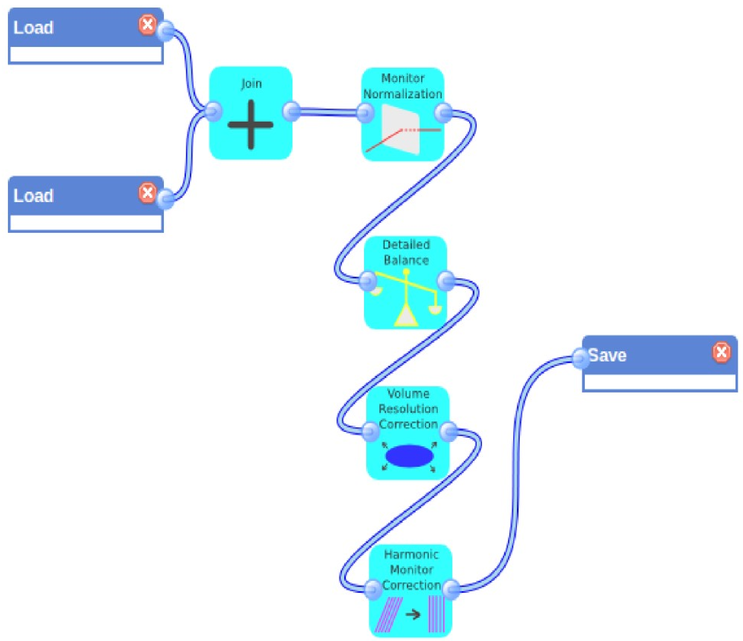


- Employed for constant-Q scans with fixed initial Energy
- Collimators are imperfect and define a range of momenta
- Corrects detector counts for this varying neutron resolution



- Employed for constant-Q scans with fixed final Energy
- According to Bragg's Law, higher harmonics of the neutron beam may be included, such as λ/2 or λ/3 for a target wavelength λ
- Corrects detector counts for the monitor over-counting of excess harmonics

Dataflow



Modules can be added, removed, and arranged as desired. Reductions begin with a load module, which loads a data file for reduction. A save module can be added at the end of a reduction to save a reduced data file.

In a reduction pipeline, modules may receive inputs from a wire connecting to their left, and may produce output which is sent along any wires connecting to their right.

Each wire stores the data at its position in the reduction. For example, an input wire for a Monitor Normalization module will have the data before the monitor normalization reduction is applied, and an output wire will have the data after the monitor normalization reduction is applied.

Clicking on a wire will show a plot for that wire's data. This allows users to easily view data at any stage in the reduction. In the diagram to the left, clicking the wire after the Join module will give the data before any reductions, and clicking the wire before the Save module will give the data after all four reductions.

References

Shirane, G., Shapiro, S. M., & Tranquada, J. M. (2002). Neutron Scattering with a Triple-Axis Spectrometer. Uni: Cambridge University Press.