Scientific Data Reduction at SNS

J. Bilheux, S. Campbell, M. Doucet, M. Hagen, W. Heller, J. Kohl, V. Lynch, D. Mikkelson,
R. Mikkelson, S. Miller, P. Peterson, M. Reuter, A. Savici, C. Tang, R. Ward, L. Yang, J. Zikovsky

NEUTRON SCIENCES

DATA REDUCTION

Our work on data reduction and analysis software for the beamlines in NSSD is based on 3 science and beamline focus areas: *Inelastic, Diffraction and Low-Q*, and on 3 Generations of software development for these areas.

Generation I – Is focused on the SNS beamlines, and its aim is 1) to provide operating beamlines with efficient data reduction software, and 2) to ensure that upcoming beamlines will have software available. In order to do this we are adapting existing software packages, ISAW for Diffraction and IDL/C++ code packages for Inelastic and Low-Q. Progress in Generation I is shown on the right.

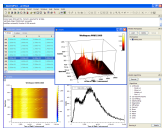
Generation II – Is to produce a coherent high performance data reduction workbench for the suite of instruments at SNS and HFIR, with a number of features planned at the outset. These include, automated/parametric/live data reduction capabilities, parallel processing for large data sets, visualization of high dimensionality data sets, Open Source cross platform (Windows, Macintosh, Linux) distributions for users, GUI's for standard reduction with scripting capability for users to customize reduction. And, of course, learning the lessons from Generation I.

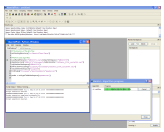
Generation III – Is to transition to a group that connects between neutron scattering, theory and the computational resources at ORNL. Connecting advanced analysis methods with our neutron scattering data reduction codes.

NEXT GENERATION

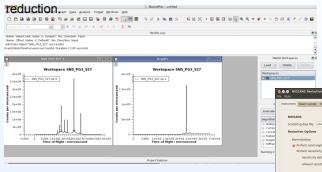
MANTID

In the second generation of data reduction software we will implement new features for automated, parametric and real time data reduction. We will also establish a single coherent workbench for our data reduction software, which will allow us to re-use code across different beamline programs and provide users with a single location to visualize all of their data from different experiments. We propose to do this in partnership with the ISIS Facility using a workbench package known as MANTID.

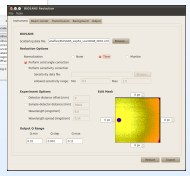




MANTID is a Python, C++ and Qt based software, and will have versions for Windows, Macintosh and Linux (which is important for high performance parallel computing on clusters). It will be Open Source software and freely distributed to users. It has both a GUI interface for "standard" reductions and a scripting interface for users who wish to customize their data reduction.



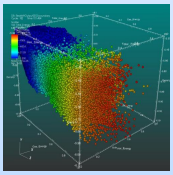
POWGEN data displayed using MANTID

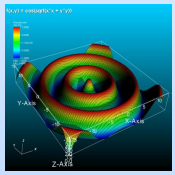


New reduction GUI for SANS instruments at HFIR

CANVAS

We have begun work on a more powerful visualization package called CANVAS. This package will allow any projection or slice in the 5D space. It uses a 4D rebinning package being developed by computer graphics experts at UTK. The visualization library to be used is the VisIt library used at ORNL for visualization of climate data and supercomputer simulation results



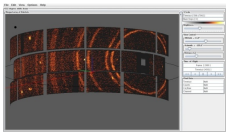


Screenshots showing the capabilities of the VisIt visualization software

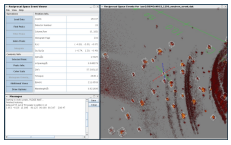
INELASTIC

Real/Reciprocal Space Views

For viewing data in real space, or for single crystal alignment ISAW can be used.



ARCS 3D view of raw data

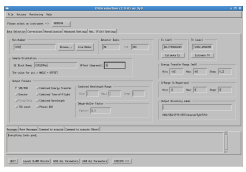


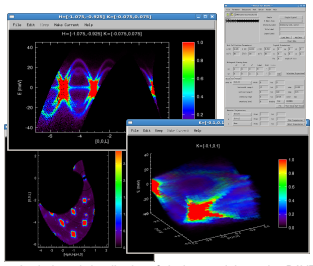
ARCS Single crystal data viewed in reciprocal space via ISAW

New visualization and planning tools are being designed to work in the Mantid framework.

Direct Geometry [ARCS, CNCS, SEQUOIA, HYSPEC]

An IDL GUI which can launch distributed (parallel) C++ code has been created to reduce the data collected in time of flight and pixel number to energy and wavevector transfer. The program, known as *DGSreduction*, allows the standard data corrections; Vanadium normalization, time independent background, sample can background, T0 (E_i), k_f/k_i, monitor or proton charge normalization etc., to obtain the dynamic structure factor, density of states, etc…





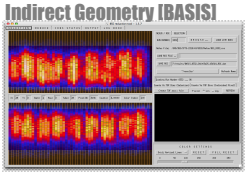
Analysis and visualization of single crystal data using DAVE

The current visualization tool used for inelastic data is DAVE from NCNR. Based on feedback from users, the speed of DAVE for the large SNS data sets has been a problem. We have optimized DAVE to increase the visualization speed by a factor of 40x. All of this has been submitted to NCNR and is included in the DAVE distribution.

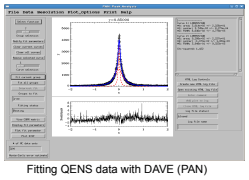
D.A.V.E.

DAVE is an IDL based package from NCNR that we use for visualization and fitting.

Indirect Geometry [BASIS]



BSSreduction GUI which allows the user to select regions of interest and perform standard data corrections.



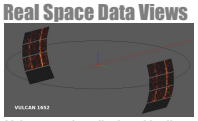
Fitting QENS data with DAVE (PAN)

DIFFRACTION

ISAW

The ISAW program was originally developed for use at the IPNS facility. The creators of the ISAW package are working as part of the Scientific Data Reduction Group to enable ISAW to read and process SNS data files with a concentration on reducing diffraction data.

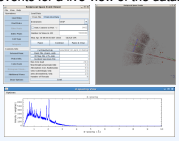
Real Space Data Views



Vulcan raw data displayed in direct space, showing detector geometry

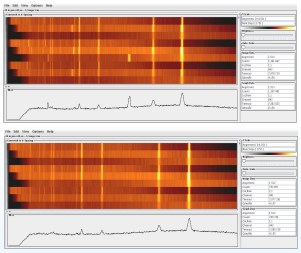
Live Data Processing

A connection between DAS and analysis computers echoes the raw data events. IsawEV (Event Viewer) can reduce and plot these events for a live view of the data.



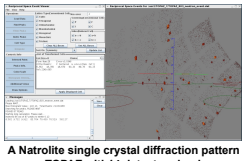
Powder Diffraction

Time focusing and grouping of data is done in ISAW using the event data directly for increased speed. It can correct for detector ghosting and single crystal peaks from sample environment. Data can be written out for both GSAS and FullProf.

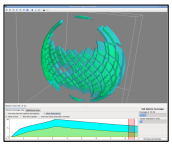


SNAP powder data with (top) and without (bottom) single crystal peaks from the anvil

Single Crystal Diffraction

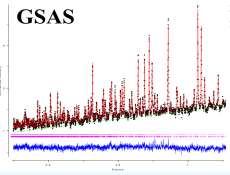


A Natrolite single crystal diffraction pattern on TOPAZ with14 detectors in place

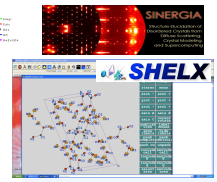


CrystalPlan – an experiment planning tool for TOPAZ.

Single-crystal peaks are located and their intensities are integrated using ISAW. The intensities are then converted to hkl positions using a UB matrix also determined by ISAW.



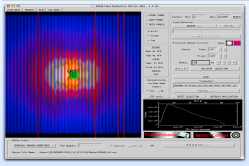
GSAS refinement of $GeZn_2O_4$ on POWGEN



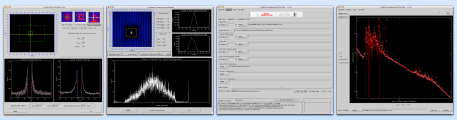
Using WinGX (SHELX wrapper) to analyze single crystal data

LOW-Q

EQ-SANS



The EQ-SANS data reduction interface is written in IDL. The interface determines the data reduction parameters, such as beam center and transmission. These parameters are built into the call of the python/C++ code that performs the data reduction.



Horizontal and vertical beam centers are determined by the center of mass of the scattered pattern.

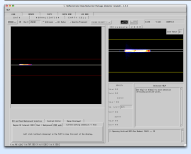
The direct beam flux provided by a hole in the beam trap is used to determined transmission.

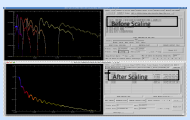
The remainder of the parameters, such as background, dark current, detector efficiency, are specified in a series of tabs.

The final step provides a plot of the result to the users. Simple fits such as Guinier can be performed in the data reduction.

REFLECTOMETRY

The reflectometry data reduction for both instruments is also written in IDL and is designed to provide reduction across the series of angles required to produce a complete reflective curve. For each angle measured, the direct beam and the background regions are selected.

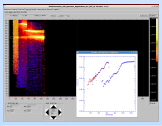




Once extracted, the specular reflectivity profiles from the different angles are merged using an automatic tool called REFscale to produce the full reflectivity profile.

Additional parameters such as normalization can be specified for use by the python/C++ data reduction.

These parameters are saved to provide reusable reduction parameters for reducing multiple samples and spin states in batch mode.



Data reduction and merging for off-specular reflectivity is under active development. It is anticipated that will become the default data reduction for specular and off-specular data.