New Developments in Data Analysis at IPNS

T. G. Worlton[1], ,D. J. Mikkelson[2], R. Mikkelson[2], J. P. Hammonds[1], J. Tao[1], A. Chatterjee[1]
[1]Argonne National Laboratory, Argonne, IL
[2]University of Wisconsin-Stout, Menomonie, WI

Abstract
The ISAW software development project at IPNS has produced software now used to visualize, correct, and transform data for several classes of instruments at IPNS and ISAW software is beginning to be used elsewhere. During the last year improvements have been made which greatly enhance the usefulness of ISAW. Recent advances include 1) a data analysis package for Single Crystal Diffractometers, 2) a data reduction package for small angle scattering, 3) a data reduction package for total powder diffraction, and 4) a newly designed set of viewers which work with basic data arrays and thus do not require the more complex data objects used for the first generation of viewers. The new viewer design allows more general use of the ISAW viewers, but still allows building complex views from basic view components. The NeXus team has included these new viewers into the NXValid program which reads, validates, and displays the contents of NeXus files (See http://www.neutron.anl.gov/nexus/NXvalid.html). The SCD software provides a method for indexing peaks based on identifying planes of peaks in reciprocal space as well as interactive two and three-dimensional viewers for reciprocal space.

1. Introduction

IPNS was the first fully instrumented proton-pulsed spallation neutron source. It began operation in 1981 with a Data Acquisition System (DAS) using what was then state of the art computing—DEC VAX and PDP-11 computers [1]. The DAS hardware was based on DEC Q Bus and CAMAC and Multibus crates [2]. A unified design for the hardware and software for different instruments was used to minimize retraining and support costs [1].

A decision was made a few years ago [3] to replace the old IPNS DAS, which was based on obsolete technology, with new systems based on Linux and VME. Experimental Physics and Industrial Control System (EPICS) software was chosen for instrument control in order to take advantage of the considerable EPICS expertise developed for Argonne's Advanced Photon Source [4]. EPICS, Linux, and VME/VXI were chosen because of the flexibility and freedom of open source development on standard hardware.

Shortly after starting development of the new DAS, a project was begun [5] to develop new data reduction and visualization software using the Java language. We also used some of the Java code from the analysis software project to support additional data acquisition functions. Our choice of Java has the benefit of portability across all standard computing systems (Windows, Macintosh, UNIX, Linux) and online availability of free development kits [6]. Java is developing rapidly and becoming the language of choice on the internet and at universities.

This new IPNS data reduction and analysis software was given the name “Integrated Spectral Analysis Workbench” (ISAW) [7]. A fruitful collaboration between Professors Dennis and Ruth Mikkelson and their students at the University of Wisconsin-Stout and staff at IPNS has enabled us to develop the ISAW package that is in use on several IPNS instruments.

ISAW is now a fairly mature software package, but new developments continue. Recent advances in ISAW include 1) a complete analysis package for Single Crystal Diffractometers, 2) wizards--a new method of operation which allows the user to step through a series of input forms to do a complete analysis, 3) a complete data reduction package for small angle scattering, 4) a newly designed set of viewers which work with basic data arrays and thus do not require the more complex data objects used for the first generation of viewers, 5) the ability to substitute the Python scripting language for the built-in scripting language. The new viewer design will allow more general use of the ISAW viewers, but still allow building complex views from the basic view components. The ability to use Python scripts will simplify use by people familiar with that language and facilitate integration into other packages such as DANSE [8].

ISAW was designed as a highly interactive and user friendly system for reading, viewing, transforming, and saving data. ISAW can read IPNS run file format files and can read and write NeXus files (see http://www.neutron.anl.gov/nexus/ for details on NeXus). Support for NeXus has allowed ISAW to be used at other laboratories which write their time-of-flight neutron scattering data in NeXus format. It will also facilitate exchange of data with other institutions and use of other general software packages to analyze IPNS data.

Object-oriented programming techniques were used from the beginning in the design of ISAW. These techniques allow menus to respond to selections of objects and allow different views of the data to be coordinated. Basic data objects in ISAW include the spectrum or “Data” block and the “DataSet”. These data objects include the data as well as associated metadata needed to list properties, perform transformations, and generate specialized views. The factory methods which build DataSet objects add operations appropriate for the type of instrument to the data objects, and the names of these operations appear as submenus of the Operations menu item on the menu bar.

Viewers for ISAW are designed for a highly interactive user environment, with views and data linked but independent as in the Model-View Controller design pattern [9]. Each view is a particular way of looking at a data set and the cursor may be used to point at a datum in one view and have that perspective reflected in other views. This is accomplished by having each view of the DataSet register as an observer of the data object and having the data object notify all observers when the pointed at datum changes.

2. ISAW Graphical User Interface and script editor

For ease of use, ISAW was initially designed to interact with the user through a graphical user interface (GUI) as shown in Fig. 1. The tree view panel of the ISAW GUI shown in Fig. 1 lists the DataSets which have been loaded into ISAW. The “Attributes” tabbed pane shows the attributes of the data object which has been highlighted by clicking on it.

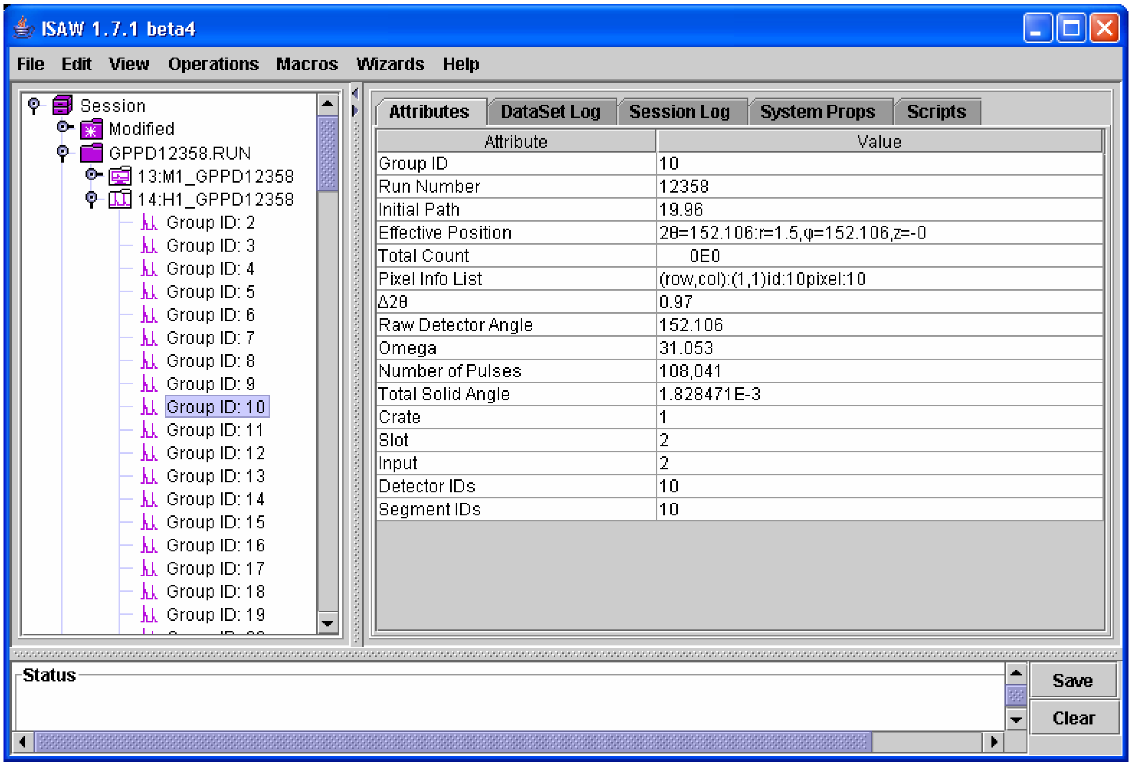

Figure 1. The ISAW graphical user interface. The interface includes a menu bar, tree view of loaded data, tabbed panes for attributes, logs, and scripts, and a Status panel.

For repetitive operations a script is preferable to a graphical user interface, so a scripting language is included as part of the ISAW package, and many sample scripts are distributed with ISAW. When a script is run, the command processor automatically generates an input dialog box to prompt for any specified input parameters. The script writer only has to specify the needed parameters, their type, and (optionally) default values. When the script calls for file input, browse buttons are automatically placed in the input dialog box alongside the text boxes for entering file names. The script may also ask the user to choose one item from an enumerated list.

The script partially shown under the ISAW Script tabbed pane in Fig. 2 can be used to load and merge data from a set of runs to be specified by the user.

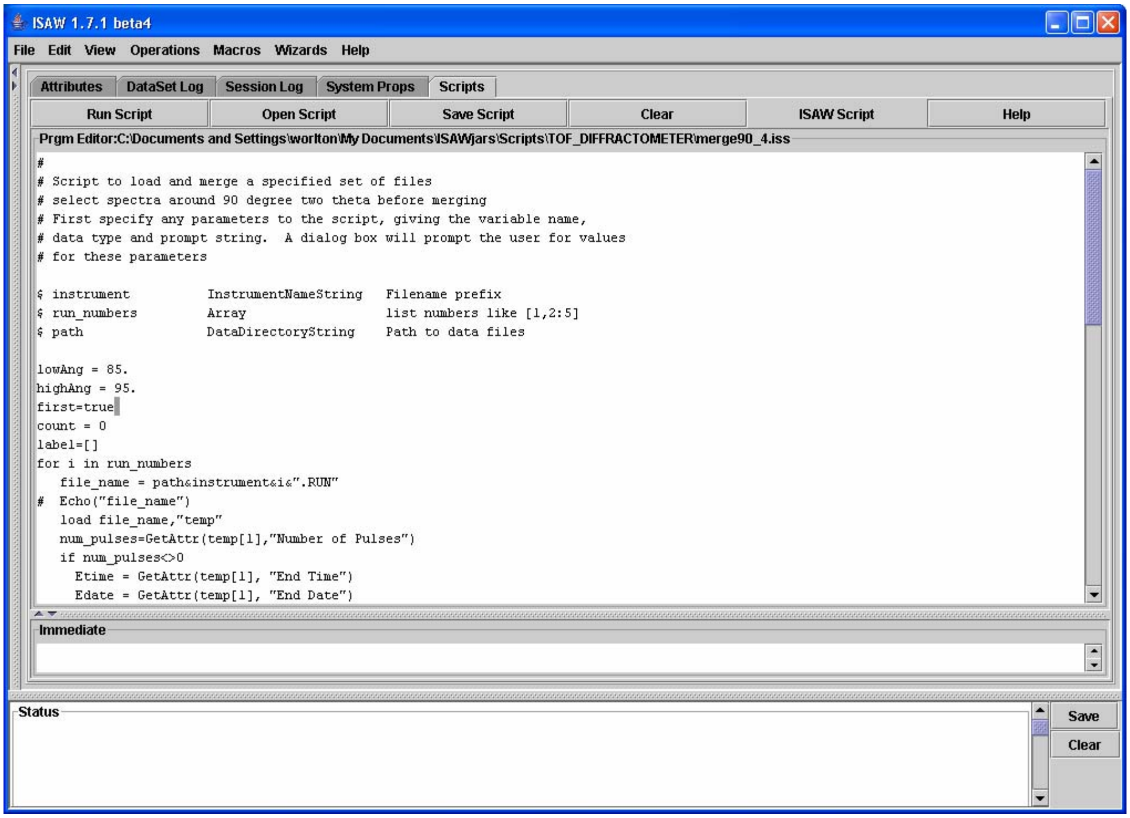

Figure 2. The ISAW GUI with an ISAW Script ready to run. Lines which start with a dollar sign specify parameters to prompt the user for.

The specified input parameters are automatically prompted for when the script is run as shown in Fig. 3a. The last step in the script is the display of all the merged data as shown in Fig. 3b.

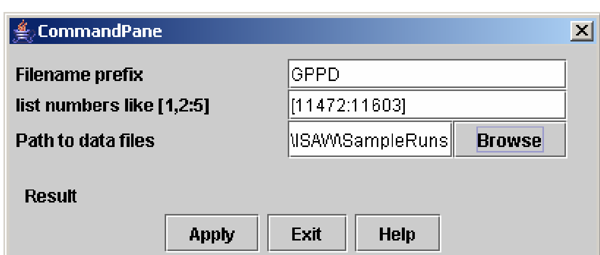

Figure 3a. The dialog box automatically generated by the script shown in Fig. 2

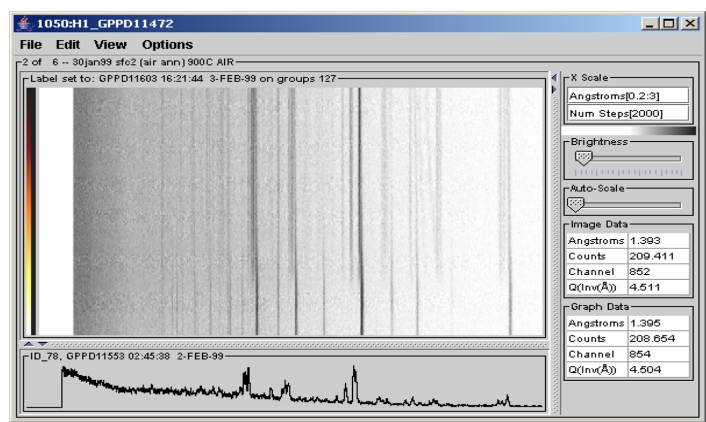

Figure 3b. An image produced by merging spectra from many measurements. This clearly shows a phase transition in the material.

In order to facilitate the use of ISAW at other laboratories, support has been added for the Python/Jython scripting language. As part of this work, an “ISAW Lite” was developed to allow using many of the features of ISAW with a script and no GUI.

Extensive documentation has been included with ISAW in order to facilitate future upgrades and collaboration with others on future developments. Each software module or class is documented using "Javadoc" style comments which are later compiled into a complete set of documentation using the Sun Javadoc tool [10]. Besides this detailed HTTP format documentation of the Java classes, there is an extensive "Help" system built into ISAW.

3. The New SCD Analysis Package in ISAW

Recent developments in ISAW provide support for the IPNS single crystal diffractometer [11] and small angle diffractometers [12]. The IPNS SCD was upgraded during the first half of 2003 to replace the single area detector at -90 degrees from the beam direction with two area detectors at angles of -75 degrees and -120 degrees. Before there were two detectors, we could integrate the SCD analysis with ISAW by running the original FORTRAN codes from an ISAW script with communication through files. After the hardware changes, we had to rewrite the software to support the second detector and add new methods, so the entire nine step Fortran data reduction and analysis suite. Because these changes required extensive revisions, the code was rewritten in Java for access through ISAW. A new calibration algorithm was developed to find calibrated values for the parameters, including detector size, position and orientation, offset of sample from goniometer center, initial flight path and T zero. During the initial stages of data reduction, peaks are located, indexed, and the orientation matrix refined using least squares techniques. Finally, the integrated intensities are calculated.

SCD data reduction is now controlled through a "wizard" mechanism that allows the user to step through the analysis, view intermediate results, adjust various parameters, repeat steps, etc., as needed. Wizards were developed to facilitate constructing user friendly GUI-based programs for data reduction and visualization. They manage a sequence of form objects, and simplify analysis by inexperienced users. Each form object represents one step of a multi-step reduction process. The GUI components used for the parameter I/O are built automatically based on the type of the parameter. The form just needs to implement a few standardized methods to specify the desired parameter types and prompt strings, calculate the result of the operation, provide a title, etc. The forms can be written in Java, Jython, or the ISAW scripting language.

Normal SCD data reduction and analysis can be done with two wizards. The InitialPeaksWizard is used whenever you begin studying a new crystal. It will determine the crystal orientation with respect to the instrument, etc. Subsequent measurements use the DailyPeaksWizard and take advantage of the alignment calculations from the InitialPeaksWizard.

4. Small Angle Scattering Data Reduction

Small angle neutron scattering (SANS) data reduction and analysis has also been recently added to ISAW. Time-of-flight SANS at spallation neutron sources provides data in a wide Q range because of the utilization of a wide range of wavelengths [13]. Typically, data from SANS instruments is reduced to produce I(Q) using the following steps:

1. Find beam center

2. Determine the sensitivity of detector pixels
3. Calculate the efficiency ratio of the area detector and the incident beam monitor
4. Determine transmission coefficients
5. Calculate the I(Q) correction for delayed neutrons and normalize to the sensitivity of the pixels and the efficiency ratio.

ISAW provides a collection of scripts and wizards that do all the steps in the SANS data treatment. There is also a script for batch processing of multiple runs. The Q bins can be 1d or 2d with a resolution that can be set in the scripts. Before the start of every run cycle at IPNS some standard samples like Bates Poly, Diphosil and Silver Behenate are measured and compared with data from other sources.

A number of viewers that come with ISAW can be used to look at the output files. Figure 4a shows a view of the SAND area detector with a double-wedge region selected. Figure 4b shows a graph of the data summed over the wedge as a function of Q.

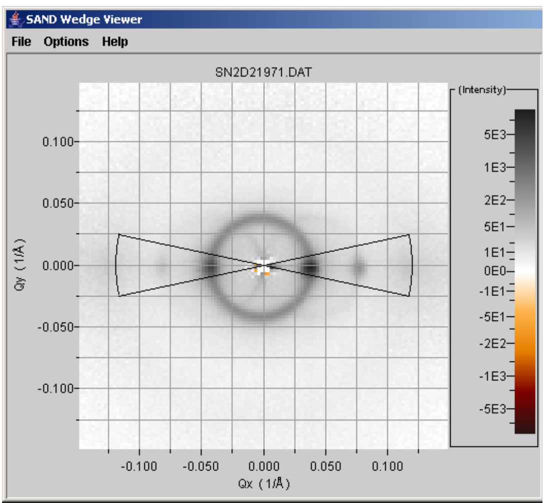

Figure 4a. A double wedge selection of the data from the SAND area detector.

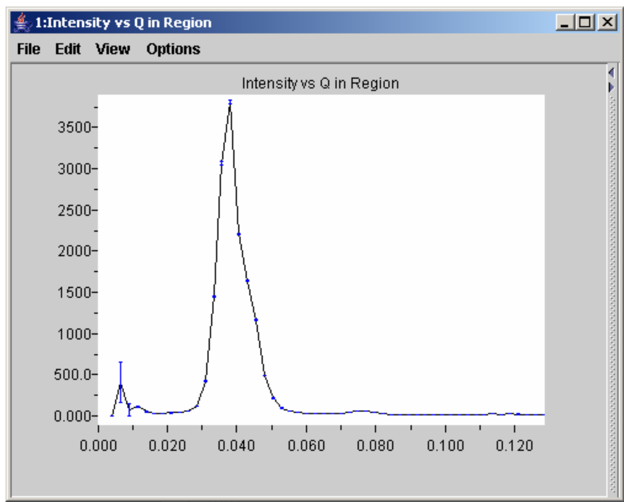

Figure 4b. A graph showing the data from the selected region in Fig. 1a summed as a function of Q.

Conclusion

The ISAW project has produced software now used to visualize, correct, and transform data for chopper spectrometers, powder diffractometers, and single crystal diffractometers and we plan to continue adapting it to new instrument types. It is currently used routinely on most IPNS instruments as well as at least one instrument at LANSCE. Prototypes for a method for indexing SCD peaks based on identifying planes of peaks in reciprocal space as well as interactive two and three-dimensional viewers for reciprocal space have been constructed. New classes of instruments being studied for ISAW support include the Glass and Amorphous Materials Diffractometer (GLAD), and the polarized reflectometers.

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