ISAW Tutorial

Tom Worlton 10/9/2003

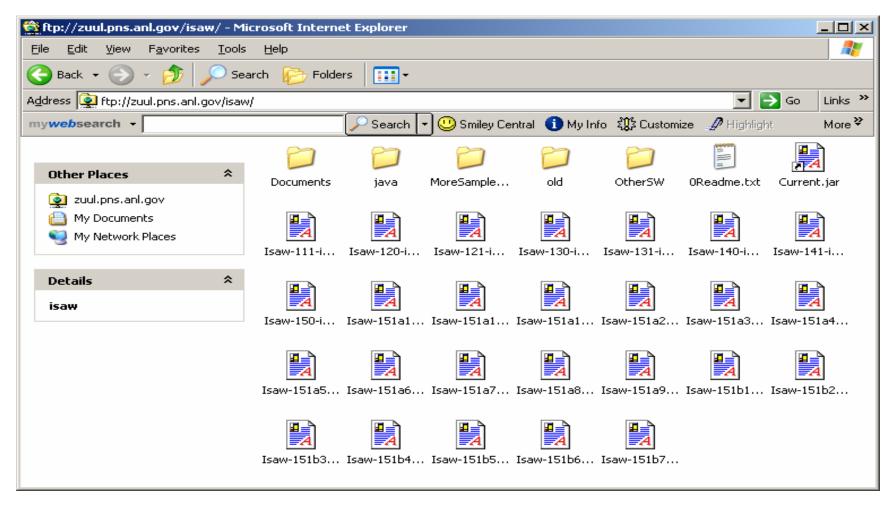
Part I

- Introduction to ISAW for New Users
 - This section teaches how to download and install ISAW and how to use ISAW with the sample data files included in the distribution. It demonstrates the use of viewers, operators and scripts.

Install ISAW

- Ensure that Java is installed on your system
 - the Java Runtime Environment (JRE) must be installed <u>before</u> installing ISAW. Java distributions are different for different platforms (see <u>http://java.sun.com/j2se/</u>), but the same ISAW installer works on all platforms
- Download and install ISAW per instructions (0Readme.txt) on the ISAW ftp site <u>ftp://zuul.pns.anl.gov/isaw</u>
 - Because of the size of the files, be patient when downloading and opening them.

The ISAW ftp site



Run ISAW

- Run ISAW following the instructions in "Test Installation of ISAW" in the "OReadme.txt" file.
- The first time you run ISAW, the IsawProps.dat file will be created in your home directory. This file will contain default locations for various files and directories used by ISAW, plus viewer defaults, etc.
- Choose "Edit Properties File" from the file menu to view and/or edit this file. Choose "save and exit" to save your changes.

A sample IsawProps.dat

🛃 IsawProperties Panel (editable)	🛃 IsawProper	rties Panel (editable)	
File	File		
#This is a properties file	IsawFileServer	1_Name=IPNS(zeus)	
ISAW_HOME=C:/ISAW/	IsawFileServer	1_Path=zeus.pns.anl.gov	;6089
Help_Directory=C:/ISAW/IsawHelp/			
Script_Path=C:/ISAW/Scripts/	IsawFileServer	2_Name=Test(dmikk-Isa	w)
Data_Directory=C:/ISAW/SampleRuns/	IsawFileServer	2_Path=dmikk.mscs.uws	tout.edu;60
Default_Instrument=GPPD			
Instrument_Macro_Path=C:/ISAW/	IsawFileServer	3_Name=mandrake	
User_Macro_Path=C:/ISAW/	IsawFileServer	3_Path=mandrake.pns.a	nl.gov;6089
Image_Path=C:/ISAW/images/			1993
neutron.nexus.JNEXUSLIB=C:/ISAW/Lib/jnexus.dll	NDSFileServer	1_Name=Test(dmikk-ND	S)
	NDSFileServer	1_Path=dmikk.mscs.uws	stout.edu;60
Inst1_Name=HRMECS			
Inst1_Path=zeus.pns.anl.gov;6088	ColorScale = C	ptimal	
	#RebinFlag=fa		
Inst2_Name=mandrake	HScrollFlag=fa	lse	
Inst2_Path=mandrake.pns.anl.gov;6088	ViewAltitudeAn	gle=5.0	
	ViewAzimuthAr	igle=180	
Inst3_Name=GPPD	ViewDistance=	4.0	
Inst3_Path=gppd-pc.pns.anl.gov;6088	ViewGroups=N	IOT DRAWN	
	ViewDetectors:	=SOLID	
Inst4_Name=UW-Stout	Brightness=40		
Inst4_Path=dmikk.mscs.uwstout.edu;6088	Auto-Scale=25	.0	
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Load some data

- From the "File" menu on the menu bar, select "Load Data", "Local" and select "sepd16837.run" from the file dialog box.
- Note that In the tree view, the file name SEPD16837.RUN appears.
- Click on the "pushpin" icon at the left of this filename to expand the view, then click on the icon to the left of H1_SEPD16837 to show the groups. You may need to change component sizes by dragging the stippled bars to see details

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	Group ID: 5	an a	End Date	+
		anna.	End Time	+
	• 🔄 21:H2_SEPD16837	a a a a	Number of Pulses	
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View Attributes

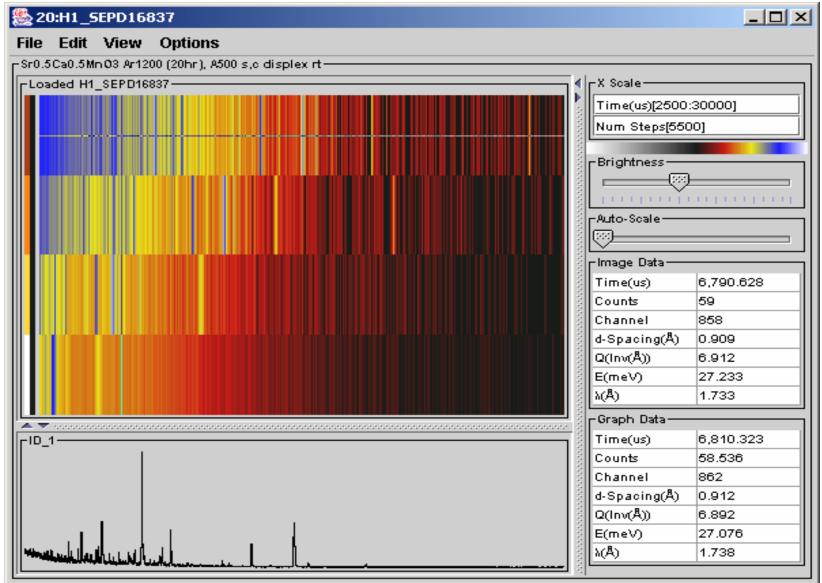
- Click on the DataSet H1_SEPD16837 and the "Attributes" tab.
- Note the attributes information for the DataSet, then click on Group #1 and note the group attributes. Detector ID's 1 through 80 (1:80) are summed together in group 1.
- Click on Group 5 and see how non-contiguous ID's are listed.

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Display an Image View

- Click on DataSet H1_SEPD16837, then select "Image View" from the "View" menu.
- Note the four bands of color in the image view. The horizontal axis refers to time-of-flight and the color indicates intensity. The four color bands represent the four detector groups. For DataSets with more groups, narrower bands will appear, down to one pixel wide. If the number of groups/spectra exceeds the number of vertical pixels, scroll bars will appear.

ISAW Image View



Test Cursor Interaction

- Put the cursor over the image and drag it to different positions while holding down the left mouse button.
- Notice how the readout information in the lower right changes as the cursor moves. Also notice that the lower graph changes when you point at different detector groups.
- Notice that the Attributes display on the ISAW GUI also responds to the cursor pointing at different groups.

Test arrow keys

- Use the up and down arrow keys to move between detector groups. Notice that the cross hairs move exactly one group for each click.
- You can also move the cross hairs left and right using the arrow keys.
- Arrow key movements will leave the cross hairs on the display.

Transform X Axis

- Select "Axis Conversions" from the "View" menu and select convert to d-spacing.
- Use the cursor to find a good range of d-values and change the range by clicking in the range following "Angstroms" in the upper right of the image view and editing the numbers. A colon separates the minimum and maximum values.
- You can also use an operator selected from the menu bar sub menus to convert axes. This creates a new DataSet and puts it in the "Modified" folder of the tree view.

Test zoom function

- Hold down the middle mouse button and drag the cursor over the image to select an area to zoom into. Double-click on the image to unzoom. Select again to zoom multiple times.
- If you don't have a middle button, use the shift key with the left mouse button to select the zoom region.
- The graph region will not change until you drag the cursor on the image with the left mouse button down.

View all data points

- In the default image view the data is compressed horizontally to allow the full spectrum to be shown in the view area. To see all points, select "Horizontal Scroll" from the "Options" menu. You will now probably need to use the scroll bar to see all of the data for each spectrum.
- Uncheck "Horizontal Scroll" to return to the default (compressed) view.
- From the View menu on the image view, select "Axis Conversions"→ "None" to return to time-offlight axes.

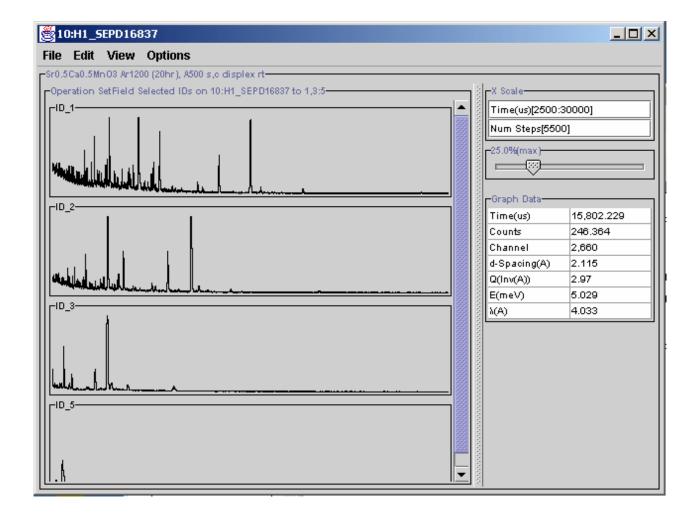
Test Viewer Controls

- There are several display controls on the right of the image display.
 - "num steps" is initially equal to the number of channels of data, but the data may be rebinned into fewer steps by editing the number.
 - The "Brightness" slider controls image brightness.
 The lower half of the brightness bar above the slider shows the scale colors for negative numbers.
 - The "Auto-Scale/%(max)" slider controls the percentage of maximum for the graph display.

Test Scrolled Graph View

- With H1_SEPD16837 still highlighted on the tree view, create a "Scrolled Graph View" from the "View" menu, or select "Additional View" from the View menu and use the View menu a second time to change the view type.
- Drag the new view window so both views can be seen.
- In the scrolled graph view, the spectrum for each detector group can be seen individually by dragging the scroll bar.
- Drag the cursor over the scrolled graph view and watch the response on the Graph Data cursor readout and the Attributes panel of the ISAW GUI.

Scrolled Graph View



Spectra selection

- Spectra can be marked as "Selected" through the tree view, image view, or scrolled graph view.
 - On the tree view, spectra are "selected" through a right-click operation as shown at the right.
 - On the viewers, the spectra are "selected" through typing "S" to select a single spectrum or "shift-S" to select a range of spectra.

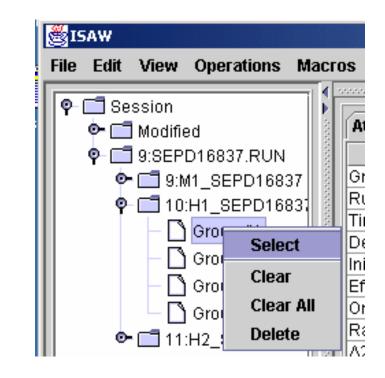
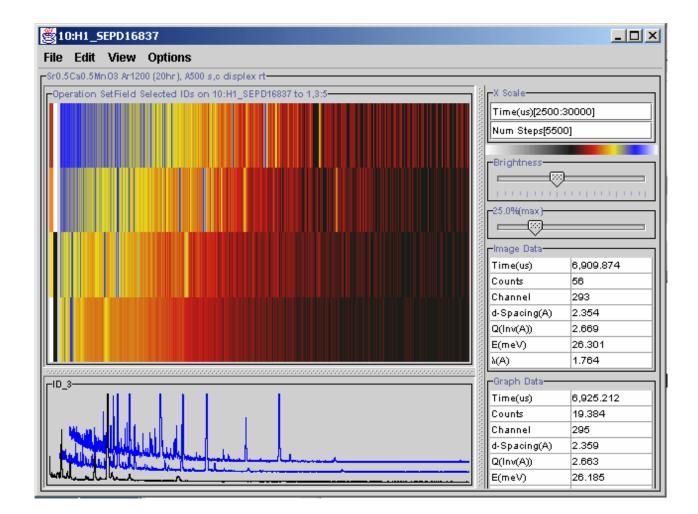


Image View selected graphs



"GRX_Y" Table View

- With H1_SEPD16837 still highlighted, select two or more spectra/groups. On the menu bar, choose "Selected Table View" and "GRX_Y" from the "View" menu. In this view, spectra are listed one at a time, serially.
- The first column is the x value (initially time-of-flight) and the second column is the counts or other intensity value. The second selected spectrum will be listed after the first and so on.
- Click on "Options" and "Show Errors" on the table view menu bar. Before any data manipulations, the errors are just the square root of the counts in each channel.

"GRX_Y" Table View

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2545.0	198.0	14.071247	
2560.0	137.0	11.7046995	
2575.0	129.0	11.357817	
2590.0	120.0	10.954452	
2605.0	105.0	10.246951	
2620.0	133.0	11.532562	
2635.0	132.0	11.489125	
2650.0	184.0	13.56466	
2665.0	148.0	12.165525	
2680.0	125.0	11.18034	
2695.0	82.0	9.055386	
2710.0	97.0	9.848858	
2725.0	129.0	11.357817	
2740.0	135.0	11.61895	
2755.0	103.0	10.148891	
2770.0	101.0	10.049875	
2785.0	85.0	9.219544	
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"Parallel y(x)" Table view

- Use the View menu to choose "Parallel y(x)" from the Selected Table View menu.
- In the "Parallel y(x)" view, ISAW will attempt to list selected spectra/groups in parallel columns following the x value column. Empty cells may appear due to differences in X axes for different spectra/groups. This view can follow the pointed at cursor position from other views.

Image view selected graphs

- When there are spectra selected, the image view graph area shows up to 16 of the selected spectra plus the spectrum pointed at by the cursor.
- Try the different options under "Options", "Graph Selected (16 Max)".
- Use the Viewer "File" menu to close the DataSet viewers.

Load spectrometer data

- Use the ISAW GUI File menu to load file HRCS2447.RUN.
- Click on the push-pin icons to expand the tree view of the file, then select DataSet H1_HRCS2447.
- Compare the "Conversion" operations for this DataSet with the operations for DataSet H1_SEPD16837.

Spectrometer/Diffractometer operations

- The operations menu adjusts to the selected DataSet, so each DataSet has different operations.
- Note the difference in operations for spectrometer and diffractometer DataSets.

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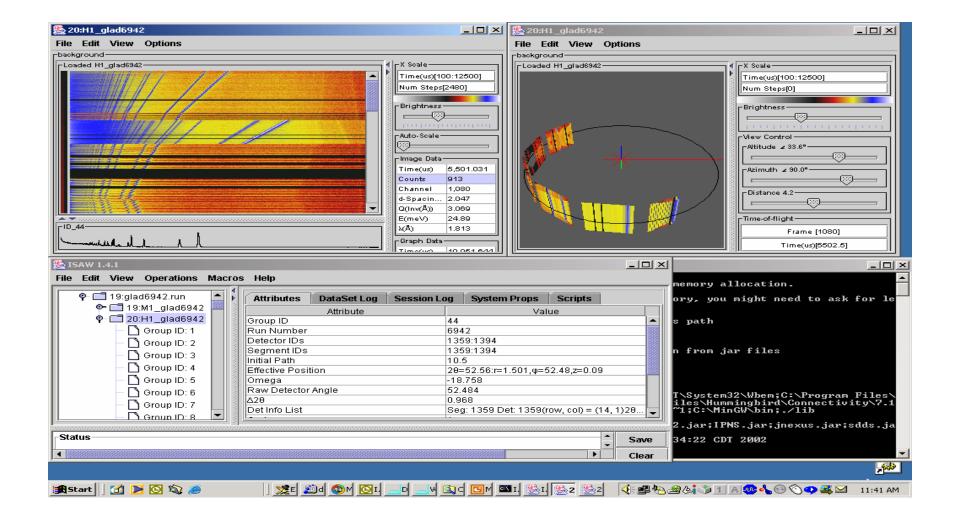
Load large DataSet

- Use the file menu to load file GLAD6942.RUN, click on the push pin to expand the tree view and select DataSet H1_GLAD6942.
- Note that this DataSet has almost a thousand groups/spectra.
- In Attributes for the groups, note that many of the groups (spectra) include data from a number of detector elements.
- When many large data sets are loaded, Java may run out of memory. If this ever happens, stop and restart ISAW.

H1_GLAD6942 views

- Create an Image View of H1_GLAD6942.
- Create an additional view which is a 3D View of H1_GLAD6942
- Click on the title bar and drag the 3D view to uncover the Image View.
- Notice how the 3D view changes as you adjust the view controls.
- Notice how the VCR-like controls at the bottom allow you to step through frames/time-channels.

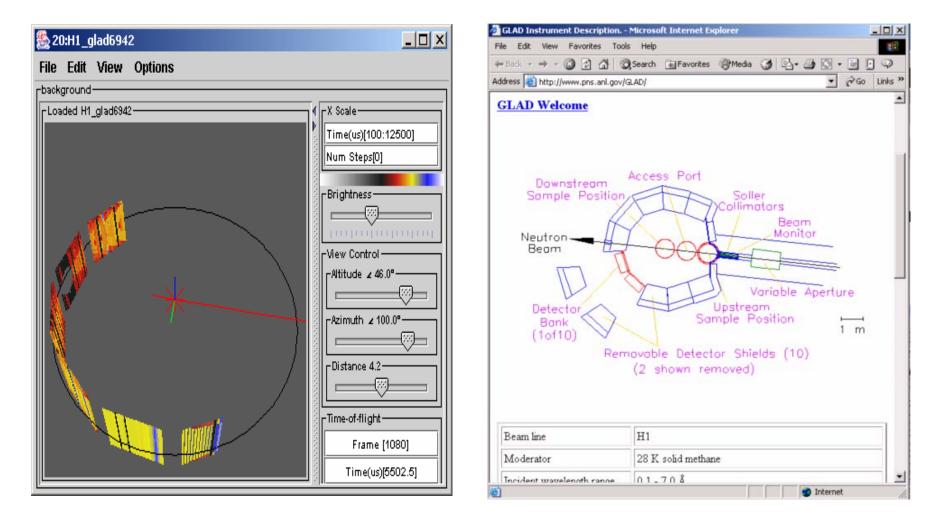
Image and 3D views



Test 3D View

- Drag the cursor over the Image view and notice the response on the cursor readout area, the 3D View, and the ISAW GUI Attributes display.
- Select the "GLAD" link from the "Instrument Info" submenu of the ISAW GUI "View" menu.
- On the 3D view, change the azimuthal angle to about 100 degrees and the altitude to about 45 degrees, then compare the instrument sketch with the 3D view.

GLAD 3D View and sketch



3D view of GLAD6942.RUN

Sketch of GLAD instrument

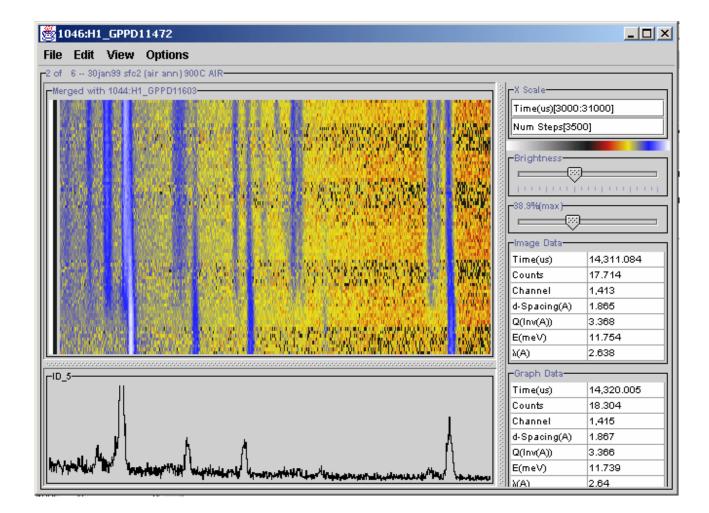
Scripts

- Scripts simplify operating on a large number of files or repeating complex operations.
- Download files: gppd11472:11603.run from the "MoreSampleData" folder at <u>ftp://zuul.pns.anl.gov/isaw/</u>
 - These files are a parametric study of one sample

Use a Script to merge files

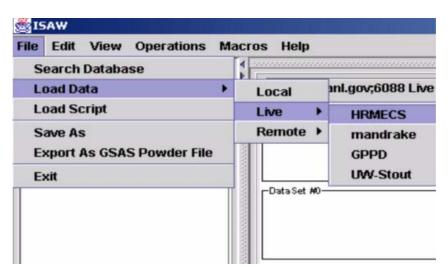
- Select the ISAW GUI "Scripts" tab.
- Select "Open Script" and open the "merge90_4" script.
- Select "Run Script" and enter 11472:11603 between the square brackets. Make sure "instrument" is "GPPD".
- ISAW should start loading 132 files (on Windows, watch the DOS window for load messages).
- When loading finishes, an image display showing one group (angle -95 to -85) from each run should appear.
- Select "EXIT" on the script dialog box.
- Use the cursor to zoom in and examine the phase transition.

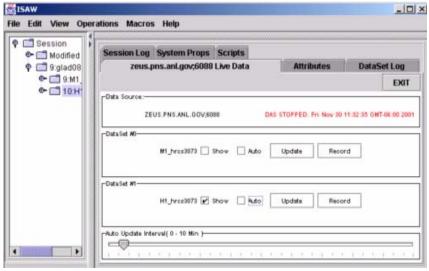
Image view of phase transition



Connect to live data server

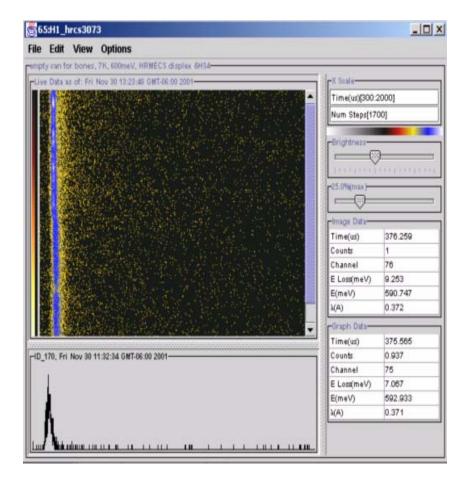
- From the ISAW menu bar, select File, Load Data, Live, DMIKK.
- DMIKK is a test data server.
- Select the tab labeled "DMIKK live data".
- Click the "Show" button on dataset #1.





View Live Data

- When the show or auto buttons are clicked on the live data server panel, an image view is generated.
- To copy the live data set to the ISAW tree, click "Record"

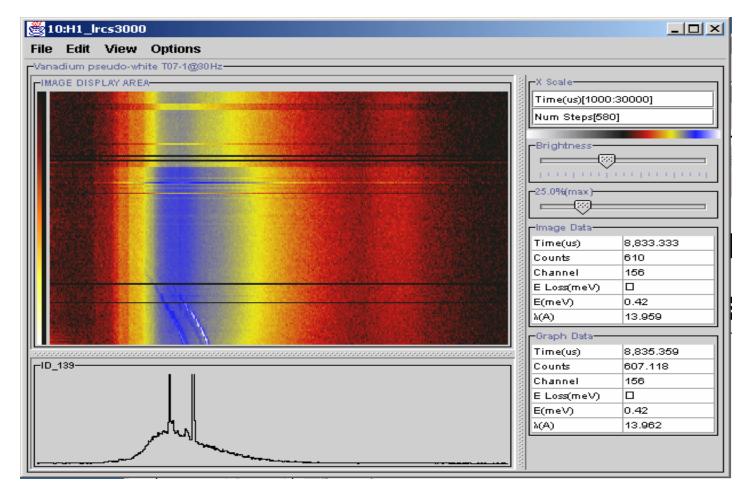


Load Remote NeXus File

- From the ISAW menu bar, select File, Load Data, Remote, Test(dmikk-Isaw)
- Enter file name lrcs3000.nxs.
- <u>Wait</u> for "Operation completed" message
- Exit "LoadRemote" Operation and view dataset H1_Ircs3000
- NeXus files can also be loaded through an NDS server, but this is much slower.

<u>×</u>
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dmikk.mscs.uwstout.edu
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WORLTON
IPNS
Ircs3000.nxs
NDS File Server 🔹
Apply Exit

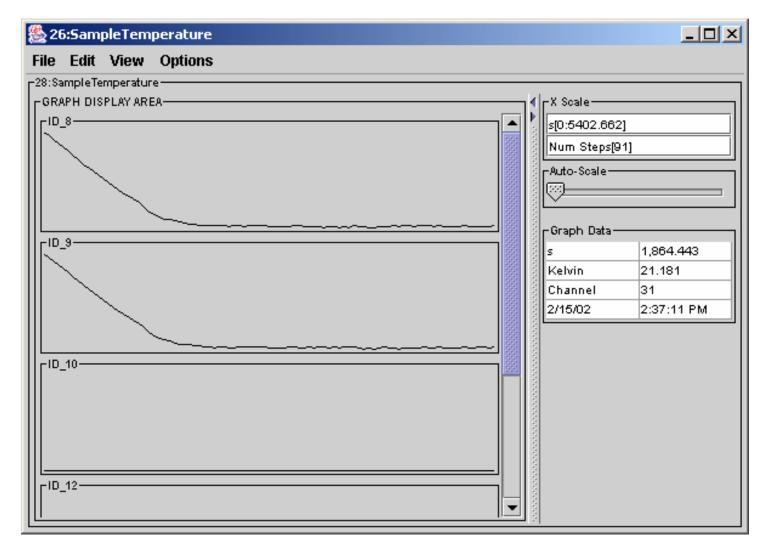
LRCS3000 from Remote NeXus File



View a Log File

- Load the file hrcs3118.sdds
 - (you will have to change the file filter in the file chooser to allow seeing sdds files)
- Expand the tree node for the file and select the sample temperature dataset
- Create an image view or scrolled graph view of the dataset
- Drag the cursor over the plot and notice the readout of temperature versus time

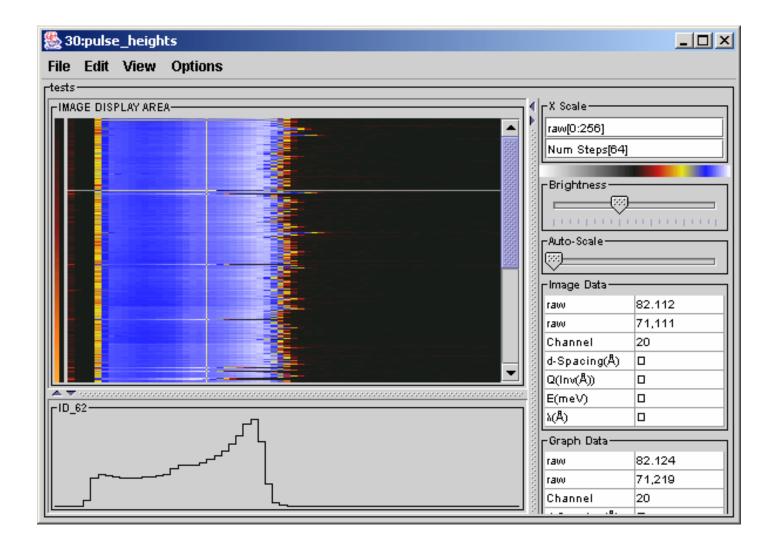
An IPNS temperature log file



View Pulse Height Spectra

- Download the file new_smarts-o4.12.o2.nxs.gz from "More Sample Data" on zuul and unzip it.
- Load the file new_smarts-o4.12.o2.nxs
- Expand the tree view to show the datasets included in the file
- Click on the DataSet "pulse_heights"
- Create an image view of the specified dataset
- Notice the typical pulse height shape of the spectra
- Also notice that this is data from LANSCE!

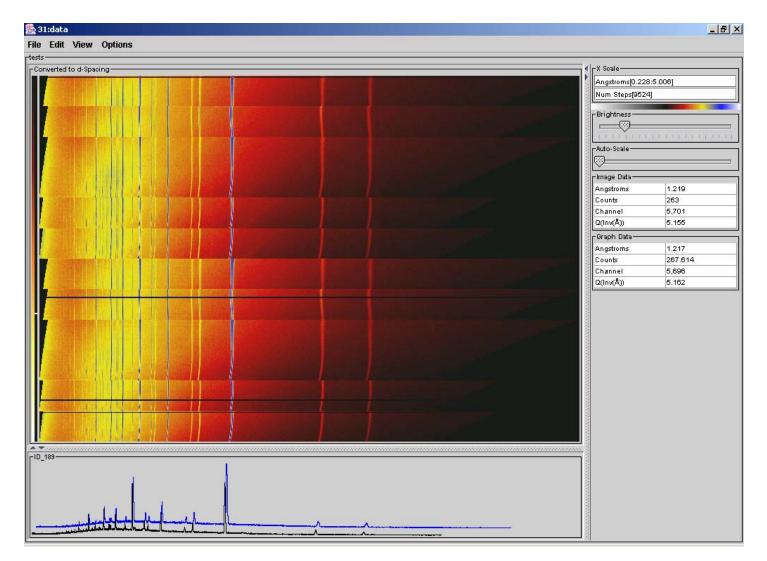
Pulse Height data from LANSCE



View LANSCE SMARTS Data

- Click on the "data" smarts DataSet
- Create an image view
- This is data from the SMARTS instrument at LANSCE (Los Alamos).
- Choose "View", "Axis Conversions", "d-spacings"
- By looking at all spectra you can see that the lines are curved--indicating a calibration problem, but this was their first data file in this format.

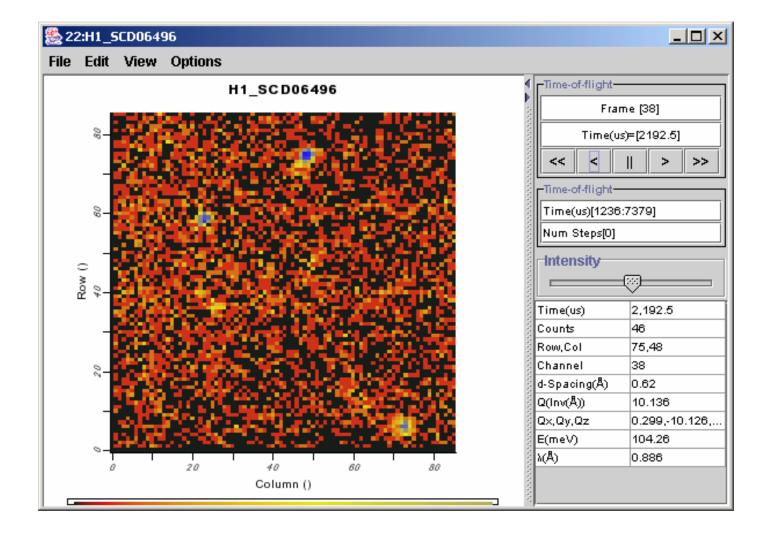
SMARTS Data



View Area Detector Data

- Load file SCD06496.RUN
- Select DataSet H1_SCD06496
- Create a Contour View which shows time slices of the area detector surface
- The cursor interaction in this view now works the same as the other views
- Use the arrow buttons to step to frame 38 to compare with the image on the next slide. You can step one slice at a time (>) or continuously (>>). Clicking on ">>" a second time pauses stepping.

Area Detector View



Part II

- Be an ISAW Developer!
 - Teaches more advanced users how to write scripts and operators. This requires use of the Java Software Developer Kit (SDK). This section teaches how to modify and recompile operators, and how to find documentation on using existing operators in scripts.
 - This section uses MS Windows examples, but most parts apply to other platforms.

Be an ISAW Developer!

- Install the Java Developer Kit
 - Download the Java Standard Edition (j2se)
 Software Developer Kit (SDK) without
 NetBeans from http://java.sun.com/j2se/
 - Install the SDK using the installation instructions for your computing platform
 - The j2se download page at the time this was written is shown on the next slide which highlights areas of interest.

The j2se SDK download page

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	Solaris SPARC® (.bin)	DOWNLOAD			
	Solaris x86 (.bin)	DOWNLOAD			
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	Release Notes	VIEW			
	License	VIEW			
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Test the Java compiler

- Create a command window at the ISAW folder (If you have the PowerToy "Command Prompt Here" installed in Windows, you can create a command window by right-clicking on the ISAW folder icon and selecting "Command Prompt Here".)
- Enter the command "javac" in the command window
 - This is the Java compile command.
 - If the software developer kit is installed correctly, you should get Java compiler information. If you don't, correct the installation.

Unpack the ISAW jar files

- Enter the command "jar -xvf Isaw.jar"
- Repeat for the "jhall.jar" file in the ISAW distribution.
- Edit the Isaw_exec.bat file and add "rem" in front of the first java command and remove the "rem" from the second java command.
 - This will cause the compiler to look in the folders before looking in the jar files for sources.

Modify an Operator

- Edit the "HelloOperator.java" file in the "Operators" folder in the ISAW directory.
- Find the "getResult" method
 - (find public object getResult)
- Change the return text from "Hello" to "Good day".
- From the ISAW folder command window, enter the command: "javac Operators/HelloOperator.java"
- This should produce a new version of "HelloOperator.class"

Test new Operator from ISAW GUI (Windows platforms)

- Double-click on Isaw_exec.bat to start the ISAW GUI.
- Select "Macros", then "Generic" and "Hello Operator".
- Click the "Apply" button.
- Your modified return text should appear.

Determine the command for scripts

- Start the "Hello Operator" dialog box as in the last slide.
- Click the "Help" button.
- Scroll to the top of the Help Window.
- Notice the "Command: " specification "SayHello(String Name)"
- This tells you how to use the command in a script

Write to Status pane

- From the tabbed panes in the ISAW GUI, select the tab "Scripts"
- In the "Prgm Editor" pane enter Display SayHello("your name")
- Click on the "Run Script" tab
- The Status pane should show a message with the text from the operator.
- Also try it with "Display SayHello()"
- Also use the immediate pane to enter the same command.

Write to command window

- Change "Display" to "Echo" in the script.
- Put parentheses around the command and text—for instance: Echo (SayHello("Master"))
- Run the modified script
- Try with text added--for instance: Echo (SayHello("Master") & " How may I serve you?")

Load DataSets

- Open the script "LoadTree.iss"
- The three lines starting with "\$" will generate a dialog box to request parameters
- The first argument has a type, "DataDirectoryString", which will result in a Browse button on the prompt, while the other two are just Strings.
- These three parameters are combined in the "load" command to make a complete file specification.
- The "load" command is a built in subroutine of the ISAW command processor. For documentation, click on the "Help" item on the ISAW menu bar and select "Command pane"

Script variable types

- String (see LoadTree.iss)
- int (see find_multiple_peaks.iss)
- Float (see Denn1.iss)
- Array (see AutoplotSA.iss)
- Choice (see ChoiceTest.iss)
- Boolean (see find_multiple_peaks.iss)
- InstrumentNameString (see AutoplotSA.iss)
- DataDirectoryString (see convert_gsas.iss)
- LoadFileString (see find_multiple_peaks.iss)
- SaveFileString (see efficiency.iss)
- MonitorDataSet (see find_peaks.iss)
- SampleDataSet (see find_peaks.iss)
- ServerTypeString (see SUMRUNS.iss)

Loading DataSets

- The first argument to the load command is a file name
- The second is a variable to receive the array of DataSets from the file. The return value is the number of DataSets loaded from the file.
- The "LoadTree.iss" script also illustrates how to "send" a DataSet from a script to the ISAW GUI tree view.

Send DataSet to Viewer

- A script can send a DataSet to a specific viewer. For viewer names, see the View menu.
 - In LoadTree.iss, add the line: display(vnam[i], "Image View") after the "send" line.
- Run the script again and notice that image views of each DataSet are generated.