ISAW Tutorial

Tom Worlton 10/30/2002

Install ISAW

- Download and install ISAW per instructions (0Readme.txt) on the ISAW ftp site, <u>ftp://zuul.pns.anl.gov/isaw</u>
 - Either the Java Runtime Environment (JRE) or Java Development Kit (JDK) must be installed <u>before</u> installing ISAW. Java distributions are different for different platforms, but the same ISAW installer works on all platforms.
 - Because of the size of the files, be patient when downloading and opening them.

The ISAW ftp site

😭 ftp://zuul.pns.anl.gov/isaw/ - Microsoft Internet Explorer											
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WARNING: This is a United States Department of Energy computer system, which may be accessed and used only for official Government business by authorized personnel. Unauthorized access or use of this computer system may subject violators to criminal, civil, and/or administrative action. All information on this computer system may be	Isaw-120-install.jarIsaw-121-install.jarIsaw-130-install.jarIsaw-131-install.jarIsaw-141-install.jarIsaw-141a2-install.jarIsaw-141a3-install.jarIsaw-141a5-install.jarIsaw-141a5-install.jar	9.73 MB 9.74 MB 9.74 MB	Executable Jar File Executable Jar File	3/4/2002 12:00 AM 3/12/2002 12:00 AM 4/8/2002 10:18 PM 4/29/2002 4:52 PM 8/15/2002 7:53 PM 9/10/2002 10:07 PM 9/11/2002 3:12 PM 9/13/2002 3:17 PM 9/27/2002 7:26 PM							
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Run ISAW

- Run ISAW following the instructions in "Test Installation of ISAW" in the "0Readme.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. Restarting ISAW is necessary to use new values.

A sample IsawProps.dat

😹 IsawProperties Panel (editable)	×
File	
#This is a properties file	
ISAW_HOME=C:/ISAW/	
Help_Directory=C:/ISAW/IsawHelp/	
Script_Path=C:/ISAW/Scripts/	
Data_Directory=C:/ISAW/SampleRuns/	
Default_Instrument=GPPD	
Instrument_Macro_Path=C:/ISAVW	
User_Macro_Path=C:/ISAW/	
Image_Path=C:/ISAW/images/	200
neutron.nexus.JNEXUSLIB=C:/ISAW/Lib/jnexus.dll	
Inst1_Name=HRMECS	
Inst1_Path=zeus.pns.anl.gov;6088	
Inst2_Name=mandrake	
Inst2_Path=mandrake.pns.anl.gov;6088	
Inst3_Name=GPPD	
Inst3_Path=gppd-pc.pns.anl.gov;6088	
Inst4_Name=UW-Stout	
Inst4_Path=dmikk.mscs.uwstout.edu;6088	
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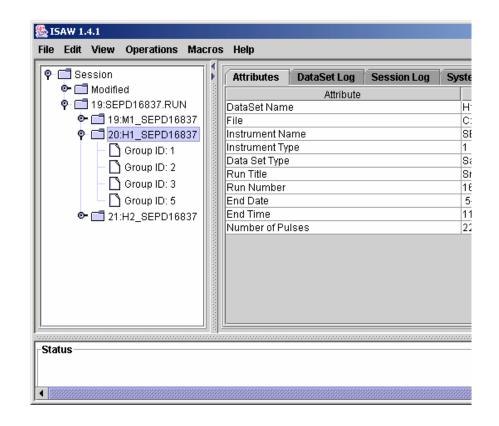
uFiloConcert.

IsawProperties Panel (editable)	×
File	
IsawFileServer1_Name=IPNS(zeus)	•
IsawFileServer1_Path=zeus.pns.anl.gov;6089	
IsawFileServer2_Name=Test(dmikk-Isaw)	
IsawFileServer2_Path=dmikk.mscs.uwstout.edu;60	
IsawFileServer3_Name=mandrake	
IsawFileServer3_Path=mandrake.pns.anl.gov;6089	
NDSFileServer1_Name=Test(dmikk-NDS)	
NDSFileServer1_Path=dmikk.mscs.uwstout.edu;60	
ColorScale = Optimal	
#RebinFlag=false	
HScrollFlag=false	
ViewAltitudeAngle=5.0	
ViewAzimuthAngle=180	
ViewDistance=4.0	
ViewGroups=NOT DRAWN	
ViewDetectors=SOLID	
Brightness=40	
Auto-Scale=25.0	
-	-

►

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_SEPD16937 to show the groups. You may need to change component sizes to see details



View Attributes

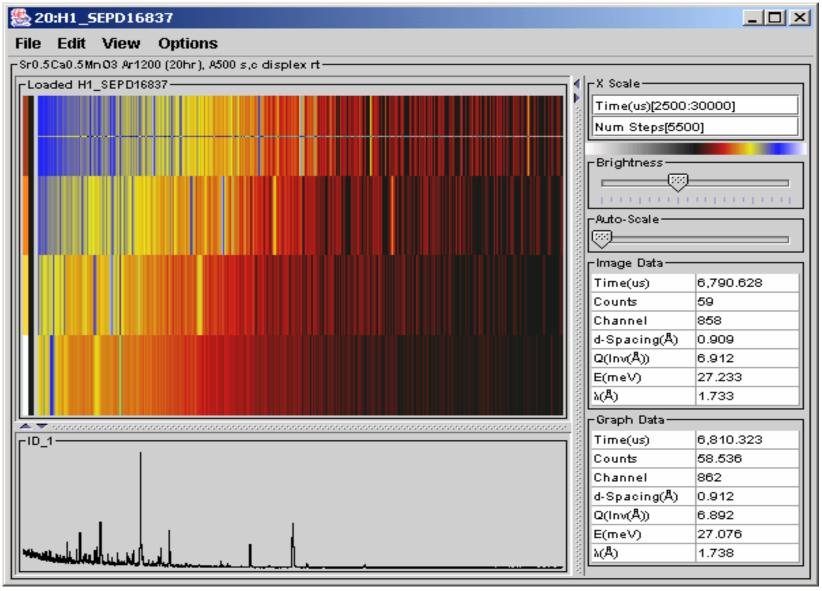
- Click on the DataSet H1_SEPD16837 and the "Attributes" tab.
- Note the attributes information for the DataSet, then click on Group #1 and note the group attributes. Detector ID's 1 through 80 (1:80) are summed together in group 1.
- Click on Group 5 and see how non-contiguous ID's are listed.

P 🗂 Session	Þ	Session Log System	n Props Scripts
💁 🗖 Modified	and an	Attributes	DataSet Log
🗣 🗂 19:SEPD16837.RUN	1000	Attribute	Value
🗢 📑 19:M1_SEPD16837	1000	Group ID	1
💡 🛄 20:H1_SEPD16837	1000	Run Number	16837
— 🗋 Group ID: 1	1000	Detector IDs	1:80
- Group ID: 2	1000	Segment IDs	1:80
	1000	Initial Path	14
— 🗋 Group ID: 3	1000	Effective Position	2θ=144.85:r=1.5,φ=-144.85,z=-0
🗕 🗋 Group ID: 5	4444	Omega	62.577
💁 🗂 21:H2_SEPD16837	-	Raw Detector Angle	-134.795
	1000	Δ2θ	0.97
	1000	Det Info List	Seg: 1 Det: 1(row, col) = (1, 1)28=1
	1000	Crate	1
	1000	Slot	1:10
	1000	Input	1:8
	1000	Total Solid Angle	0.346
	1000	Efficiency	1
	4444	Number of Pulses	22806
	200	Total Count	182,640

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. For larger numbers of groups, vertical 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 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.

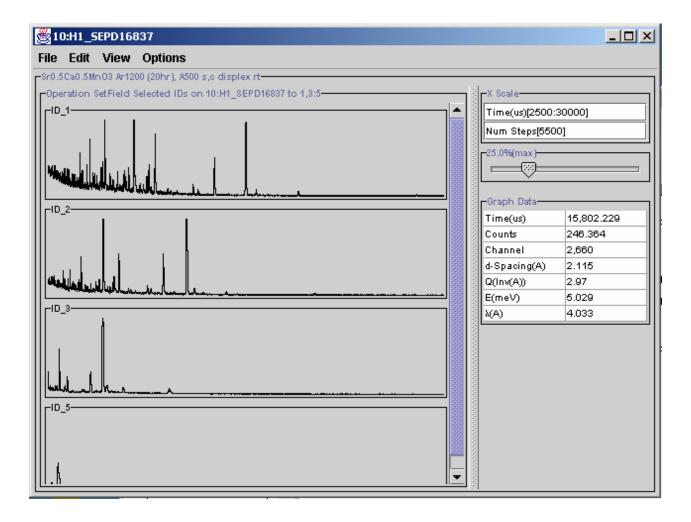
Test Viewer Controls

- There are several display controls on the right of the image display.
 - The number of 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 scale is for negative numbers.
 - The percentage 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.
- 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



Test Table View

- With H1_SEPD16837 still highlighted, choose "SelectedTable View" and "Group x versus y" from the "View" menu. By default, the Table view shows just the first spectrum.
- Right-click on Group #3 of H1_SEPD16837 in the tree view and choose "select". Note changes in viewers.
- 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.

ISAW Table View

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2500.0	486.0	22.045408
2515.0	472.0	21.725561
2530.0	300.0	17.320509
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
2800.0	83.0	9.110434
2815.0	81.0	9.0

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.

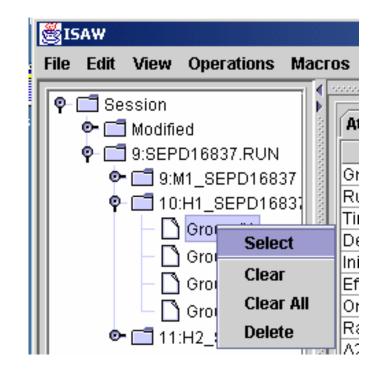
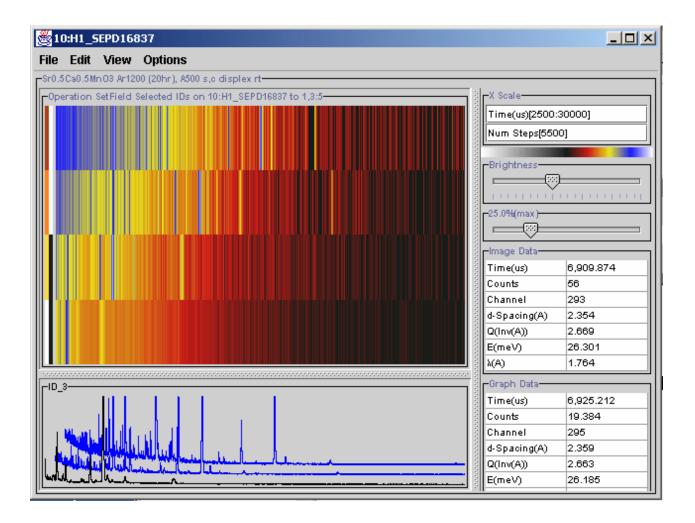


Image view selected graphs

- 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. Each selected spectrum will show in blue unless the cursor also points at it.
- Try the different options under "Options", "Graph Selected (16 Max)".
- Use the Viewer "File" menu to close the DataSet viewers.

Image View selected graphs



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 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.

Operations Macros Help								
Math → Edit List →	Attributes DataSet Log Session Log System Props Sc							
Conversion 🕨	Attribute							
Attribute 🕨 🕨	DataSet Name							
Data Plotter	File Instrument Name							
Special 🔹 🕨	Remove Bad Detectors Data							
1_HRCS2447	Scale Using Monitor 1 DataSet							
1_HRCS2447	HRMECS Macro: Calibration, Evaluation, Grouping & Tof~E							
H2_HRCS2447	Double Differential Crossection							

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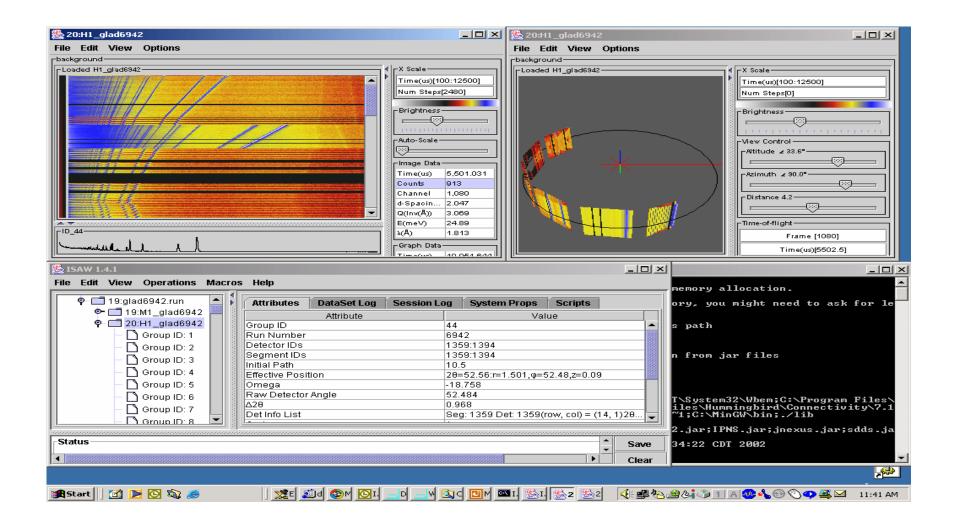
Load large DataSet

- Download GLAD6942.RUN from the "MoreSampleData" folder on the ISAW ftp site to the Data_Directory (Use the "Data_Directory" listed in properties file, IsawProps.dat).
- Use the file menu to load this file.
- Note that there are more than a thousand spectra in DataSet H1_GLAD6942.
- In Attributes for the groups, note that many of the groups (spectra) include data from a number of detector elements.

H1_GLAD6942 views

- Create an Image View of H1_GLAD6942.
- Create 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 time channels.

Image and 3D views

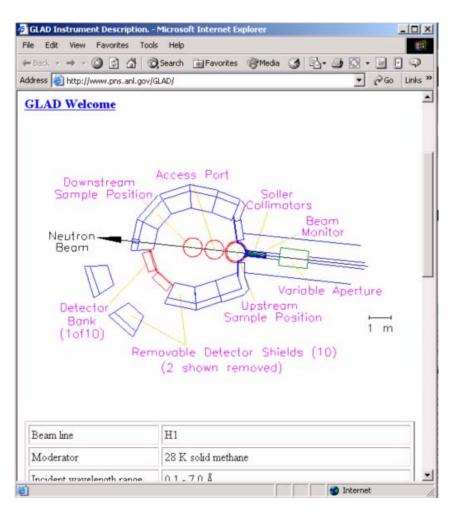


Test 3D View

- 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 "GLAD Link" from the "Instrument Info" submenu of the ISAW GUI "View" menu.
- On the 3D view, change the azimuthal angle to about -50 degrees and the altitude to about 45 degrees, then compare the instrument sketch with the 3D view.

GLAD 3D View and sketch

8 21):H1_g	jlad694		
File	Edit	View	Options	
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				Time(us)[100:12500]
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Sketch of GLAD instrument

3D view of GLAD6942.RUN

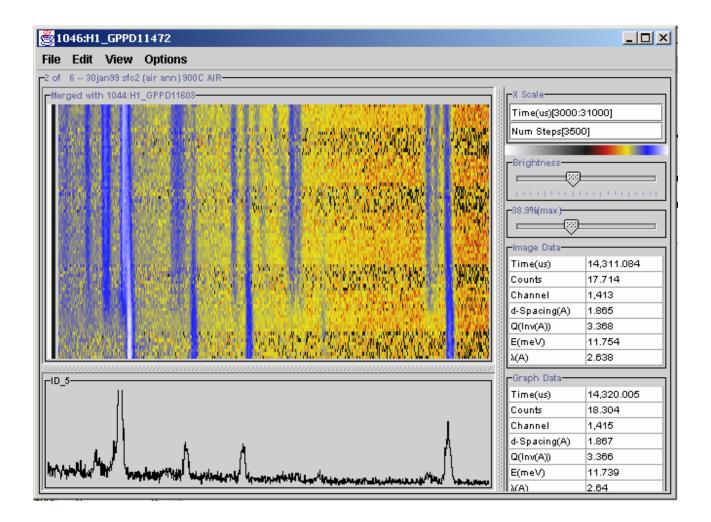
Scripts

- Scripts simplify repeating complex operations or operating on a large number of files.
- 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 dialog box.
- Use the cursor to zoom in and examine the phase transition.

Image view of phase transition



Connect to live data server

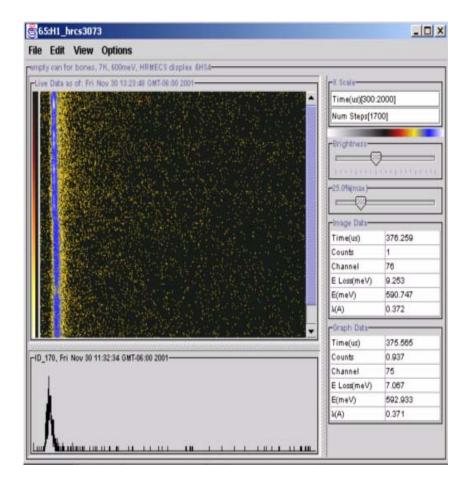
- From the ISAW menu bar, select File, Load Data, Live, HRMECS.
- Select the tab labeled "zeus.pns.anl.gov"
- Click the "Show" button on dataset #1.

File Edit View Operations Search Database	M		
Load Data	•	Local	anl.gov;6088 Live
Load Script		Live 🕨	HRMECS
Save As		Remote >	mandrake
Export As GSAS Powder File Exit	-	and a second	GPPD UW-Stout
		Data Set #0-	L

♥	Session Log System Props Scripts zeus.pns.anl.gov;6088 Live Data Attributes I	DataSet Log
		EXIT
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	ZEUS.PNS.ANL.GOV;6088 DAS STOPPED; Fri Nov 30 11:32	35 GMT-06 00 20
	Data Set NO	
	M1_hros3073 Show Auto Update Record	
	DataSet M	
		1
	H1_hros3073 🖌 Show 🗌 Ruto Update Record	

View Live Data

- When the show or auto buttons are clicked on the live data server panel, an image view is generated.
- To save the live data set in the 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.

Оре	ration LoadRemote
Host name	dmikk.mscs.uwstout.edu
Port (eg. 6088)	6008
User name	WORLTON
Password	IPNS
File Name (eg. hrcs1797.run)	Ircs3000.nxs
Server Type	NDS File Server
Operation completed	
	kpply Exit

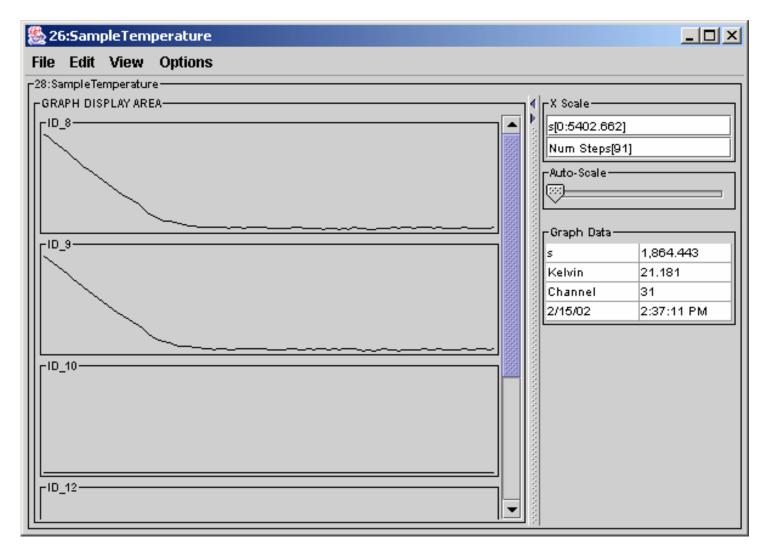
LRCS3000 from Remote NeXus File

😤 10:H1_lrcs3000		
File Edit View Options		
-Vanadium pseudo-white T07-1@30Hz-		
IMAGE DISPLAY AREA	X Scale	
	Time(us)[1000	
	Num Steps[58	0]
	Brightness	a
	25.0%(max)	
	Image Data	
	Time(us) Counts	8,833.333
	Counts	156
	E Loss(meV)	
	E(meV)	0.42
	λ(A)	13.959
	Graph Data	
		8,835.359
LID_133	Counts	607.118
	Channel	156
	E Loss(meV)	
	E(meV)	0.42
الماليم ا	λ(A)	13.962

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

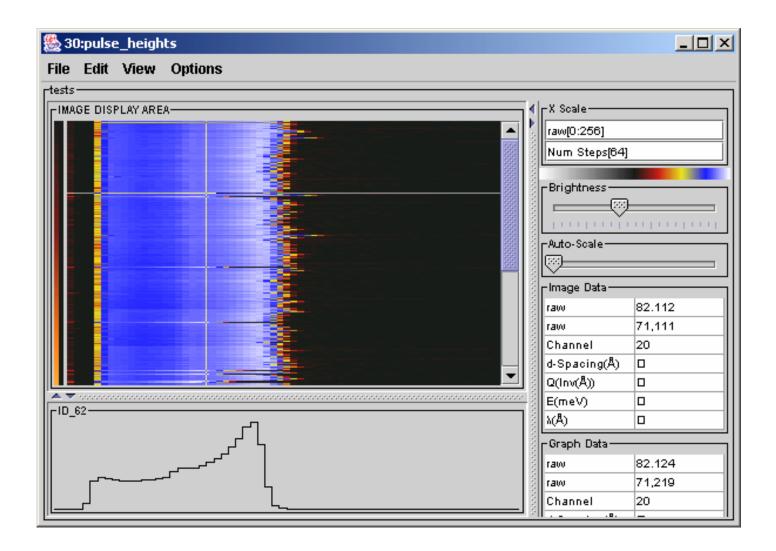
An IPNS temperature log file



View Pulse Height Spectra

- 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!

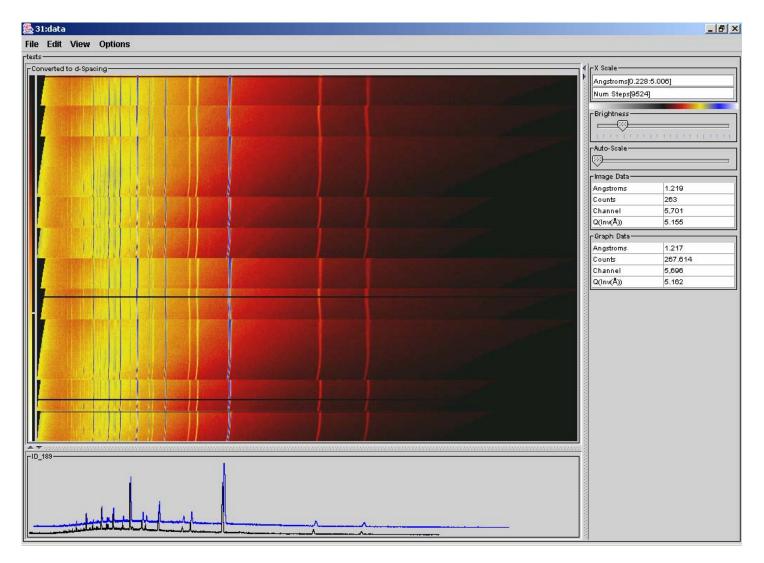
Pulse Height data from LANSCE



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-value"
- By looking at all spectra you can see that the lines are curved--indicating a calibration problem, but this is their first data file in this format.

SMARTS Data



View Area Detector Data

- Load file SCD06530.RUN
- Select DataSet H1_SCD06530
- Create a Contour View
- Cursor interaction does not work the same way on this view as the other views
- Click on a point for cursor readout
- Dragging the cursor with the left button down selects a zoom region
- Shift plus click of the center mouse button unzooms
- Forward and backwards buttons step through time-slices either one at a time (>) or continuously (>>)

Area Detector View

