• **VSANS Data Reduction Documentation**

v 0.1 Sep 2019
v 0.2 Jun 2020
v 0.3 Mar 2021

All operations and instructions are subject to improvemet, pending user feedback

This tutorial guides you through reduction of VSANS data using Igor Pro.

If you use this software to reduce or analyze your data, please reference:
"Reduction and Analysis of SANS and USANS Data Using IGOR Pro"
S. R. Kline, *J. Appl. Cryst*. **39** (2006) 895–900.

Videos containing abbreviated instructions and more tips for use of the macros are available at the NCNR web site: (VSANS videos coming soon)
<https://www.nist.gov/ncnr/sans-usans-reduction-video-tutorials>

VSANS Reduction Using Igor

System Requirements

• Macintosh or PC

• Igor Pro installed <http://www.WaveMetrics.com> As of 2/2020, v.8.04 is the current Igor version, and these macros require Igor Pro v. 7.0 or higher. As always, the macros will work with free Demo versions of Igor. These macros do work with the beta version of Igor 9.

NOTE: You DO NOT need to purchase Igor Pro to reduce your data. You can use either the (free) Demo version of Igor Pro, or the full version. Igor 7.0x or higher is required.

The Igor Pro Demo software is fully functional for the first 30 days. After the trial period, the NCNR macros are still functional, but those using the demo version for reduction will have the obvious limitation that they will not be able to save, or copy/paste into other programs. Some specialized operations that use the clipboard will not function since saving and copy/paste is of course, not allowed. Printing also has an Igor watermark overlay. Thus, the only real limitation is that reduction needs to be done in one sitting (without quitting Igor), and that publication graphics must be generated in another software package.

During the reduction process (even with the Demo version):
- All corrections to raw data headers are written directly to the files on disk.
- Reduced and averaged data files are written to disk as ASCII output that can be plotted and analyzed with Igor or with other software.
The ONLY special step that demo users may want to do is:
- Protocols for data reduction are usually saved with the experiment. Since this is not allowed, protocols must be exported (see Build a VSANS Data Reduction Protocol) and imported again if you quit the demo version.

• SANS, USANS, and VSANS Reduction Macros, plus Analysis Macros, and Tutorial data are available on our website:
<https://www.nist.gov/ncnr/data-reduction-analysis/sans-software>
Follow the instructions on the webpage for downloading and installing the NCNR_SANS_Package.

(The use of certain trade names or commercial products does not imply any endorsement of a particular product, nor does it imply that the named product is necessarily the best product for the stated purpose.)

Installation Note for VSANS

Igor v7 or v8 is required to run these macros. Please use the 64-bit version of the Igor Application. The 64-bit version allows larger event files to be loaded and processed. The 32-bit version of Igor may not be fully supported in the future.

*** as of the package release 8.02 (Jan 26, 2021), the installation of the HDF5 XOP is done automatically (Thanks, Jeff) so there is no need to follow these steps, but they are left here just in case something goes wrong.*

> After installing the NCNR Macros, the HDF5 XOP needs to be activated (the 64-bit version). To do this, follow the instructions from the WaveMetrics help file:
>
> If you press the shift key while clicking the Help menu, you can choose Help->Show Igor Pro Folder and User Files. Igor then opens the Igor Pro 7 (or 8) Folder and the Igor Pro User Files folder on the desktop, making it easy to drag aliases/shortcuts into "Igor Pro User Files/Igor Extensions". Go to the folder More Extensions (64-bit), open the folder, and make a shortcut for the file HDF5-64.xop. Cut that shortcut and paste it into the folder Igor Extensions (64-bit). You may leave the "-shortcut" in the name if you want. Pasting ".xop" shortcuts into Igor Extensions (64-bit) is a general way to activate additional WaveMetrics XOPs for a given user.
>
> Once you have placed an alias/shortcut of the “HDF5-64.xop” in the “Igor Extensions (64-bit)” folder, quit and restart Igor. You are now ready to reduce VSANS data.

*** There is also a known issue with some NCNR-authored XOPs and MacOS 10.15 (Catalina) where the OS will refuse to allow these to be loaded. There is a workaround, verified by WaveMetrics (the authors of Igor Pro) that can be found at: <https://www.wavemetrics.com/node/21088>*

Initialization

Once the macros are installed, start a reduction experiment by selecting "Load NCNR VSANS Reduction Macros" from the Macros menu. This step sets up the internal folder structure, global variables and constants, and opens the main panel. This is done automatically at the start of each new VSANS experiment. On startup, you will be asked if you are “using the back detector” – if so, answer “yes”, if not, choose “no”. If you did not use the back detector in the experiment, then selecting “no” will provide a significant speedup in most operations since the back detector can be ignored.

General - VSANS Data Handling Overview

*If you are new to VSANS, start with the VSANS Tutorial Instructions. You can simply follow along with the instructions and use your own data or use the example data supplied in the NCNR Data Reduction Package (in the NCNR_SANS_Utilties folder).

For more specific functions and their explanations and descriptions of the operation of all panels, see the links in the section Additional VSANS Operations

VSANS Overview
VSANS Data Reduction Overview
What's New in VSANS
VSANS Instructions for the Impatient

VSANS Tutorial Instructions

This tutorial guides you through the basic steps needed to reduce VSANS data. The example data uses the converging beam collimation and thus uses all the detectors available on VSANS. There are many other collimation configurations available, but all will follow this basic reduction sequence.

The tutorial covers the basic steps necessary. Many other operations are available, and descriptions are either linked in the help file or can be accessed directly by help buttons on the respective panels.

VSANS Experiment Planning Tools

Additional VSANS Operations

VSANS Event Mode

General - VSANS Data Handling Overview

VSANS Overview

The processing of VSANS data has been implemented such that it behaves as much like the reduction of SANS data as possible to make the processing easy for longtime SANS users as well as those new to VSANS. While VSANS is essentially a SANS instrument that can reach much lower angle than a traditional SANS instrument, there are some differences. Most notable is that the data is collected simultaneously on multiple detector panels. In this way, a large angular range is covered all at once and is all saved into a single (large, approx 4 MB) data file. In addition, important identifying tags are added to the data files as part of the data acquisition process. Having all the data housed in a single data file, plus the additional metadata identifiers greatly simplifies the data reduction process.

Raw VSANS data file names are of the form: sansNNNNN.nxs.ngv where NNNNN can be any number, no leading zeros needed, no restriction on number of digits. Data files are stored in Nexus format, which is based on the HDF5 format. VSANS files are loaded into folder structures following the Nexus definition. These folder structures are carried throughout the WORK file process. Nexus attributes and the DAS_log (generated by NICE) are not routinely loaded to improve speed. These can be read in if necessary.

VSANS Data Reduction Overview

The basic correction steps in reduction and the process of converting to absolute scale are identical to SANS. See the SANS Reduction help topic: Data Reduction Overview for the details and equations. There are some differences in the details of the processing steps. For example, VSANS absolute scaling requires only a single open beam measurement (two if the back detector is used) since the collimation is not changed - all the data is collected at once.

Some of the data handling for VSANS is also slightly different. Many of these differences are due to the different types of detectors used at VSANS. The four panels on each of the front and middle detector carriages are made of individual tubes. The high-resolution detector on the back carriage uses a scintillator process. Each requires a set of initial corrections somewhat different than the gridded area detectors currently in use on the 30m SANS instruments.

Initial correction when RAW data is loaded in:

The only correction that is done is calculation of the non-linear corrections so that the beam center and the pixel locations are all known in real-space distance (mm) rather than in pixels. This is so that q-values can be properly calculated. The raw data counts are not changed in any way when the raw data is loaded.

When converting RAW data to a WORK file - (SAM, EMP, etc):

Corrections are done in this order, and all are applied to the full, 2D data panels:

(1) For the back detector only – if the ReadNoise file has been loaded, it is subtracted, otherwise a constant read noise value is subtracted. The back panel image is also shifted to register the three CCDs of the back detector..
(2) The detector sensitivity correction is applied (this is different than the order for SANS data). The DIV correction is applied on a “pixel” basis for each panel before any non-linear effects are corrected.
(3) (re)Calculate the non-linear corrections. This generates lookup waves that match each detector pixel to a real space x and y distance. (count data is not affected)
(4) Apply the dead time correction to the data – the dead time correction needs to be applied before the count values are altered by other operations, since it is based on the raw count rate seen by each tube. The dead time correction does alter the count values.
(5) Calculate the solid angle per pixel and apply it to the data values. The result is that each pixel is on a counts/solid angle basis. This makes the pixel values significantly larger than the original “count” values since the solid angle per pixel is a small value.
(6) Calculate and apply the angle-dependent tube shadowing.
(7) Calculate and apply the angle-dependent efficiency correction.
(8) Calculate and apply the downstream window transmission correction.
(8) Calculate and apply the angle dependent sample transmission correction.
(9) The detector counts are normalized to 1E8 monitor counts.

What's New in VSANS

For details of the latest changes to the VSANS macros and to all of the NCNR Reduction Macros, please go to our github page:
<https://github.com/sansigormacros/ncnrsansigormacros/wiki>

The latest version of the package can always be found at:
<https://github.com/sansigormacros/ncnrsansigormacros/releases/latest>

VSANS Instructions for the Impatient

1) "Load VSANS Procedures" and pick the data path
2) List VSANS Data Files
3) Calculate Transmissions in VSANS
3) Build a VSANS Data Reduction Protocol
4) Reduce Multiple VSANS Files
5) Write journal article

VSANS Tutorial Instructions

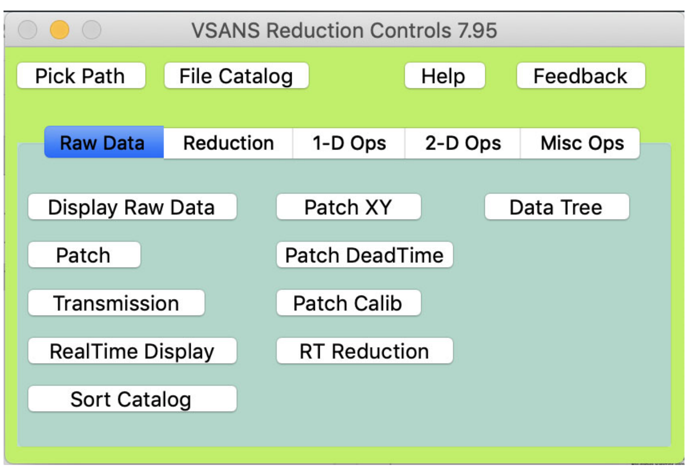
Main VSANS Panel

What: Upon opening a blank experiment for VSANS data reduction, this main control panel is the starting point for viewing your data, performing the data reduction, plotting the averaged data, and performing some simple analysis. It organizes the essential controls for VSANS data reduction in one location.

How: The Main Panel of VSANS Reduction Controls is automatically created. If you've lost this panel on the screen, selecting VSANS->Find Windows->Main Control Panel from the main menu bar will bring this window to the front. Clutter can be minimized by closing auxiliary panels when not in use. Panels are automatically re-created on demand.

Use the "Pick Path" button, which brings up a standard open dialog where you pick the folder on disk where the data files are located. Save the experiment (typically in the same folder), and the data path will also be saved.

For new experiments, the current version number of the NCNR macros will be displayed in the window title. Old experiment files that are opened with a newer version of the macros will not update the version in the title.



The buttons are:
(always visible)

Pick Path: presents a dialog to select the folder that contains your data. This only needs to be set once, at the beginning of a data reduction session.

File Catalog: after the data path has been set, this will generate a table of information about each file in the data folder. The table is very useful to identify each file and for building reduction protocols.

Help: will display this help file.

Feedback: will automatically direct you to a web page that is a form where you can submit a bug report or a feature request.

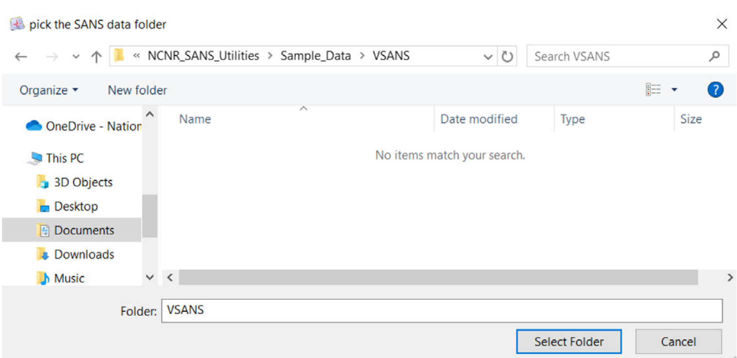
Tutorial -- Proceed to List VSANS Data Files

There is also a VSANS Menu that is always visible on the main menu bar. Menu selections will generate the input panels as if the corresponding button had been pressed on the Main Panel, or simply bring the window to the front if it has been misplaced. The Initialize step is run automatically as the experiment is launched but can be re-run at any time to ensure that the VSANS Preference values are reset to their default values. For a detailed description of the buttons contained on all the tabs, see:
Raw Data Tab - VSANS
Reduction Tab - VSANS
1-D Ops Tab - VSANS
2-D Ops Tab - VSANS
Misc Ops Tab - VSANS

List VSANS Data Files

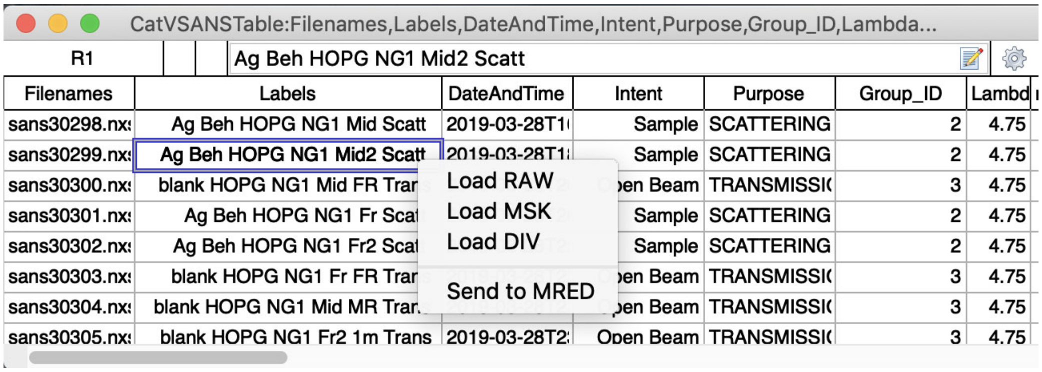
What: Set a path to your data folder. Then create a "Catalog" table with information about your data files, available for use in building data reduction protocols.

How: All the raw data files, detector sensitivity files, mask files, etc. must be kept in a single folder for IGOR to access them. From the main panel, click "Pick Path" to set the path to this folder. Depending on your OS (Mac or Windows) the dialog may look slightly different.



After you have set the data folder path using "Pick Path", click on the File Catalog button to generate a table listing all the data files in the folder. This operation gets a listing of all the data files in the folder selected by "Pick Path". Details about each file are added to a table, including the file name, sample label, its purpose and intent, its group_id, and the assigned transmission and thickness of each sample. The table is sorted by file name by default but can also be sorted by other fields using the Sort Catalog Panel.

On the CatVSANSTable window, there is now a contextual popup menu for loading data. This is a quick way to load the RAW VSANS data from the selected row. The DIV file or MASK file can also be loaded this way by selecting the correct file. You do not need to click on the filename. A click anywhere on that row will work. (The behavior of the popup always appearing with every click can be rather annoying – simply click anywhere else off the menu to get rid of it).



CatVSANSTable:Filenames,Labels,DateAndTime,Intent,Purpose,Group_ID,Lambda...

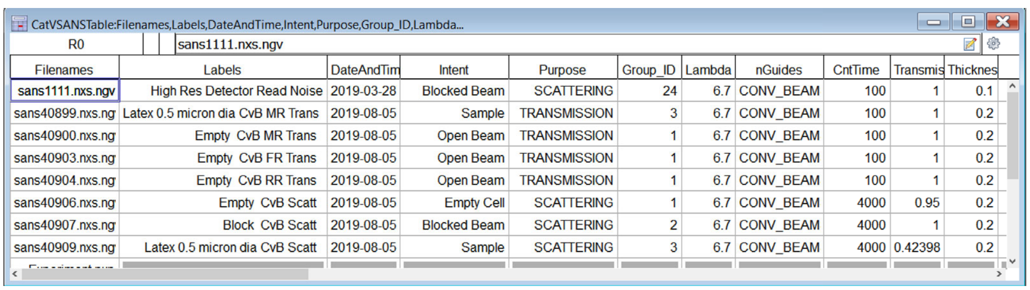
R1 | Ag Beh HOPG NG1 Mid2 Scatt

Filenames	Labels	DateAndTime	Intent	Purpose	Group_ID	Lambd
sans30298.nx	Ag Beh HOPG NG1 Mid Scatt	2019-03-28T1	Sample	SCATTERING	2	4.75
sans30299.nx	Ag Beh HOPG NG1 Mid2 Scatt	2019-03-28T1	Sample	SCATTERING	2	4.75
sans30300.nx	blank HOPG NG1 Mid FR Trar		en Beam	TRANSMISSI(	3	4.75
sans30301.nx	Ag Beh HOPG NG1 Fr Scat		Sample	SCATTERING	2	4.75
sans30302.nx	Ag Beh HOPG NG1 Fr2 Scat		Sample	SCATTERING	2	4.75
sans30303.nx	blank HOPG NG1 Fr FR Trar		en Beam	TRANSMISSI(	3	4.75
sans30304.nx	blank HOPG NG1 Mid MR Trar		en Beam	TRANSMISSI(	3	4.75
sans30305.nx	blank HOPG NG1 Fr2 1m Trans	2019-03-28T2	Open Beam	TRANSMISSI(	3	4.75

Load RAW
Load MSK
Load DIV
Send to MRED

(Load RAW will load file 30299)

Some reduction operations need to access information from the file for identification and grouping. With the larger file size (≈ 4 MB for VSANS vs. 33 KB for SANS), this can be unacceptably slow. To speed things up, information is often read from the file catalog. As more data files are collected, or if header information has been patched, be sure to refresh the file catalog. Before any refresh, a progress bar is shown as the old file information is being cleaned out, and then another progress bar as the refreshed file catalog is generated. Keep in mind that the data files are more than 100x larger than for SANS, so don't expect the file catalog refresh to be instantaneous.



CatVSANSTable:Filenames,Labels,DateAndTime,Intent,Purpose,Group_ID,Lambda...

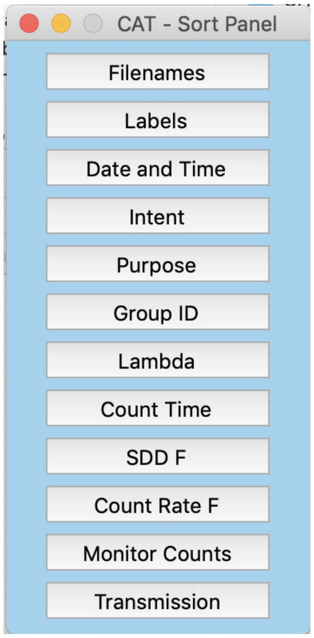
R0 | sans1111.nxs.ngv

Filenames	Labels	DateAndTim	Intent	Purpose	Group_ID	Lambda	nGuides	CntTime	Transmis	Thicknes
sans1111.nxs.ngv	High Res Detector Read Noise	2019-03-28	Blocked Beam	SCATTERING	24	6.7	CONV_BEAM	100	1	0.1
sans40899.nxs.ng	Latex 0.5 micron dia CvB MR Trans	2019-08-05	Sample	TRANSMISSION	3	6.7	CONV_BEAM	100	1	0.2
sans40900.nxs.ng	Empty CvB MR Trans	2019-08-05	Open Beam	TRANSMISSION	1	6.7	CONV_BEAM	100	1	0.2
sans40903.nxs.ng	Empty CvB FR Trans	2019-08-05	Open Beam	TRANSMISSION	1	6.7	CONV_BEAM	100	1	0.2
sans40904.nxs.ng	Empty CvB RR Trans	2019-08-05	Open Beam	TRANSMISSION	1	6.7	CONV_BEAM	100	1	0.2
sans40906.nxs.ng	Empty CvB Scatt	2019-08-05	Empty Cell	SCATTERING	1	6.7	CONV_BEAM	4000	0.95	0.2
sans40907.nxs.ng	Block CvB Scatt	2019-08-05	Blocked Beam	SCATTERING	2	6.7	CONV_BEAM	4000	1	0.2
sans40909.nxs.ng	Latex 0.5 micron dia CvB Scatt	2019-08-05	Sample	SCATTERING	3	6.7	CONV_BEAM	4000	0.42398	0.2

Tutorial -- Proceed to The VSANS Data Display Window

Sort Catalog

From the Raw Data tab on the Main Panel, there is a button for Sort Catalog – this allows sorting of the file catalog by a variety of different fields. This operation is useful for grouping files by intent or group_ID. Sorting by Filenames is the default.



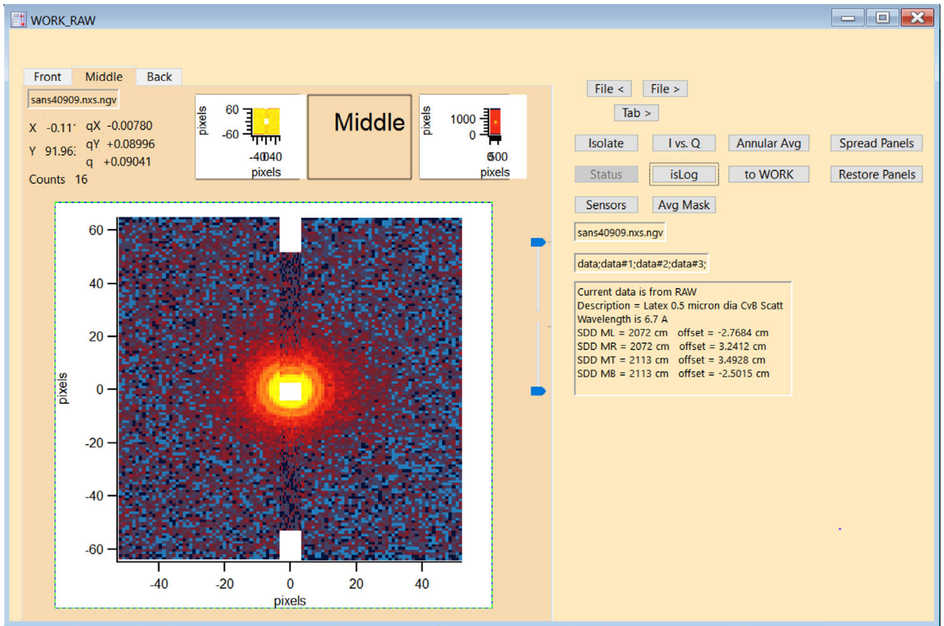
The VSANS Data Display Window

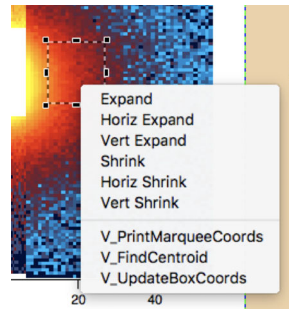
What: This is the main data display for viewing the data from the 9 detector panels. Front, Middle, and Back carriages are displayed separately.

How: Load a RAW VSANS data file by either clicking on "Display Raw Data" in Raw Data tab on the Main VSANS Panel, or select the file from the CatVSANSTable and load it using the popup contextual menu (by clicking on the file row and selecting "Load RAW".

When selected, the data file will be loaded and displayed. In addition to displaying images of the count data for each detector panel, there is also limited status information about the file, counts, cursor position and panel SDD and panel offset. More metadata may be added as needs arise. There are also basic marquee operations to print out box coordinates for summing, finding the centroid of an open beam for beam center values, and updating box coordinates for calculation of transmission.

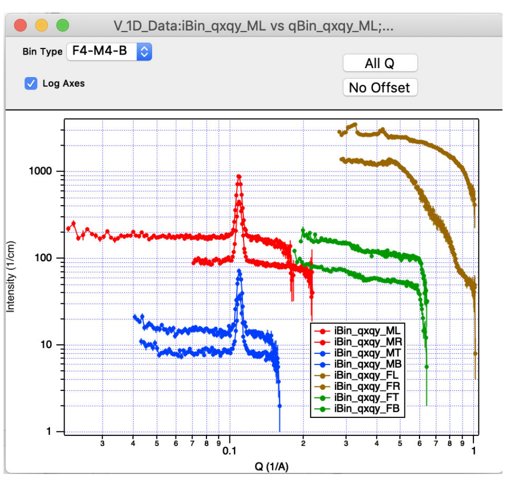
Clicking the tabs “Front – Middle -- Back” or the “Tab >” button scrolls through the detector carriage sets. The display axes for the panel images is “pixels” scaled in relation to the common center of (0,0) and the panel offset value. Pixels are used only for display, and not for any calculations.

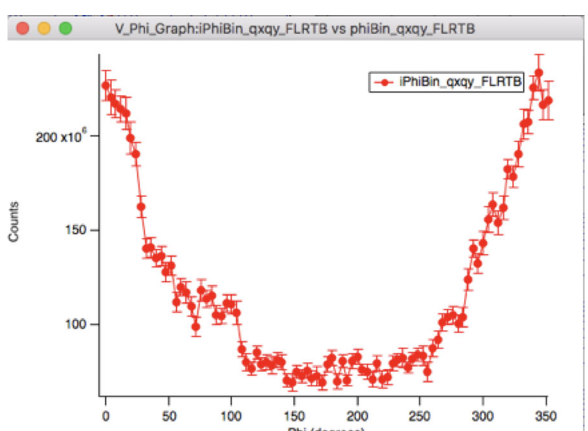




File < and File > -- buttons scroll to the previous / next raw data file, loading data and updating the display.
Tab > -- toggles through the carriage groups.
Isolate – using the current RAW data, opens a new panel to display single panels. Also allows for toggling of detector corrections to see the effect on the data. Allows for closer, individual inspection of each panel.
I vs. Q – plots the data in I(q) representation. Nonlinear corrections are always used, as they are calculated on loading of every data file. For the best representation, a mask file is needed, since much of the T/B panels are obscured and adversely affect the I(q) average. Select the binning type and the new binning is plotted. "B" data is on the actual scale of the data, and other detector groups are offset for easier visualization. See Bin Types for more description.

Annular Avg – will do an annular average, as specified by the dialog (see VSANS Annular Average below for more detail)





To WORK – converts RAW data to a WORK file. Applies the detector corrections and plots the new data. This step is largely for testing but is useful to see how well data overlaps before doing full data reduction.

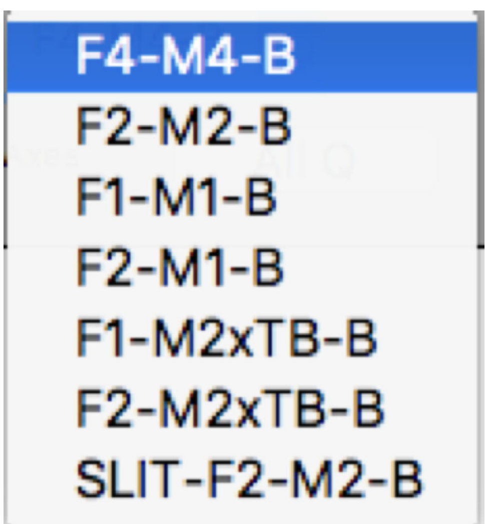
Status – currently inactive, may or may not be kept, as status is automatically updated.
isLog/isLin – as for SANS, toggles the display between log and linear color scaling. The default display preference can be set in the VSANS preferences. Unlike SANS, color scaling is changed entirely on the display. No transformation of the data values is done.
Spread Panels – spreads the panels out so that the T/B panels are a little easier to see. No function other than giving a better view of what is really happening on the T/B panels. The amount of the spread is arbitrary.
Restore Panels—restores the panels to their relative locations based on their offset relative to the common beam center.
Sensors - opens a new panel where the sensor data is displayed for the current data file. Currently only temperature sensor data is stored in the file. Multiple temperatures can be monitored and stored.
AvgMask - opens a panel where the current mask can be overlaid on the current data set. Masks for Sector and Annular averages can be displayed to determine the best input parameters for defining protocols. See Averaging Mask.

All 9 panels are not on a common color scale, but rather scaled as carriage groups. The display is in pixels (images are plotted an even grid). However, given the non-linearity of the detector tubes, all calculations behind the scenes (beam centers, q-values) are carried out using the real space distances corrected for the non-linear effects, which are calculated as the RAW data is loaded.

The two sliders to the right of the detector images adjust the color scale. The Upper slider adjusts the upper limit of the scaling, and the Lower slider adjusts the lower range of the scaling.

Tutorial -- After you have investigated the data display -- Proceed to Averaging Options for VSANS

Bin Types



F4-M4-B = Treat the Front as 4 separate panels (F4), Middle as 4 panels (M4), and Back. I(q) sets are tagged with FL, FR, FT, FB, ML, MR, MT, MB, B
F2-M2-B = Treat the Front as 2 separate panels (F2) pairing T/B and L/R, Middle as 2 panels (M2), and Back. I(q) sets are tagged with FLR, FTB, MLR, MTB, B
F1-M1-B = Treat the Front as 1 panel (F1) combining T/B/L/R, Middle as 1 panel (M1), and Back. I(q) sets are tagged with FLRTB, MLRTB, B
F2-M1-B = Treat the Front as 2 separate panels (F2) pairing T/B and L/R, Middle as 1 panel (M1), and Back. I(q) sets are tagged with FLR, FTB, MLRTB, B
F1-M2xTB-B = Treat the Front as 1 panel (F1) combining T/B/L/R, Middle as 2 panels (M2) but

exclude the T/B pair from the output (xTB), and Back. I(q) sets are tagged with FLRTB, MLR, B

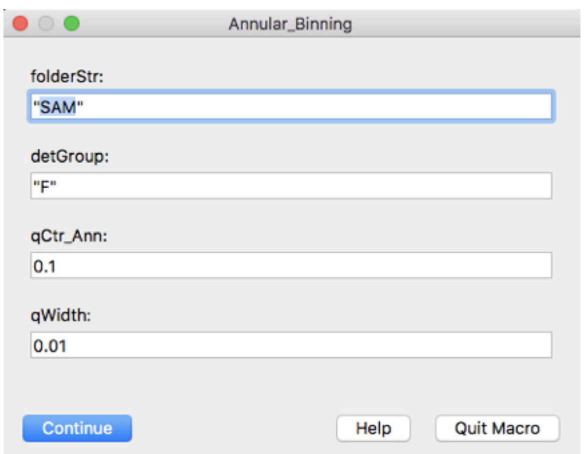
F2-M2xTB-B = Treat the Front as 2 separate panels (F2) pairing T/B and L/R, Middle as 2 panels (M2) but exclude the T/B pair from the output (xTB), and Back. I(q) sets are tagged with FLR, FTB, MLR, B

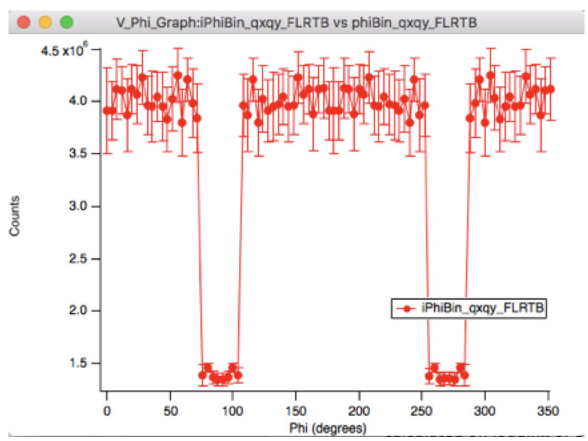
SLIT-F2-M2-B = Treat the Front as 2 separate panels (F2) pairing T/B and L/R, Middle as 2 panels (M2), and Back. In SLIT mode, the T/B detector panels are not useful in this representation since their q-range in the qy direction is far too limited and thus are automatically excluded from the output. I(q) sets are tagged with FLR, FTB, MLR, B

More averaging modes can (and will) be added as needed, and nomenclature may change for clarity. If data has been converted to a work file, then the pixel data is on a per solid angle basis and all the 1D data should overlap (if the trace offset is removed).

VSANS Annular Average

A dialog is presented, to choose the data type, the panel set (carriage), and the q center and delta q (+/-). As with SANS, zero is at the positive x-axis (3 o'clock), and proceeds CCW around the data. The dialog and resulting plot, I(phi) look like:





Note that the "dips" at 90° and 270° are from the different observed count rates on the T/B panels when averaging RAW data. After the solid angle correction, all the pixels are on equal footing and the "dips" should disappear. This definition of delta is different than for SANS, where annular averages were specified in terms of a q center and a number of pixels (+/-) as delta. VSANS uses a q-center and (+/-) qWidth since pixels do not provide a consistent definition.

Averaging Options for VSANS

What: This feature allows you to perform different types of averages on your data, and allows you to see what regions of the detector will contribute to the average. The regions to be included in the averaged data set are shown graphically on the data and can be easily adjusted. The desired numerical vales of pixels, angles, etc. can be used later in reduction protocols.

In addition to choosing the type of averaging, the combination of detector panels that are grouped together during the binning is also chosen.

How: The "I vs Q" button on the Display window will perform a standard circular average of the currently displayed data.

The "Annular Avg" button will perform an VSANS Annular Average based on input ranges

The Averaging Mask panel will open a panel that allows easy visualization of the exact detector regions that contribute to annular, sector, and circular averaged data.

• "Circular" is the default average type. It will perform and average in constant q-rings around the (x,y) pixel location of the beam center. The default bin width is fixed at approximately one pixel width. This bin width can be reset in the VSANS Preferences. Other than the bin width there are no other options to set when doing a circular average.

• "Rectangular" is not yet implemented for VSANS.

• "Sector" is very similar to Circular, except that the angular range around the beam center is limited, specified in degrees (+/- delta phi) each direction from a specified central angle (phi).

• "Sector_PlusMinus" is not yet implemented for VSANS.

• "Annular" will perform an average centered at a single q-value (q-center), and averaged over a width of a specified +/- delta q. The data is returned as a function of angle (phi) in degrees. If a normal x-y coordinate system is drawn through the beam center, zero angle is defined as the positive x-axis and proceeds counter-clockwise. Therefore 270 degrees corresponds to the negative y-axis. The number of angular steps (phi) is set by default to 90 but can be changed in VSANS Preferences.

• "2D ASCII" is not yet implemented for VSANS.

• "QxQy ASCII" saves the currently displayed data in 2D form in a 9 column format, converting each detector pixel into Qx and Qy and its corresponding intensity. This data format cannot be re-read into the VSANS macro set.

• "Narrow Slit" option will averaged the data appropriately for narrow slit collimation. For each vertical tube (L/R panels only) the y-values are summed as the infinite slit approximation integrates over all y-values. Data from the T/B panels does not cover enough of a y-range to be correctly approximated as an infinite slit, so this data is automatically discarded.

The different panel binning options for data sets can be found in the discussion of Bin Types.

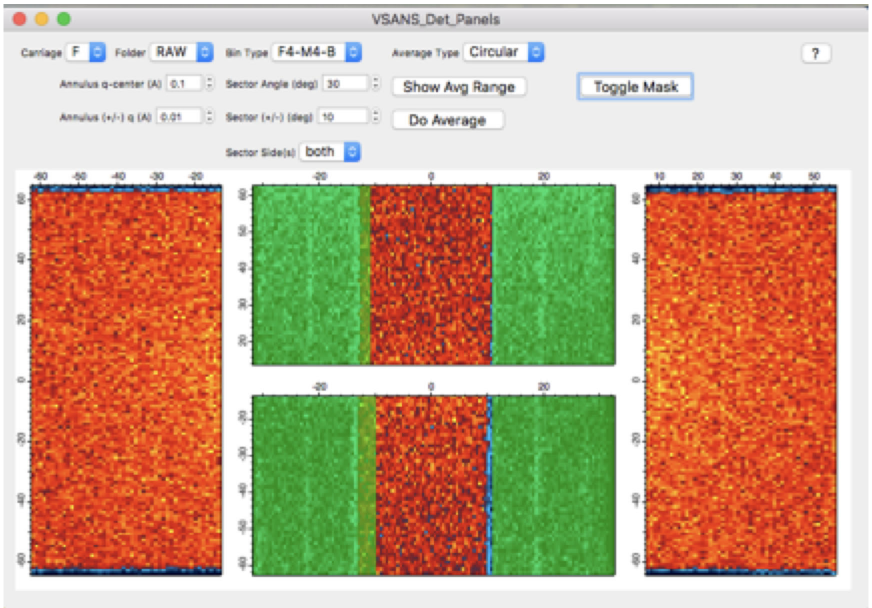
VSANS Annular Average and 2D output as QxQy_ASCII are also available.

Tutorial -- Proceed to Calculate Transmissions in VSANS

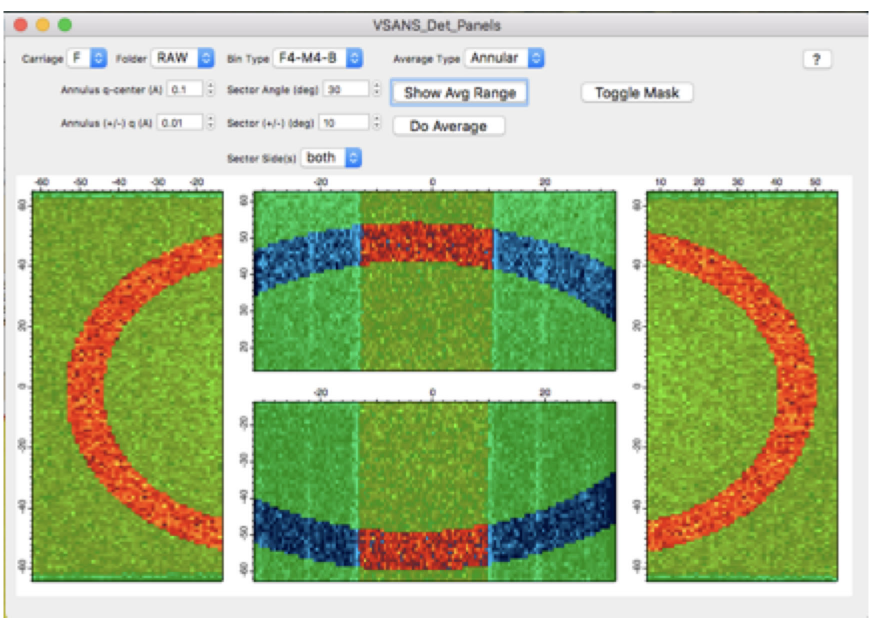
Averaging Mask

This panel shows (1) the extent of the mask as drawn on each of the panels or (2) the regions of the detector that will contribute to the averaged data for various options when selecting annular or sector averages. No drawing is done on this panel for the normal mask file. That is done through a separate panel. This is simply for easier visualization of sector and annular average parameters.

During the data reduction, if the average type is "circular", only the standard mask is applied. If the average type is either "annular" or "sector", then both masks - the standard mask and the defined annulus or sector.



For sector or annular averages, enter the conditions (q-center, angles, sector sides, etc.) and Show Avg Range. A mask will be drawn showing what regions of the detector will be masked out and which will contribute to the averages. You may need to click a few times to toggle the mask on/off. Note that the panels are not to scale, and not scaled relative to each other. Inspect each individually. To average the current data with the selected values, “Do Average”. You do not need to save this mask as part of a protocol. The appropriate mask is drawn and applied to the data based on the numerical input you supply in the averaging options section of the protocol. It is exactly these numbers that you will need to enter there.



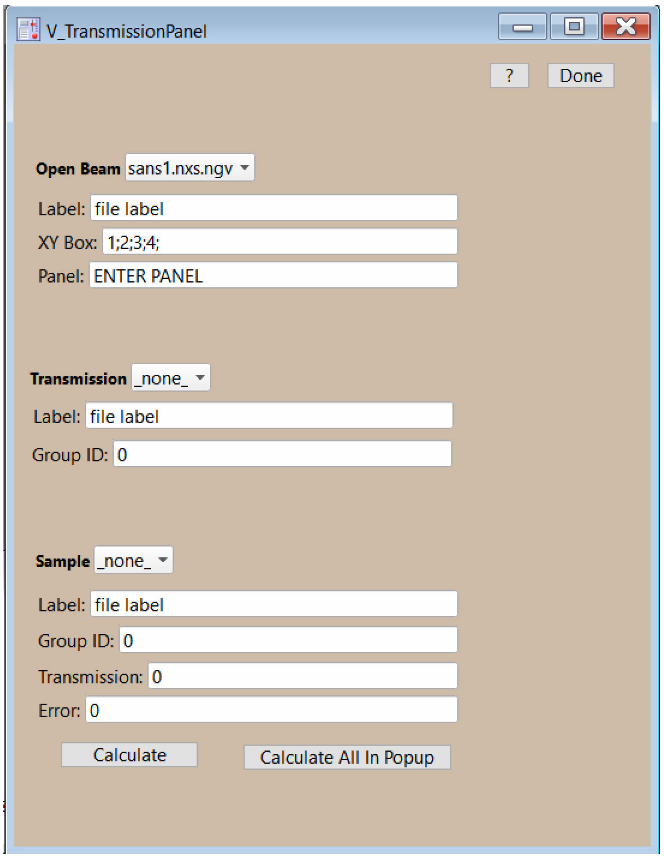
Calculate Transmissions in VSANS

What: Transmission of samples and sample containers must be calculated and entered into the headers of the raw data files for proper subtraction of non-sample scattering during data reduction.

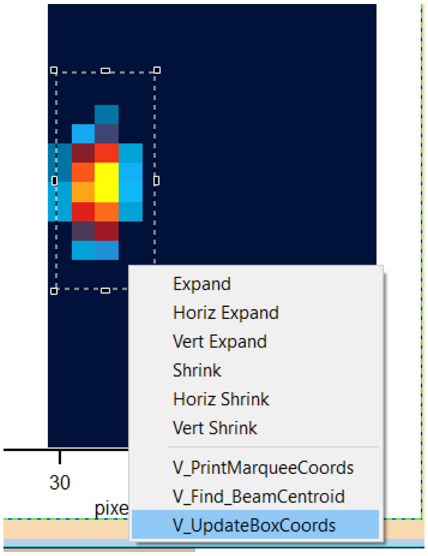
Here we will create the "associations" between the transmission measurements and the scattering files to which they correspond. Transmissions will then be calculated and automatically patched to the file headers.

How: 1) Open the Transmission panel by clicking "Transmission" on the Raw Data tab of the main panel. The following new panel will appear:

The transmission panel for VSANS operates very differently than for SANS. For VSANS, calculating transmission hinges on the correct metadata being present in the VSANS files to make the task of matching up files much easier. These fields are the “intent” and “Group_ID”. These data fields unambiguously identify the intent (as an *Open Beam* file, *Transmission* file, or *Sample* file), rather than having to guess from the file name or depend on user intervention to identify each file at each step of the process.



Begin by selecting an Open Beam file from the first popup. Initially, the Open Beam file will not have the box to sum over set correctly and will not even know which of the 9 panels contains the direct beam. So, to correct this, you will need to manually display the Raw Open Beam file. For the tutorial data, go to the File Catalog and select file sans40900 to load it, then draw a marquee around the direct beam. In this case, the direct beam is on the MR panel and all the sample transmissions have been measured on the MR panel. Finally, use the marquee popup menu to “V_UpdateBoxCoords”. This defines the box coordinates and defines the panel containing the direct beam. These values are automatically patched into the Open Beam file. Re-select this Open Beam file from the popup and the correct values will be present. If not, you may need to refresh the file catalog and re-pop the menu.



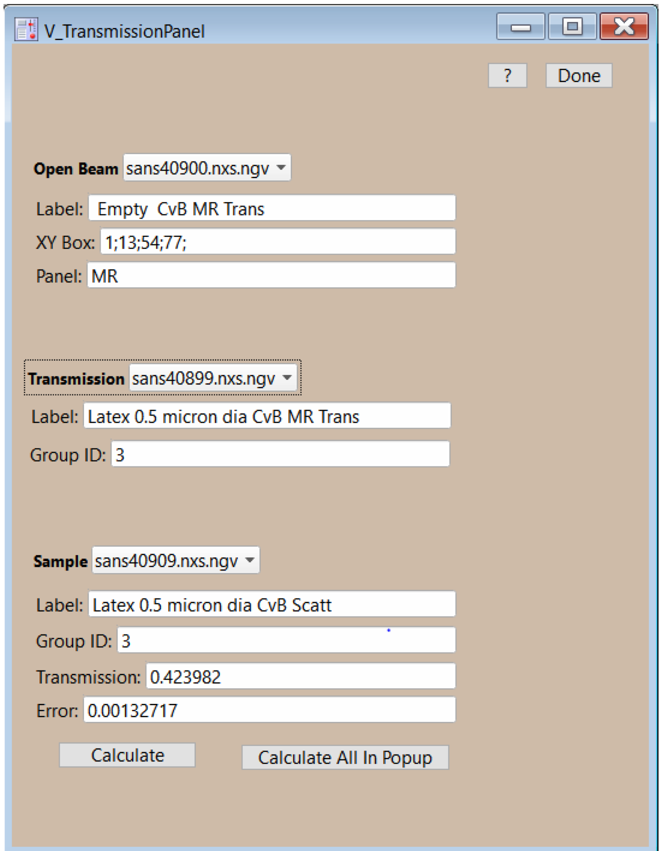
Next, select a transmission file from the second popup. Only sample transmission files taken at a matching configuration to the open beam file will be shown. When the sample transmission file is selected, the label and group_id for the transmission measurement will be updated. The sample scattering file popup menu below will simultaneously update, finding any scattering files with the same group_id. Click (or scroll) through the list of sample files. Clicking “Calculate” will calculate (and patch) the transmission of the top file in the popup. If all the files in the popup are correct, then “Calculate All In Popup” will automatically calculate the transmission for the top file and patch this value to all files in the popup (without wasting time re-calculating the value). As each is calculated, the scattering files are cleared from memory so that the next access will read the new transmission. You will, however, need to manually refresh the File Catalog to see the new values.

* Only files that are "Intent = Open Beam" are listed in the Open Beam Popup.

* Only files that are: "Intent = Sample" and "Purpose = Transmission", match the wavelength, guides, and panel offsets as the Open Beam file will be displayed in the transmission file popup.

* Only files that are: "Intent = Sample" and "Purpose = Scattering", match the Group_ID, and wavelength of the transmission file will be displayed in the Sample file popup.

After selecting a transmission file and calculating the transmission of the automatically located scattering file, the panel shows the results of the calculation:



Repeat the process of selecting the transmission files and calculating the transmissions.

* If files are missing, you will need to check the File Catalog to see why they are missing from the lists. If the file intent was not set correctly at the time of data collection, it can be reset now. See the Nexus File Corrections submenu under the VSANS Menu Items

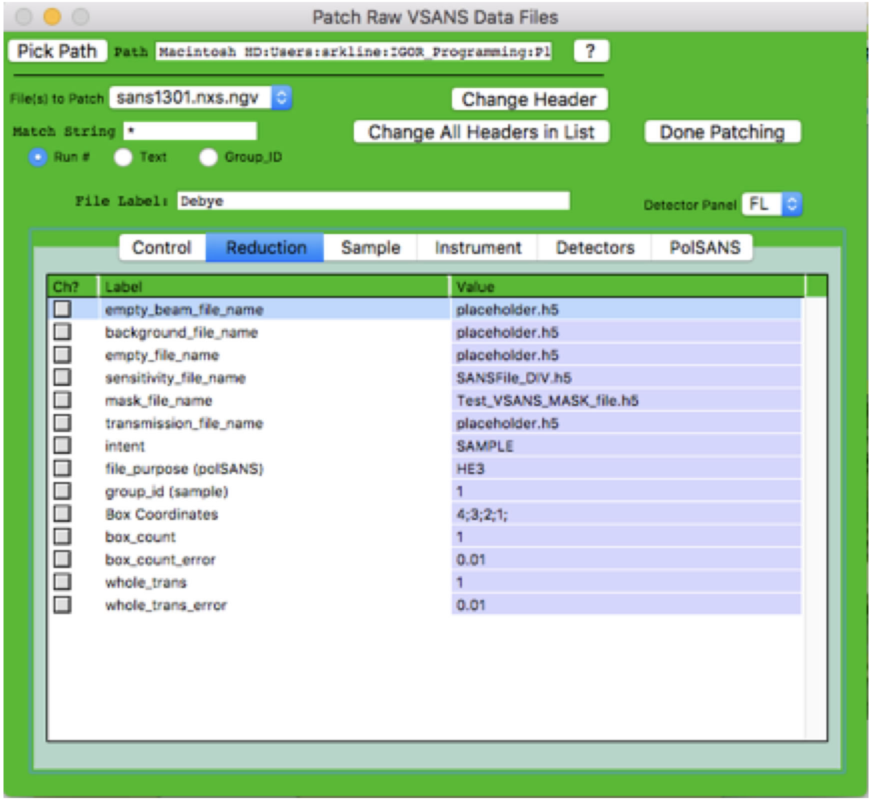
The option of "Total Transmission" as can be done in SANS using the whole detector (=Total Transmission) and compared to the transmission in a small box around q = 0 as a method to estimate multiple scattering has not yet been implemented. The meaning of "whole detector" is somewhat nebulous for the configuration of the VSANS instrument.

Tutorial -- Proceed to Patching VSANS File Headers

Patching VSANS File Headers

What: Some of the information in the file header may have been incorrectly set at the time of data collection and must be updated before data can be correctly reduced. Here we can change header values in the raw data files. Typically, no information needs to be changed here if the beam center values were set correctly at the time of acquisition, and the sample transmissions were calculated in the previous step. If you think he beam centers are not correct or if you want to verify that they are, go to: Calculate VSANS Beam Centers

How: From the Raw Data tab on the main panel, click "Patch". This will display a new panel that can be used to verify and change certain fields in the raw data headers. If the data path is not set, do it now using the "Pick Path" button. The "Match String" field has a single asterisk present. Click into the field and hit <return> to populate the file popup with all the data files.



The main patch panel operates in a similar way to the SANS panel but has been greatly expanded to match the needs of VSANS data files where there is much more metadata.

If, for example, you want to change the sample label, you simply enter the new text into the box, check the "change" box next to it, and click "change header". If the "change" box is not checked, that field cannot be changed in the file header. This feature prevents accidentally changing values you don't intend to change. To patch the same information to a series of data files (like the beam center X and Y) enter the new values and check the "change" boxes. You can use the match string to trim the file popup to include the files that you want to change (you may have to change the files in a few batches to change just the ones you want). Then click "change all headers in list". You will be warned that it will change more than just the top file, and say "yes" to change all the files in the list. Transmissions were calculated previously using the Transmission panel, and should all be correct here.

For more efficient filtering of the files:

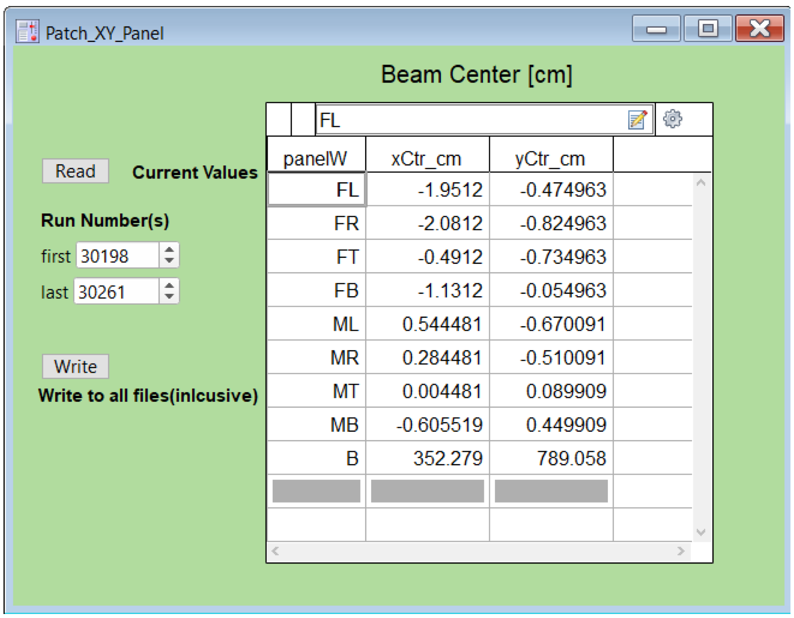
<u>By Run#:</u>
- Enter a list of run numbers (comma delimited) or a range of run numbers specified by a dash.
<u>By Text:</u>
- Enter some text (no wild card needed) and grep will search the entire file for the text match. The file name is also in the file header, so these are searched too.
<u>By Group_ID</u>
- Enter the group_ID to get all matching files.

Note that for VSANS, header changes must be written per tab. If you fill in all the information and switch tabs without saving, that information will be lost. To see the changes, be sure to refresh the catalog listing. The internal Igor folder of RawVSANS data will be cleared when the panel is closed, forcing a re-read from disk the next time data is accessed.

Several additional panels are available for operations where all (or many) of the data files require patching for each of the detector data blocks. These are operations such as defining the beam center, the dead time, or calibration constants. They are available as separate panels called from their respective buttons on the Raw Data Tab - VSANS on the Main VSANS Panel.

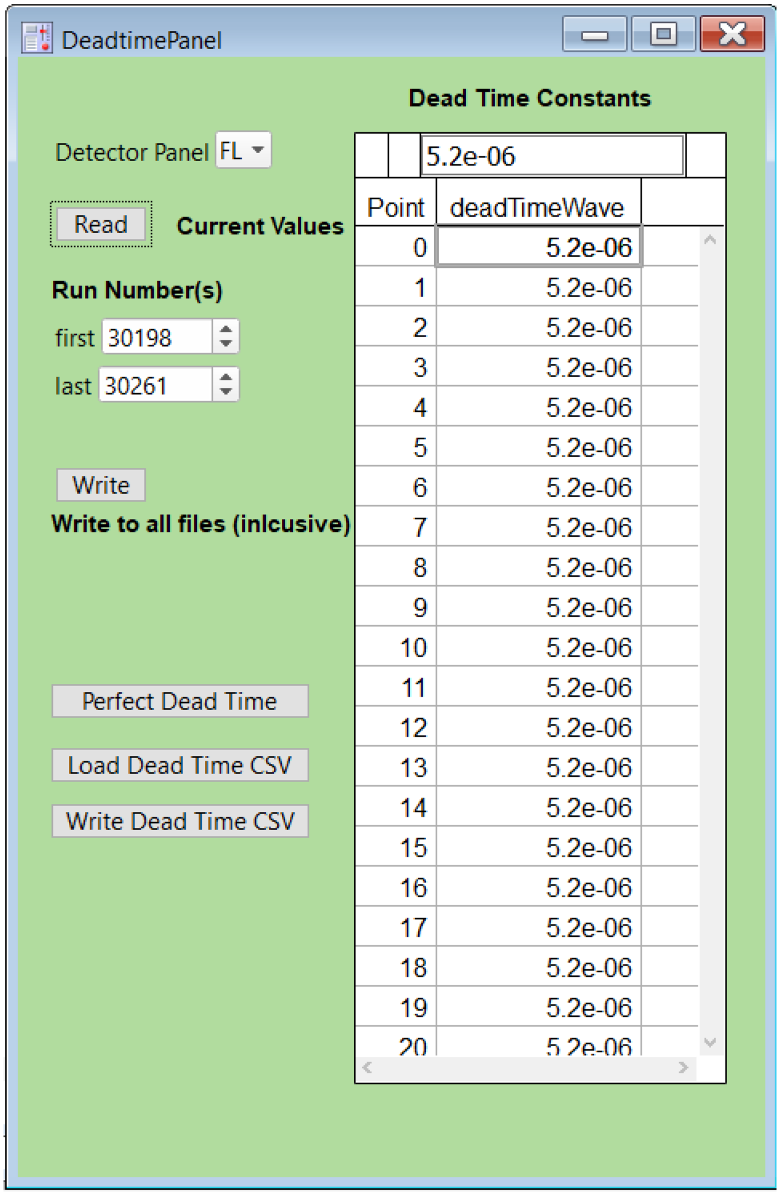
Patch XY

This is a separate panel to allow bulk patching of all (9) of the beam centers to multiple data files at once, rather than one-by-one. The Read button will read the XY center values from the file number listed as “First”. Only that file will be read in. Write - will write the table of beam centers to all the file numbers defined by first and last, inclusive. Missing numbers in the sequence are OK, they will simply be skipped. This panel is most useful to patch all the data files with the correct beam center once the beam centers have been derived from the centroid values.



Patch DeadTime

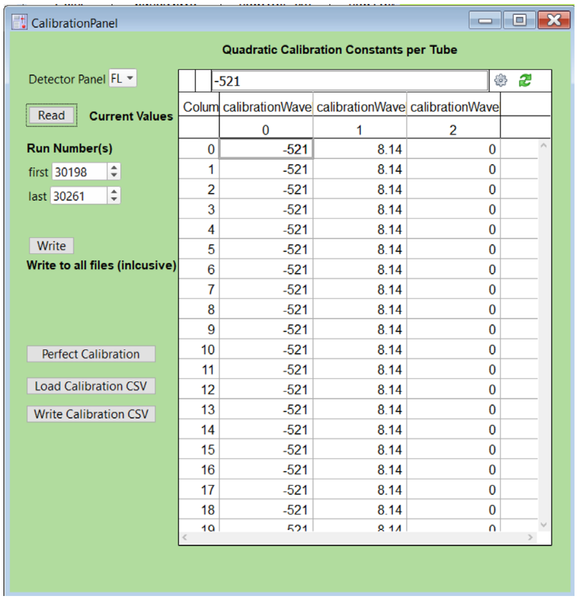
This is a separate panel to allow bulk patching of the dead time for the tube detectors (8 panels) to multiple data files at once, rather than one-by-one. You can read in a “good” set of dead time values from a file, then apply this set to other files, or read in the CSV file of dead time values.
(Sept. 2017: first measurements yielded a dead time of 5.2e-6 s per tube.)



Patch Calib

This is a separate panel to allow bulk patching of the nonlinear calibration values for the tube detectors (8 panels) to multiple data files at once, rather than one-by-one. You can read in a "good" set of calibration values from a file, then apply this set to other files, or read in the CSV file of calibration values.

(Sept. 2017 – As a result of the reasonably good linearity behavior of the tubes, we are using "perfect" calibration values that essentially don't apply any non-linear correction.)



Tutorial -- Proceed to [Draw a Mask for VSANS]

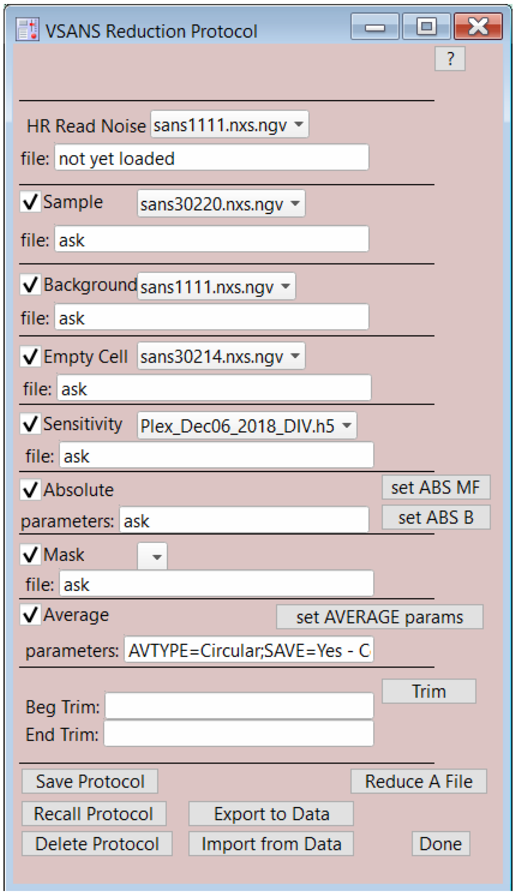
Build a VSANS Data Reduction Protocol

What: Building and saving a protocol allows you to repeatedly reduce raw data files for a given configuration using the same exact sequence of corrections. Here, you can identify the files and steps necessary to correct your data for non-sample scattering, detector sensitivity, convert to absolute scaling, eliminate "bad" detector pixels, and produce output in a variety of formats. Once a protocol is constructed for a specific instrument configuration, it can be saved and recalled for later use. Setting up a reduction protocol for VSANS is similar to SANS, but a bit different in that essentially, only one protocol needs to be set up, and once the data trimming is set up, there should be no need for the separate NSORT step. Reduction should proceed directly from raw data to the final I(q).

How: Click "Build Protocol" on the Data Reduction tab of the main panel. This will present a new panel with a list of reduction steps that can be used. The panel takes a few seconds to open, since in that time it's sorting through all the data files to determine which are sample, background, empty cell, sensitivity, and mask files. In the protocol, steps that are checked will be performed, steps that are not checked will be skipped (except that you will always supply a sample file, or be prompted for one). For this example, we will use nearly all the data reduction steps. Click "Show File Catalog" to bring the listing of files to the top and arrange the windows so the list and the panel are visible.

Before defining a protocol be sure that these steps have been completed:

- Calculate the transmissions
- Verify the beam center for each detector panel has been correctly patched
- Draw a mask (and save the file)
- Use the marquee to update the box coordinates for the open beam file



Any checked steps will be used, unchecked steps will be skipped. Although a file shows in each popup menu, you need to pop the menu to fill the text field below, indicating which file is actually used.

1) If you collected data on the high-resolution (back) detector, there is an additional step to do before reducing the data. The high-resolution detector uses a different neutron detection method than the tube detectors on the other panels. The high-resolution detector data includes "read noise", which is a relatively constant background that is independent of the counting time that must be subtracted from each data file. This can be accomplished by either loading a pre-collected data file containing this read noise data, or if this file has not been loaded, a pre-set constant value will be subtracted from the data. Both methods seem to be equally effective.

-- Pick the High-Resolution Read Noise file by "popping" the HR Read Noise popup. The file: field below initially reads "file not yet loaded". Once the menu is popped, the file is immediately loaded and the loaded file name is listed. This operation only needs to be done once for any and all reduction protocols. This file is "sans1111.nxs.ngv", numbered so that is will not conflict with your data. This file can be obtained from your local contact along with the detector sensitivity file.

2) Pick the Sample File (be sure to pop the menu to fill the field). You can also simply enter a run number here. You can also do this in other fields where a numbered run is appropriate.

sans40909.nxs.ngv is a sample scattering file.

3) Pick the Blocked Beam (background) (pop)

sans40907 is the blocked beam file. (sans1111 is a special file, noted below)

4) Pick the Empty Cell (pop)

sans40906 is the empty cell file.

5) Pick the DIV file (pop)
FMBi_VSANS_DIV_file_12NOV19.h5 is the sensitivity file.

6) Set the ABS parameters:
Using an open beam file is the most common choice and is quite reliable. Only a single open beam is required (either Front or Middle carriage) since the collimation is constant and the geometry is known. However, if you are using the back detector, you *do* need to set a second ABS parameter for that detector, since the detectors use a different method for neutron detection.
You can use file 40900 or 40903 for the scaling of the middle and front carriages, and 40904 for the scaling of the back detector.

7) Pick the MASK (pop)
if you haven't drawn a mask yet, Draw A Mask for VSANS, otherwise you can select it from the popup menu. There's typically only one choice.

8) Set the Average settings
Since there is little data on the MT and MB panels, I have chosen to ignore them, averaging the data as F2-M2xTB-B.

9) Set the trim values – if not set, default values will be used. See the separate instructions for this new step at Combine 1D Files. The number of points to trim from each set needs to be done as part of the data reduction protocol with VSANS, since the data reduction is completed all in one step. There is no need to identify, trim, combine, and sort reduced data from multiple detector distances as in SANS.

10) Reduce a file…
Click the button at the bottom of the protocol panel. Watch as the steps are completed.

11) Save the protocol
If all the steps look correct, and the number of data points trimmed is good, save the protocol.

You can Save/Recall/Delete Protocols. Protocols are kept locally within the Igor experiment to make them available for Multiple Reduce.

Export/Import protocol will write the reduction protocol to a selected data file on disk (to the reduction block). This can be a record of what steps were used to reduce that file. Import will prompt for a file to read a protocol from.

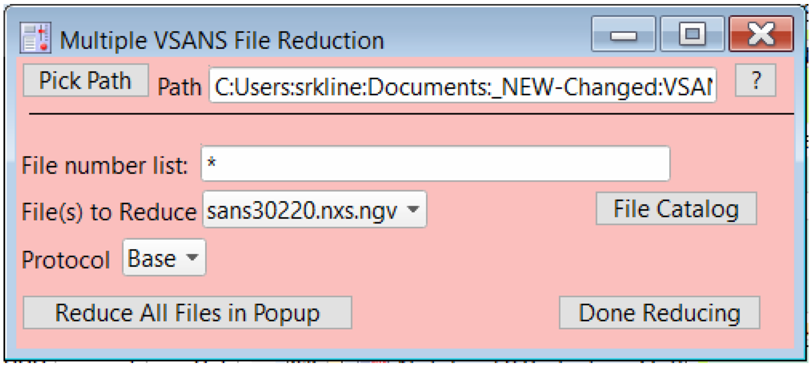
Tutorial -- Proceed to Reduce a VSANS File

Reduce a VSANS File

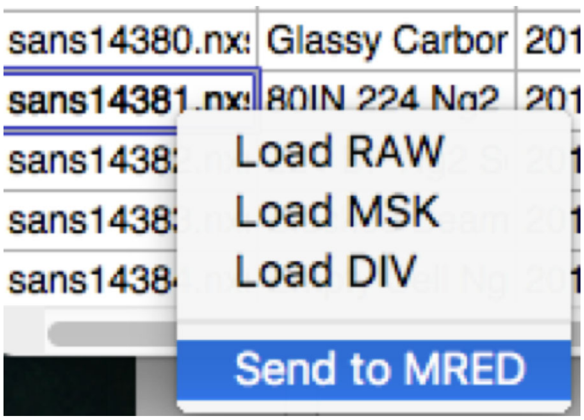
On the Protocol panel, click "Reduce A File". You just did this. How quickly you forget.

Tutorial -- Proceed to Reduce Multiple VSANS Files

Reduce Multiple VSANS Files



Once a protocol has been saved, files can be reduced in batch mode. The file list popup uses a run number list, in the same way as the equivalent panel in SANS. Entering "*" for the list returns all files with "scattering" as the intent.



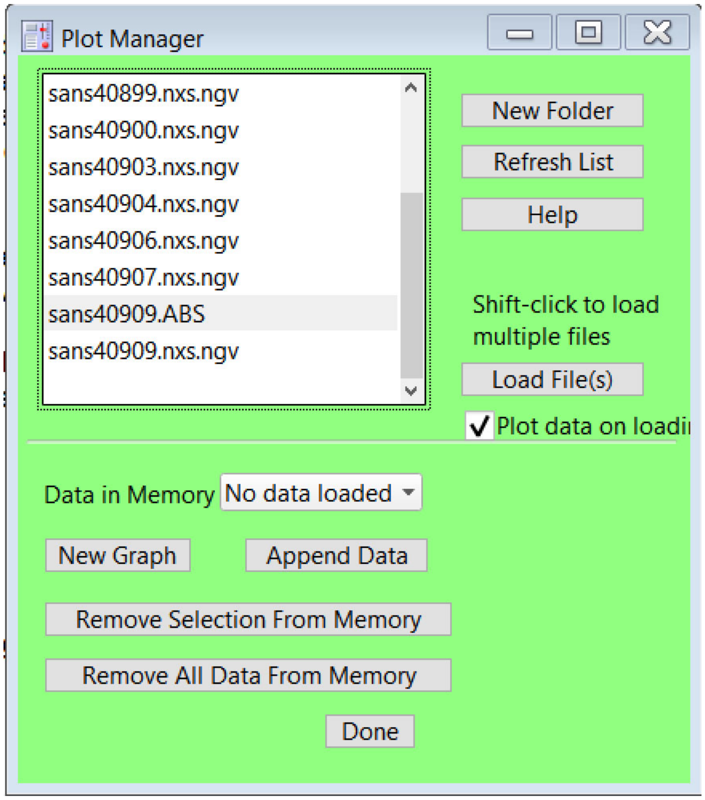
An alternate method to populate the list of files to reduce is to select a file (or group of files) from the file catalog. From the contextual menu, choose "Send to MRED". If the Multiple REDuction panel is open, the selected files will appear in the list and in the popup, ready for reduction. Select a protocol to use and reduce all the files in the popup. Additional files can be added to the list by selecting additional files and "Send" again. Sorting the catalog to group the scattering files is helpful to find everything that needs to be reduced. To clear the list, either triple-click on the list (to select all) and delete the list, or simply close the MRED panel and re-open the panel.

Tutorial -- Proceed to Plot Averaged VSANS Data

Plot Averaged VSANS Data

What: Plots 1-D averaged data files in a nice graph, allowing you to plot multiple datasets on the same graph. No change in functionality from SANS.

How: Click "Plot" on the 1-D Ops tab on the main panel, and the Plot Manager panel will appear

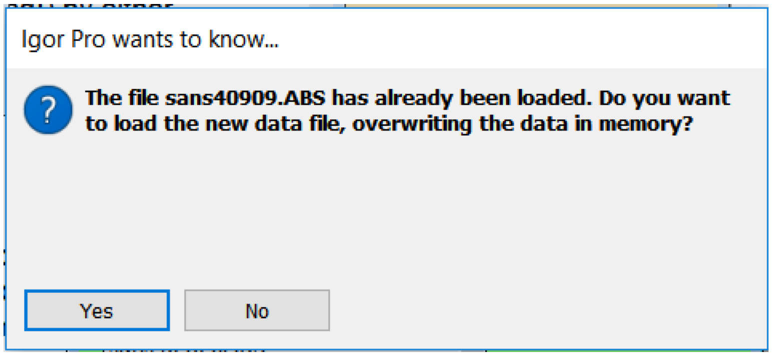


Initially, there is no data loaded in memory, so use "Load File(s)" to load and plot the data that you have reduced. Data placed on absolute scale will have the extension "abs". The listing of data files is from the same data path that you set from the Main Panel. Leave the checkbox selected to automatically graph all the selected files on the same, new graph. Shift-click to select both data files, then "Load Files" to load and graph both data sets on the same plot:

If you don't want all the data on the same graph, uncheck the box, and you will be able to graph and append data as you choose from the Plot Manager Panel. "New Graph" will create a new graph using the data set selected in the popup menu. "Append Data" will do just that to the topmost graph. Unwanted data files in the popup list can be removed from memory (the data on disk is NOT removed!) by either removing the selected file, or all files. Any data that is "in use" in a table or a graph won't be removed and will remain in the popup list. You will have to close (and Kill) any open graphs to then be able to remove the data from memory.

NOTES:

• If you try to load a data set that is already in memory, you will see the dialog below. Clicking yes will load a fresh copy from disk into IGOR's memory. Clicking no will leave the data in memory unchanged. If you know that the data sets are the same, there is no harm in overwriting the data set in memory.

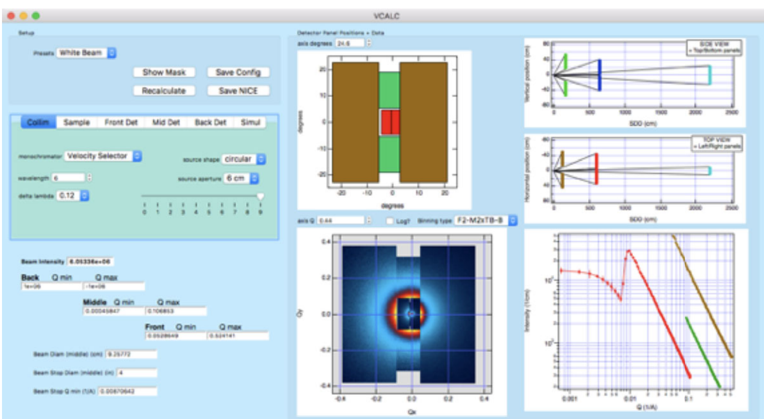


• If you load a data set that was reduced as Narrow Slit data, you will be prompted for a "slope" as it is treating the data as smeared with an infinite slit and is preparing the smearing matrix.

VSANS Experiment Planning Tools

<u>VCALC</u>

The VSANS simulator is currently in progress. Its function is similar to SASCALC.



Features:

Flux, q-ranges, projected beam stop diameter
Views of the detector panels from top/side/sample perspective
Views of the detector in angle and q-space
Averaged data I(q) representative of the real, shadow-corrected output
Masking that accounts for hard and soft shadowing of panels
Separate panel to visualize the extent of shadowing, represented as masks
Multiple collimation presets
Export of configurations to ASCII and NICE formats

Future additions:

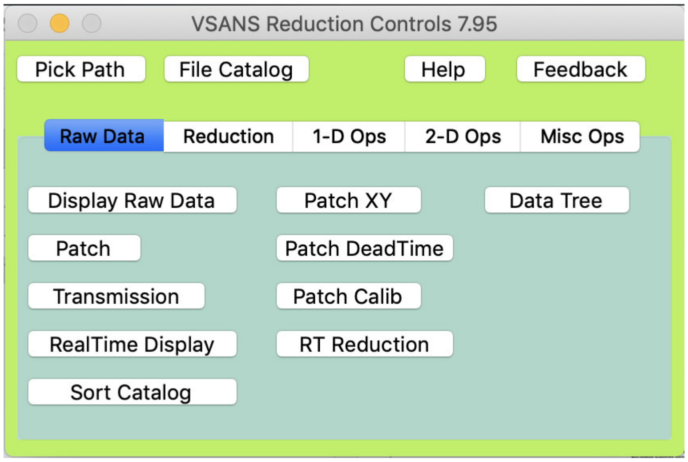
More preset configurations
Save and import of user configurations

Additional VSANS Operations

<u>Main Panel Tabs - VSANS</u>

See: Main VSANS Panel

Raw Data Tab - VSANS



Display Raw Data – presents a standard open file dialog, then loads raw data into the RAW work folder, and displays the data. The only math operation done as raw data is loaded is the non-linear calibration values are used to calculate a matrix of real space distances. This is done so that true q-values can be calculated. The data values are not altered.

Patch: Opens a panel where a large list of metadata fields in the raw VSANS data file headers can be corrected. See: Patching VSANS File Headers

Transmission: Operation to calculate sample transmission and patch the value to file headers for use during data reduction. See: Calculate Transmissions in VSANS

Real Time Display: Operation to display VSANS during data acquisition. Only available within the NCNR. See: Real Time VSANS Data Display

Sort Catalog: Opens a panel where the data catalog can be sorted by different fields rather than the default sort by file name (number). See: Sort Catalog

Patch XY: Opens a panel where the XY beam center for all 9 panels can quickly be patched. Either a single file can be patched, or a range of run numbers can be patched. See: Patch XY

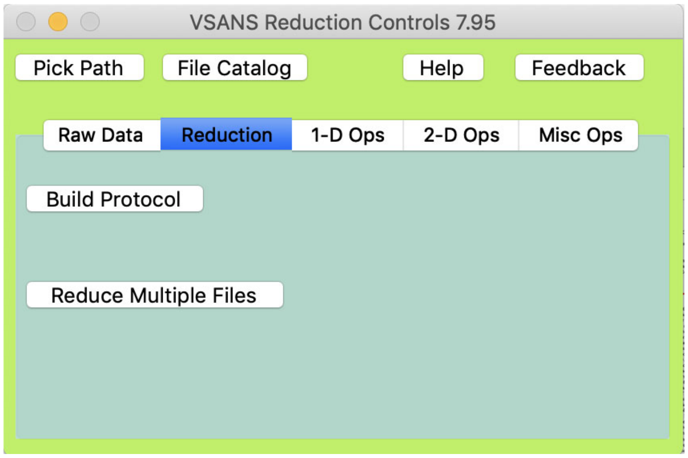
Patch DeadTime: Opens a panel where the dead time constant for all 9 panels can quickly be patched. Either a single file can be patched, or a range of run numbers can be patched. See: Patch DeadTime

Patch Calib: Opens a panel where the non-linear calibration constants for all 9 panels can quickly be patched. Either a single file can be patched, or a range of run numbers can be patched. See: Patch Calib

RT Reduction: Operation that will perform a specified reduction protocol on the Real Time data display to allow visualization of the "final" processed data as more neutron counts are being accumulated. See: Real Time VSANS Data Reduction

Data Tree – not needed for general use, but rather used for troubleshooting the data tree structure as it is read in by Igor / defined by NICE. Gives a quick view of the folder structure and data types.

Reduction Tab - VSANS



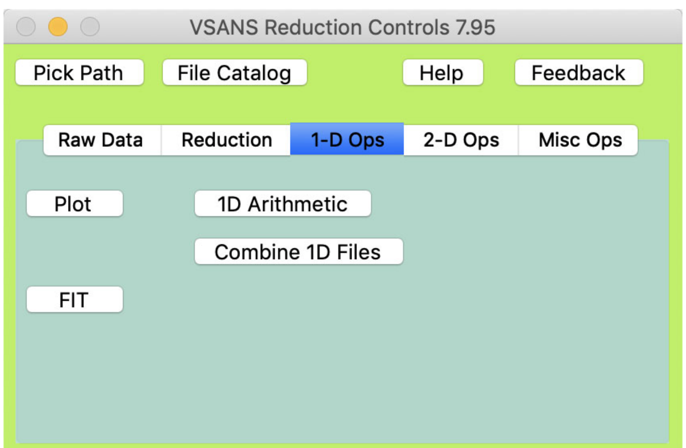
Build Protocol

Opens a panel to set up the steps and files needed for data reduction.
See: Build a VSANS Data Reduction Protocol

Reduce Multiple Files

Opens a panel to allow batch reduction of data files.
See: Reduce Multiple VSANS Files

1-D Ops Tab - VSANS



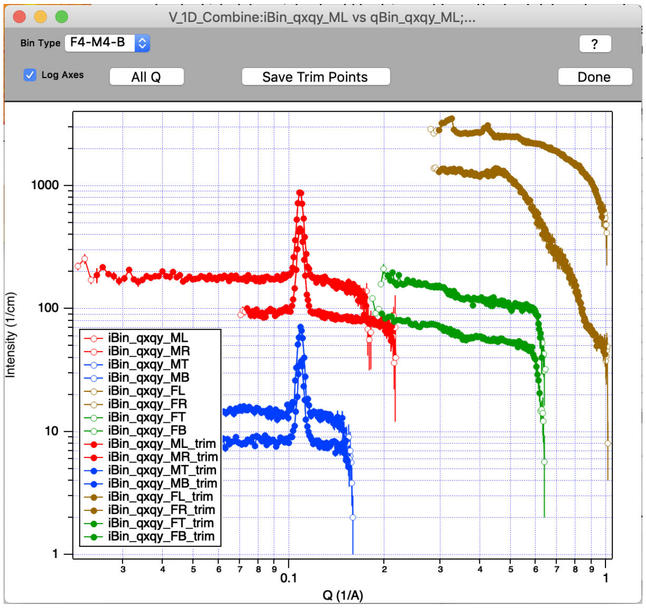
Plot – behaves as usual to load and plot reduced data (.ave, .abs). Plot will not load the individual sets that are saved in ITX format. These ITX files are a temporary format read in manually and is rarely used.

FIT - (to be filled in and linked to the appropriate SANS code)

1D Arithmetic - (to be filled in with SANS code, may be re-written to accept separate VSANS data sets)

Combine 1D Files – A data set reduced to I(q) can be inspected and a judgement can be made about which data points should be trimmed from the final data set, as done in the NSORT function of SANS. For VSANS, this decision is a bit more complex since there are a lot more individual I(q) sets. Also, this information is an integral part of the VSANS reduction protocol, not a separate step as for SANS.

Combine 1D Files



V_TrimPointsTable:PanelNameW,Beg_pts,E

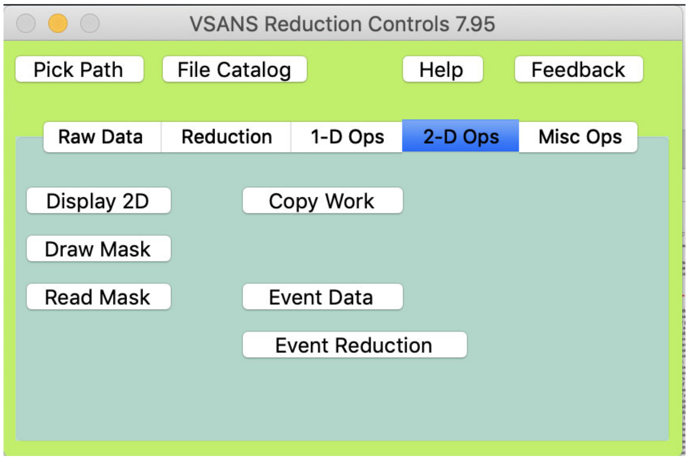
R0 | B

Point	PanelNameW	Beg_pts	End_pts
0	B	5	10
1	FT	6	9
2	FB	6	9
3	FL	6	9
4	FR	6	9
5	MT	6	9
6	MB	6	9
7	ML	6	9
8	MR	6	9
9	FTB	7	8
10	FLR	7	8
11	MTB	7	8
12	MLR	7	8
13	FLRTB	8	7
14	MLRTB	8	7
15			

Steps to use:
(1) Reduce a data set to the desired level. Often simply converting raw data to a work file is sufficient to be able to define what points to trim out. Whatever data file is in the current data display is what will be used as the example for trimming. Using raw data is not recommended since the data has not been corrected for instrument effects or non-sample scattering.
(2) Click “Trim” on the Protocol Panel or “Combine 1D Files” from the main control panel. A graph and table will open.
(3) Select the BinType, and the data is plotted.
(4) In the table of points, enter the number of points to trim from the specified set. Open circles in the plot will be discarded, solid points will be kept. The table and the plot are linked to automatically update.
(5) Zoom, pan, scroll as needed to view the data as you set the points.
(6) “Save Trim Points” will copy the trim values to global strings that can be used in the definition of a reduction protocol. If you adjust the trim values, use “Save Trim Points” again, and the values in the Protocol Panel will update.
(7) Be sure to save the protocol once you have the set of trimming values that you want.

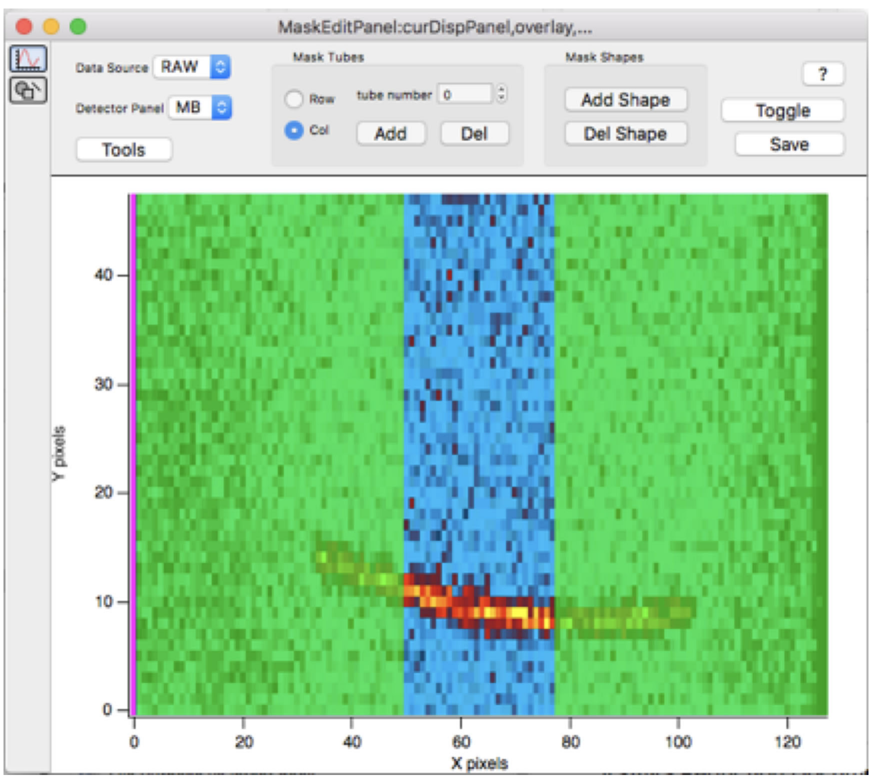
Using a reduction protocol with properly selected trim values is the preferred method for generating and saving a final I(q) data set ready for analysis.

2-D Ops Tab - VSANS



Display 2D – as expected. More work folders will be added to the popup as needed. Currently, MASK files can only be viewed through the Draw Mask operation, and DIV files can only be viewed from the Isolate operation (on the main data display).

Draw Mask - Opens a panel where a mask can be drawn for each of the 9 panels. All 9 masks are saved into a single HDF5 file that has a similar structure as the raw data, but significantly stripped down to only what is necessary to define a mask. Mask drawing operations allow you to mask/unmask individual tubes, or arbitrary shapes. See Draw a Mask for VSANS.



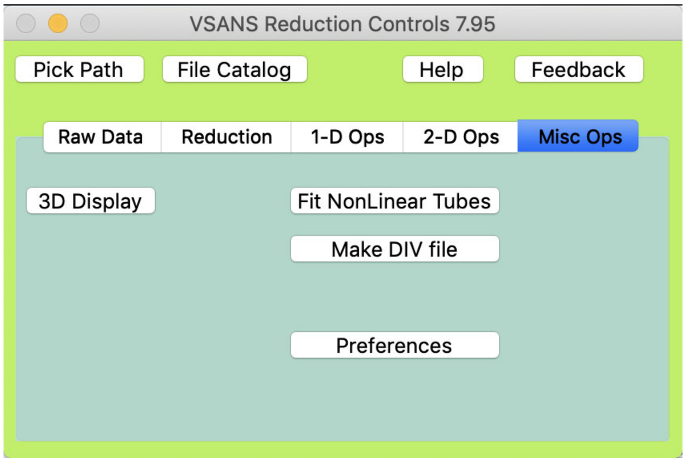
Read Mask – loads in Mask data into the work file. Mask data must be of the HDF5 format as generated from these functions.

Copy Work – as expected. More work folders will be added to the popup as needed.

Event Data – opens up the event mode panel. Panel looks and operates similar to SANS, but all functions are custom for VSANS. More features will be added as needed.

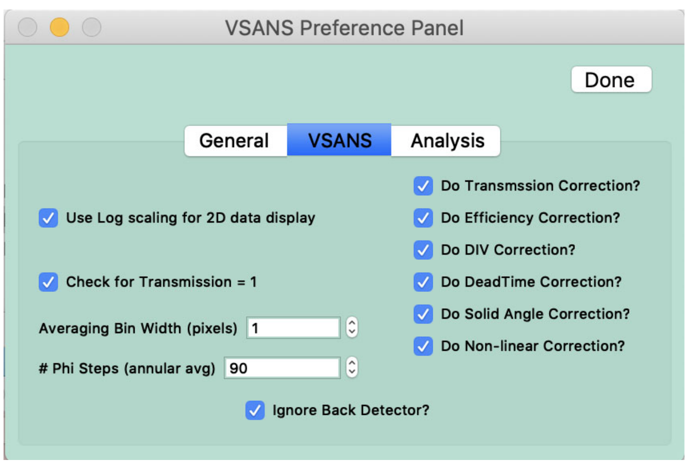
Event Reduction – opens a new panel where event mode data that has been binned and saved can be reduced without generating individual “raw” data files. See Processing VSANS Event Data.

Misc Ops Tab - VSANS



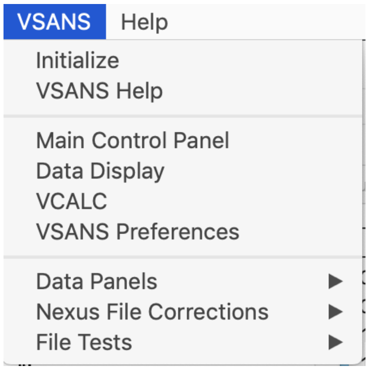
3D Display - (currently not used)
Fit NonLinear Tubes - (see details below)
Make DIV File - (See separate documentation – this operation is typically only performed by an instrument scientist. Users will be given the current DIV file for use in reduction.)
Preferences – Currently used to toggle the different corrections as raw data is converted to a work file. Binning steps is currently active, and non-integer step values are allowed. Note the check box at the bottom to "Ignore Back Detector", which will prevent the "blank" data from the back detector to be written to reduced data files. If the back detector is not used, you do not want this blank data to be written out, or waste time processing the very large panel (number of pixels).

See: VSANS Preferences

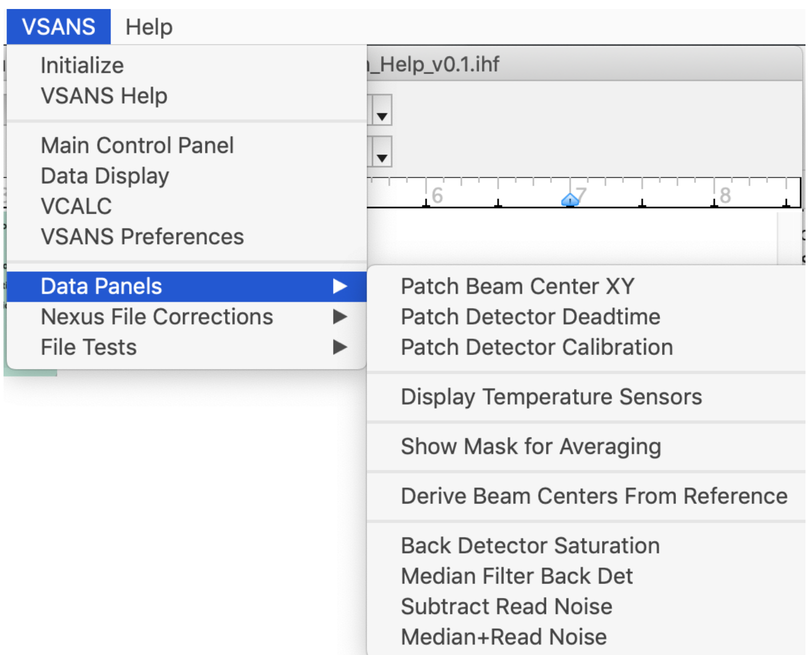


VSANS Menu Items

There are many useful operations on the VSANS Menu. What is described here is likely out-of-date with the current version of the macros. Many of the most useful operations eventually become their own panels and are linked to the appropriate data display. Other new test functions are constantly being added to improve the process of VSANS data reduction.



Initialize - (re)initialize global values and constants.
VSANS Help – link to this help file.
Main Control Panel - bring the main control panel back to the top.
Data Display – brings the RAW data display to the top.
VCALC - initialize and open the VCALC panel.
VSANS Preferences – panel to set various preferences, especially if the back detector is used or ignored.



Data Panels Submenu:

Patch Beam Center XY – brings up panel for batch-wise patching of the beam center.
Patch Detector Deadtime – brings up panel for batch-wise patching of the detector dead time.
Patch Detector Calibration – brings up panel for batch-wise patching of the detector non-linear calibration constants.
Display Temperature Sensors - opens a new panel where the sensor data can be displayed for the current data file. Currently only temperature sensor data is stored in the file. Multiple temperatures can be monitored and stored.
Show Mask for Averaging – brings up a panel that shows averaging options and the associated masks. Masks can be either the shadowing as predicted from VCALC or a mask defined by annular or sector averaging. Unmasked areas are the portions of detector panels that will contribute to the final data sets. See below for more explanation.
Derive Beam Centers From Reference – given the reference beam centers found from centroid measurements, this panel will calculate the beam centers for the other panels, correcting for the

relative panel geometry and variation in the tube zero points.

Back Detector Saturation – for the back (high-resolution) detector, identify if there are any saturated pixels present. If so, report the number of saturated pixels and color them in the detector image as bright green. The data is not actually changed but is colored to highlight if there is an issue with the data file. Currently with the pre-processing of the high-resolution detector, the saturation level is 262384 counts in any individual pixel.

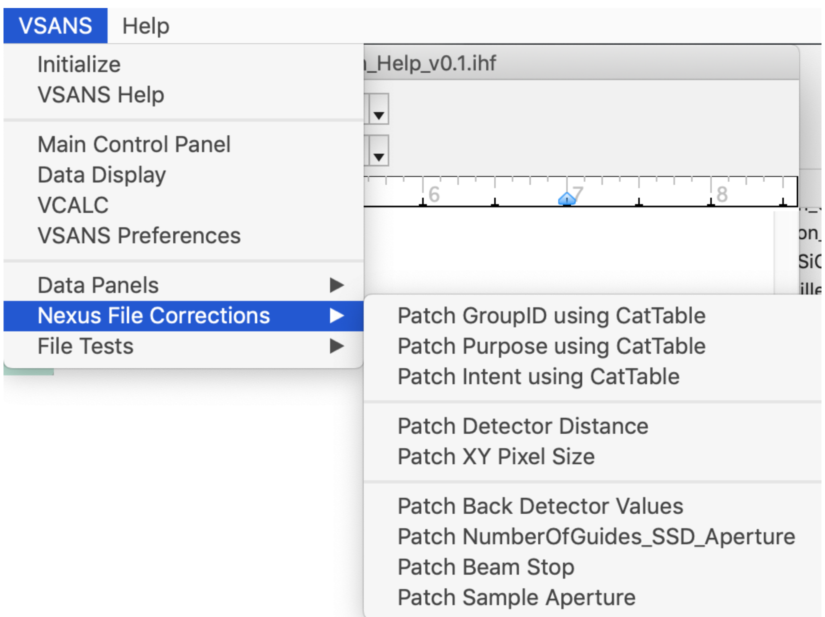
Median Filter Back Det – will apply a median filter to the back detector to reduce noise. Only for testing. Currently all filtering is done during the pre-processing and no filtering is done during the data reduction.

Subtract Read Noise – will subtract a constant value of read noise from the back detector. Currently the constant = 3160 counts and is independent of counting time. This procedure is only for testing. This read noise is automatically subtracted during data reduction.

Median+Read Noise – apply both median filter and read noise subtraction in a single step. Again, only for testing.

Nexus File Corrections Submenu:

This submenu has a growing number of routines that allow patching of the metadata. Most of these fields are critical for automation or for correct reduction of the data. Patching of Group_ID, Purpose, and Intent of files is done in a new way. For these fields, directly update the values in the file catalog and run the appropriate command. Updating the values in the table does nothing, and these values are not written to the file until the command is run.



Patch GroupID using CatTable – writes the Group_ID of files after updated have been made directly to the file catalog.

Patch Purpose using CatTable - writes the Purpose of files after updated have been made directly to the file catalog.

Patch Intent using CatTable - writes the Intent of files after updated have been made directly to the file catalog.

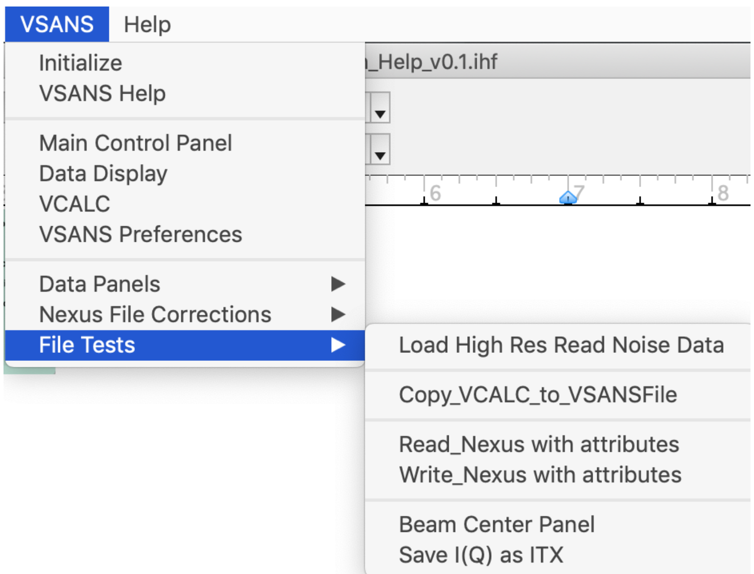
Patch Detector Distance – patches the sample to detector distance (actually gate valve to detector) for all three of the detector carriages.

Patch XY Pixel Size – patches the XY pixel sizes for all the front and middle panels. The back detector is not changed.

Patch Back Detector Values – patches the calibration constants, number of pixels, pixel size, dead time, and nominal (cm) beam center for the back detector panel.

Patch NumberOfGuides_SSD_Aperture – patches the number of guides (or CONV_BEAMS, NARROW_SLITS), source to sample distance (tabulated) and the source aperture diameter. Currently the source aperture is assumed to be circular, but this will be changed in the future to accommodate narrow slit apertures.
Patch Beam Stop – patches the shape and dimensions of the beam stop on either the middle or back carriage. CIRCLE or RECTANGLE shapes can be used.
Patch Sample Aperture – patches the shape and dimensions of the sample aperture (external). CIRCLE or RECTANGLE shapes can be used, filling in the diameter or height+width as appropriate.

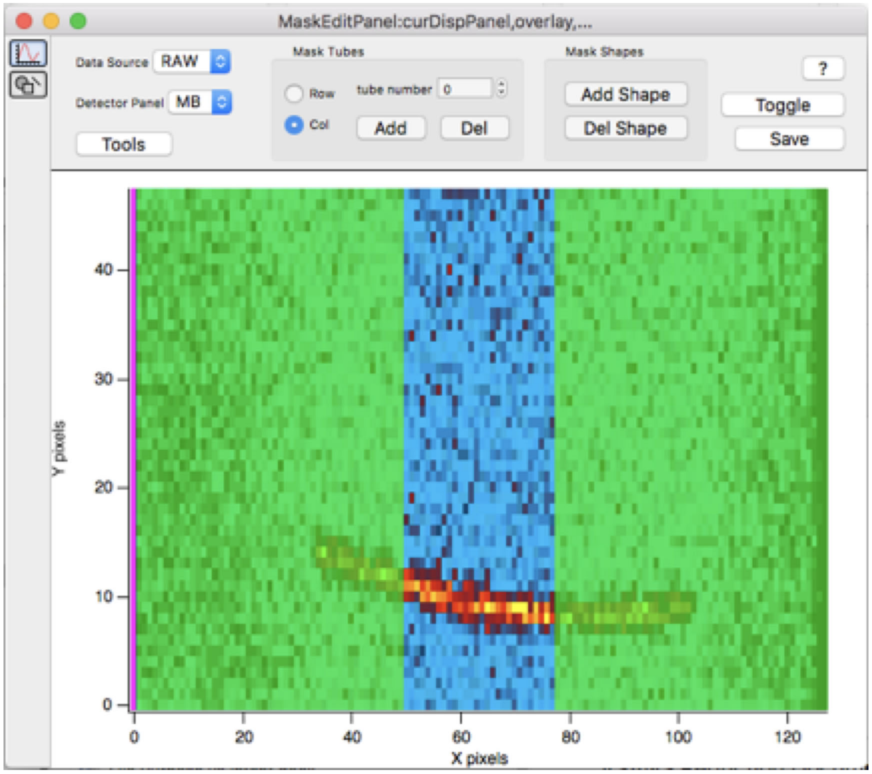
File Tests Submenu:



Load High Res Read Noise Data – Loads in a "Read Noise" data file for the high resolution detector. Used to correct the per-file read noise during data reduction. If this file is not present, a constant value will be subtracted.
Copy_VCALC_to_VSANSFile – Copies the settings and simulated data from a VCALC configuration to a previously duplicated raw VSANS data file. This operation WILL OVERWRITE the detector data and metadata in the file. Before using this, be sure to duplicate a “good” VSANS data file and give it a new (much larger) file number. This is meant only as a testing procedure to make “fake” data for testing.
Read Nexus with Attributes - reads everything in the Nexus file. Slow, but this loads in all the information in the file, including the attributes.
Write Nexus with Attributes - writes everything to a new Nexus file. Writes everything in the folder structure, including attributes.
Beam Center Panel – opens a separate panel where raw data can be fitted to determine the beam center for each panel. Currently, beam center is fitted in pixels and converted to real-space dimensions [cm] for the Front and Middle carriages. The beam center is kept in pixels for the Back detector. More details of beam center corrections are given in a separate document.
Save I(Q) as ITX – a simplistic save of the data that bins the data as specified by the I vs Q panel and saves the data. No trimming, no scaling, just all lumped together. Data is saved in Igor text (ITX) format and cannot be loaded with the usual Plot routines. This format contains multiple I(q) sets and is meant for troubleshooting.

Draw a Mask for VSANS

A mask will always need to be drawn for VSANS, since the panels that are closer to the sample naturally shadow those at longer detector distances. Opening the Draw Mask panel will automatically generate a "default" mask based on the relative geometrical positions of the panels within a carriage, and between the carriages.



To draw a mask:
(1) Open the Draw Mask panel. Either the default mask (automatically generated) will be displayed or the currently loaded mask. Green areas are masked and will not be part of the final data set, transparent areas represent data to be kept. The mask overlay is semi-transparent so that the data can be seen through the mask. You can mask individual tubes (rows or columns) or arbitrary shapes, or any combination. The data displayed is the current data set in the data display window. The log/lin scaling of the data here is set by the VSANS preference, not the current state of the button on the data display window.

<u>To mask tubes:</u>
(2) Choose the Data Source and the Detector Panel, then either “row” or “col” radio button as appropriate for the orientation of the panel.
(3) L/R arrow keys will move the (pink) cursor line, no matter which orientation (row/col) is selected. “Add” will turn the line under the cursor green, “adding” it to the mask. “Del” will delete it from the mask. Up/Down arrows will Add/Delete from the mask, respectively. (This method of control may be kept/removed/altered)

<u>To mask shapes</u>:
(4) Click on the “shapes” in the top left to enter “draw mode”. Draw the shape(s) that you want to mask (or unmask).
(5) Click on the “graph” in the top left to return to “operate mode”. The buttons are now active. Click on either Add Shape or Del Shape. The mask will be updated and the shapes you drew cleared.
(6) “Toggle” will toggle the mask on/off from the view.
(7) Continue masking all the different panels. If the panel is kept open, you can return to any panel as needed to continue editing. Once done, click “save” to save the mask file. The mask for all 9 panels will

be saved in a single file.

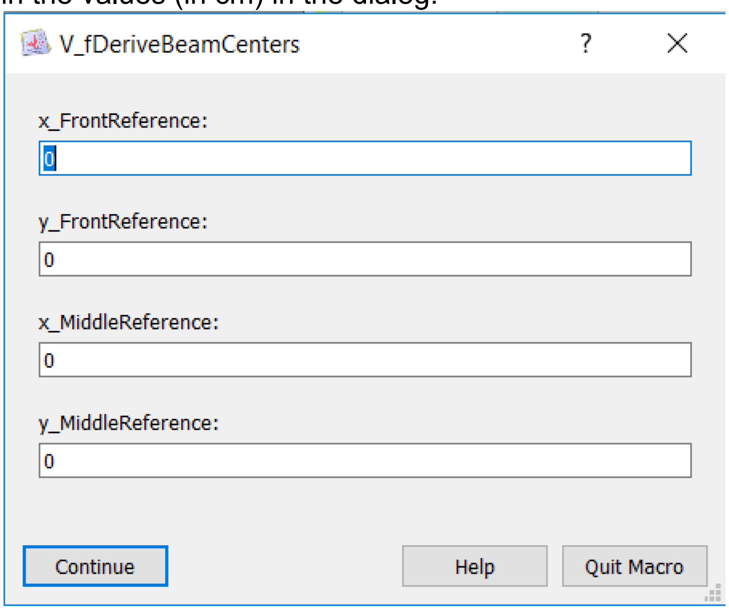
Calculate VSANS Beam Centers

For VSANS, each of the 9 detector panels will have its own associated beam center value. During data collection, the direct beam will not be on most of the detector panels. To determine the beam centers for the four panels on the front carriage, one of the panels (L or R) is offset laterally so that it catches the direct beam. The "beam center" for this offset configuration is determined from the Marquee Operation "V_Find_BeamCentroid" and converted to a "Reference Beam Center". The reference beam center (x,y) is written to the command window. Note these values. Then repeat this process for the Middle carriage and Back carriage. The reference centers for front and middle are reported in units of [cm]. The back, high-resolution detector has its beam center defined in pixels.

Then with the reference beam centers for front and middle in hand, select the following option from the VSANS menu:

VSANS->Data Panels->Derive Beam Centers From Reference

and fill in the values (in cm) in the dialog:



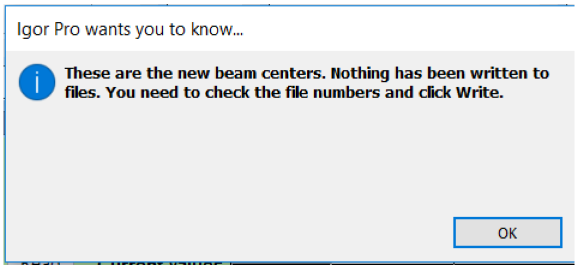
The result of the calculation is a table of beam centers for each panel. Be sure to enter the values for the beam center for the Back detector into the table (in pixels).

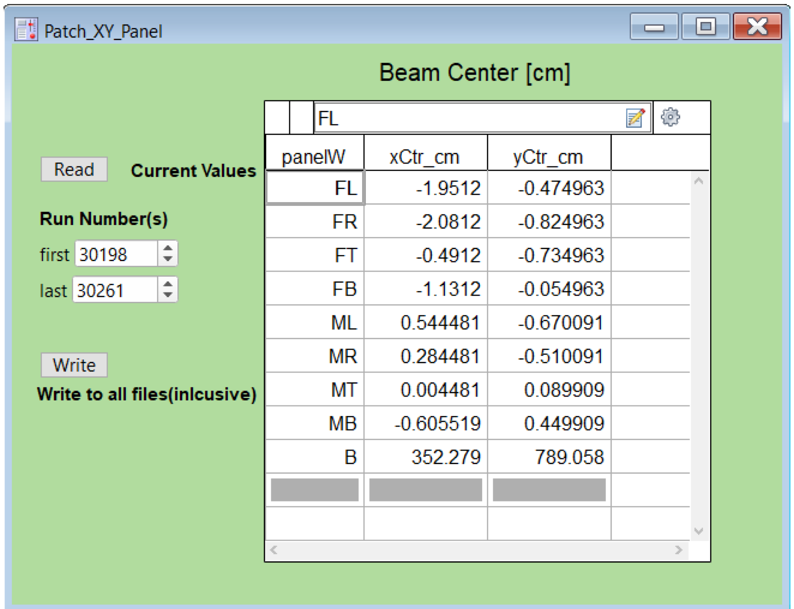
The last step is to patch all these values into the file headers. Do this by clicking on the "Patch XY" button on the Raw Data tab on the Main VSANS Panel. This brings up a new panel where these beam centers can be copied, and then written to a range of run numbers (default is all data files).

Alternatively, once the centroid has been calculated for each of the carriages using the marquee option, you can choose from the VSANS Menu:
VSANS menu:

VSANS->Data Panels->Derive Beam Centers From Open Beam Files

This presents dialogs to select all three open beam files (the back panel will be ignored if you're not using it), and the beam centers are all calculated. Then proceed with patching all the beam centers using the "Patch XY" panel as above.



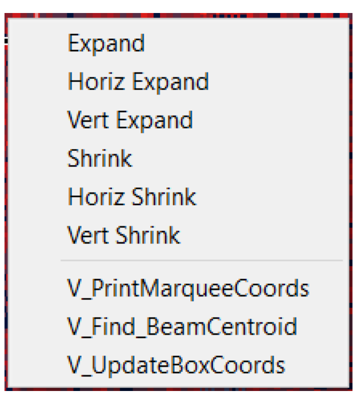


Tutorial -- Return to Patching VSANS File Headers

Marquee Operations in VSANS

What: The marquee menu, invoked from a marquee selection on the VSANS Data Display provides several operations.

How: Click and drag a marquee region in the VSANS Data Display window. Then move the cursor inside the selection (to get an upside-down hat cursor) and click to get a new menu:



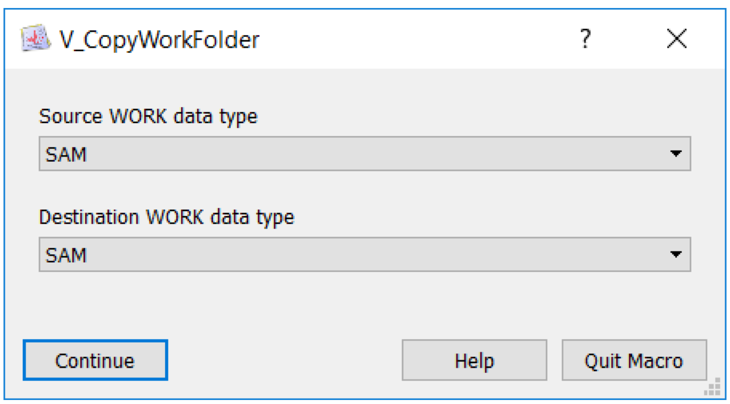
The operations are:

V_PrintMarqueeCoords: prints the (X,Y) extent of the selection in terms of pixel coordinates, and prints the total number of counts, and the average number of counts in the selected region.
V_FindBeamCentroid: reports the centroid (intensity-weighted) of the selected region. Calculates the centroid in pixels and in real-space distances. Reports the beam center in terms of the reference beam center for the current carriage that is needed for calculation of the other three beam centers on the carriage. Writes the reference beam center to the reduction block of the data file for future use.
V_UpdateBoxCoords: writes the selected box coordinates to the reduction block of the data file for use in calculation of the transmission. Also writes a string representing the carriage+panel where the open beam is located.

Copy VSANS Work Folder Contents

What: This operation duplicates the contents of any data folder into another folder. It is often useful to keep a fresh copy of a 2-D dataset when performing math operations on 2-D data.

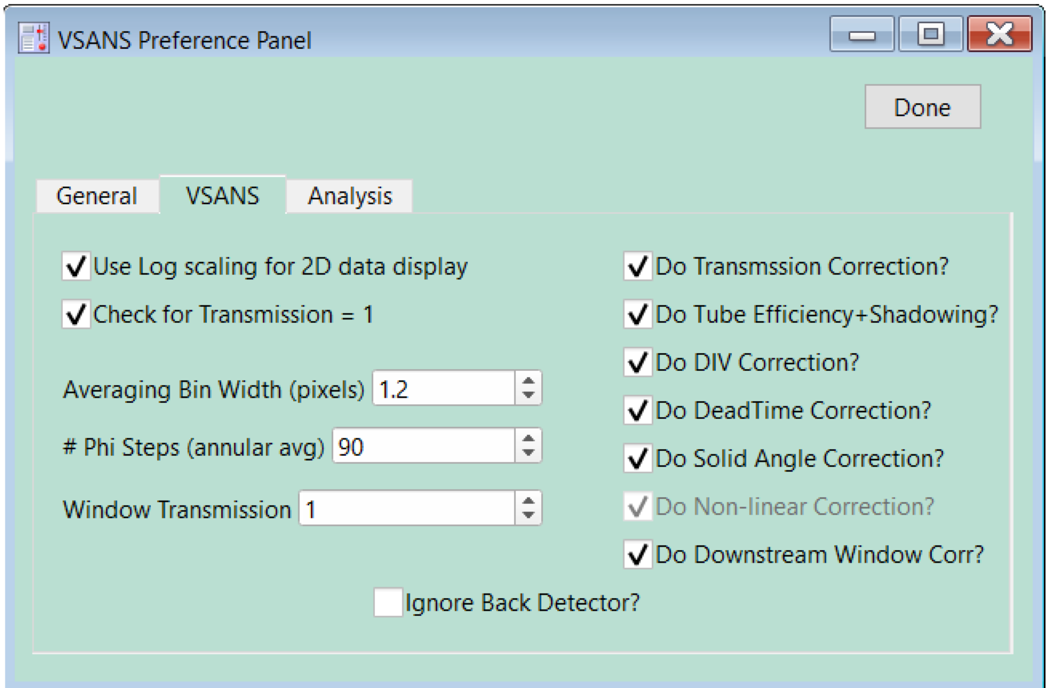
How: Click the "Copy Work" button on the 2-D Ops button on the main panel. You will be presented with the following dialog, prompting you for the source and destination data folders. Data in the destination folder will be overwritten, and you will not be warned. You can view the new contents of the destination folder by choosing "2D Display" on the same tab of the main panel.



VSANS Preferences

What: Set a few display and averaging preferences, and control which data corrections are applied.

How: From the Misc Ops Tab on the Main VSANS Panel, click on "Preferences", or by selecting the item "VSANS Preferences" from the VSANS Menu. The values shown in the panel are the default values. The default values can be reset by selecting "Initialize" from the SANS Menu.

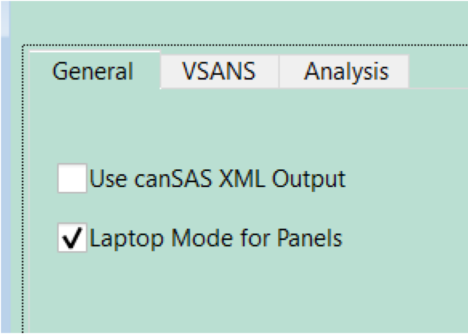


Most of the important settings are on the VSANS tab:

- Use Log scaling for 2D data display: This sets the default view for the VSANS data display.
- Check for Transmission = 1: checks during reduction if the sample transmission is 1, which may be an indication that the transmissions have not properly been calculated.
- Averaging Bin Width (pixels): the bin width is set in q-space as the width of a single tube on a panel. This is set to a slightly larger multiple of a tube width to avoid artifacts in the reduced data when combining data from multiple panels.
- # Phi Steps (annular average): this sets the number of angular bins used when performing an annular average. The default number of bins is 90.
- Window Transmission: this field sets the total transmission of all of the windows that are downstream of the sample. Talk to your local contact about this value. The default value is 1, meaning that there are no transmission losses. In the future, this value may be stored in the data header.

The following are flags that toggle different corrections on/off. The default (and correct) choice is to have all of these corrections applied to the data sets. However, there may be some non-standard experiments or testing conditions where these corrections may be temporarily turned off. Be sure to turn them back on when done!
- Do Transmission Correction?: the angle dependent sample transmission correction
- Do Tube Efficiency+Shadowing?: the angle dependent tube efficiency and the angle dependent tube shadowing correction. These are technically two separate corrections, but they are calculated together.
- Do DIV Correction?: the detector sensitivity correction (note that turning the correction off here supersedes any choice made in the data reduction protocol)
- Do DeadTime Correction?: the per-tube dead time correction.
- Do Solid Angle Correction?: the solid angle correction per pixel.
- Do Non-linear Correction?: the non-linear corrections per tube (this can't be turned off)
- Do Downstream Window Corr?: the angle dependent downstream window transmission correction.

- Ignore Back Detector?: this flag tells the reduction to ignore the high-resolution detector. If you did not collect data using the high-resolution detector, be sure that this box is checked. Ignoring the back detector will provide a significant speedup during processing and will also prevent null data from the back detector being written to reduced data files.



There are two settings on the General Tab:

- Use canSAS XML output. Checking this box will write out reduced data in the canSAS XML output format if the XOP has been installed. Leaving this unchecked is the default, standard NCNR ASCII output style.
- Laptop Mode for Panels: this will draw smaller panels that can be easier to work with on the small screen of a laptop. This selection can be toggled at any time.

There are currently no settings for VSANS on the Analysis tab.

3D Display of VSANS Data

This can be done through Igor's built-in functionality "Gizmo". Simply right-click on the panel you'd like to have a 3D plot and choose "3D surface from data". The plot and the Gizmo controls will appear, and can be modified as you wish. There are a plethora of viewing options that are available as well as needs for viewing data that I cannot anticipate. Gizmo help is available within Igor's Help menu, or discuss this with your local contact.

VSANS Detector Sensitivity Files

This operation is for instrument scientists to generate a detector sensitivity file for use in data reduction. Each detector panel is normalized individually and saved into a single file in the same format as the raw data files.

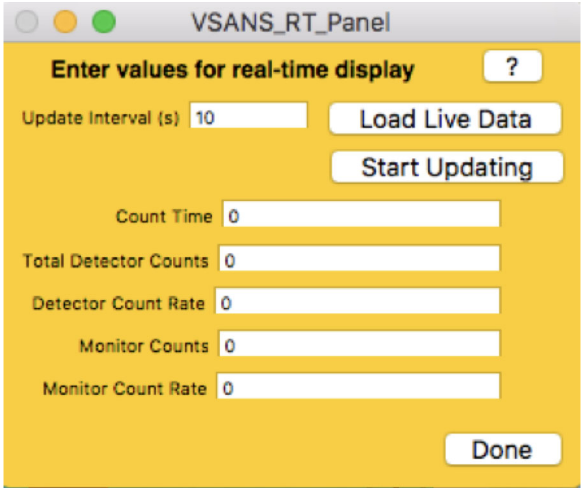
See your local contact for the latest copy of the detector sensitivity file. If your experiment used the back (high-resolution) detector, be sure that the sensitivity file includes this detector. The sensitivity of the back detector is not measured as frequently as the other carriages, so the file may be not as recent as expected. As such, we have not yet seen any significant time dependence of the sensitivity of any of the detector panels.

Real Time VSANS Data Display

This is the usual RT display as in SANS. Pick the periodically updated file from NICE that is stored at:

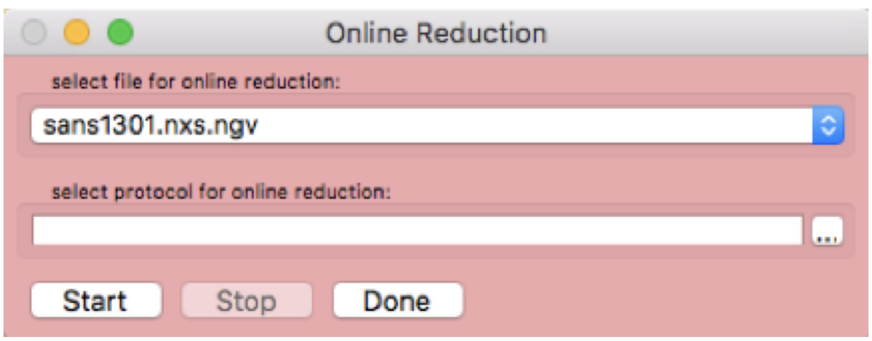
charlotte.ncnr.nist.gov/Sans Data/VSANSCurrent/vsans1.nxs.ngv

This file is updated at an ≈ 5s interval, and the update will display the file and vitals. Start/stop as needed. Note that this operation and the Real Time VSANS Data Reduction are available only within the NCNR.



Real Time VSANS Data Reduction

With a defined reduction protocol, this will periodically load the RT data (again, from charlotte), and reduce the data (you may not want to have "save" as the last step – or maybe you do? to get "simple" kinetic data?). If backgrounds have been collected, this will give a true view of what the final data set will be. It may also prove useful to smooth out non-linear and sensitivity effects, or at least convert to a WORK file so that the solid angle per pixel correction is calculated and the averaged data will overlap. The timing of the refresh period may need some adjustment if there are network speed issues.



VSANS Event Mode

Updated MAR 2021 SRK

[Processing VSANS Event Data]

VSANS event mode data is neutron scattering data that is collected in a mode where every neutron event is recorded with its XY position, detector panel, and its arrival time. This results in a file that is a stream of events, each an encoded 64-bit binary word. This package allows processing of the event stream into any number of time bins, spaced as needed for the experiment conditions.

In VSANS, there are two event files associated with each raw VSANS file, one for the Front carriage and one for the Middle. The Back (high-res) detector does not support event data collection. Each event file contains data from all four panels on a given carriage, stored in an interleaved fashion. Both filenames are stored in the raw VSANS data files, making data processing more convenient.

Other useful operations for event processing:

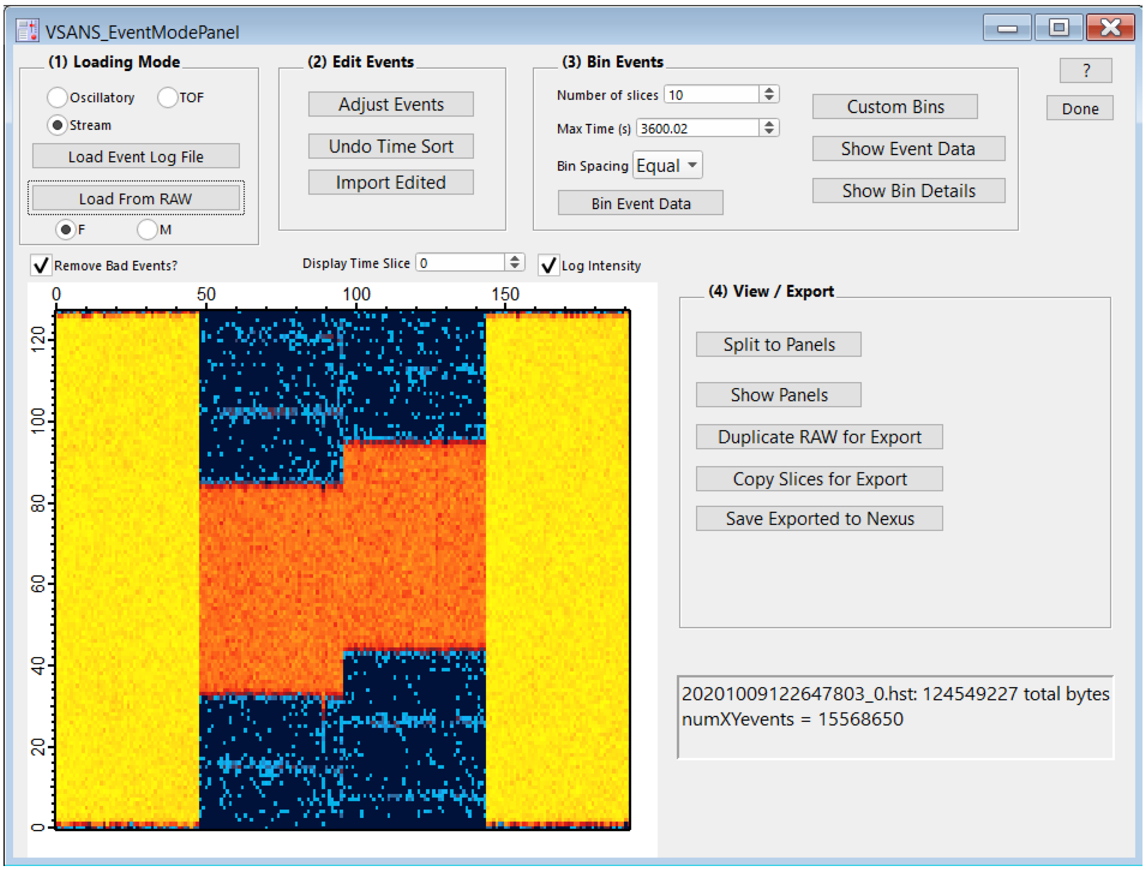
Correcting Errors in VSANS Event Data

Types of VSANS Event Data

Setting up Custom Bin Widths - VSANS

Reducing VSANS Event Data

Processing of VSANS Event Data:



Processing VSANS Event Data

To start, from the VSANS control panel, choose 2D Ops -> Event Data
The processing steps generally flow as the sections in the panel are numbered:

(1) Loading Mode
Using the radio buttons, select the "mode" of the data you have collected. This will set how the data is processed and presented. With the proper mode selected, click either

-- Load Event Log File: to load the XY neutron events versus time for processing. Select the raw ".hst" event file. If you are attempting to load previously edited event data, skip to "Import Edited" in the next section.
-- Load from RAW: This is the preferred method, and based on the currently loaded RAW VSANS file and the (F) or (M) radio buttons - the proper event file will automatically be loaded (if the event file is in the same folder on disk as the raw data files).

(2) Edit Events
These sections allow you to adjust the stream of the events, correcting for mis-encoded data. If "Remove Bad Events?" is checked (it is by default), then this step can usually be skipped.

-- Adjust Events: opens a panel to allow you to inspect all of the event versus time data and make "adjustments" to the data, correcting for mis-encoded times, noise, and other obvious instrumental artifacts. See Correcting Errors in VSANS Event Data. The corrected data can then be saved to disk and re-loaded later (see Import Edited).
-- Undo Time Sort: will "un-sort" the data into the original timing of the events as they arrived. If the data is oscillatory, you'll see the oscillations again. Only the first 1500 events are shown, but you can change this by modifying the graph. But be careful if you try to plot everything - as there can be millions of points, making things slow and obscuring all of the oscillations.
-- Import Edited: will load in data that you have saved from the "Adjust Events" panel. This is saved in Igor text format, not the binary event stream format. Once imported, proceed with binning.

(3) Bin Events
-- Number of Slices: enter the number of slices that you want to use. You can change this later after you see what results you get. Using slice=1 is a valid choice and puts all of the events into a single bin.
-- Max Time: you can manually enter a Maximum time on the panel, and this will be the maximum time binned.
-- Bin Spacing: use this popup to select the type of bin spacing. Currently the spacing can be linear(equal), Fibonacci, or Custom.
-- Bin Event Data: processes the data based on the mode checkbox, number of slices, maximum time, and bin type.
-- Custom Bins: opens the panel to set up custom bin widths for the currently loaded data set.
-- Show Event Data: Displays the RescaledTimeGraph, showing the first 1500 points of the event file by default (for speed). It should be monotonically increasing. For oscillatory data, if you've processed the data and want to see the oscillations, you need to "un-do" the sorting. For either mode, it is very instructive to see all of the data, since there may be millions of events and the first 1500 are likely to look good. Ctrl-A or Cmd-A will show all of the data. Be patient as re-drawing all of the data is sometimes slow.
-- Show Bin Details: This brings up a bar graph of the number of event in each bin as a function of the bin width. There is also the tabulated data showing the numbers and the bin edges. Note that the single zero values at the opposite ends are for display purposes only.

(4) View / Export
Saving the binned event data is a multi-step process since there is a separate data file for each carriage. The processed output file will contain data from both event files and mimic the raw data file structure. This will make the reduction of the sliced data more convenient.

-Split to Panels: Events from all four panels of a carriage are interspersed in the event stream. This step separates the binned data into each individual panel.
-Show Panels: shows a view of the data in a more traditional view.
-Duplicate RAW for Export: This step makes a copy of the currently loaded raw data file read for the addition of the sliced data from each panel and the details of the bin time widths. It is local in Igor and has not yet been saved to disk.
-Copy Slices for Export: This copies the time slices (histograms) for each detector panel to the correct detector block in the export file. Only the slices from the current event file (either F or M) are copied.
-Save Exported to Nexus: Saves the sliced event data (along with the original raw data) is a file with the name "Events_" prepended to the original file name "sansNNNNN.nxs.ngv"

To bin and save event data slices for reduction:

1) Once the first carriage event file is processed and binned (it does not matter which one, F or M), then “Duplicate RAW for Export”. This generates a copy of the raw data file as loaded where the binned data and bin width details will be appended.

2) Then “Copy Slices for Export” will copy a 3D wave of “slices” to the appropriate detector folders. Waves of binEndTime, timeWidth, and binCounts are also copied to the Reduction folder for later use.

3) Then, load the second event file, bin it in the same way. Be sure to not change the binning details.

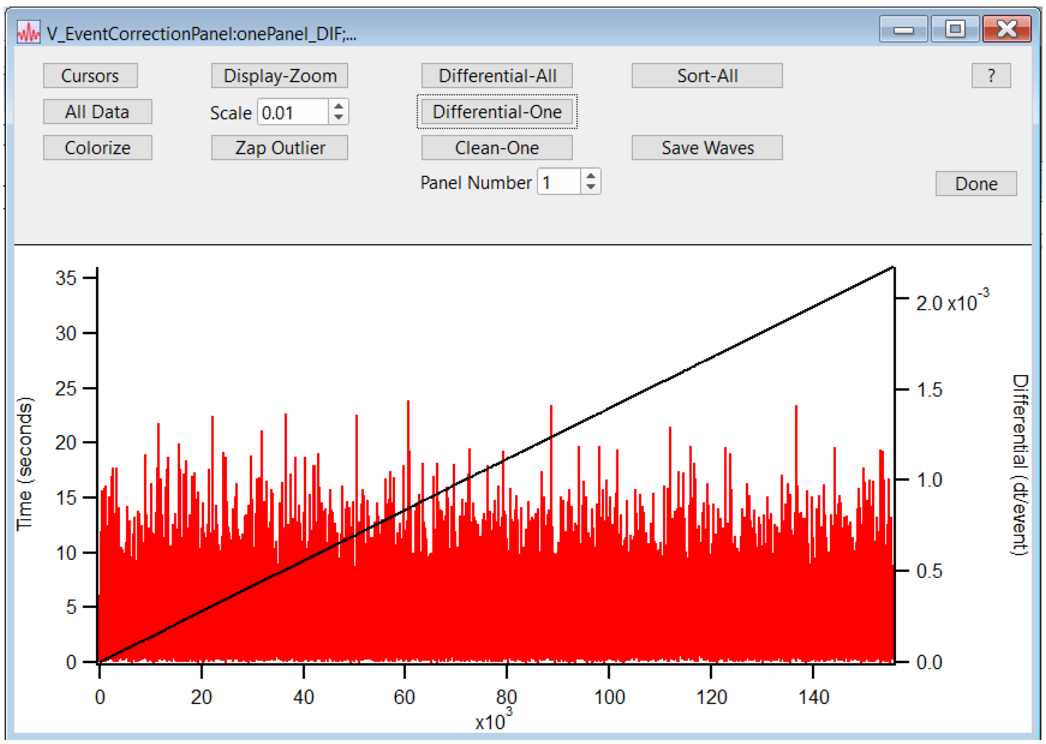
4) Next, “Copy Slices for Export” again, and it will put the slices in the correct detector folders. (Don’t “Duplicate RAW for Export” again – it is not needed until you start with another raw file). You also do not need to "Split to Panels". This is done automatically when the "Copy" step is done.

5) Last, “Save Exported to Nexus” will save the events (and the original raw data) in a file with the name “Events_” prepended to the original file name sansNNNN.nxs.ngv.

If you re-bin the same raw data file with different time bins, be sure to re-name the "Event_sans..." file with a different name to prevent it from being overwritten.

The "Events_sansNNNNN.nxs.ngv" file is essentially a copy of the original data file where each of the 8 detector panels has been binned into time slices giving a 3D data set I(x, y, t). The new data file contains both the original raw data, plus the 3D time sliced detector data. The time slices can then be reduced using a reduction protocol that you define.

Correcting Errors in VSANS Event Data



Adjusting Events allows you to inspect the event stream and remove any "bad" or misencoded data. For the VSANS event stream, corrections are usually not necessary, but if need, require some special steps due to the way the events are written to the file. The controls on the panel are:
-- Cursors: Puts cursors on the graph, either rescaledTIme, or onePanel
-- All Data: Shows all of the data
-- Colorize: Colorizes the data from the four different panels in the graph. Zoom in to see the time reversals form the different buffers of data from each panel (in sequence).
-- Display Zoom: Zooms (expands) the display to the percentage scale factor shown. Use All Data to revert to the full data set
-- Zap Outlier: If the cursors are on the graph, and both cursors are on the same data point, Zap Outlier will delete that point. Otherwise, it does nothing.
-- Differential-All: Computes the differential of the entire set of event data.

-- Differential-One: Computes and displays the differential for the numbered panel. Time data for other panels is set to NaN (temporarily) so that the differential is only of the selected panel.
-- Sort-All: Sorts the data so that time is always increasing. An index is produced so that the sort can be un-done if necessary
-- Save Waves: Saves the adjusted waves as Igor Text. This operation can take a very long time to write out the data files, especially if there are millions of events.

NOTES - adjusting events

Zoom and shrink as needed:
- drag a marquee and right-click (horiz expand) (repeat)
- double-click on the bottom axis and on the "Axis Range" tab, enter the min and max values (you may want to make sure that the "Live update" checkbox is NOT checked).
- "All Data" will show you all of the data again.

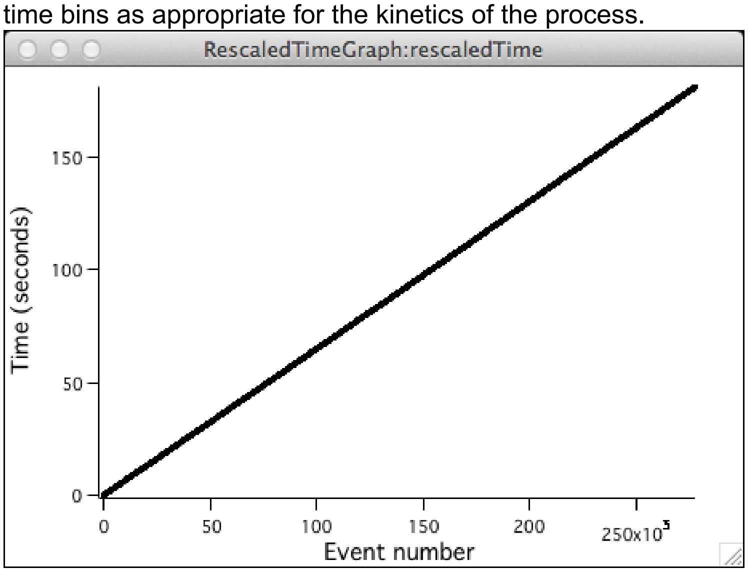
Move cursors faster:
- click and drag them. If you place them on an "edge" they'll and up at one end of the step or the other.
- if a cursor is "solid" in the information bar at the bottom of the graph, if can be moved with the arrow keys, or the "slider". if both are "solid", both cursors move in tandem. To make a cursor not solid - and then not move with the arrows. click on its icon in the status bar at the bottom of the graph to toggle its solid/open state.

Read out where the cursors are:
- the status bar at the bottom of the graph shows where the cursors are, reporting the point number, x and y values, and also the delta(x) and delta(y). When there is a step in the time, set the cursors at each edge to read the delta t.

There is NO UNDO
Trimming the points is not reversible. Once they're gone, they're gone.

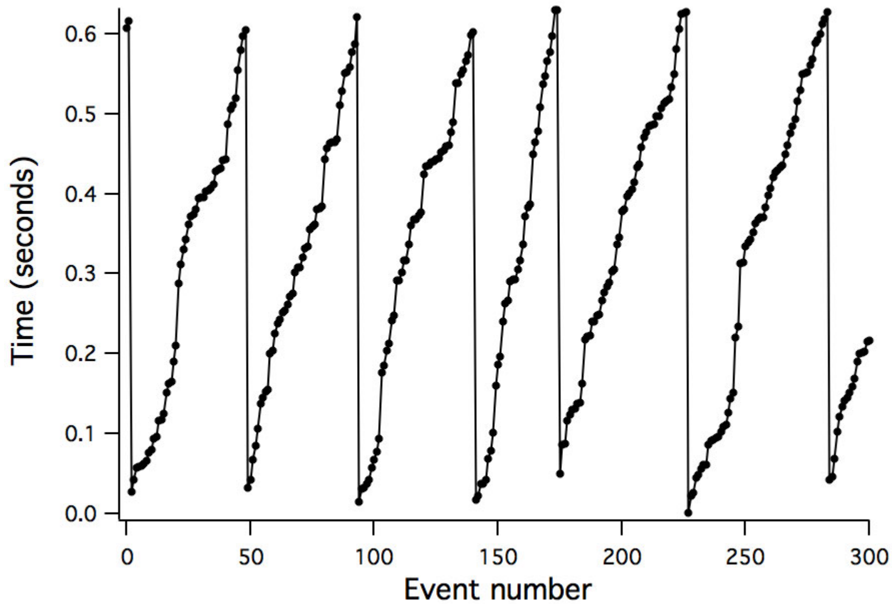
Types of VSANS Event Data

-- Stream data details:
This is a "stream" of data events where no T0 signal is sent. A possible application of this file type is a single, long relaxation process over several minutes or longer. The full time is collected in a single file, and then sliced into time bins as appropriate for the kinetics of the process.

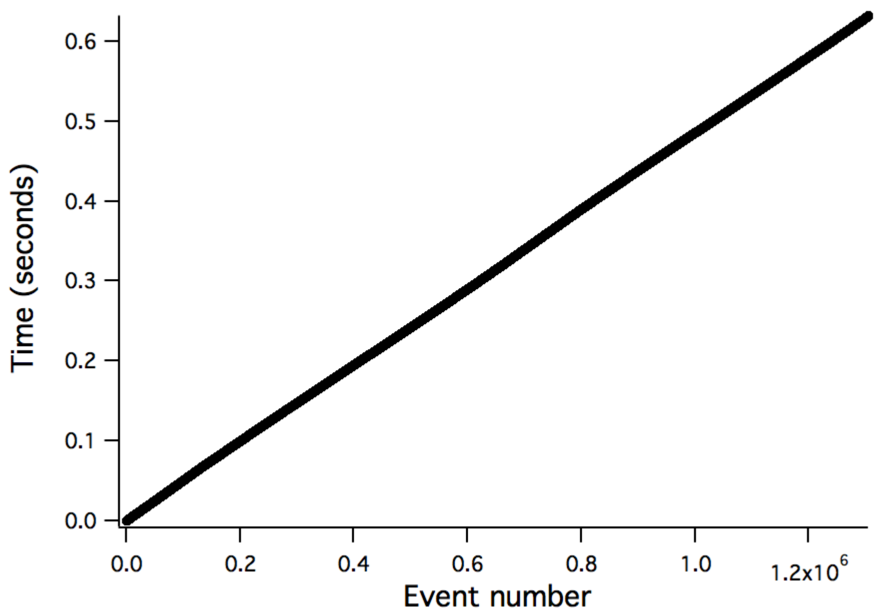


-- Oscillatory data details:

At the T0 signal, the clock is reset on the hardware side, so there is nothing to interpret when reading the data (as long as the period of the oscillation is less than 6.7s. In this example, it's about 0.6s. So time only ever reads a value between zero and 0.6s. In the graph, only the first few hundred events are shown, to show the sawtooth nature of the data. So upon loading, the data looks like:



Then in processing, the data is sorted by time to collapse all of the XY events into a single time "frame" of 0s -> 0.6s. Then it's easily binned from here. It can also be "un-sorted" to return to the original event stream. After processing, the rescaled time graph looks like: (and this is now all 1,300,000+ events)

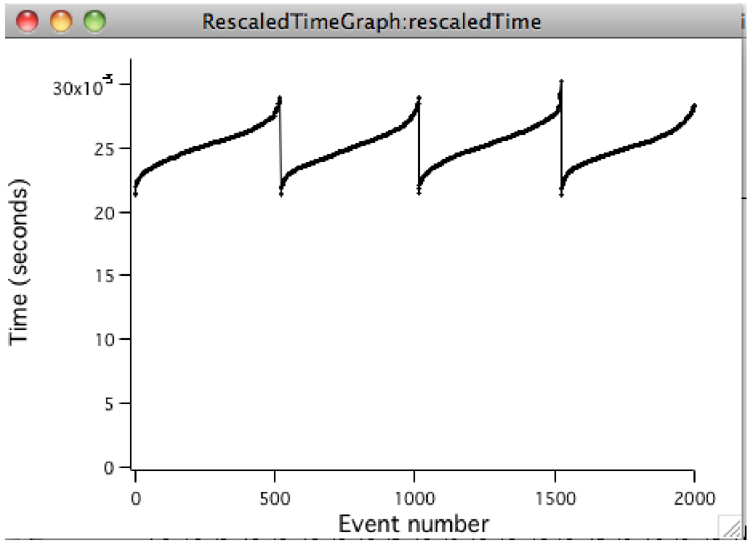


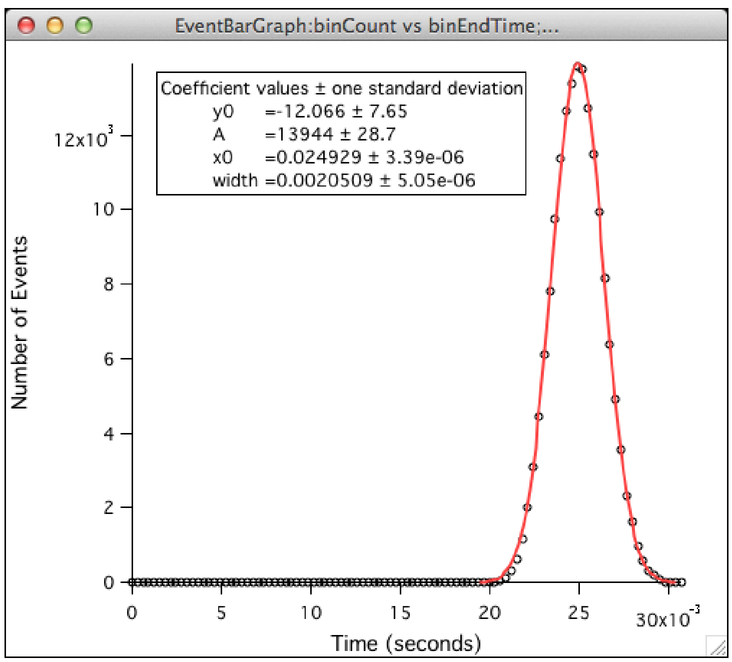
-- TISANE data details:

Details and an example to be added.

-- Time-of-flight data details:

An example of TOF data is shown below. I don't know the actual setup here, but there is a chopper in the beam, chopping the beam into non-overlapping pulses. The event stream looks like below with regular oscillations. Note that the mean time for an event is around 25 ms and is in a narrow band, set well away from zero. Note also the sigmoidal shape of the event arrival times in each pulse. When histogrammed (following graph), the result is a gaussian(ish) distribution of arrivals. This example file may be a TOF measurement of the wavelength distribution, which could be calculated if the sample to detector distance were known.





For time-of-flight data (TOF) for calibration of the wavelength, load in the event file (as TOF mode), and bin the events, using a large number of slices – several hundred, maybe a thousand, depending on the count values. Then “show bin details”. Right-click on the data and change the Mode to “markers”, then right-click again, choose “quick fit” from the bottom of the menu, and choose “gauss” as the fit type.

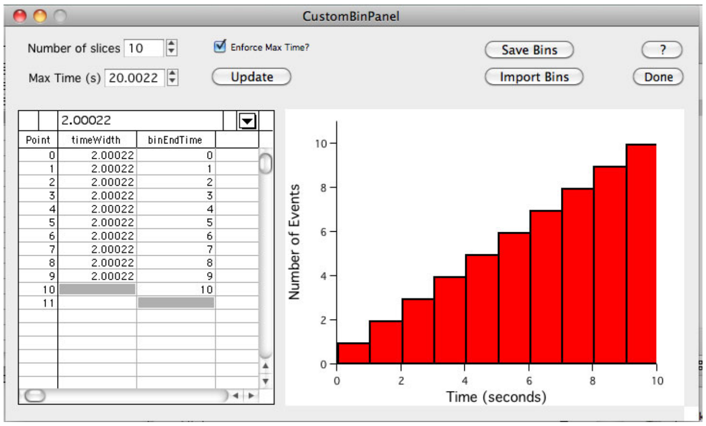
X0 is the center of the Gaussian, and width = sqrt(2)*(std. deviation of Gaussian)

The time unit is not seconds, but is in 1e-7 seconds. The actual value is in the header of the data file, and is reported in the command window when the file is loaded.

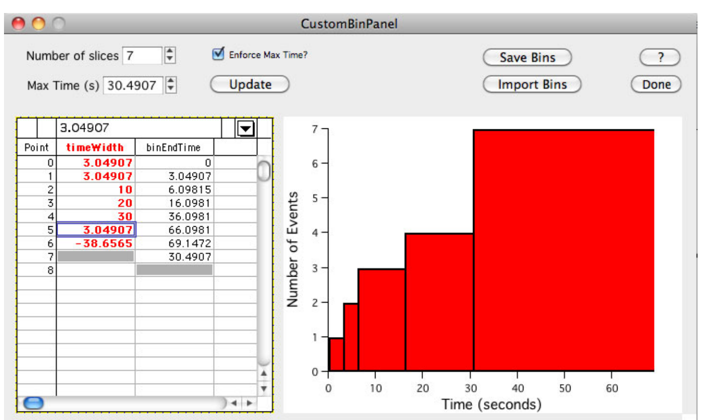
Setting up Custom Bin Widths - VSANS

Currently, there are three choices for the bin spacing: Equal, Fibonacci, and Custom.
Equal - splits the time from 0->t_max into equal bin widths.
Fibonacci - sets the bins from 0->t_max based on the Fibonacci series (neglecting the first zero)
Custom - lets you set the number of bins and the width of each bin. Details are below.

When you select "Custom" from the popup, a new panel is presented:

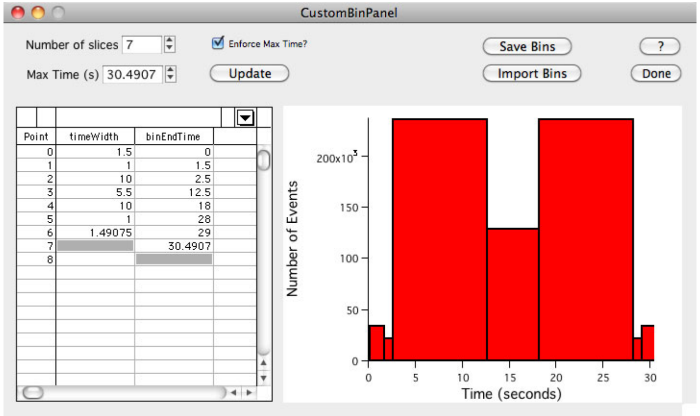


On this panel you can set the number of slices and the maximum time to use. These are the same values that are on the main event loader panel. The table contains two columns. timeWidth is the width of each time bin in seconds. binEndTime is the ending time of each bin, also in seconds. There is one extra point in the binEndTime column. The first point here is zero, simply for display in the bar graph. Therefore the delta(t) for bin[p] is (binEndTime[p+1]-binEndTime[p]). A bar graph of the bin widths is also shown, with dummy values for the number of events. (the # of events = the bin number)
Now you can simply enter the number of bins (slices) that you want. The length of the waves in the table automatically adjusts. Next, be sure to enter a timeWidth for all of the bins.
--Then click "Update" to recalculate the binEndTime and update the bar graph.
By default, bins of equal widths are filled in, and the maximum time is enforced. What this check box means is that the calculation of the binEndTime will use the entered timeWidths up until the last one - then it will CHANGE what you have entered to make the delta(t) work out so that the last bin ends at the maximum time. Note that this WILL CHANGE the value that you entered, and if the total of the bins exceeds the maximum time, then the last bin width will be negative - which is bad - and the column will turn red and bold to warn you to fix the timing.



You must click "Update" to recalculate every time you make a change. It doesn't update automatically.
Now, when you process the data (and Custom is still selected in the Bin Spacing popup), the bins that you made will be used, and the bar graph of bins will now reflect the actual number of counts.
You can save the bins that you generated by clicking "Save Bins". This will save and Igor text file that

you can read back in using "Import Bins"



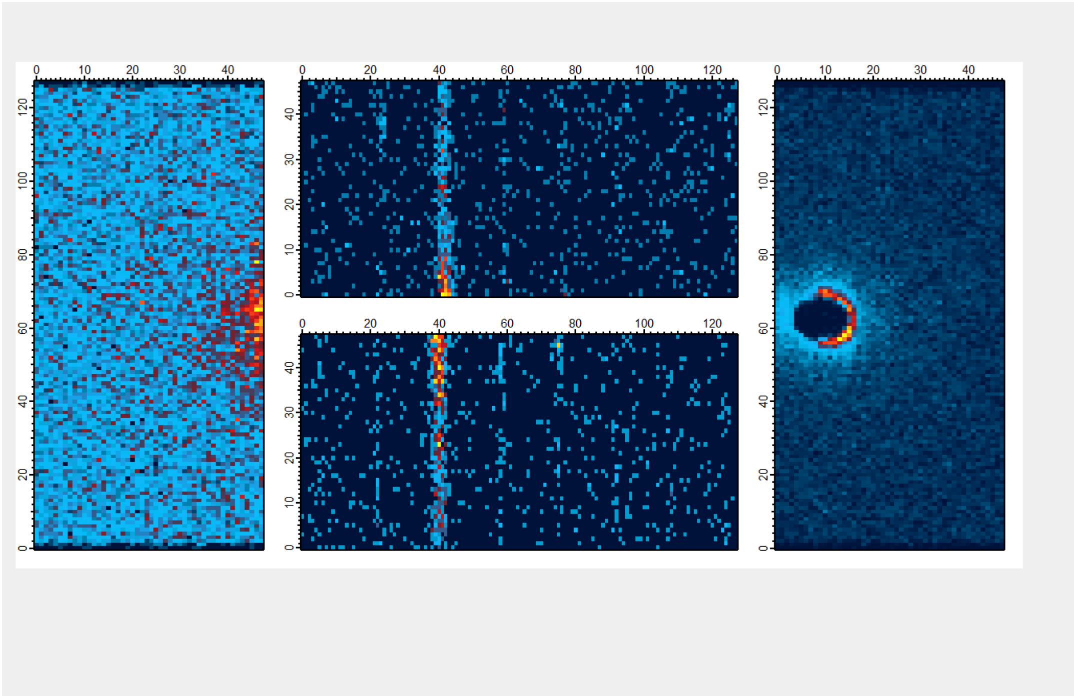
Structure of VSANS Event Files

The VSANS Event files are 64-bit encoded words, with a short header on the file. The 64-bit words are easily processed with built-in Igor functions, so no external XOP is necessary to load and process VSANS event data. See the Event-related procedures for details of the header and the encoding.

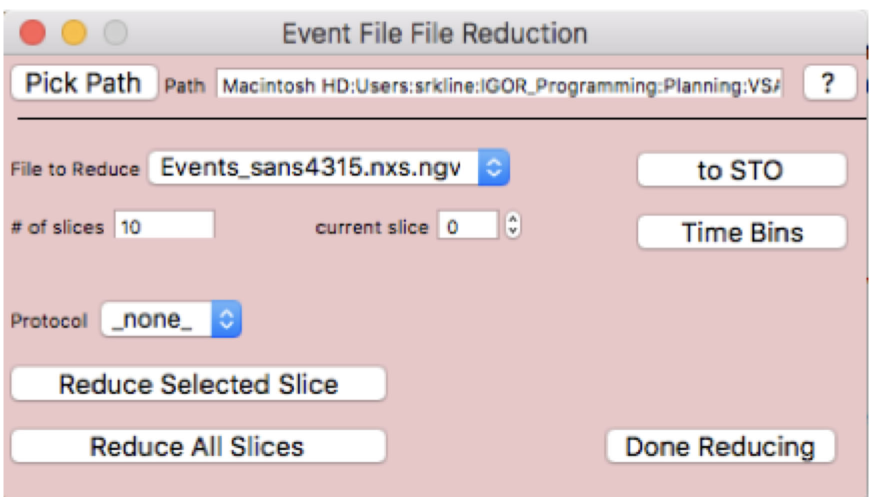
As a consequence of having events from all four panels written to a single event file, the events must be assigned to proper panels for viewing. The raw event 2D data display is (192, 128) as all four panels of the (M)iddle or (F)ront carriage, hence 48 tubes (x 4) = 192 in the x-direction. The encoded tube number assignment is:

Right = (0, 47)
Top = (48, 95)
Bottom = (96, 143)
Left = (144, 191)

That means that the view of the detectors is jumbled from the expected view of the panels. “Split to Panels” and “Show Panels” will take the binned data and display slice[0] as the “normal” view.



Reducing VSANS Event Data



Opening the “Event Reduction” panel allows reduction of all the slices at a single time. Files with event slices are recognized from the “Event_” tag at the beginning.

1) Select one of these files in the popup and click “to STO”. This loads the data file (which is essentially a RAW data file) and copies it to the STO work folder. The number of slices found in the data is displayed.

2) Clicking on “Time Bins” displays a table with the cumulative bins and the width of each (in seconds). This is the binning that was used to slice the data.

3) You must have a pre-defined protocol to use here – no default protocols that will stop for input are

allowed. Also, when setting up the protocols, remember that you do not need to take slices of the empty or background measurements. These can (and should) be used with the full statistics.

4) Be sure to set “Ignore Back Detector” in the VSANS preferences before doing the reduction since there is no event data for the back detector. Otherwise, each reduced slice will have the time-averaged back detector data included.

5) When you “Reduce Selected Slice”, the named slice and appropriate count time and rescaled monitor counts are copied over to RAW from the STO folder. This slice then appears like a standard raw data file, ready for reduction. You can either reduce just the selected slice number (counting from zero) or reduce all the slices as a batch using "Reduce All Slices". Reduced data files will be automatically named “Events_sansNNNN_SLx.ABS” where SLx is the slice number (or .AVE if no absolute scaling).

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