

- **SANS and USANS Simulation**

04/2010 Vers. 1.0 (Package 7.0)  
03/2012 Vers. 1.0 (Package 7.10)  
06/2014 Vers. 1.0 (Package 7.2+)  
12/2014 Vers. 1.0 (Package 7.2+)

These modules provide utilities for simulation of SANS and USANS instrument configurations and scattering. They can help you to decide what is the "best" instrument configuration for the experiment you are performing. Setting up the instrument configuration is in general a task of optimizing the flux on the sample while maintaining a measured q-range and resolution that is sufficient for your sample.

With a little knowledge and some educated guesses about your sample, the scattering can also be simulated. This level of simulation can show the general shape and features of the scattering, the level of signal above background, and even provide estimates of the countrate on the detector, required counting time, and statistical error in the data. While this is optional, it can provide important feedback to ensure that both the instrument configuration and sample conditions are truly optimized for your sample and the type of analysis that you plan to carry out.

For even more help in designing a complete experiment, full sets of experimental "runs" can be set up in a manner very similar to a real SANS experiment. In this way, you can optimize the configurations, sample conditions, experimental counting times, etc. to get the best possible data. You can even run through the steps of analysis that you are planning to use to see if you get the results you expect. A little investment in planning can eliminate a lot of wasted sample preparation, travel time, and beam time.

Remember that when setting up configurations, what is "best" is still often a judgment call. At the very least, some very bad choices can be weeded out before it's too late. Your local contact can provide additional help and advice.

These macros are designed to provide an easy to use, graphical interface for the simulation, reduction, and analysis of scattering data. As of 10/2009, USANS Reduction macros require IGOR Pro v. 6.1x. As always, the macros will work with the free Demo version of IGOR.

If you use this software to simulate, 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.

\* John Barker of the NCNR provided the code that is used in the 2D Monte Carlo simulation and the algorithms to efficiently simulate 1D scattering.

Videos containing abbreviated instructions and more tips for use of the macros are available at the NCNR web site:

[http://www.ncnr.nist.gov/programs/sans/data/movies/reduction\\_analysis\\_movies.html](http://www.ncnr.nist.gov/programs/sans/data/movies/reduction_analysis_movies.html)

2/2012:

- In this release, gravity, wavelength spread, and initial trajectory have been added to the 2D monte carlo simulation.

6/2014:

- Calculation of multiple scattering probability for USANS-sized structures is improved.  
- Real-space structures can now be used as the "model" function for simulation. Draw the real space structure first, then plot the model "GenericFFT". Set N=256 and T=5 for a reasonable q-range.

6/2014:

- Added the Run List Panel to allow a full experiment to be easily simulated through generating configurations, samples, and finally a run list for the experiment. Simulations can be run for 1D or 2D, saving results as a real experiment would. Currently limited to SANS experiments.

## **Experiment Planning Tools**

[SASCALC](#)

[UCALC](#)

[Plotting a Model for Simulation](#)

[Simulation of 1D SANS Data](#)

[Simulation of 2D SANS Data](#)

[Simulation of USANS Data](#)

[Simulating a Run List](#)

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## **SASCALC**

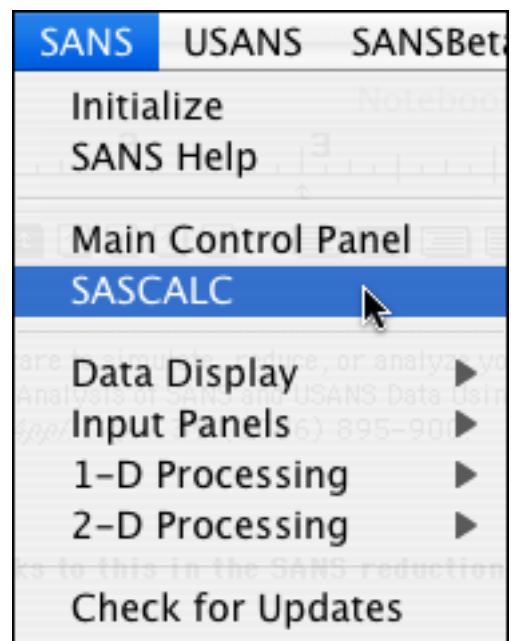
The SASCALC module allows you to simulate the collimation and sample configurations on the NG3 and NG7 SANS instruments. By doing this, you can optimize the setup of the instrument to provide the "best" quality data in the "shortest" collection time. There are many ways to define "best" and "shortest" since the collimation is a tradeoff between good q-resolution and higher flux.

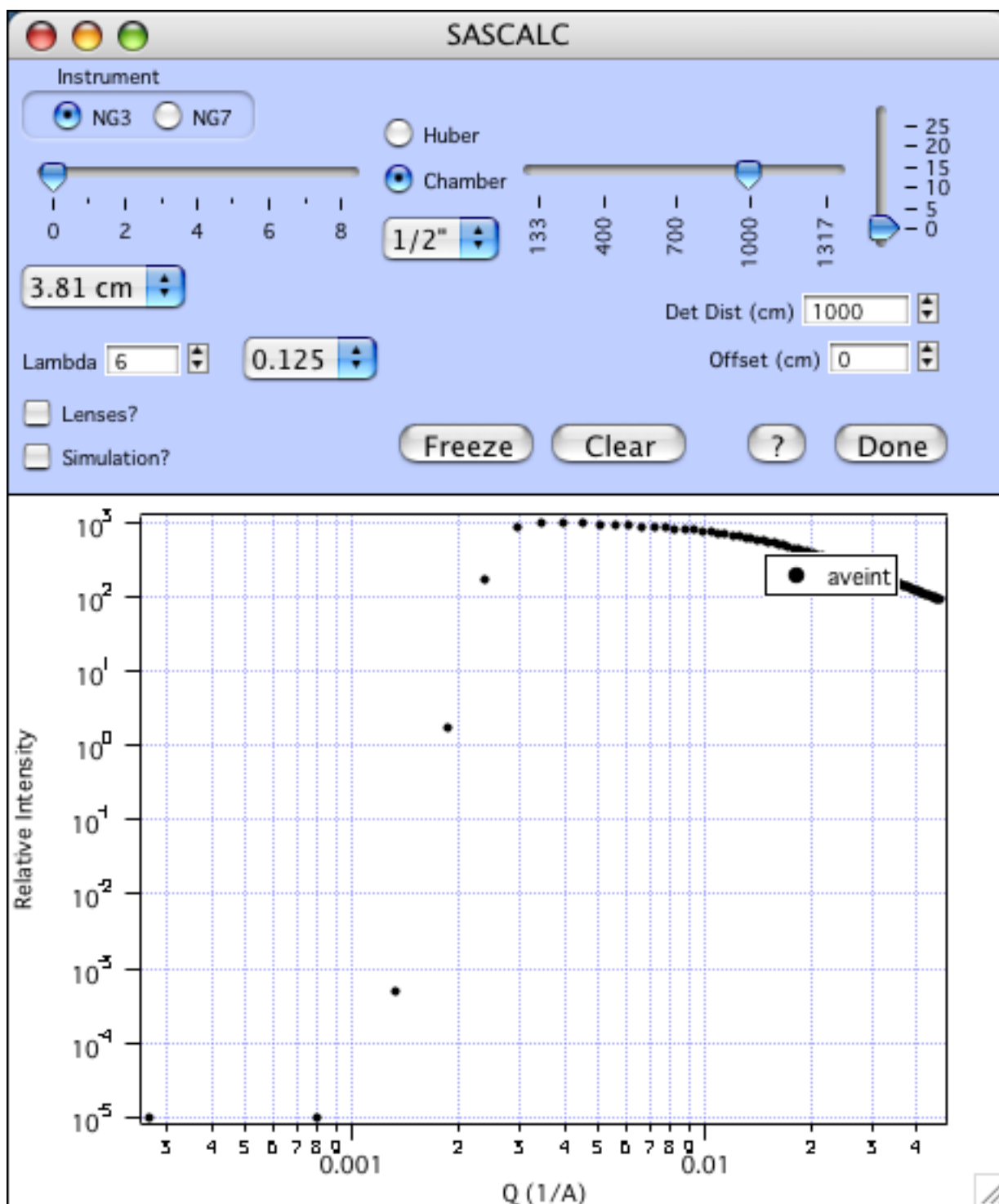
Start by thinking about the real-space length scales present in your sample, largest and smallest. Q is an inverse length scale, so you'll want to set up the SANS instrument to cover **at least**  $Q = 1/D_{\text{max}}$  to  $Q = 1/D_{\text{min}}$ . Then adjust the instrument settings to get the q-range that you want, while maximizing the beam intensity on sample. It may (it usually does) take more than one configuration to measure the necessary q-range. In this case, you want to make sure that there is sufficient overlap in q between each of the configurations. Keep in mind that for overlap, some of the data points will be trimmed from each data set when they are combined.

If you want to simulate scattering from a particular sample at the same time as optimizing the instrument configuration, see [Simulation of 1D SANS Data](#) or [Simulation of 2D SANS Data](#), after you are comfortable with optimizing the collimation.

### **To Optimize the SANS Instrument Collimation:**

- Open up the SASCALC Panel (the SANS Reduction Macros must be loaded). From the SANS menu, choose "SASCALC". Two windows will open up. One will have the controls and a plot of the data range, and the other will be the text of the numerical results.

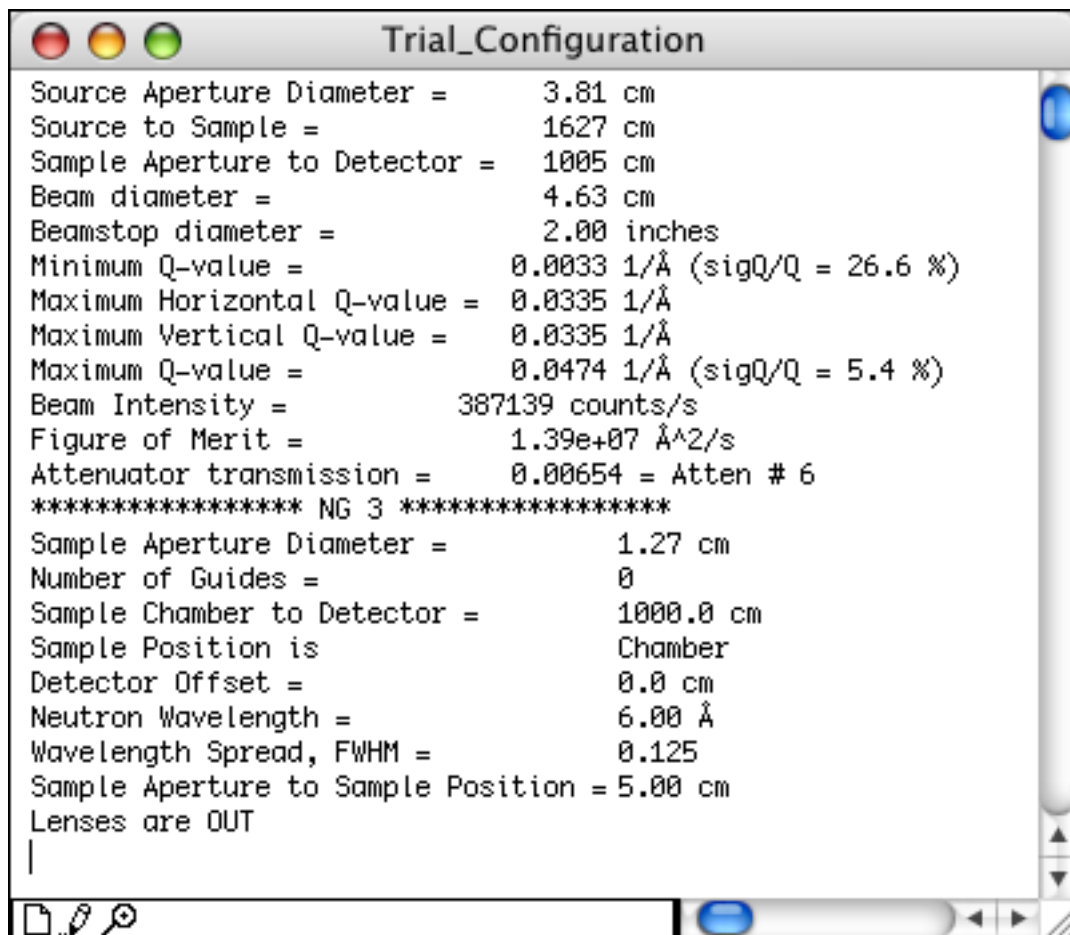




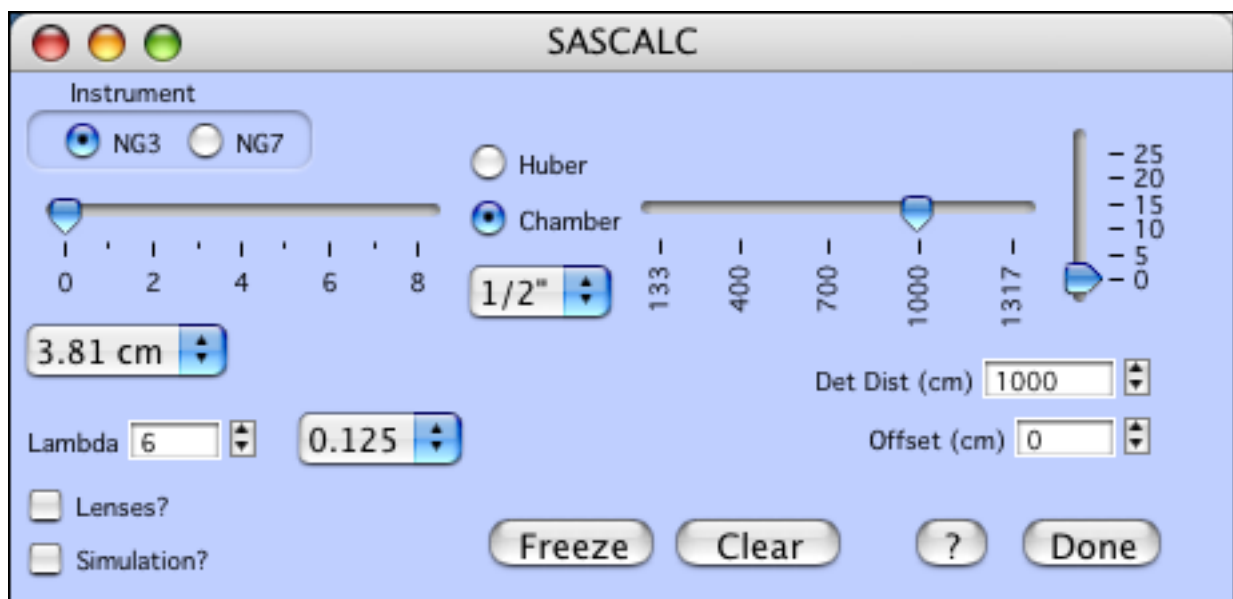
The details are displayed in the Trial\_Configuration. The most important values for comparison are:

- Minimum Q-value
- Maximum Horizontal Q-value
- Beam Intensity
- Beamstop Diameter

The instrument is equipped with beamstops that are discrete diameters, and must be larger than the Beam diameter.



What are the controls and what do they mean?



Since each instrument is slightly different:

-Select the instrument: using the radio buttons, either NG3 or NG7.

Then after adjusting the configurable parts of the instrument collimation, the 1D-averaged data that

would result from the set instrument collimation is plotted as a function of Q. A Debye function is used for the relative intensity. The presence of the beamstop and its shadowing effect is visible at the lowest q-values for each configuration. The graph and Trial\_Configuration is updated with every collimation change.

Working from left to right / top to bottom:

- Guide Slider: This sets the number of neutron guides inserted in the pre-sample collimation. Zero to eight guides can be inserted. More guides means more flux on sample, but a larger divergence of the beam. Note that on NG3 6 guides is not allowed as there is a beam polarizer installed.
- Source Aperture: This popup is below the guide slider. There are three choices of diameters when zero guides are inserted. All other guides give only one choice, 5 cm. The one exception is the 7-guide configuration on NG3 where there are two source diameter options.
- Lambda: Set the wavelength in Angstroms. 5 Å, 6 Å, and 8 Å are the most common choices as they are at or near the maximum in neutron flux from the cold source.
- Wavelength spread: The popup to the right of the wavelength is the wavelength spread. There are typically three choices, and the "middle" setting (~0.13) is most commonly used on each instrument. A smaller spread improves the q-resolution, but at a cost of lower neutron flux. Similarly, increasing the wavelength spread increases the flux, but at the expense of poorer q-resolution.
- Lenses?: This check box sets all of the required instrument settings for using focusing lenses to reach the lowest q-values. Note that this will also change the wavelength to a value near 8 Å, depending on the focus condition for each instrument.
- Simulation?: Opens an input dialog for setup of simulation of the scattering from a model sample that can give a more realistic view of what data might be collected at the current instrument conditions.

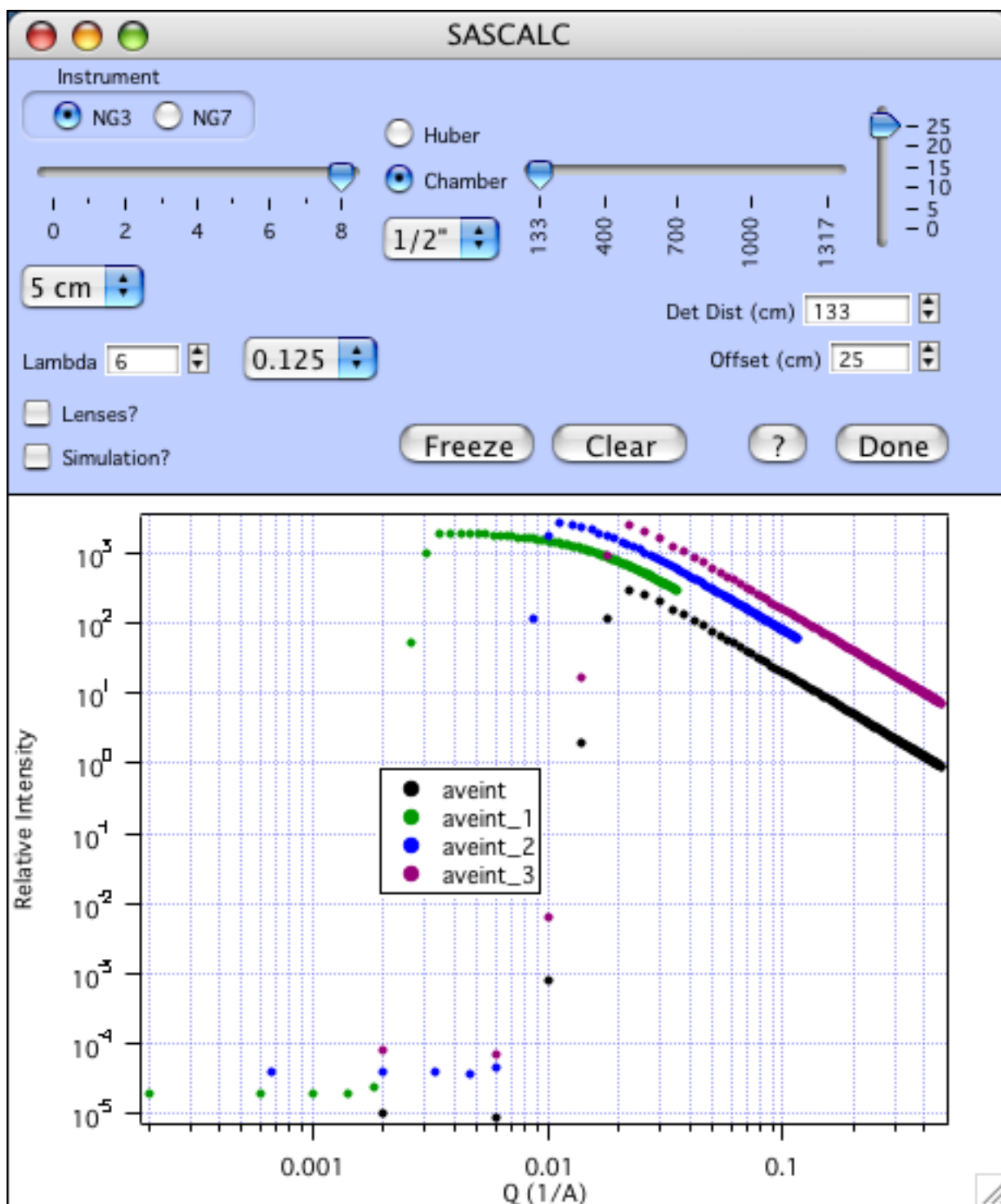
In the middle:

- Huber/Chamber: These radio buttons select the sample position. Normal configurations with multiple sample changers are mounted in the Chamber position. Large equipment (magnets, cryostats, shear cells, etc. ) is mounted on the Huber stage.
- Sample Aperture: this is the popup below the sample position selector. 1/2" diameter is typically used for standard SANS sample cells, either the titanium cells or quartz banjo cells.
- Sample to Detector Distance: This slider (or type in the value) sets the distance from the sample *chamber* position to the detector. Note that the Huber sample position is offset by 55 cm. Also, note that the detector position limits are different for each instrument.
- Detector Offset: This slider (or type in the value) sets the horizontal offset of the detector from 0 cm to 25 cm maximum. Offsetting the detector gives a wider q-range for a given sample to detector distance. However, if the sample scattering is expected to be anisotropic, half (or more) of the scattering will not land on the detector.

At the bottom:

- Freeze: this button "freezes" the current configuration on the graph, and saves the numerical results to a Saved\_Configurations window. The data on the plot is offset for easier viewing.
- Clear: clears all of the test configurations from the graph, and clears the Saved\_Configurations text.
- ?: Displays this help file.
- Done: Closes the panel and the configuration text windows.

Once you're happy with the configurations, you can print out the Saved\_Configurations. An example of three configurations is shown below:



### General tips for use

- The beamstop diameter is not set, but rather derived from the collimation optics. The instruments only have 1", 2", 3", and 4" beamstops, even though SASCALC recommends a larger one.
- To cover the full q-range of the instrument, typically three separate sample-to-detector distances are required. Two may look like they overlap, but it is usually not sufficient for real data that is noisy (especially at the high-Q end of each configuration) and shows the effect of resolution smearing (worst near the beamstop of each configuration).

- Use no detector offset if anisotropic scattering is expected.

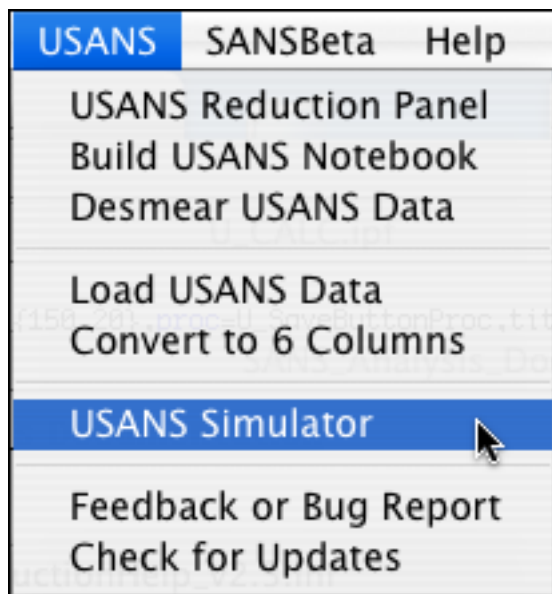
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## **UCALC**

Simulating the scattering that would be measured from a particular sample is a valuable tool for optimizing your experiment, from the time spent in instrument setup, data collection, and in the overall quality of the data. For the USANS instrument, data collection is point-by-point. So, in the planning of your experiment, think very carefully if that data point is necessary, if that high  $q$  is necessary (USANS and SANS can't truly overlap), and if that density of points is necessary. For example, power-law or fractal scattering generally has no sharp features, meaning that they can be effectively measured with fewer points per interval, significantly reducing the measurement time per sample. So measure just what you need to get the data you need, and you'll often be able to measure more samples.

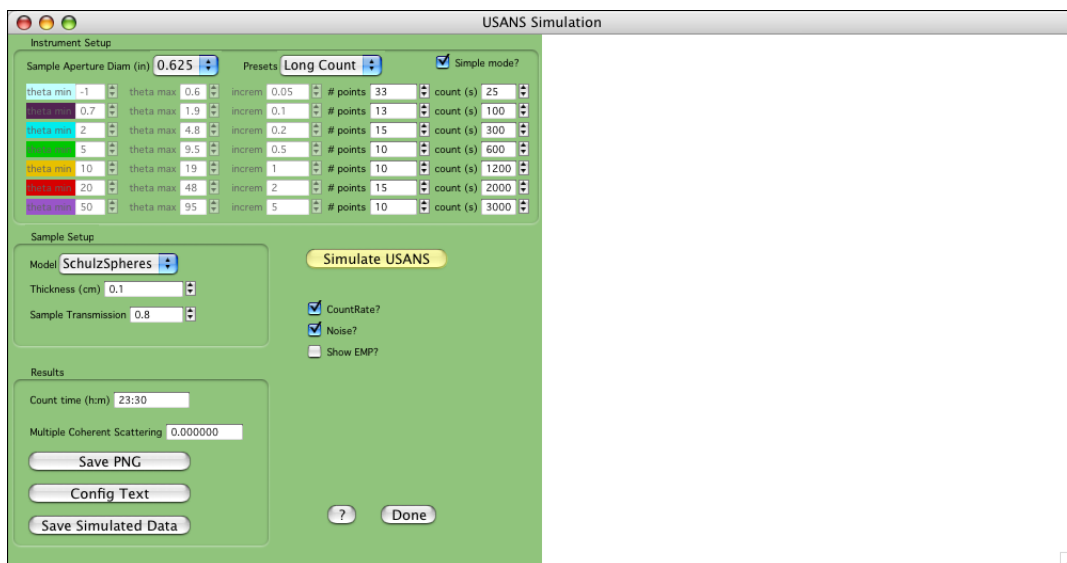
Since the counting time per point is very often sample-specific, optimizing the configuration and collection time is best done with sample specific information. If you want to simulate scattering from a particular sample at the same time as optimizing the instrument configuration, see [Simulation of USANS Data](#).

Open the USANS Simulation panel from the USANS Menu:

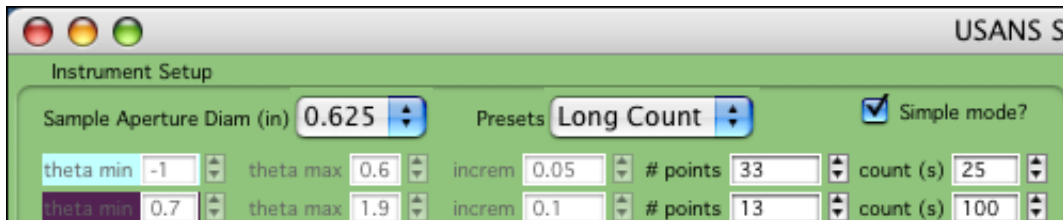


The simulation panel will open, with a setup section to the left, and a (blank) space for the graph of the results on the right.

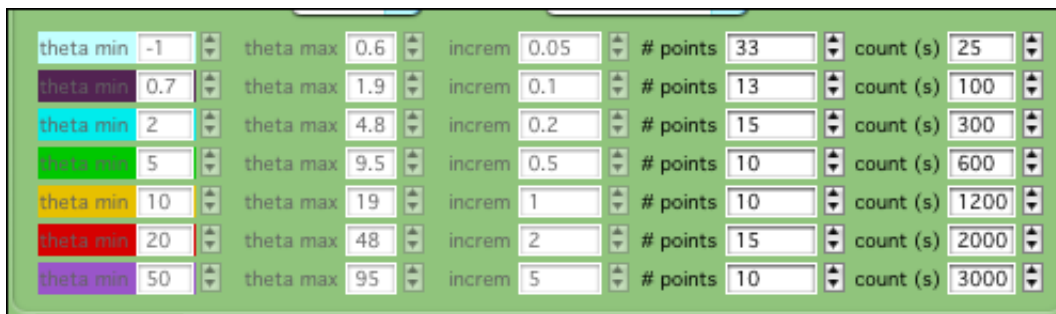




When the panel opens, in the (green) Instrument setup section:



- Sample Aperture: Set this depending on the size of your sample. This is really the only configurable part of the instrument. The larger the aperture diameter, the larger the flux on sample. 0.625" is typical for the standard SANS demountable or banjo cells.
- Presets: these are for quick setting of the number of points and counting time for each angular range. In general, you will want to tweak values for your own experiment.
- Simple Mode: When checked, theta min, theta max, and the angle increment are not editable, simplifying the choices of what to adjust. Typically, you will only need to adjust the number of points, and the counting time.

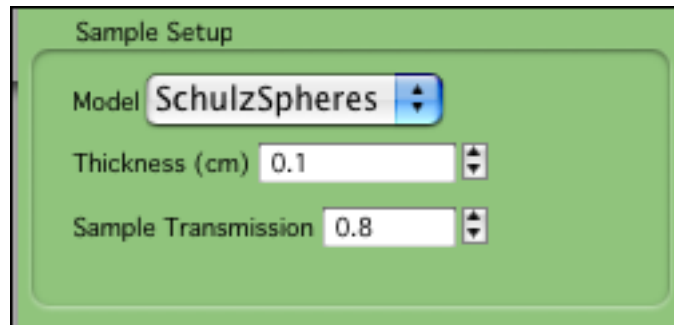


For each angular range (denoted by different colors)

- Set theta min: the starting angle for the range
- Set theta max: the ending angle for the range
- Set the increment: sets the delta between points, with the result that the theta max increases if the increment is increased for a fixed number of points. (these are typically not editable)

- Set the number of points: changes the number of points in that angular interval. The increment and counting time will change in response. The plot will not be updated until "Plot" is clicked.
- Set the counting time: Sets the counting time per point in that angular range. Setting the time to zero results in no counts and that interval is not plotted. The total counting time is adjusted, but the plot is not updated until "Plot" is clicked.

Much longer counting times are usually required at the larger angles since the scattered intensity of most samples falls off very steeply at larger angles (larger Q values). The total counting time for all (nonzero) intervals is reported in the results section. It is clear that most of the counting time is spent on a few points at the highest angles.

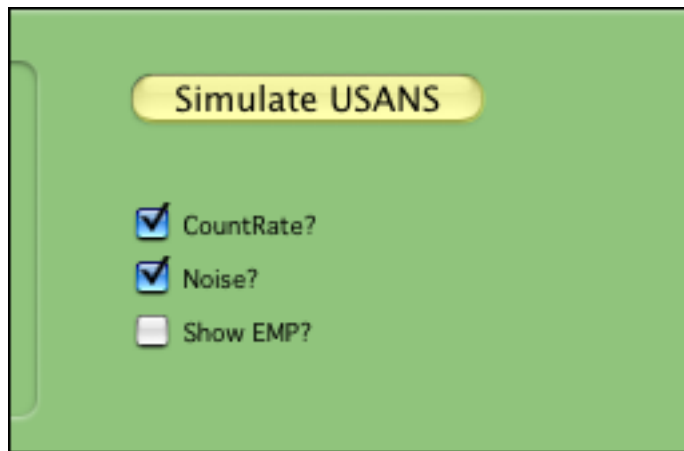


In the Sample Setup:

- Set the function. This must be the unsmeared model. The parameters used for the simulation are those set in the fit manager panel. Be sure to select the model function that you want (even if it already looks like it's selected). If you do not select a function, a default power law will be plotted.
- Set the sample thickness.
- Set the sample transmission (use your best guess). Remember that if you increase the sample thickness, you should also decrease the transmission. Transmissions for USANS will in general be a bit higher than for SANS since the wavelength used is shorter. For reference, at the USANS wavelength, transmissions (roughly) are:

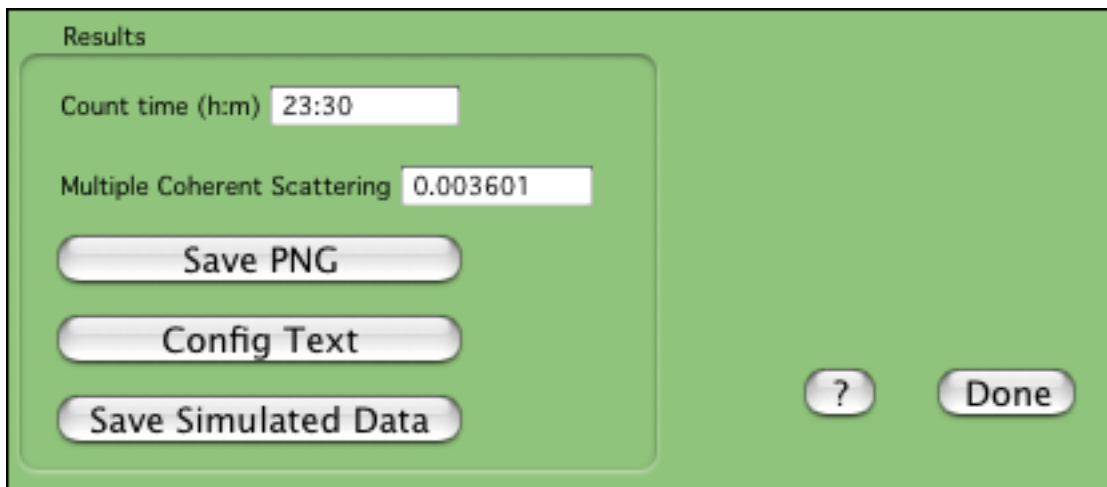
1mm H<sub>2</sub>O = 0.64  
2 mm H<sub>2</sub>O = 0.41

1 mm D<sub>2</sub>O = 0.95  
2 mm D<sub>2</sub>O = 0.90  
5 mm D<sub>2</sub>O = 0.76  
10 mm D<sub>2</sub>O = 0.58



And in the checkboxes:

- CountRate?: When checked, this will plot the simulated data as a function of count rate. This is the preferred way, so that the separate angular ranges display continuously, and the empty cell count rate can be directly compared. When unchecked, raw counts are plotted and the data from different ranges will appear staggered.
- Noise?: Will add noise to each data point within the counting statistics of the simulation.
- Show EMP: Will plot the experimentally measured count rate from an empty aperture at the specified sample aperture diameter (if it exists).



Values reported are:

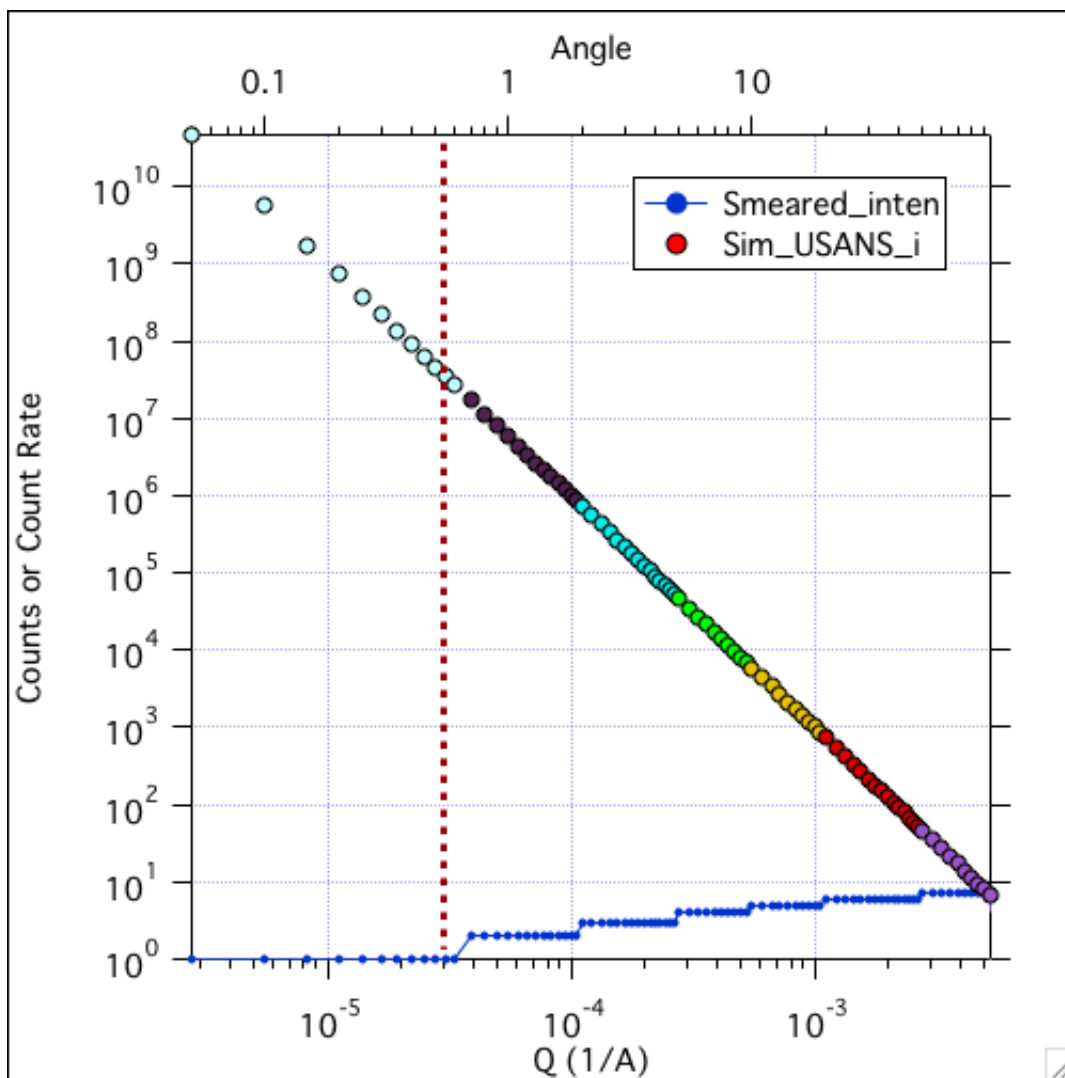
- Count Time: the total counting time for all of the angular intervals.
- Multiple Coherent Scattering: the fraction of the beam that is multiply scattered. Only coherent scattering is considered. If this number is more than 10% talk to your local contact. Excessive multiple scattering can make analysis difficult.
- Save PNG: will save a PNG image of the panel and the graph. Won't work with the demo version of Igor.
- Config Text: will generate a printable text file with the USANS setup information - the angle ranges, number of points, and counting times. Very useful to have on hand when the instrument is set up.
- Save Simulated Data: The 1D data for each of the angular intervals can be saved as simulated BT5 raw data files.
- ?: Displays this help file.
- Done: Closes the panel.

--Clicking "Simulate USANS" will simulate the counts you would get, based on the model and the instrument setup. Since the slit-smearing calculation can be lengthy, you must manually update the plot any time you change the setup of the instrument or the coefficients of the model function.

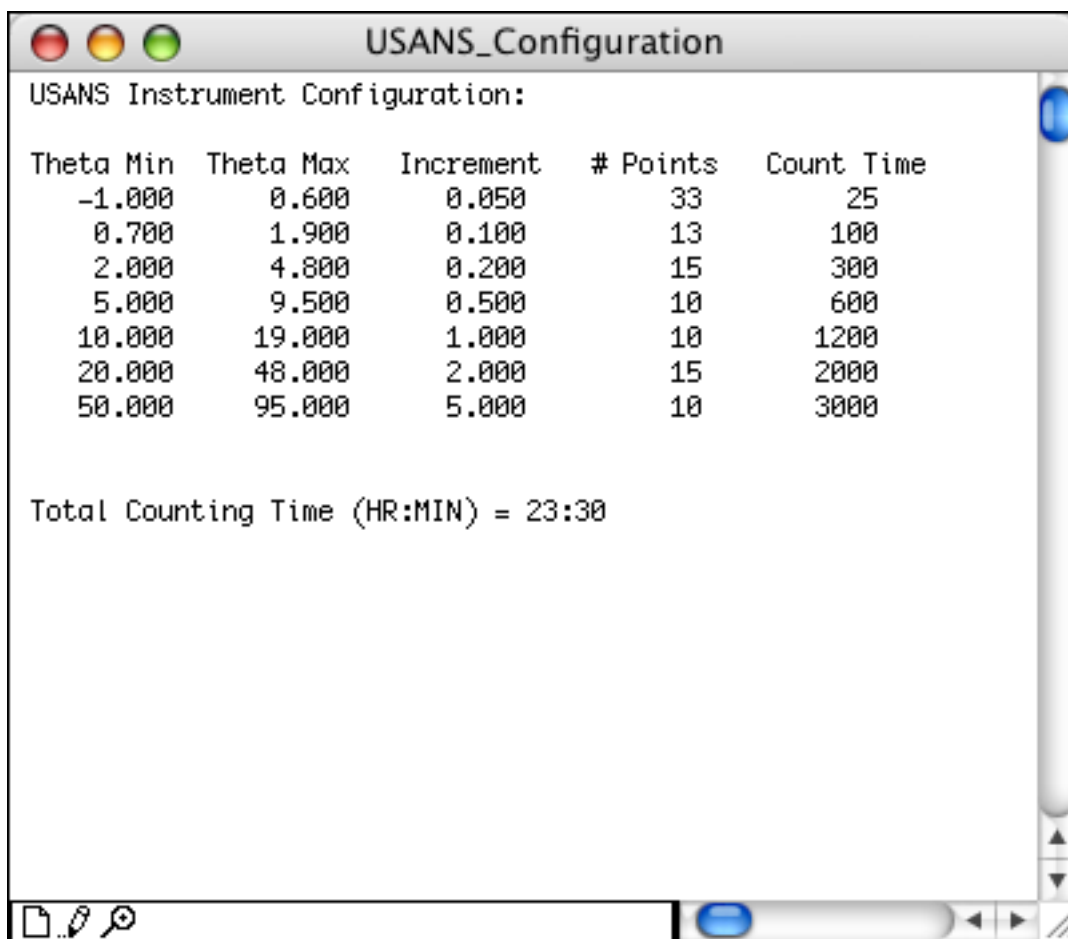
#### What the results are:

The main result is the simulated 1D data set, as if you measured the "sample" specified by the model function at the specified angular ranges and times. The simulated data points are color coded for each angular range. "Smeared\_inten" is the expected smeared intensity, but is NOT plotted on the same scale as the simulated data, which is typically plotted as count rate on the detector. "CR\_n", if plotted, is the countrate from an empty sample aperture of the size you selected.

Since no model function was selected here, a default power-law scattering is shown. The "Smeared\_inten" has no meaning, and the "Sim\_USANS\_i" simply shows the density and spacing of the points that result from the angular ranges. No meaning can be drawn from the statistics of the simulation since it is not a real sample.



-- Clicking "Config Text" creates a printable notebook with the details of the current configuration:



USANS Instrument Configuration:

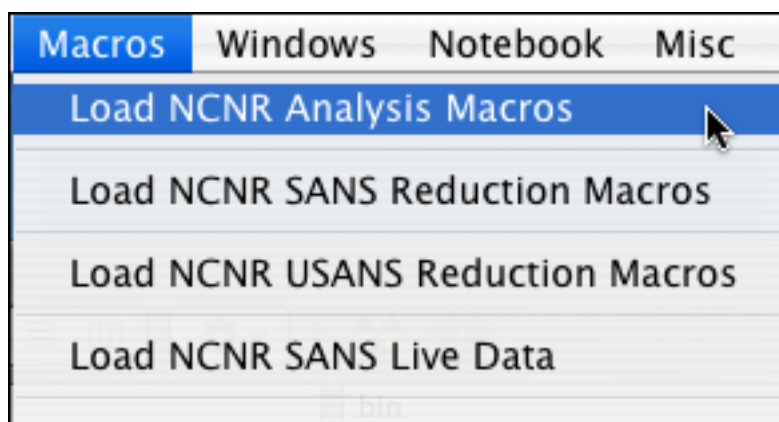
Theta Min	Theta Max	Increment	# Points	Count Time
-1.000	0.600	0.050	33	25
0.700	1.900	0.100	13	100
2.000	4.800	0.200	15	300
5.000	9.500	0.500	10	600
10.000	19.000	1.000	10	1200
20.000	48.000	2.000	15	2000
50.000	95.000	5.000	10	3000

Total Counting Time (HR:MIN) = 23:30

### **Plotting a Model for Simulation**

(new for 2014) - Real-space structures can now be used as the "model" function for simulation. Draw the real space structure first, then plot the model "GenericFFT". Set N=256 and T=5 for a reasonable q-range.

SANS and USANS instrument simulations can be done with default model functions. However, to better refine the setup and to get solid estimates of expected counting times and statistics, a more detailed simulation can be carried out. The simulation is only as realistic as the input model function. You can choose from any of the model functions available for analysis, entering parameter values that are close to what you expect for your sample. To get started, load the analysis package:



Then pick any model function that is appropriate for your experiment (see [SANS Model Picker](#)) and then plot that model (See the [Fit Manager](#), and the description of the "Plot 1D Function Button"). The section [Plotting a Model Function](#) shows these steps in detail. You only need to plot the unsmeared model, and the q-range is not that important, unless you want to append the model to the simulation for comparison. You can append the model function to the SASALC window if you like. A smeared version is automatically appended to the UCALC window. Once you have plotted the function then simply adjust the coefficients in the table to appropriate values. During the simulation, you can change the parameters and re-run the simulation. That's an important part of the experiment design process.

To get a true feel of whether an experiment is "feasible" - that is you have enough signal above background, you need to add in an appropriate incoherent background. As a general rule of thumb (NOT a hard and fast rule):

- For a sample with fully deuterated solvent (D2O or d-organics), use a value of 0.05 (1/cm)
- For a sample with fully hydrogenated solvent (H2O or h-organic), use a value of 1.0 (1/cm)
- If your sample is a mixed solvent, use a linear combination of the above values. That is if you have a solvent that is 70:30 D2O:H2O, the incoherent background will be approximately 0.3 (1/cm)

Once you've plotted an appropriate model, proceed to:

[Simulation of 1D SANS Data](#)

[Simulation of 2D SANS Data](#)

[Simulation of USANS Data](#)

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### **Simulation of 1D SANS Data**

For the 1D simulation of SANS data:

Start with an analysis model that represents your expected scattering. See [Plotting a Model for Simulation](#). The q-range is not that important. The parameters are, however, since they must correctly represent the concentration, size, contrast, incoherent background, etc. of your sample. In this example, we'll use the LogNormalSphere model function, representing polydisperse spheres. The Fit Manager window looks like:



- Set the sample transmission: (use your best guess). Remember that if you increase the sample thickness, you should also decrease the transmission.

**Checkboxes:**

- Yes Offset: When checked, this will offset the frozen 1D traces so that they do not overlap
- Abs Scale?: When checked, the simulation is converted to absolute scale rather than raw detector counts.
- Noise?: Will add noise to each data point within the counting statistics of the simulation.

--Then - clicking "Do 1D Simulation" or changing any of the instrument configuration parameters will simulate the counts you would get, based on the setup.

**What the results are:**

The main result is the simulated 1D data set, as if you measured the "sample" specified by the model function at the specified configuration and time.

**Values also reported are:**

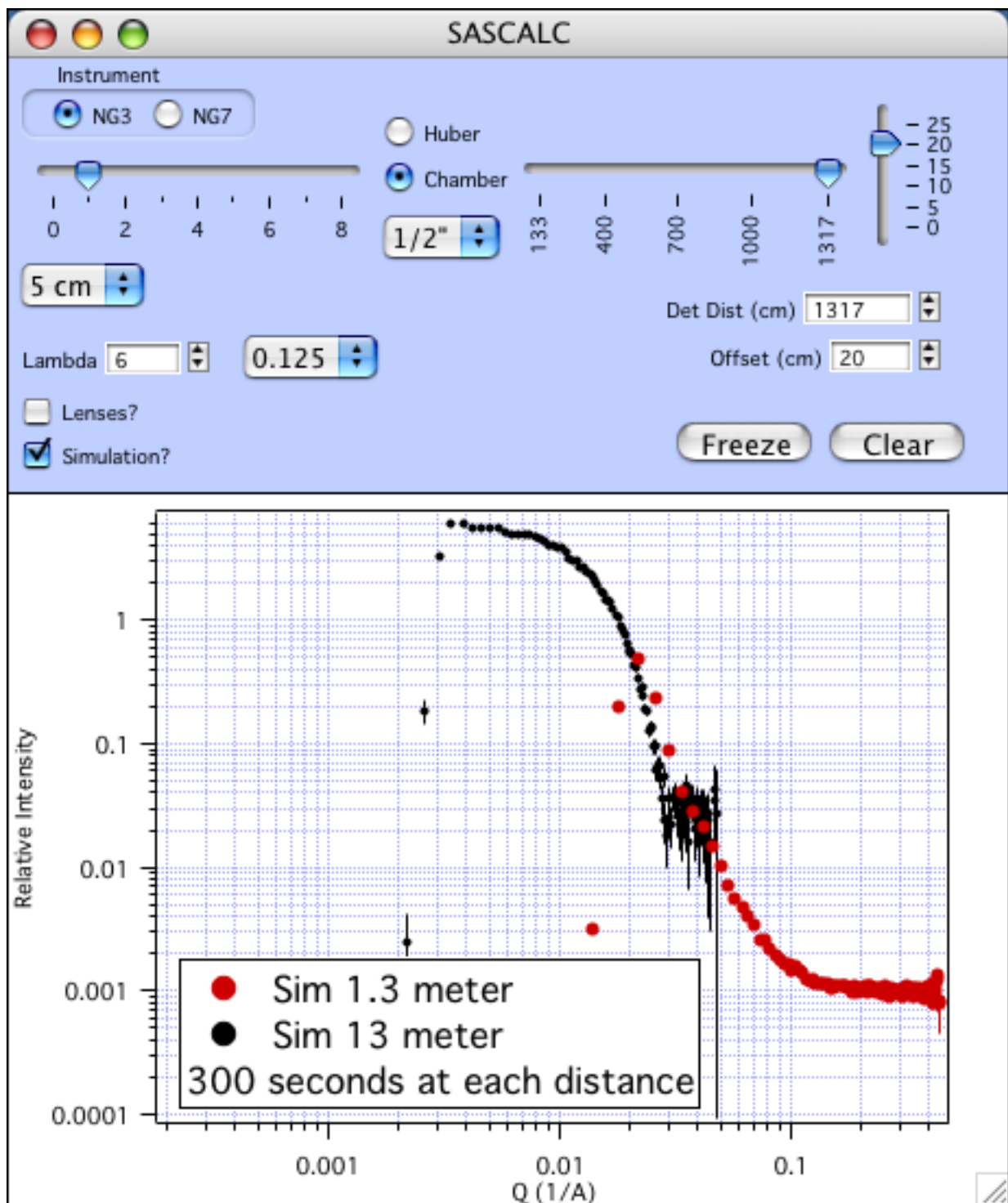
- Total Detector Counts: as would be collected on the 2D detector
- Estimated count rate: an estimate of the total detector count rate
- Fraction of the beam scattered: This is the fraction of the beam that is scattered coherently. It should be a rather low number.
- Estimated transmission: this is an estimate of the transmission due simply to small angle scattering. No effect of absorption or incoherent scattering is included here, so this number may have little correlation with the true, measured transmission.

These are the results for a typical 13 m sample-to-detector configuration:

The screenshot shows the '1D SANS Simulator' window. On the left, under 'Model Function', 'LogNormalSphere' is selected. Below this is the 'Sample Setup' section with input fields for 'Counting time(s)' (300), 'Thickness (cm)' (0.1), and 'Sample Transmission' (0.8). At the bottom left are two buttons: 'Do 1D Simulation' (green) and 'Save Simulated Data' (grey). To the right of these buttons are three checkboxes: 'Yes Offset' (unchecked), 'Abs scale?' (checked), and 'Noise?' (checked). On the right side of the window is the 'Simulation Results' section, which displays four values in text boxes: 'Total detector counts' (47226.6), 'Estimated count rate (1/s)' (157.422), 'Fraction of beam scattered' (0.000336411), and 'Estimated transmission' (0.999664).

And then overlapped with a 1.3 m sample-to-detector configuration:





**These simulated configurations need improvement in a number of areas:**

- The counting statistics at the high-q end of the 13m configuration is very poor. To improve this, plan to count for longer than 300 seconds, use a thicker sample, or try to improve the flux on sample. You'll quickly find out that you need to count a lot longer to significantly improve the statistics at the highest q-values (3600 s or more!), while the lowest q-values need only a fairly short counting time (maybe 900 s) to collect very good statistics.
- The overlap region is not good. There are oscillatory features in the data right at the overlap. There

are not many data points in the overlap. The 13 m data is (and will be) noisy there, and the 1.3 m data is significantly resolution-smeared at its low-q end, which is very close to the beam stop. All of these reasons make for very bad overlap. The remedy here is to measure at a third sample to detector distance, in between 1.3 m and 13 m (try near 4 m). Then only the "good" data from each configuration is kept.

#### What happens in the calculation is:

- A "fake" work data folder is created named "SAS" to hold a blank 2D detector image and its associated waves. It is then "averaged" to 1D, to a folder named "Simulation", so that this has all of the associated waves and resolution information. (nCells, Simulation\_q, Simulation\_i, etc. are needed here, so the simulation can fill them in)

The probability,  $p$ , that a neutron is scattered into a  $q$ -value (or equivalently a  $q$ -bin centered at  $q$ ) is:

$$p(q) = T_{sam} d_s (\Delta\Omega) I_{smeared}(q)$$

where  $T_{sam}$  is the sample transmission,  $d_s$  is the sample thickness,  $\Delta\Omega$  is the solid angle of the detector pixel, and  $I(q)$  is the expected (model) scattering at that  $q$ -value, smeared with the resolution.

The simulated intensity is then:

$$I_{sim}(q) = i_{beam} \cdot t \cdot p_i(q)$$

where  $i_{beam}$  is the beam intensity from SASCALC (counts/s) and  $t$  is the counting time. Then from the 1D averaging of the "fake" 2D detector as specified by SASCALC, the number of detector pixels that contribute to each  $q$ -bin are known. So then before noise is added or absolute scaling is done, the total detector count is calculated as:

$$total\ counts = \sum_{N_q} I_{sim}(q) \cdot N_{cells}(q)$$

The standard deviation of the intensity for each  $q$ -bin is not  $\sqrt{counts}$ , but is properly treated as the standard deviation of the intensity that has been measured  $N_{cells}$  times at each  $q$ -value. See John Barker's memo from 8/9/99 for details.

$$\sigma(q) = \sqrt{\frac{I_{sim}(q)}{N_{cells}(q)}}$$

If desired, random noise is added to the simulated data at each  $q$ -value by selecting a new point based on a Gaussian (normal) distribution at each point. If absolute scaling is desired,  $\kappa$  is calculated as:

$$\kappa = T_{sam} d_s (\Delta\Omega) i_{beam} \cdot t$$

which essentially "un-does" all of the sample and instrument information that led to the simulated data.

Although not directly used in any of the simulation, some additional parameters are calculated and

reported in the results section. The total cross section due to small angle scattering is calculated using the unsmeared model function and the coefficients with the last point set to zero (the incoherent background).

$$\Sigma_{SAS} = \lambda \int_0^{q_u} \left\{ \frac{\sin \left[ 2 \arcsin \left( \frac{q\lambda}{4\pi} \right) \right] I(q)}{\sqrt{1 - \left( \frac{q\lambda}{4\pi} \right)^2}} \right\} dq$$

In practice, the numerical integration is carried out from [1e-4,qu\*(1-1e-10)] to avoid numerical issues. Then the total scattering probability is:

$$\tau \equiv d_s \Sigma_{SAS}$$

Tau is the average number of times that any neutron is scattered. The sample transmission can be estimated as:

$$T = \exp(-\tau)$$

Note that this is the transmission due to small angle scattering only. Absorption, incoherent scattering, and inelastic scattering are ignored. So then the fraction of the beam that is small angle scattered is what is not transmitted, and is simply (1-T)

### What assumptions are behind all of this?

- Only single scattering is considered. No multiple scattering effects are included. A full 2D simulation is required for multiple scattering.
- The empty cell is not included as part of the sample.
- Background is not included.
- Incoherent scattering is included, to the extent it is entered in the model function.
- Resolution smearing is incorporated in the simulated data set
- The unsmeared model is used only for estimation of transmission and fraction of coherent scattering
- The number of pixels on the detector at each q-value is taken into account when determining the total count on the detector and the count rate.

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### **Simulation of 2D SANS Data**

The 2D Monte Carlo Simulation of SANS Data is a normally hidden feature. It's slow, and results must be interpreted carefully. It however, does give information about multiple scattering that the 1D simulation cannot. The simulation of the scattering is done in 2D. Then the 1D averaged data is shown in the SASCALC graph, and the 2D data can be viewed.

Start with an analysis model that represents your expected scattering. See [Plotting a Model for Simulation](#). The q-range is not that important. The parameters are, however, since they must correctly represent the concentration, size, contrast, etc. of your sample. (But not the incoherent background -- this is set separately - see below). In this example, we'll use the LogNormalSphere model function,

representing polydisperse spheres. The Fit Manager window looks like:

parameters_Ins	coef_Ins	Hold_Ins	LoLim_Ins	HiLim_Ins	epsilon_Ins	
Volume Fraction	0.1	0			1.0001e-06	
exp(mu)=media	100	0			0.006	
sigma	0.1	0			2.00001e-05	
SLD sphere (A-	1e-06	0			2e-10	
SLD solvent (A-	6e-06	0			3e-10	
bkg (cm-1 sr-	0.065	0			1e-10	

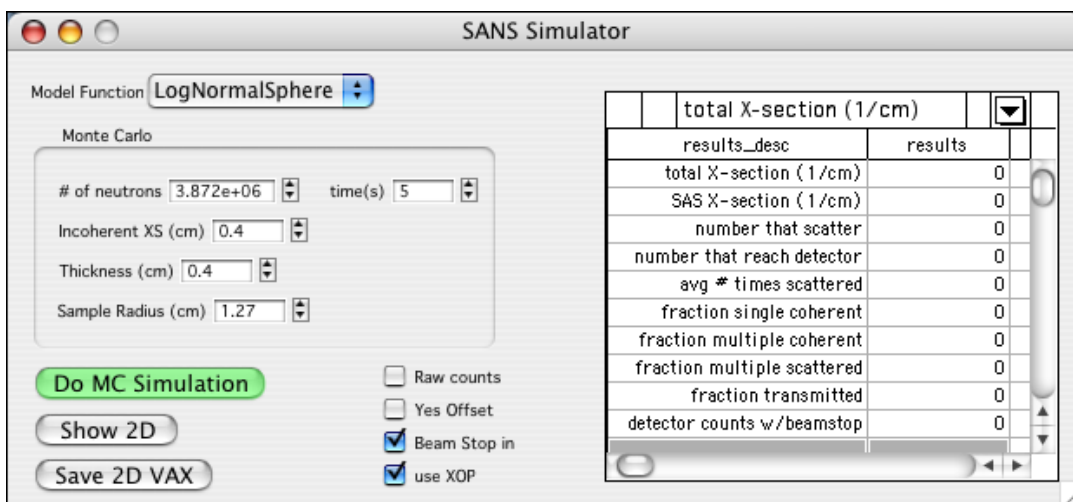
--Open the [SASCALC](#) panel, and set the instrument to a new configuration.

--Click here to set the flag to allow 2D simulation:



Set\_2DMonteCarlo\_Flag(1)

--Check the "Simulation" checkbox in the SASCALC panel, and the SANS Simulator panel will open (If the title has "1D", it's the wrong panel)



Now you can adjust the collimation as usual with the SASCALC controls. The additional panel (plus the function and coefficients set in the Fit Manager) controls the details of the model that is plotted or simulated. Note that adjusting the collimation parameters plots a resolution-smeared version of the model and does not do a simulation. Since the simulation can be very slow, you must manually initiate the simulation.

#### What you can set in the panel:

- Set the function: This must be the unsmeared model. The parameters used for the simulation are those set in the fit manager panel. If you see an alert that "no model function is plotted...", re-select the model function from the popup list even if it looks like it's selected.
- Set the # of neutrons OR the counting time: Setting the number of neutrons uses just that number of neutrons for the simulation. Setting the time multiplies the beam flux (at the current configuration) to get the total incident number of neutrons. You in general won't ever want to do a simulation of a real counting time (unless you can wait until tomorrow).
- Set the incoherent cross section (per unit volume): Empirically, for H<sub>2</sub>O in a 1 mm cell, use XS=3.9 (1/cm). For D<sub>2</sub>O in a 1 mm cell, use XS=0.33 (1/cm). Solvent mixtures and different path lengths will give different results due to incoherent multiple scattering. Don't even think of calculating the "proper" value to use. There are too many real issues with the incoherent scattering from water to include in the simulation. See [Approximate Incoherent Cross Section](#) for other empirical values to use.
- Set the sample thickness: (in cm)
- Set the sample radius: this is the sample radius, not the sample aperture radius. Use 1.27 cm for a (1" diameter) banjo cell, and 0.95 cm radius for a 3/4" diameter titanium cell.

#### Checkboxes

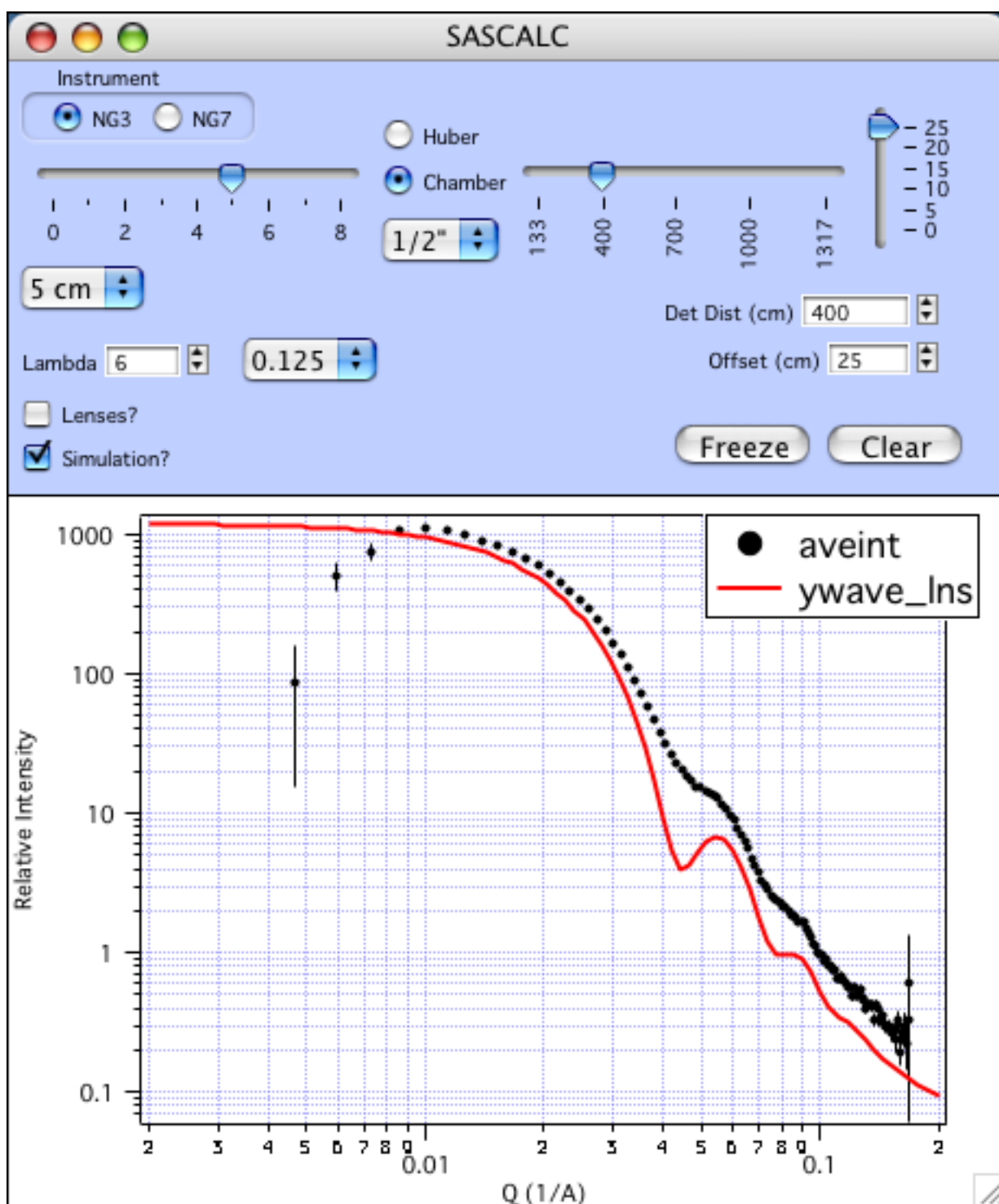
- Raw counts: This should typically be checked; to simulate the total detector counts. Otherwise, it will convert the simulated data to absolute scale.
- Yes Offset: When checked, this will offset the frozen 1D traces in the SASCALC graph so that they do not overlap.
- Beam Stop In: masks out the SASCALC-specified beam stop area in the 2D simulated data, effectively cutting out the transmitted beam.
- Use XOP: Always leave checked to use the much faster XOP code. Unchecked uses the development code in Igor.

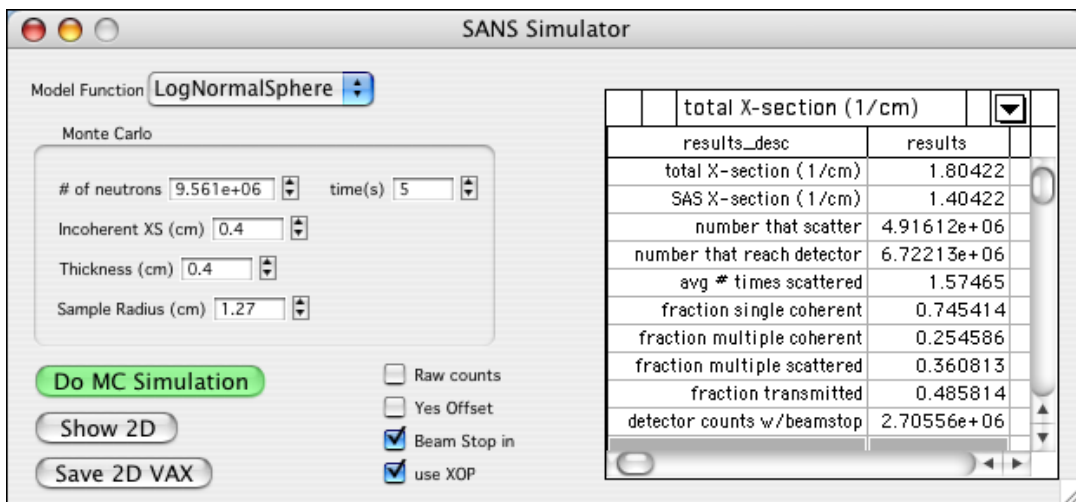
To do the simulation - click on "Do MC Simulation". If the calculation is going to be lengthy, you will be warned and given the chance to abort the simulation.

**NOTE:** the Monte Carlo simulation is ONLY done if you click the button. Changing the instrument configuration parameters in SASCALC will trigger a recalculation, which will be a plot of the smeared model intensity, not a simulation.

**What the results are:**

The main result is the simulated 2D (and 1D) data set, as if you measured the "sample" specified by the model function at the specified configuration and time. In the plot below, the "perfect" model calculation has been appended to the SASCALC graph. Note that both of the data sets are on absolute scale, even though the simulated data points are offset to higher intensity. This is a direct consequence of multiple coherent scattering (25%) and has a very detrimental effect on the data. The sample conditions should definitely be changed. Measuring under these conditions will yield data that cannot be correctly analyzed. Using a thinner sample, reducing the concentration, or reducing the contrast are all ways to reduce the scattering probability and obtain better data.



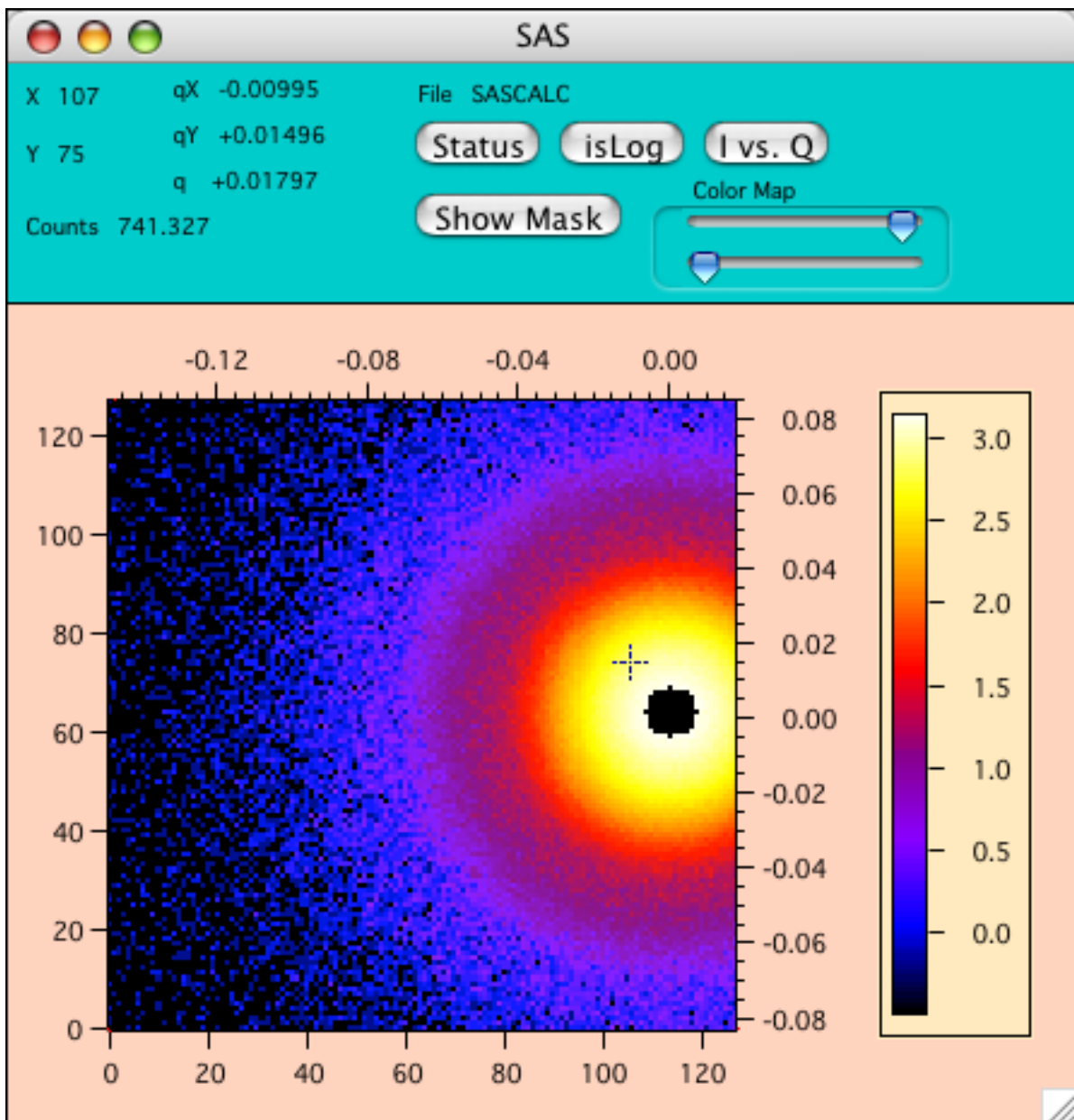


#### Values reported in the table:

- Total X-section: the sum of the coherent and incoherent scattering cross sections.
- SAS X-section: The coherent small angle scattering cross section as calculated from the model scattering function (as detailed below).
- Number that scatter: This is the total number of neutrons that scatter at least once, either coherently or incoherently. With the number of incident neutrons, it can be used for calculating the transmission.
- Number that reach detector: This is the number of neutrons that reach the detector minus the number of neutrons at  $Q=0$ . Since there is no beam broadening, this is the single pixel [xCtr][yCtr].
- Avg # times scattered: Of those neutrons that are scattered, the average number of times that it is scattered. Calculated as the total number of scattering events divided by the number of neutrons that scatter. Coherent and incoherent scattering events are both included and not differentiated. This number should be not much larger than one.
- Fraction single coherent: This is the fraction of coherently scattered neutrons that are scattered coherently, once.
- Fraction multiple coherent: This is the fraction of coherently scattered neutrons that are scattered coherently, more than once.
- Fraction multiple scattered: This is the fraction of scattered neutrons that are scattered more than once. Scattering can be either coherent or incoherent, or a mixture.
- Fraction transmitted: This is the fraction of unscattered neutrons.
- Detector counts w/ beam stop: this is the total number of detector counts outside the area shadowed by the beam stop. Directly comparable to the total detector counts you would expect in a scattering experiment.

"Show 2D" plots the 2D data as you are used to seeing.





#### What happens in the calculation is:

- A "fake" work data folder is created named "SAS" to hold a blank 2D detector image and its associated waves. It is then averaged to 1D, to a folder named "Simulation", so that this has all of the associated waves and resolution information. (nCells, Simulation\_q, Simulation\_i, etc. are needed here, so the simulation can fill them in).

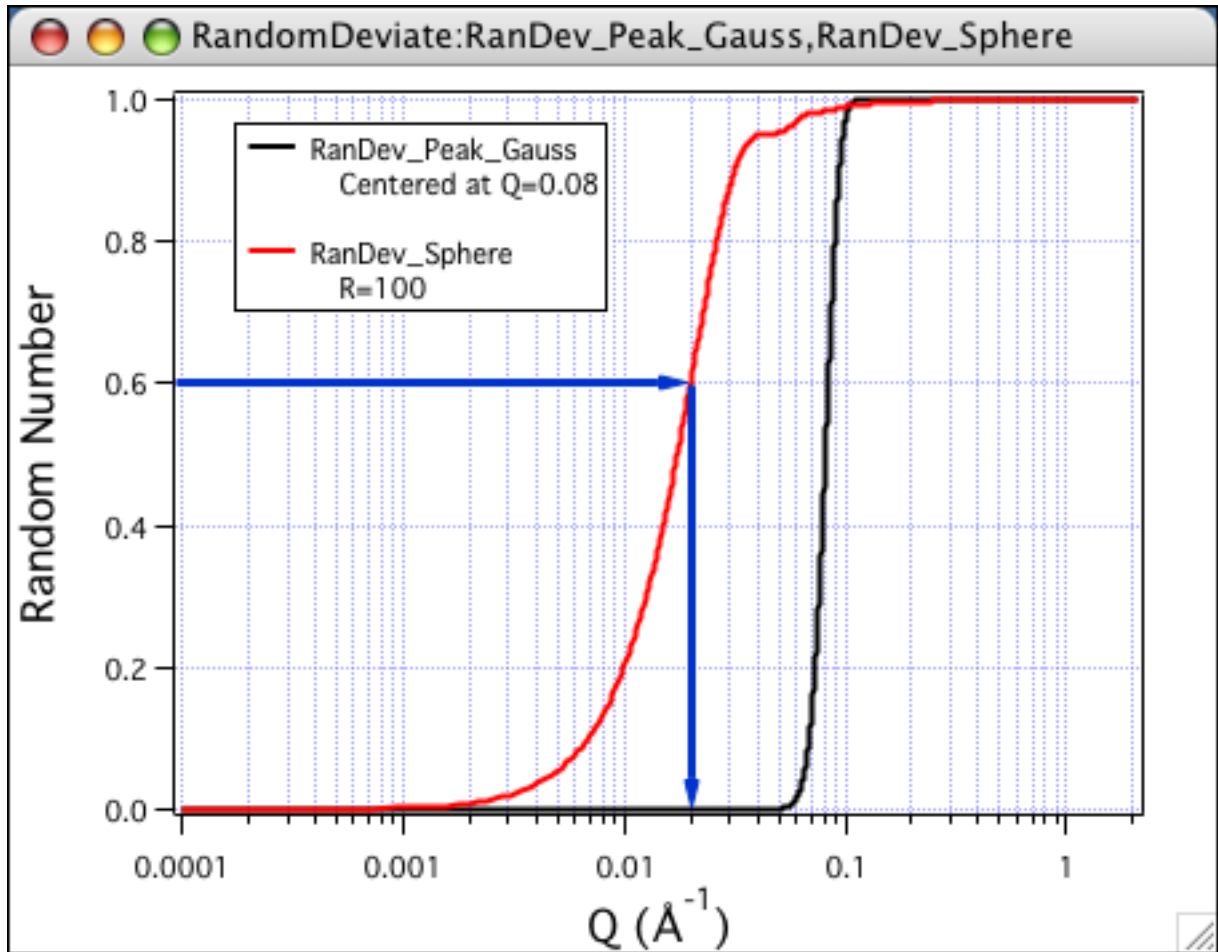
The most important calculation is the random deviate,  $R$ , a cumulative probability function that maps a random number  $[0,1]$  to the probability of scattering at a given  $q$ -value.

$$R = \frac{G(q)}{G(q_u)}$$

$$G(q) \equiv \lambda \int_0^q \left\{ \frac{\sin \left[ 2 \arcsin \left( \frac{q\lambda}{4\pi} \right) \right] I(q)}{\sqrt{1 - \left( \frac{q\lambda}{4\pi} \right)}} \right\} dq$$

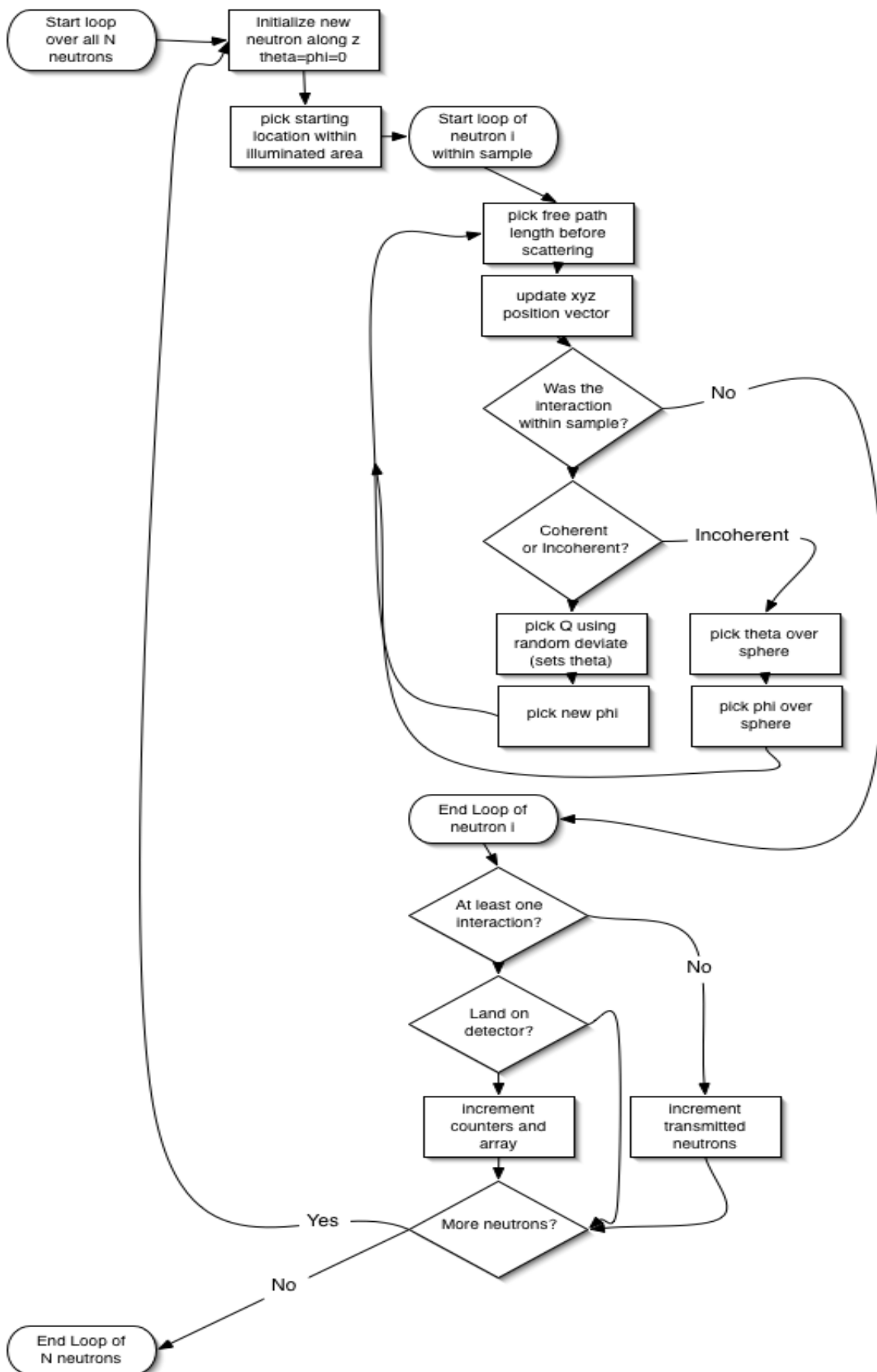
$$q_u = 4\pi / \lambda$$

In practice, the numerical integration is carried out from  $[1e-4, q_u*(1-1e-10)]$  to avoid numerical issues. Two examples of the random deviate function, R, are plotted below. For the case of a gaussian peak centered at  $Q=0.08$ , it is clear that most random numbers will map to scattering at a  $q$ -value near 0.08, the most likely  $q$ -value for scattering to occur. The probability of scattering at other  $q$ -values is low, needing a random number very close to zero, or very close to one. The mapping for a sphere scattering is somewhat different, and has some features of sphere scattering, but is monotonic after the calculation so there is a 1:1 mapping.



Then the Monte Carlo simulation begins. The flowchart describes the progress as a neutron passes through the sample and interacts. For each of the choices, random numbers  $[0,1)$  are generated and mapped to the range as needed.





Once the simulation is complete, the simulated 2D data file is averaged to 1D as usual and displayed on the SASCALC graph.

#### **What assumptions are behind all of this?**

- Multiple coherent and incoherent scattering is included, but not all of the subtle instrumental resolution effects are. So the resolution smearing may be slightly different than a real instrument since not all of the instrumental imperfections can be included.
- The wavelength spread is explicitly included, choosing the wavelength of each incoming neutron based on the wavelength spread.
- Divergence of the incoming beam is included. The incoming angle is calculated based on the incoming neutron trajectory through the source and sample apertures. This allows for a realistic view of the transmitted beam.
- Gravity fall of the neutrons is included, accounting for the wavelength spread.
- Absorbance is not included
- The empty cell is not included
- Background is not included
- Incoherent scattering is included, to the extent that the incoherent cross section is correctly entered

#### **Approximate Incoherent Cross Section**

Incoherent scattering as calculated typically does not agree with measured levels. That is certainly the case in this simulation which does not capture every aspect of scattering. So empirical values for the input incoherent cross section have been determined based on the known hydrogen content of the sample. If you know the fraction of hydrogenated material in your sample, then the estimated background to use (1/cm) is in the second column. Here I've assumed that D<sub>2</sub>O or some other deuterated material is the remainder of the sample. Mass fraction or volume fraction is fine, since this is an estimate. Then the next three columns give the suggested incoherent cross section to input to the simulation to give the expected level of background in the output. A lower input cross section is needed to give the same output level for thicker path length, possibly due to the increased multiple incoherent scattering.

fraction_H	estimated_BKG	use_incXS_1mm	use_incXS_2mm	use_incXS_4mm
1.0	1.0	3.9	3.1	2.6
0.9	0.9	3.6	2.9	2.4
0.8	0.8	3.3	2.7	2.2
0.7	0.7	2.9	2.5	2.1
0.6	0.6	2.6	2.2	1.9
0.5	0.5	2.3	2.0	1.7
0.4	0.4	1.9	1.7	1.4
0.3	0.3	1.5	1.3	1.1
0.2	0.2	1.0	0.92	0.79
0.1	0.1	0.54	0.48	0.42
0.0	0.06	0.33	0.3	0.26

-----

#### **Simulation of USANS Data**

For the simulation of USANS data:

Start with an analysis model that represents your expected scattering. (See [Plotting a Model for Simulation](#)) Plot the unsmeared model function. The q-range is not that important. The parameters are, however, since they must correctly represent the concentration, size, contrast, incoherent background, etc. of your sample. This example is using a model of Schulz polydisperse spheres for the simulation. Once you have a model function plotted and some reasonable parameters entered, the Fit Manager

window looks like:

R6	parameters_sch	coef_sch	Hold_sch	LoLim_sch	HiLim_sch	epsilon_sch	
	Volume Fraction (sca)	0.01	0			1.0001e-06	
	mean radius (A)	8000	0			0.006	
	polydisp (sig/avg)	0.1	0			2.00001e-05	
	SLD sphere (A-2)	1e-06	0			2e-10	
	SLD solvent (A-2)	3e-06	0			4e-10	
	bkg (cm-1 sr-1)	0.001	0			1.001e-07	

--Open the [UCALC](#) panel, and set the angle ranges or choose a preset.

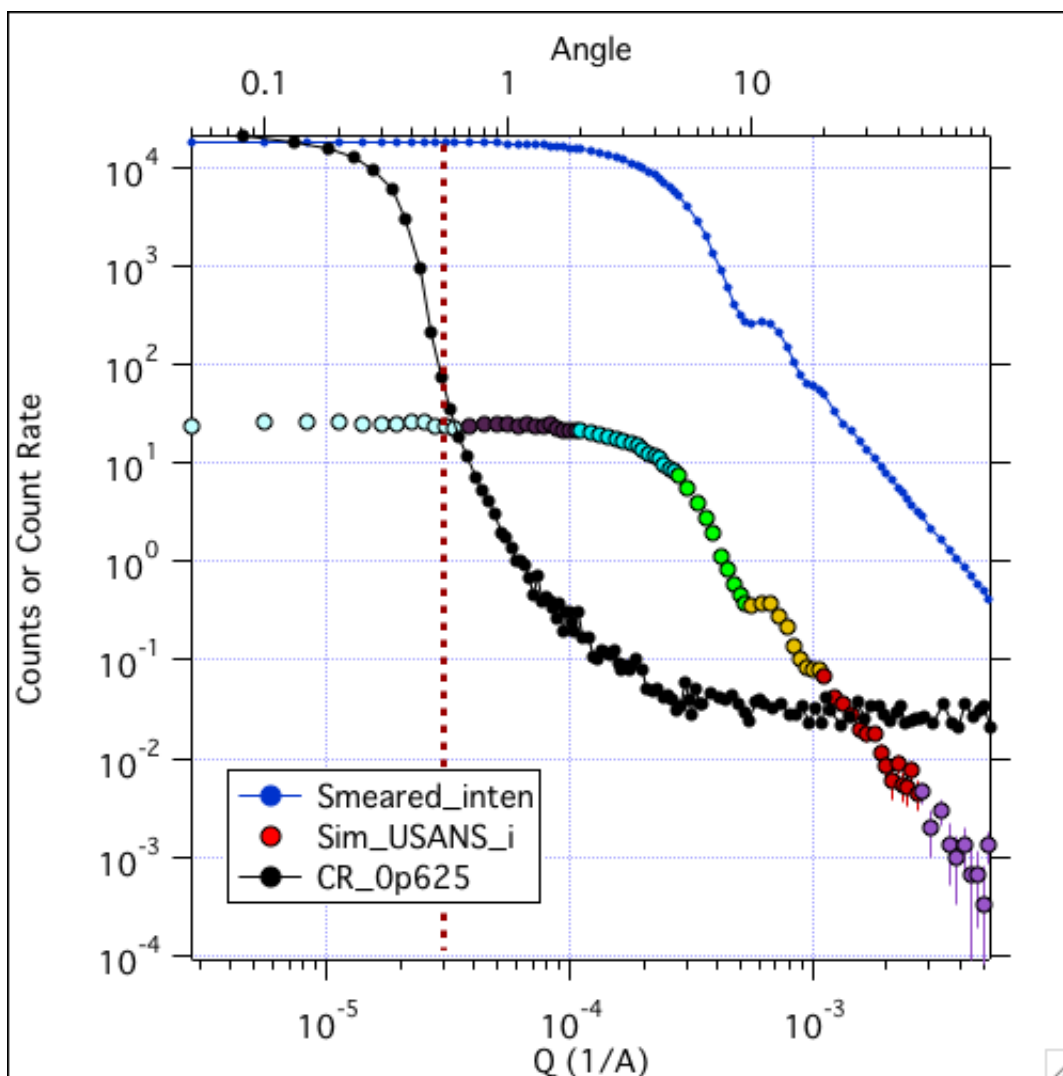
-- Then in the Sample Setup, be sure to select the function, sample thickness, and transmission:

--Clicking "Simulate USANS" will simulate the counts you would get, based on the model and the instrument setup. Since the slit-smearing calculation can be lengthy, you must manually update the plot any time you change the setup of the instrument or the coefficients of the model function.

### What the results are:

The main result is the simulated 1D data set, as if you measured the "sample" specified by the model function at the specified angular ranges and times. The simulated data points are color coded for each angular range. "Smeared\_inten" is the expected smeared intensity, but is NOT plotted on the

same scale as the simulated data, which is typically plotted as count rate on the detector. "CR\_n", if plotted, is the countrate from an empty sample aperture of the size you selected.



### How do I interpret the results?

- The dotted vertical line is at  $q = 3e-5$  (1/A) and represents the minimum q-value that can be measured in practice. Your sample may not do this well.
- The interval centered on zero angle is necessary to measure transmission and to establish  $q=0$ .
- At higher  $q$ , the simulated sample count rate approaches or is below the count rate of the empty aperture. At this point, don't bother counting to larger angles, or for longer times. (A thicker or more concentrated sample might help, though, so change your sample conditions and re-run the simulation). In the above example, nearly 16 hours of the 23.5 hours of counting are spent on the largest two angle ranges. Since the scattering is expected to be at or below the empty scattering, it is best to not measure these intervals. Then only 7 hours are required, rather than 23.5 hours.

### What happens in the calculation is:

- The angular ranges and count times specified by the Instrument Setup are "loaded" as individual files as if they were raw BT5 files, generating the necessary files to carry along. As for "real" data, the data is loaded into a SWAP folder, then concatenated into the SIM folder.

- All the angular ranges are sorted and the angle is converted to Q.
- Then a fake data folder "Sim\_USANS" is created as if a reduced USANS data set was loaded. No matrix is generated since the smearing calculation must be done point-by-point using the trapezoid rule (since it can only be done per interval).

Once the folders are created, the simulation can be carried out. The probability,  $p$ , that a neutron is scattered into a  $q$ -value (or equivalently a  $q$ -bin centered at  $q$ ) is:

$$p(q) = T_{sam} d_s (\Delta\Omega) I_{smeared}(q)$$

where  $T_{sam}$  is the sample transmission,  $d_s$  is the sample thickness,  $\Delta\Omega$ , is the solid angle of the detector (=  $7.1 \times 10^{-7}$  steradians), and  $I(q)$  is the expected scattering at that  $q$ -value, slit-smeared (since this is what the detector sees).

The simulated intensity is then:

$$I_{sim}(q) = i_{beam} \cdot t \cdot p_i(q)$$

where  $i_{beam}$  is the beam intensity (counts/s, based on the aperture diameter) and  $t$  is the counting time. The number of counts is rounded to an integer. The standard deviation of the intensity for each point is then  $\sqrt{\text{counts}}$ .

If desired, random noise is added to the simulated data at each  $q$ -value by selecting a new point based on a Gaussian (normal) distribution at each point, again rounding the count value to an integer.

To plot as count rate, the simulated intensity and errors are divided by the counting time.

#### **What assumptions are behind all of this?**

- Only single scattering is considered. No multiple scattering effects are included. A full 2D simulation would be required for multiple scattering.
- The contribution of the empty cell is not included in the simulated data set (just shown). There is little difference between the empty aperture and an empty cell.
- Instrumental background is not included
- Incoherent scattering is included, to the extent it is entered in the model function. It is typically not important in the  $q$ -range of USANS.
- Resolution smearing (slit smearing) is incorporated in the simulated data set

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#### • **Simulating a Run List**

SRK NOV 2014

This is a control panel that makes it much easier to simulate SANS from any type of sample over a variety of sample conditions and instrument configurations. In this way, a complete experiment can be simulated either in 1D or 2D. Like a real SANS instrument, a run list can be built up from samples and configurations, and run unattended.

#### Quick Overview

From the Macros Menu, choose "Load Simulation Run Builder". This will load both the SANS Reduction package, and the Analysis package. These are both necessary for simulation.



Then from the Macros Menu, choose "Simulation Scripting - Beta -> Run List Panel". This will open the main control panel for building a run list. Once all is open and compiled, save the experiment so the data you generate will have somewhere to go.

(1) First, adjust the instrument configurations to those you would like to test, and save each of them from the Configurations tab, click "Store Config". Add a descriptive tag to identify the configuration ("Config\_" will be automatically added as a prefix). You will want to do this in conjunction with step (2), setting the samples.

(2) Next, set the different samples. Plot the desired model and adjust the coefficients to match what you want the sample to be. Then from the "Setup Samples" tab, enter all of the following information:

Sample Label: be descriptive, this will be the label in the raw data file.

Thickness

Sample Transmission (only used for 1D)

Incoherent XS (only used for 2D)

Sample radius (only used for 2D)

Then "Store Sample" ("Sam\_" is added as a prefix). Treat each different set of coefficients, sample thickness, incoherent XS, etc. as a separate "sample"

(3) Setup the runs. From the "Setup Runs" tab. Pick the configuration and sample (the sample label will show up). Edit the sample label as needed. Check ABS or noise as desired, enter the count time, and the file name to use (only for 1D data - 2D data is named using the run index)

Last, click "Add to Run List", and it will add the sample at the selected configuration, check the run, and step to the next run.

(4) Run the "experiment". Click "Run Selected 1D" (or 2D).

(5) Do what you wish with the output. If 1D, plot it. If 2D, you can inspect the raw data, and reduce it as normal data (with a few important points to remember - see below)

Below is a detailed listing of everything on the panel, followed by an example simulated experiment of particles as a function of concentration that shows the effect of multiple scattering.

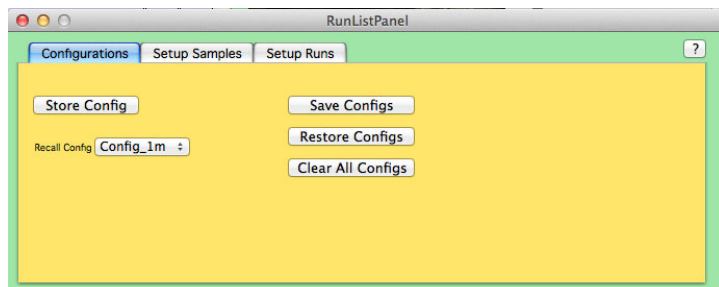
### The Run List Panel

Run	Config	Sample	Sample Label	Count Time	Save Name	Abs ?	Noise
0	Config_1m	Sam_mine	My favorite sample	300	Simulation.abs	1	1
1							
2							
3							
4							
5							
6							
7							
8							
9							
10							
11							
12							
13							
14							
15							

Initially, the popup menus will show "error" and the run list will be blank until you have configurations and samples to populate the menus. A detailed description of what is on each tab is below. Help is always available from the "?" button on the upper right corner of the panel.

### What's on each tab?

#### Configurations Tab



Store Config: Button to store (in memory) the current instrument configuration as defined by SASCALC. "Config\_" is added as a prefix to whatever descriptive name you enter.

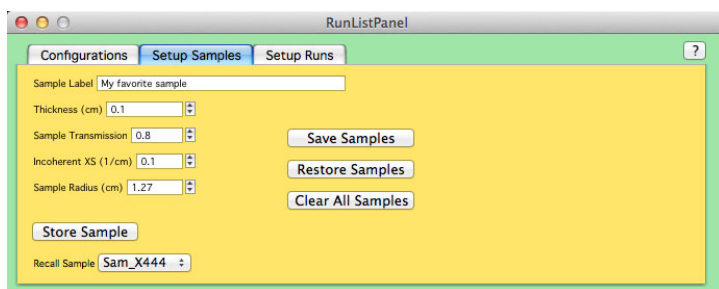
Recall Config: A popup list of all of the stored configurations (those with names starting in "Config\_"). When a configuration is selected, SASCALC moves to that configuration and recalculates the scattering from the current model function.

Save Configs: Save all of the configurations to an Igor text file, for later recall.

Restore Configs: Load a set of configurations from an Igor text file.

Clear All Configs: Clear all of the stored configurations from memory.

#### Setup Samples Tab



Sample Label: Enter a descriptive sample label. This will be the sample label saved to either the 1D or 2D data files

Thickness (cm): as it says.

Sample Transmission: set this for samples you plan to run as 1D simulations. For 2D simulations the actual transmission is simulated, and this value is ignored.

Incoherent XS (1/cm): see the simulation help file (or the 2D simulation panel) for more details of how to properly set this cross section to match the expected macroscopic incoherent background. This value is only used for 2D simulation, and ignored for 1D simulations. For 1D simulations, the

incoherent level is taken from the background value as set by the model coefficients.

Sample Radius (cm): The actual sample radius, not the sample aperture radius. This is typically 1.27 cm for a 2.54 cm diameter quartz cell. Titanium cells have a slightly smaller inner ring.

NOTE: These 5 items to fill in are part of each "sample". If you want a thicker/thinner sample, different incoherent cross section, etc., change the values and store as a separate sample.

Store Sample: Button to store (in memory) the current sample conditions as defined by the parameters above and the coefficients of the current model on the Curve Fit Setup Panel. "Sam\_" is added as a prefix to whatever descriptive name you enter.

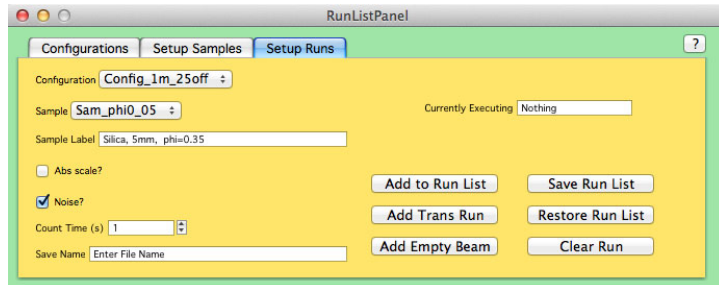
Recall Sample: A popup list of all of the stored samples (those with names starting in "Sam\_"). When a sample is selected, The Curve Fit Panel is reset to that sample condition, and SASCALC recalculates the scattering from this selected model function.

Save Samples: Save all of the configurations to an Igor text file, for later recall.

Restore Samples: Load a set of samples from an Igor text file. It is up to you to be sure that the proper model functions are loaded and plotted before trying to "run" a sample.

Clear All Samples: Clear all of the stored samples from memory.

## Setup Runs Tab



Configuration: Pick the configuration you want to use from the popup

Sample: Pick the sample you want to "measure" from the popup. The sample label for this sample will update in the field below

Sample Label: Change the sample label as needed. Add any other specifics about the simulation time, etc. or change the label to reflect that it is a transmission or empty beam run.

Abs Scale?: Check this for output in absolute scale. Typically use absolute scale for 1D simulations and un-check for 2D simulation to obtain "RAW" SANS data that can be directly compared with real experimental data.

Noise?: Keep this checked for 1D simulations to get a realistic level of statistical noise in the output data. This is ignored for 2D simulation where noise is inherent in the MC simulation.

Count Time (s): Set the counting time for the run. Note that this is not the actual time it will take for the computer to run the simulation.

Save Name: Enter the file name to save the 1D simulation. For 2D simulation, default "VAX" filenames are generated using the starting Run Index (found above the Run List).

Add to Run List: With the run conditions set, this will add the run to the selected row of the run list.

Add Trans Run: This will add a transmission run at the set conditions. Be sure to change the sample label to reflect that this is a transmission measurement. This will set the count time to 1 s and automatically remove the "beam stop" from the simulation. This is only meaningful for a 2D simulation.

Add Empty Beam: This will add an empty beam run at the set conditions. Be sure to change the sample label to reflect that this is an empty beam measurement. This will set the count time to 1 s and automatically remove the "beam stop" from the simulation. This is only meaningful for a 2D simulation.

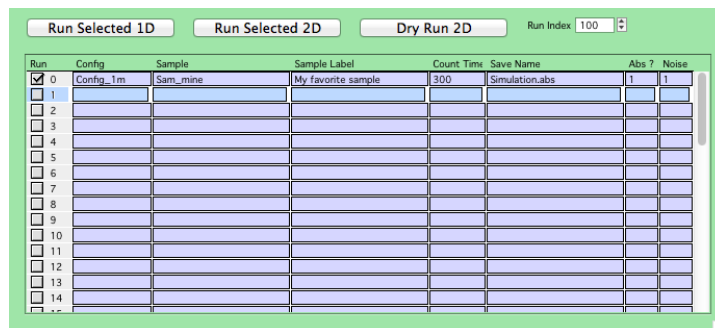
Save Run List: This saves the entire run list to an Igor text file for later recall.

Restore Run List: Restores the run list from a previously saved run list. This will overwrite anything currently in the list.

Clear Run: Clears the selected row in the run list. Clears one row only.

Currently Executing: while a 2D simulation is in progress, this field will update with the currently running row.

## The Run List



Run	Config	Sample	Sample Label	Count Time	Save Name	Abs ?	Noise
<input checked="" type="checkbox"/> 0	Config_1m	Sam_mine	My favorite sample	300	Simulation.abs	1	1
<input type="checkbox"/> 1							
<input type="checkbox"/> 2							
<input type="checkbox"/> 3							
<input type="checkbox"/> 4							
<input type="checkbox"/> 5							
<input type="checkbox"/> 6							
<input type="checkbox"/> 7							
<input type="checkbox"/> 8							
<input type="checkbox"/> 9							
<input type="checkbox"/> 10							
<input type="checkbox"/> 11							
<input type="checkbox"/> 12							
<input type="checkbox"/> 13							
<input type="checkbox"/> 14							
<input type="checkbox"/> 15							

The Run List: Labels at the top of the columns are self-explanatory. Sample Label, count time, Save Name, Abs, and noise are all editable so you can correct the information before running the samples. Config and Sample are editable, but you must exactly match the stored configuration or sample. Checked runs are those that will be "run". They need not be contiguous.

Run Selected 1D: Does the 1D simulation for selected runs.

Run Selected 2D: Does the 2D simulation for selected runs.

Dry Run 2D: Does a Dry Run of the 2D simulation for the selected runs and reports the projected total counting time to the command window. Always run this before actually running a 2D simulation to see how long it will take, making sure that your simulation will finish before the sun runs out of hydrogen.

Run Index: Set the starting run number for the VAX file naming of the raw 2D simulation files. This

number automatically increments after each run. Same numbered files will be overwritten - so be sure that this is not reset if you close/reopen the panel.

### An Example Simulated Experiment

For an example, we can carry out a simulation of silica particle scattering similar to the SANS reduction tutorial. The tutorial sample is silica particles that are approximately 14 nm in diameter, and relatively dilute, in deuterated water. We can duplicate the instrumental configurations, but let's ask the question of what sample conditions are free(\*) from multiple scattering, and how does multiple scattering affect the data?

(\*) scattering is a probability, so there is technically always some multiple scattering.

The two configurations are defined with SASCALC. I used NGB30:

- (1) SDD = 4 m; 0 cm offset; 5 guides; 6 A, dL/L=0.125; 1/2" aperture
- (2) SDD = 1.33 m; 25 cm offset; 7 guides; 6 A, dL/L=0.125; 1/2" aperture

For the model function, the silica is well represented as a polydisperse sphere model, SchulzSpheres with  
coef\_sch = {0.01,72,0.2,3.4e-6,6e-6,0.1}  
and is reasonably close to reality (since I do have the experimental data).

(1) Start by setting up the two configurations as listed above, and store them both. Save them to disk if you wish.

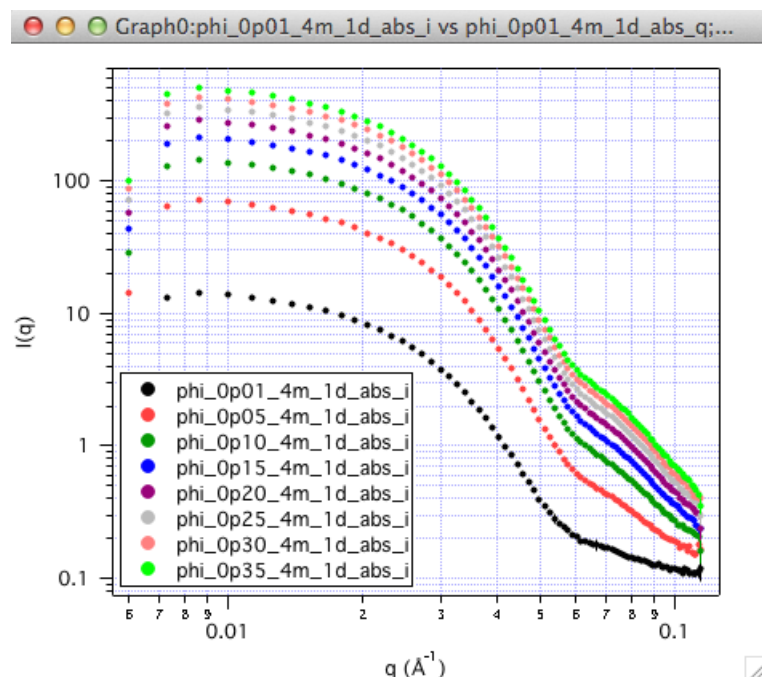
(2) Next, move to the "Setup Samples" tab. If you haven't plotted the SchulzSpheres model, do it now and set the coefficients to the values above. Then return to the Setup tab. Enter a sample label like "Silica, 5mm, phi=0.01". Then set the thickness to 0.5cm, transmission to 0.6, incoherent XS to 0.4 (1/cm) and a radius of 1.27 cm. Store the sample and give it a name like "phi0.01", as we'll make a series of samples that are identical except for larger volume fraction. So now change the volume fraction to 0.05, keeping the sample thickness the same, change the sample label and make (store) this sample with phi=0.05. Repeat this process of changing the volume fraction and storing the new sample for phi = 0.10, 0.15, 0.20, 0.25, 0.30, and 0.35. Then you'll have a set of samples from dilute to concentrated to test (yes, a model function that includes interparticle interactions is more realistic, but that's an exercise left for the reader). Save the set of samples to disk when you're done storing all of the samples.

(3) Now move to the "Setup Runs" tab. Here we build up a run list, just like in a real experiment. Pick the configuration and sample from the popup (4m config, and phi=0.01 to start). At first, we'll run the simulation in 1D, where multiple scattering is not considered, so we can leave "Abs" checked, and leave noise checked too. Set the count time to 300 s, and change the save name to "phi\_0p01\_4m\_1d.abs" or something similar, to identify the data set. Click "Add to Run" to add it to the list. Repeat for all of the other samples at 4m. Then repeat for the 1m configuration. You should end up with 16 runs (0->15). Save this run list as we will modify it later for the 2D simulation.

(4) Next, Run the simulation in 1D. This will save all of the 16 data files to disk, in the same format as a normal reduced data file. It should also be relatively quick to do the simulation, since it's all in 1D. Click "Run Selected 1D"

(5) Plot the results, just for the 4 m data, to see how the scattering increases as expected with

volume fraction. Within the statistical noise and the approach to a constant background of 0.1 (1/cm), the data scales in proportion to volume fraction.



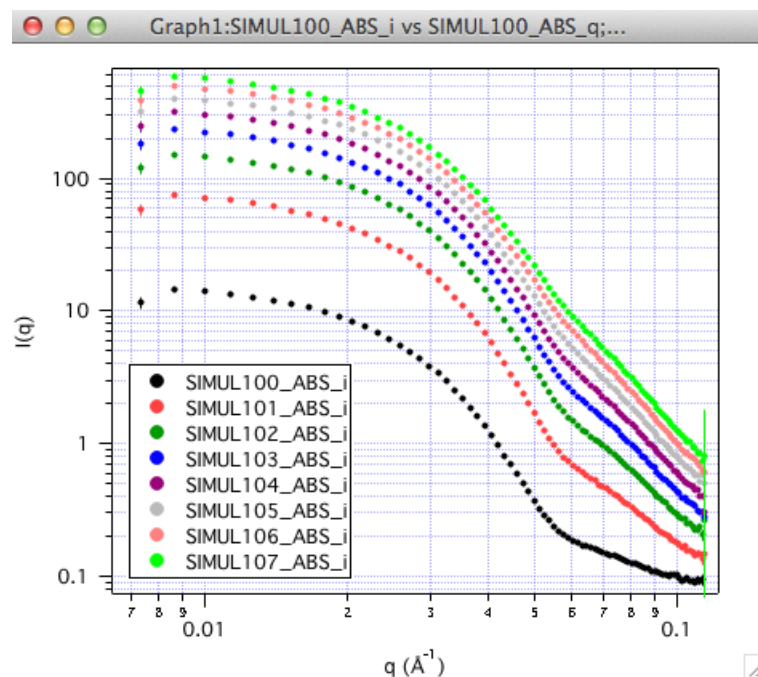
(6) Now prepare for the 2D simulation. We can modify some of the runs that were set up for 1D to use for 2D, and add more runs in as needed. For the 2D runs, we want these to be in raw counts, not on absolute scale (yet). So uncheck the box, and for all of the runs on the list, edit the "1" in the Abs column and change it to "0". In addition to running the samples at both detector configurations, we also want to run "empty beam" measurements for each configuration. You can also run transmission measurements for each sample, but the correct transmission will automatically be entered into the RAW data file as a direct result of the simulation. So, to add the two empty beam measurements, select the configuration. The selected sample does not matter. Change the sample label to "Empty Beam(and the correct distance)". Save name is not used for 2D simulations. Then highlight the empty row at the bottom of your run list, and click "Add Empty Beam". The run will be entered with a count time of 1s. When the empty beam is actually "run", the sample conditions will be set to an empty sample and no beamstop in place. Repeat for the second configuration

(7) Next, we need to do a "Dry Run" of the 2D simulation to see how long this will take. Runs can be checked for time individually using the simulation panel (be sure you've got the 2D SANS Simulator open). It's very helpful to run a few short simulations manually to get a feel for how long simulations take at each configuration, and the quality of the data obtained. For the nominal 300 s "beam" time set for each of the samples, on my computer a spot check of a few samples predicted 2 min and 4 min of CPU for 4 m and 1 m simulations, respectively. That means a total time of  $(2 \times 8 + 4 \times 8) = 48$  minutes + empty beam runs. Or - I could click "Dry Run 2D". This takes a few minutes to run a short simulation of each of the runs (so it'll catch errors now rather than later) and report the total predicted time to the command window (I got  $t=2552$  s = 42 min). So this is a "lunchtime" simulation, rather than overnight. If your simulation has an excessive run time, adjust count times as needed. Once you're happy with the run list, save this list too.

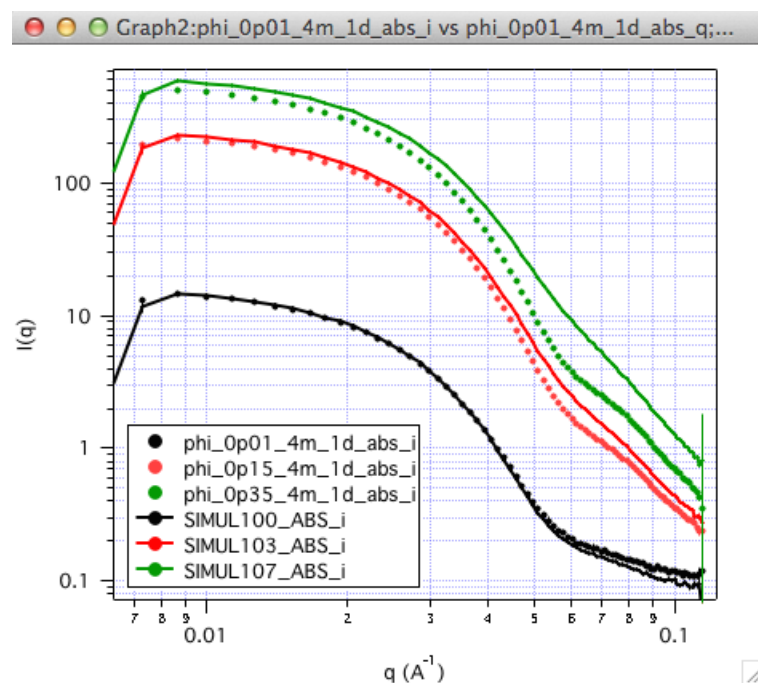
(8) Finally, we are ready to run the 2D simulation and go get some lunch. Be sure that the run Index is set to what you want. This is the run number used to name the raw data files. If this is your first simulation, 100 is fine. If you're re-running anything, be sure that this number is larger than the largest in the folder where you're saving data. The index automatically increments, but verify. Click "Run Selected 2D". Progress is reported in the command window and the "Currently Executing" number.

(9) The output of the 2D simulation is raw data. Reduce it like any other raw data, with the exception that since the simulation has a perfect detector, from the Macros Menu, choose:  
Simulation Scripting->Turn Off Dead Time Correction

then set up protocols and reduce the data as usual. The 4m data from the 1D simulation (free from multiple scattering) can be compared to the 4m data from the 2D simulation (which contains multiple scattering effects):



The 2D simulated and reduced data (plotted above) is very similar to the 1D result, but upon closer inspection by plotting the  $\phi = 0.01, 0.15$ , and  $0.35$  data together, we see some clear effects of multiple scattering:



The lines are the 2D simulation, and deviate from the 1D simulation at  $\phi > 0.15$ . The high  $q$  deviation of the  $\phi=0.01$  data is due to a slight mismatch of the incoherent scattering. Without even plotting the data, the data files can be opened (the 1D are text files) and the fraction of multiple scattering is reported in the header. It's also in the txt file of data that is generated with the 2D data files. For many samples, 10% multiple scattering is where significant deviations occur, but that can vary greatly with the type of sample. For these samples, it is clear that if you really wanted to measure the scattering from samples with  $\phi \geq 0.15$ , you'll want to change the sample conditions to reduce the scattering probability. (thinner samples, reduce the scattering contrast, smaller wavelength - all will help.)

<u><math>\phi</math></u>	<u>fraction multiple coherent scattering</u>
0.01	0.0073856
0.05	0.036562
0.10	0.072212
0.15	0.10695
0.20	0.14078
0.25	0.1737
0.30	0.20572
0.35	0.23685

What else can be done with the simulations? Any experimental planning should make use of some simulation to convince yourself that you're running the right set of samples to answer the questions that you have. Then with the right set of samples, you can optimize the configurations, sample conditions, experimental counting times, etc. to get the best possible data. You can even run through the steps of analysis that you are planning to use to see if you get the results you expect. A little investment in planning can eliminate a lot of wasted sample preparation, travel time, and beam time.

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