

Data Reduction User Manual for ORNL SANS Instruments

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DATA REDUCTION USER MANUAL FOR ORNL SANS INSTRUMENTS

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Prepared by
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, TN 37831-6283
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Data Reduction User Manual for ORNL SANS Instruments

Updated 9/14/20

Introduction

This document presents the different user-friendly software approaches offered to users by the SANS suite of instruments to reduce SANS data. All the reduction approaches are script-based and developed to cover execution of scripts in different environments from within and outside the analysis cluster. Among the different options, command-line execution and Mantid workbench environments require the user to be logged into the analysis cluster, while the Jupyter notebook environment does not. Overall, the reduction scripts detailed in this document allow to reduce data for the most routinely performed experiments with minimal input from users. Furthermore, these scripting methods provide flexibility to reduce data obtained from complex experiments including expert-user-driven atypical experiments. Video tutorials are provided for several guides with links available at the beginning of the sections.

Table of Contents

| | |
|--|----|
| Data Reduction User Manual for ORNL SANS Instruments | 2 |
| 1. EQSANS Data Reduction with drtsans—Quick Reference for the Data Reduction Parameters | 3 |
| 2. EQSANS Data Reduction with drtsans—Quick Reference for Script Mode | 16 |
| 3. EQSANS Data Reduction with drtsans—Quick Reference for Working in MantidWorkbench | 22 |
| 4. Bio-SANS Data Reduction with drtsans—Quick Reference for the Data Reduction Parameters | 27 |
| 5. Bio-SANS Data Process Guide—Quick Reference for using Jupyter Notebook to Reduce Data | 39 |
| 6. GP-SANS Data Reduction With drtSANS – Quick Reference for the Data Reduction Parameters | 47 |
| 7. GP-SANS Data Process Guide—Quick Reference for Using Jupyter Notebook to Reduce Data | 60 |
| 8. Neutron Imaging—Extract Metadata from SANS ReductionLog | 72 |

1. EQSANS Data Reduction with drtsans—Quick Reference for the Data Reduction Parameters

Editors: Changwoo Do, Gergely Nagy, William Heller

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Introduction

The various parameters required by drtsans are listed below with a brief description of their meaning, the acceptable values, and appropriate format for the information. An example is shown here.

```
{"schemaStamp": "2020-05-26T22:28:16.336908", "instrumentName": "EQSANS",
"iptsNumber": "24184", "sample": {"runNumber": "111524", "thickness": 1,
"transmission": {"runNumber": "111522", "value": ""}}, "background": {"runNumber":
"111523", "transmission": {"runNumber": "111521", "value": ""}}, "emptyTransmission":
{"runNumber": "111520", "value": null}, "beamCenter": {"runNumber": "111520"},
"outputFileName": "EQSANS_111524", "configuration": {"outputDir":
"/SNS/EQSANS/shared/codereview/acceptance/wt3_final/ipts24184/", "useTimeSlice":
false, "timeSliceInterval": 300, "useLogSlice": false, "logSliceName": null,
"logSliceInterval": 10, "cutTOFmin": "500", "cutTOFmax": "1500", "wavelengthStep":
"0.1", "wavelengthStepType": "constant Delta lambda", "sampleOffset": "314.5",
"useDetectorOffset": true, "detectorOffset": 80.0, "sampleApertureSize": "10",
"sourceApertureDiameter": null, "usePixelCalibration": null, "maskFileName":
"/SNS/EQSANS/shared/codereview/acceptance/wt3_final/mask_bs60_morebanks2.nxs",
"useDefaultMask": true, "defaultMask": null, "useMaskBackTubes": false,
"darkFileName":
"/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/EQSANS_108764.nxs.h5",
"normalization": "Total charge", "fluxMonitorRatioFile": "/SNS/EQSANS/IPTS-
24769/shared/EQSANS_110943.out", "beamFluxFileName":
"/SNS/EQSANS/shared/instrument_configuration/bl6_flux_at_sample",
"sensitivityFileName":
"/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/Sensitivity_patched_thinPM
MA_4m_108772.nxs", "useSolidAngleCorrection": true, "useThetaDepTransCorrection":
true, "mmRadiusForTransmission": "25", "absoluteScaleMethod": "standard",
"StandardAbsoluteScale": "5.0719320777245", "numQxQyBins": "80", "1DQbinType":
"scalar", "QbinType": "log", "numQBins": "100", "LogQBinsPerDecade": null,
"useLogQBinsDecadeCenter": false, "useLogQBinsEvenDecade": false,
"WedgeMinAngles": "-30, 60", "WedgeMaxAngles": "30, 120", "autoWedgeQmin": null,
"autoWedgeQmax": null, "autoWedgeQdelta": null, "autoWedgeAzimuthalDelta": null,
"autoWedgePeakWidth": null, "autoWedgeBackgroundWidth": null,
"autoWedgeSignalToNoiseMin": 2.0, "AnnularAngleBin": 5.0, "Qmin": null, "Qmax":
null, "useErrorWeighting": false, "smearingPixelSizeX": null, "smearingPixelSizeY": null,
"useSubpixels": null, "subpixelsX": null, "subpixelsY": null, "useSliceIDxAsSuffix":
true}, "dataDirectories":
"/SNS/EQSANS/shared/codereview/acceptance/wt3_final/ipts24184/"}
```

Below is the same configuration file expanded into a more readable format.

```
{
  "background": {
    "runNumber": "111523",
    "transmission": {
      "runNumber": "111521",
      "value": ""
    }
  },
  "beamCenter": {
    "runNumber": "111520"
  },
  "configuration": {
    "1DQbinType": "scalar",
    "AnnularAngleBin": 5.0,
    "LogQBinsPerDecade": null,
    "QbinType": "log",
    "Qmax": null,
    "Qmin": null,
    "StandardAbsoluteScale": "5.0719320777245",
    "WedgeMaxAngles": "30, 120",
    "WedgeMinAngles": "-30, 60",
    "absoluteScaleMethod": "standard",
    "autoWedgeAzimuthalDelta": null,
    "autoWedgeBackgroundWidth": null,
    "autoWedgePeakWidth": null,
    "autoWedgeQdelta": null,
    "autoWedgeQmax": null,
    "autoWedgeQmin": null,
    "autoWedgeSignalToNoiseMin": 2.0,
    "beamFluxFileName":
"/SNS/EQSANS/shared/instrument_configuration/bl6_flux_at_sample",
    "cutTOFmax": "1500",
    "cutTOFmin": "500",
    "darkFileName":
"/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/EQSANS_108764.nxs.h5",
    "defaultMask": null,
    "detectorOffset": 80.0,
    "fluxMonitorRatioFile": "/SNS/EQSANS/IPTS-24769/shared/EQSANS_110943.out",
    "logSliceInterval": 10,
    "logSliceName": null,
    "maskFileName":
"/SNS/EQSANS/shared/codereview/acceptance/wt3_final/mask_bs60_morebanks2.nxs",
    "mmRadiusForTransmission": "25",
    "normalization": "Total charge",
    "numQBins": "100",
    "numQxQyBins": "80",
    "outputDir": "/SNS/EQSANS/shared/codereview/acceptance/wt3_final/ipts24184/",
    "sampleApertureSize": "10",
    "sampleOffset": "314.5",
    "sensitivityFileName":
"/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/Sensitivity_patched_thinPMMA_4m_108772.nxs",
    "smearingPixelSizeX": null,
    "smearingPixelSizeY": null,
    "sourceApertureDiameter": null,
    "subpixelsX": null,
    "subpixelsY": null,
    "timeSliceInterval": 300,
    "useDefaultMask": true,
    "useDetectorOffset": true,
    "useErrorWeighting": false,
    "useLogQBinsDecadeCenter": false,
    "useLogQBinsEvenDecade": false,
    "useLogSlice": false,
    "useMaskBackTubes": false,
    "usePixelCalibration": null,
    "useSliceIdxAsSuffix": true,
    "useSolidAngleCorrection": true,
    "useSubpixels": null,
    "useThetaDepTransCorrection": true,
    "useTimeSlice": false,
    "wavelengthStep": "0.1",
    "wavelengthStepType": "constant Delta lambda"
  },
  "dataDirectories": "/SNS/EQSANS/shared/codereview/acceptance/wt3_final/ipts24184/",
  "emptyTransmission": {
```

```

    "runNumber": "111520",
    "value": null
  },
  "instrumentName": "EQSANS",
  "iptsNumber": "24184",
  "outputFileName": "EQSANS_111524",
  "sample": {
    "runNumber": "111524",
    "thickness": 1,
    "transmission": {
      "runNumber": "111522",
      "value": ""
    }
  }
},
"schemaStamp": "2020-05-26T22:28:16.336908"
}

```

1.1 Parameter Descriptions

Note that all key:value pairs use quotes around both the key and value unless the value is null or a mathematical constant. Also note that the file has a hierarchical structure, where {} are used to denote groupings. The descriptions of the parameters below reflect the structure of the hierarchy.

- I. "schemaStamp": "2020-05-26T22:28:16.336908"
This particular parameter is autogenerated by the scripting method for reducing data and when using MantidWorkbench. It should not be changed, even when hand-modifying the contents of the configuration file.
- II. "instrumentName": "EQSANS"
The instrument name is used by drtsans to know how to use some of the specified parameters. It must be consistent with the instrument used for the data collection (i.e. do not try to reduce data from EQ-SANS if this parameter is set to "BIOSANS"). Note that there is no dash in the name of the instrument in the drtsans parameter file.
- III. "iptsNumber": "24184"
The proposal number for the experiment allows drtsans to quickly find the data to be reduced, rather than using tools to find the data based solely on the run number. It can be left blank (i.e. "").
- IV. "sample":
This is the first parameter that contains a set of parameters grouped using {}. The various parameters in the group follow.
 - a. "runNumber": "111524"
This is the run number for the sample scattering to be reduced. It can be found via OnCat or using the catalog in MantidWorkbench. It is possible to specify a set of scattering runs for a single sample that are to be summed together into a single data set for reduction. To do so, use the following format, which uses a single pair of quotes to enclose the list.
 - i. "runNumber":{"XXXXXX, YYYYYY"}

- b. "thickness": 1
This parameter specifies the sample thickness in millimeters. Note that the value is not enclosed in quotes.
 - c. "transmission":
This is the start of another level of the hierarchical structure. Of the two key:value pairs in this grouping, only one can have an actual value: either the run number or the value of the transmission to use for the reduction. One rarely specifies a simple value for the transmission for EQ-SANS data because the transmission is wavelength-dependent.
 - i. "runNumber": "111522"
This is the run number of the transmission for the sample. There can only be a single run number specified here.
 - ii. "value": ""
This would be a numerical value for the transmission to use for the reduction, which would normally only be done for quick qualitative checks if the data needs to be viewed prior to the completion of the transmission measurement for a sample. Note that the value must be enclosed in quotes ("").
- V. "background":
The set of parameters that follow specify information required to identify the background to use for the reduction. It is possible to reduce data without a background by leaving the run numbers in this set of parameters empty (i.e. "").
- a. "runNumber": "111523",
The run number of the background data to subtract from the sample scattering.
 - b. "transmission":
The following set of parameters are used to specify either the run number for the background's transmission measurement or to specify a value for the transmission of the background.
 - i. "runNumber": "111521"
 - ii. The run number for the background's transmission measurement. If no background is specified, then this run number should not be specified (i.e. set to "").
 - iii. "value": ""
 - iv. This would be a numerical value for the transmission to use for the reduction, which would normally only be done for quick qualitative checks if the data needs to be viewed prior to the completion of the transmission measurement for a sample. Note that the value must be enclosed in quotes ("").

- VI. "emptyTransmission":

This grouping of parameters is used to specify the reference measurement, or value, used to calculate the transmission from the other specified measurements or values. If the transmissions are specified as values, the value specified here should be "1.0".

 - a. "runNumber": "111520"

The run number for the background's transmission measurement.
 - b. "value": null

A value can be specified for the reference transmission. If used, it should be "1.0", if not specify it as null, as shown above.

- VII. "beamCenter":

The beam center is specified by providing a run number for an empty beam or a transmission measurement to calculate the beam center from.

 - a. "runNumber": "111520"

This is the run number of an empty beam or a transmission measurement. It cannot be left blank.

- VIII. "outputFileName": "EQSANS_111524"

This is the base used to construct all of the file names that result from the data reduction process. In this example, all of the files will be named "EQSANS_111524*.*". The filename can be any valid string that is acceptable for filenames for a unix operating system.

- IX. "configuration":

A large number of parameters are specified within this hierarchical grouping, most of which directly impact the reduction process and results produced. Many of these parameters will be provided by your local contact and should not be changed without discussing the reasons for the change with him or her. When using the scripting or MantidWorkbench methods for data reduction, some of these parameters may not be presented to you. If they are not presented to you in either the scripts that your local contact helps set up for you or in the tool in MantidWorkbench, then you do not need to provide them directly.

 - a. "outputDir":

"/SNS/EQSANS/shared/codereview/acceptance/wt3_final/ipts24184/"

The directory to write the data reduction result to is listed here. Normally, it would be the shared directory for the particular proposal, which allows other team members and the local contact to view the results. However, it is also possible to specify a location in a user's home directory. It is left to the discretion of the user.

- b. "useTimeSlice": false
If the user wishes to parse the event stream contained in the run specified in the "sample:" parameter set, then set this value to true. If this value is true, then the parameter "useLogSlice", below, must be false.
- c. "timeSliceInterval": 300
This is the interval in seconds to use for the time slicing of the event stream. The event stream will be cut into as many consecutive portions of the event stream as exist in the file, with a final bin that contains as much time as remains in the stream. In this case, the various slices are for the following intervals: $0 \leq t < 300$ seconds, $300 \leq t < 600$ seconds, etc. Note that the value is not contained in quotation marks.
- d. "useLogSlice": false,
It is possible to divide an event stream into bins that derive from another parameter that is saved by EPICS in the NeXus file, such as temperature, pressure, magnetic field, or even a motor that continuously moves during data collection. If a user wishes to do so, set the value to true. Note that useLogSlice and useTimeSlice cannot both be true. Discuss the use of log slicing with your local contact.
- e. "logSliceName": null
This is the name of the instrument log to use for log slicing. If useLogSlice is true, change this to the name of the EPICS parameter that you wish to employ. Discuss the use of log slicing with your local contact.
- f. "logSliceInterval": 10
This parameter sets the interval of the instrument log specified in logSliceName to use. It must be in the units of the device, be it degrees, millimeters, Celcius, etc. Discuss the use of log slicing with your local contact. Note that the value is not enclosed in quotation marks.
- g. "cutTOFmin": "500"
This is an expert parameter, specified in microseconds, that makes it possible to discard neutron events that arrive between the start of the 30 or 60 Hz time window at the plane of the detector from the data reduction. This is normally set by the local contact or instrument team in the default configuration parameter sets. If you would like more information, please consult your local contact. Note that the value is enclosed in quotation marks.
- h. "cutTOFmax": "1500"
This is an expert parameter, specified in microseconds, that makes it possible to discard neutron events that arrive within this number of microseconds of the end of the 30 or 60 Hz time window at the plane of the detector from the data reduction. This is normally set by the local contact or instrument team in

the default configuration parameter sets. If you would like more information, please consult your local contact. Note that the value is enclosed in quotation marks.

- i. "wavelengthStep": "0.1"
During data reduction, the time-of-flight of the events are converted to wavelength. Neutrons are then binned into 2D patterns as a function of wavelength. The width of the wavelength bins in Å is specified by this parameter. Note that the value is enclosed in quotation marks.
- j. "wavelengthStepType": "constant Delta lambda"
This particular parameter is not actually used. Do not change the value.
- k. "sampleOffset": "314.5"
This parameter specifies the distance, in mm, that the actual sample position differs from the central axis of the large sample environment flange that can be seen on the ceiling of the downstairs sample environment enclosure of EQ-SANS. A positive number means that the sample position is offset from this axis in the direction of the detector, while a negative number means that it is offset towards the SNS target. Your local contact has either determined this number for the sample environment that you are using for your experiment, or they will work with you to determine the correct value. Note that this value is contained in quotation marks.
- l. "useDetectorOffset": true
This parameter is an expert parameter and should not be changed without consulting your local contact. If you have any questions, ask your local contact.
- m. "detectorOffset": 80.0
This parameter is an expert parameter and should not be changed without consulting your local contact. If you have any questions, ask your local contact. Note that this value is not enclosed in quotation marks.
- n. "sampleApertureSize": "10"
This parameter specifies the diameter of the sample aperture used in millimeters. While it is possible to specify the diameter of this aperture during data acquisition, specifying a different value here allows you to over-write the incorrect value saved in the data files. The sampleApertureSize impacts the calculation of the resolution information for the instrument (i.e. the uncertainty in Q), which is required to accurately analyze your data. Note that the value is enclosed in quotation marks.
- o. "sourceApertureDiameter": null
This can be used to specify the diameter of the source aperture in millimeters used for a measurement. Normally, this parameter is actually taken from the

positions of the motors of the three fixed slit wheels of the instrument. If you feel that you need to change this value, which you would specify as a number enclosed in quotation marks, consult your instrument scientist.

- p. "usePixelCalibration": null
At present, this is an unused parameter for reducing data on EQ-SANS. It is not recommended that a user changes the value of this parameter.
- q. "maskFileName": "/SNS/EQSANS/shared/codereview/acceptance/wt3_final/mask_bs60_morebanks2.nxs"
This is the name of a hand-drawn mask. Several default options are normally available during any given run cycle of the SNS, but masks may also be drawn for each experiment, such as when a non-standard sample environment is employed. Speak to your local contact about what mask to use or if a new one should be prepared.
- r. "useDefaultMask": true
On EQ-SANS, the instrument team prepares a default mask that contains information about linear position sensitive detectors that are not performing well. If this parameter is true, drtsans automatically determines the correct version of the default mask to use and applies it. This mask is applied in addition to the user-specified mask from the maskFileName parameter. If the value is set to false, any mask specified with the "defaultMask" parameter, below, will be applied.
- s. "defaultMask": null
This parameter is used to select an alternative mask in place of the file that would normally be used. It is recommended to leave this value set to null unless told to do otherwise by your local contact.
- t. "useMaskBackTubes": false
The EQ-SANS detector, like the Bio-SANS and GP-SANS detectors, consists of an array of linear position sensitive detectors that are arranged in two planes that are offset to ensure complete coverage across the area of the detector. When this parameter is set to true, the back plane of tubes, being those furthest away from the sample, are all masked. Typically, this is only done when the detector is positioned close to the sample.
- u. "darkFileName":
"/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/EQSANS_108764.nxs.h5"
This parameter specifies the name of the file that contains the "dark current" measurement, which for EQ-SANS is normally a measurement performed during regular calibrations with the facility running but the instrument shutter closed.

It is a measure of cosmic radiation and detector electronic noise. Your local contact will provide the correct file to use.

- v. "normalization": "Total charge"
The data can either be normalized by the measurement time ("Time"), the total proton charge accumulated during the measurement ("Total charge") or the beam monitor ("Monitor"), which is only appropriate when data has been collected with the choppers running at 60 Hz. The normal method for normalizing EQ-SANS data is "Total charge", which is also how the length of a measurement is normally specified. If "Total charge" is used, then the beamFluxFileName must be provided. Another option is "Monitor", which requires that the flux file and the fluxMonitorRatioFile parameter be provided. Speak to your local contact about the correct files to use.
- w. "fluxMonitorRatioFile": "/SNS/EQSANS/IPTS-24769/shared/EQSANS_110943.out"
This is a measure of the beam flux, as measured on the primary detector, relative to the beam monitor. It accounts for the different wavelength efficiencies of the two detectors. It is only used when data are to be normalized by the beam monitor. Consult with your local contact about the correct file to use.
- x. "beamFluxFileName":
"/SNS/EQSANS/shared/instrument_configuration/bl6_flux_at_sample"
This file contains the instrument flux as a function of wavelength as measured using the primary detector that is used for data normalization during data reduction. Consult with your local contact for the correct file to use.
- y. "sensitivityFileName":
"/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/Sensitivity_patched_thinPMMA_4m_108772.nxs"
The file name of the pre-processed relative pixel response of the detector is specified with this parameter. These calibration files are measured during instrument commissioning each cycle and are prepared by staff for use in data reduction. Consult your local contact for the correct file to use.
- z. "useSolidAngleCorrection": true
This parameter specifies whether or not to correct the data for the solid angle subtended by each pixel, which can be a considerable effect for configurations with the detector positioned close to the sample. It is recommended to leave this parameter set to true.
- aa. "useThetaDepTransCorrection": true
When set to true, the data reduction will correct the data in each pixel for the actual distance that the neutrons travel through the sample when performing

the correction for the transmission. The effect increases with scattering angle and can be considerable when the detector is positioned near the sample. It is recommended to leave this parameter set to true.

- bb. "mmRadiusForTransmission": "25"
This parameter allows the user to specify the radius in millimeters to use when integrating the attenuated direct beam measurements for calculating the transmissions. The instrument team has found 25 mm to perform well under most circumstances, but it is possible that certain sample environments or instrument configurations may benefit from the use of a different value. Consult your local contact if you feel that another value may be required.
- cc. "absoluteScaleMethod": "standard"
At present, the only method available for scaling data collected on EQ-SANS into absolute units of 1/cm is by using a calibrated standard. Do not change the value of this parameter. Presently, the standard is a well-characterized sample of porous silica that your local contact will provide to you during your experiment. A measurement of the standard is used to derive the absolute scale factor, which is specified with the StandardAbsoluteScale parameter, described below.
- dd. "StandardAbsoluteScale": "5.0719320777245"
This is the scale factor that must be applied to the data to place it into absolute units of 1/cm. Your local contact can help you derive it from a measurement of a standard.
- ee. "numQxQyBins": "80"
This parameter specifies the number of Q-bins in the 2D reduced data, which is always output by drtsans. Note that only a single value may be provided, which implies that the 2D reduced data is on a regular, square grid that covers the Q-range in 2D measured by the detector. The beam center is not necessarily in the center of the output data. The grid in Q-space is always linear.
- ff. "1DQbinType": "scalar"
Three options exist for the kind of 1D data that are output by drtsans. Possible values are "scalar", which is used for 1D azimuthally averaged data that most people are familiar with; "wedge" makes it possible to define wedges to perform scalar binning within, as one might do for anisotropic data and utilize the WedgeMinAngles, WedgeMaxAngles and the various autoWedge parameters described below, although automatic wedge determination is not enabled for EQ-SANS at this point in time. The "annular" binning makes it possible to visualize how data varies around the beam center within a Q-range specified by the user and requires that the parameters AnnularAngleBin, Qmin and Qmax, described below, be provided.

- gg. "QbinType": "log"
This parameter dictates whether the Q-spacing of the intensity profiles calculated when performing scalar or wedge binning is logarithmic or linear. The possible values of this parameter are "log" and "linear". The choice of binning determines how the numQBins, LogQBinsPerDecade and useLogQBinsEvenDecade parameters work.
- hh. "numQBins": "100"
This parameter must be set to an integer value if QbinType is "linear", but can also be used if it is "log". The value is the number of Q-values that are in the 1D data that is binned as "scalar" or "wedge" and their spacing is determined by the value of QbinType. This parameter must be null if LogQBinsPerDecade is set to an integer value. Note that the value is enclosed in quotation marks.
- ii. "LogQBinsPerDecade": null
This parameter only works when QbinType is "log". The value specified here will be the number of Q-bins that are present within each decade between the minimum and maximum Q values that the reduced data contain. For example, if the value is "25", then there are 25 Q-bins between 0.01 Å⁻¹ and 0.10 Å⁻¹ and 25 Q-bins between 0.10 Å⁻¹ and 1.0 Å⁻¹ or any other decade in Q that are present in the reduced data. The parameter useLogQBinsEvenDecade must be set to true to enable this option and numQBins must be null.
- jj. "useLogQBinsDecadeCenter": false
At present, this option is no longer enabled. The Q-values when using an even number of Q-bins per decade by setting useLogQBinsEvenDecade to true and providing a value for logQBinsPerDecade to a non-zero, positive integer always have a bin centered on 0.001 Å⁻¹, 0.010 Å⁻¹, 0.100 Å⁻¹, etc.
- kk. "useLogQBinsEvenDecade": false
This parameter tells drtsans to use a fixed number of Q-bins per decade when binning the result. The logQBinsPerDecade parameter must have a non-zero integer value and numQBins must be null.
- ll. "WedgeMinAngles": "-30, 60"
- mm. "WedgeMaxAngles": "30, 120"
The WedgeMinAngles and WedgeMaxAngles are only used when QbinType is set to "wedge". The arrays provide a matched set of angles, specified in degrees and indexed from the Qx axis, within which to perform 1D Q-binning. In this particular example, 1D Q-binning will be performed in two wedges: from -30° to 30° and from 60° to 120°. The angles need not be the same size and need not be symmetric. It is also possible for the angles to overlap, should the user desire it. The only requirement is that both arrays have the same number of elements and that the minimum angle for a wedge be lower than

the maximum value for that wedge.

Parameters shown in points nn through tt, below, are required for the drtsans methods for automatically determining the correct wedges to use for binning reduced data into 1D. Development of these routines was driven by the Bio-SANS instrument team. At present, automatic wedge determination is not available for data collected using EQ-SANS.

nn. "autoWedgeQmin": null

oo. "autoWedgeQmax": null

pp. "autoWedgeQdelta": null

qq. "autoWedgeAzimuthalDelta": null

rr. "autoWedgePeakWidth": null

ss. "autoWedgeBackgroundWidth": null

tt. "autoWedgeSignalToNoiseMin": 2.0

uu. "AnnularAngleBin": 5.0

When the 1DQbinType parameter is set to "annular" this parameter specifies the size of the bins in degrees that are to be used for binning. Annular binning takes the data in a ring of Q-values and creates a profile as a function of angle around the beam center. Annular binning also requires that Qmin and Qmax, described below, be specified.

vv. "Qmin": null

ww. "Qmax": null

When performing annular binning this is the minimum and maximum Q-values, specified in \AA^{-1} , to use during the binning. These parameters are only used when 1DQbinType is set to "annular".

xx. "useErrorWeighting": false

If weighting by the experimental uncertainty is desired when binning the reduced data and propagating the corresponding uncertainties, set the value of this parameter to true.

yy. "smearingPixelSizeX": null

zz. "smearingPixelSizeY": null

The detectors used in the SANS instruments at ORNL are gas detectors. The pixel sizes are determined from parameters supplied to the hardware that

determines where a neutron is detected and can be varied by changing said parameters. In actuality, there is intrinsic uncertainty in the position of the event along the tube. Further, the arrangements of the tubes in the detector makes it possible to have a neutron in the region of overlap between a tube in the front panel and a tube in the back panel be detected in either, which also creates uncertainty in the position in which an event is encoded. The `smearingPixelSizeX` and `smearingPixelSizeY` parameters make it possible to account for this uncertainty when calculating the uncertainty in Q . The effect is small for most Q -values, but can impact data analysis when sharp features are present. Your local contact can provide suitable values for the parameters. Note that specifying values for these two parameters does not change the calculation of the value of Q or the intensity profile that results after reduction. It only alters the uncertainty in Q of the result.

aaa. `"useSubpixels"`: null

In cases where there are sharp features in the data, or a need to use as much data near the beamstop as possible, it is possible to divide the pixels defined on the detector into sub pixels to improve the quality of the results from the 1D binning process. Subpixels, if specified, will also be used in the 2D binning. To enable this feature, set `useSubpixels` to true and set `subpixelsX` and `subpixelsY`, described below, to positive integers.

bbb. `"subpixelsX"`: null

ccc. `"subpixelsY"`: null

Set these two parameters to a non-zero, positive integer to use subpixels when binning the data. The real pixels will then be divided into subpixels for the binning in the data reduction. If `subpixelsX` is set to 2 and `subpixelsY` is set to 3, then each pixel will be divided into a 2 by 3 grid for the binning process.

ddd. `"useSliceIDxAsSuffix"`: true

At present, this option is not implemented. In the future, when performing time or log slicing of an event stream during data reduction, setting the value of this parameter to true will mean that each slice is assigned a consecutive numerical value that is used to construct the output file name. If the value is set to false, the beginning and ending values of the slice will be used to construct the output file names.

X. `"dataDirectories"`:

`"/SNS/EQSANS/shared/codereview/acceptance/wt3_final/ipts24184/"`

2. EQSANS Data Reduction with drtsans—Quick Reference for Script Mode

Editors: Changwoo Do, Gergely Nagy, William Heller

Date: 07/16/2020

Video tutorial: https://www.youtube.com/watch?v=1XU_40Z8RuY&feature=youtu.be

Introduction

EQ-SANS data reduction is typically performed through two equivalent means:

- via scripts run in the terminal window or
- via mantidworkbench.

The present document details the former method. Your local contact will work with you to configure the reduction for the various instrument configurations that you use during your experiment.

Below find the step by step description of the procedure.

2.1 Visit analysis.sns.gov

- a. Data reduction can be performed both from inside and outside of ORNL
- b. Log in with your ucams ID and password
- c. Same credentials can be used for easy file transfer to personal computer via e.g. WinSCP

2.2 Populate the Shared Directory of your IPTS with the Required Reduction Tools and Activate the Reduction Environment

- a. open a terminal
- b. go to the shared folder of your IPTS
 - i. `cd /SNS/EQSANS/IPTS-*****/shared`
- c. copy `eqsans_setup.sh` from `/SNS/EQSANS/shared/usertools/`
 - i. `cp /SNS/EQSANS/shared/usertools/* .`
 - ii. or one can directly run the shell script by typing `/SNS/EQSANS/shared/usertools/eqsans_setup.sh` and enter.
- d. run `eqsans_setup.sh` by typing
 - i. `./eqsans_setup.sh`
- e. run `eqsans_activatedrtsans.sh` by typing
 - i. `source ./eqsans_activatedrtsans.sh`

2.3 Edit the Template Reduction Script, Which is Written in Python 3

- a. Use `gedit` or `pluma` to edit `reduce_template.py`
 - i. `gedit reduce_template.py &`
 - ii. `pluma reduce_template.py &`
- b. The script contains examples for:
 - i. reduction of data for a single configuration

- ii. reduction of data from 2 configurations in a single script

2.4 Example of Writing and Running a Script for a Single Configuration Reduction

- a. Update output directory

```
#####
# USER INPUT BEGINS HERE
# CHANGE THIS TOP FOLDER AS NEEDED
#####
output_path_top = "/SNS/EQSANS/IPTS-24283/shared/example/reduced/"
output_path = output_path_top + "" #fill between "" if you want to make sub-folder|
```

- i. It is recommended for the target directory for the reduced files to be empty or to not to contain reduction results from previous reductions in EQSANS_runnumber_*.nxs format because drtsans will over-write previous results without asking the user if they wish to do so.

- b. Update common reduction parameters

```
#####
# example. standard sample 4m 10a|
#####
eq = EQVar('2020A') # consult with IS for the correct value
eq._outputdir = output_path # update as appropriate
eq._absolutescale = 1 # update as appropriate
eq._thickness = 1 # update as appropriate
eq._empty = "113526" # update as appropriate
eq._bkgscatt = "113530" # update as appropriate
eq._bkgtrans = "113527" # update as appropriate
eq._qbintype = "linear" # update as appropriate
eq._numqbins = 100 # update as appropriate
```

- c. Update run numbers and names for individual scattering and transmission runs

- i. multiple samples can be inserted with comma separation
- ii. multiple runs collected from a single sample that you wish to sum together are specified as a comma-separated list enclosed in quotation marks

```
samscatt = [113531,"113532,113533"] # update as appropriate
samtrans = [113528,113529] # update as appropriate
fn_list = ['sample1','sample2'] # update as appropriate
```

- d. to look up run numbers from your experiment please refer to

- i. oncat.ornl.gov
- ii. or the catalogue method presented in the other tutorial document.

- e. Below is a complete example of how to specify data reduction for a standard sample. Note that the loop could be used to reduce data from multiple samples if the samscatt, samtrans and fn_list arrays contained more than one element. If used to reduce multiple data sets, these three arrays must have the same number of elements.

```

#####
# example. standard sample 4m 10a
#####
eq = EQVar('2020A') # consult with IS for the correct value
eq._outputdir = output_path # update as appropriate
eq._absolutescale = 1 # update as appropriate
eq._thickness = 1 # update as appropriate
eq._empty = "113526" # update as appropriate
eq._bkgscatt = "113530" # update as appropriate
eq._bkgtrans = "113527" # update as appropriate
eq._qbintype = "linear" # update as appropriate
eq._numqbins = 100 # update as appropriate

samscatt = [113531] # update as appropriate
samtrans = [113528] # update as appropriate
fn_list = ['porsil_4m10a'] # update as appropriate

for i in range(0, len(samscatt)):
    print("...reducing data set #" + str(i+1))
    eq._samscatt = str(samscatt[i])
    eq._samtrans = str(samtrans[i])
    eq._filename = str(fn_list[i])
    print("....reducing " + eq._samscatt + " for " + eq._filename)
    mreduceNow(eq) #comment this line in order to skip
    print("....reduction complete.")

```

- f. comment all unnecessary sections of the file by using either a # to remove a single line or a pair of ''' at the start and end (i.e. enclosing) of sections that you wish to comment out and save the document
 - i. this is advised to prevent time consuming re-run of already completed reduction runs
- g. Save the file and run the reduction script from the terminal. For the example template file provided, type the following.
 - i. python reduce_template.py
 - ii. Depending on the size of the data files, which can be quite large for strongly scattering samples, each data set may require several minutes to reduce because the instrument saves data in “event mode”, which results in large files. If you are reducing a large number of files, such as after an overnight script, you may want to get a cup of coffee.
- h. Reduced files can be found in the output folder in a variety of formats.
 1. Images in png format for both 1D and 2D reduced data can be displayed via the “display” command ([analysis] display filename.png), or can be opened using the Caja file browser by double clicking on the file.
 - i. I(q) files can be also displayed via launching eqsans_rungui.sh created in paragraph 3.3, clicking on the “Display IQ” button and select the data of interest.
 - ii. Analysis cluster has ‘sasview’ software, which can also display and perform fittings. To launch sasview, open a terminal and type the following.
 1. Sasview

2.5 Stitching of Individual Runs

- a. The template script also contains a section entitled “stitching” that allows data sets collected in different instrument configurations for a sample to be stitched into a single intensity profile. While the example presents stitching of two data sets, it is possible to stitch data from several different configurations together. Then, the overlap array takes the form “overlap =

[MergeAB_min, MergeAB_max, MergeBC_min, MergeBC_max, ...]", having
 2·(Num_Configurations -1) pairs of minimum and maximum Q-values for the merge regions.

```
#####
# example of stitching
#####
fn_list_low = ['porsil_4m10a_Iq.dat']
fn_list_high = ['porsil_4m205a_Iq.dat']
fn_merged = ['porasil']
suffix = '_merged.dat'
overlap = [0.06, 0.07]
for i in range(0, len(fn_merged)):
    print('.....stitching...')
    low_q_fn = output_path + fn_list_low[i]
    high_q_fn = output_path + fn_list_high[i]
    iq_low = load_iqmod(low_q_fn, sep=' ')
    iq_high = load_iqmod(high_q_fn, sep=' ')
    overlap = [0.060,0.070]
    stitched = stitch_profiles([iq_low, iq_high], overlap, target_profile_index=0)
    merged_fn = output_path + fn_merged[i] + suffix
    save_iqmod(stitched, merged_fn, sep=' ', float_format='%.6E')
    print('.....stitching completed.')
```

- b. Update the section with names of files to be stitched, with output name, stitching range etc.
 - i. The stitching ranges are generally determined by examining the data files. Feel free to ask your local contact or another instrument scientist for advice.
 - ii. The stitching ranges have to be listed in order of increasing momentum transfer (from low-Q to high-Q)
 - iii. During scaling of the independent curves target_profile_index will determine the curve to scale to. **Note that index of the first curve is 0.**
 - iv. The applied scale factor will be displayed in the terminal window during script execution.
- c. Unless another name is provided for the merged_fn variable in the save_iqmod command, the stitched file will have an ending of _merged.dat. In the example above, the output file for the stitched data is “porasil_merged.dat”.

2.6 Reducing and Stitching Two Configurations in One Go

- a. Example to be found under “# example of one-step reduction”
 - i. Comment out all sections not intended to be used
- b. Define necessary parameters. In the example below, there are two different configurations: low Q and high Q. Note that the two configurations have their own variables, which makes it possible to reduce the data from two configurations with a single script.

```
#####
# example of one-step reduction
#####
eqlow = EQVar('2020A') # consult with IS for the correct value
eqlow._outputdir = output_path # update as appropriate
eqlow._absolutescale = 1 # update as appropriate
eqlow._thickness = 1 # update as appropriate
eqlow._empty = "113526" # update as appropriate
eqlow._bkgscatt = "113530" # update as appropriate
eqlow._bkgtrans = "113527" # update as appropriate

eqhi = EQVar('2020A') # consult with IS for the correct value
eqhi._outputdir = output_path # update as appropriate
eqhi._absolutescale = 1 # update as appropriate
eqhi._thickness = 1 # update as appropriate
eqhi._empty = "113518" # update as appropriate
eqhi._bkgscatt = "113523" # update as appropriate
eqhi._bkgtrans = "113519" # update as appropriate
```

- c. Provide scattering and transmission run numbers for the samples and the overlap range for stitching

```
# define run numbers
samscatt_hi = [113524]
samtrans_hi = [113520]

samscatt_low = [113531]
samtrans_low = [113528]

fn_merged = ['porsil']
suffix = '_merged.dat'

# define overlap range
overlap = [0.06, 0.07]
```

- d. Run the reduction script and observe the results as describe above in section 3.5.

2.7 Data Reduction with Added Flexibility

- a. The template file provided serves as a reduction example for simple cases. The data reduction software is highly configurable through the various reduction parameters that can be seen in the json files created during script execution. Consult with an instrument scientist about their usage. Data reduction with more specialized needs can be achieved through modifying json parameters. A separate document describes the various parameters.
- b. The json files can be directly edited with gedit or pluma, but can be viewed easily with the prettyjson.sh script that is created during the steps described in section 3.3.
- i. Being in the output subdirectory within the shared directory the script can be run as follows:
 1. ./prettyjson.sh <name_of_jsonfile>
- c. Modify the selected json parameters by adding new lines to the reduction script. In the example below, a different sensitivity file is specified on the last line.

```
#####
# example of one-step reduction
#####
eqlow = EQVar('2020A') # consult with IS for the correct value
eqlow._outputdir = output_path # update as appropriate
eqlow._absolutescale = 1 # update as appropriate
eqlow._thickness = 1 # update as appropriate
eqlow._empty = "113526" # update as appropriate
eqlow._bkgscatt = "113530" # update as appropriate
eqlow._bkgtrans = "113527" # update as appropriate

eqhi = EQVar('2020A') # consult with IS for the correct value
eqhi._outputdir = output_path # update as appropriate
eqhi._absolutescale = 1 # update as appropriate
eqhi._thickness = 1 # update as appropriate
eqhi._empty = "113518" # update as appropriate
eqhi._bkgscatt = "113523" # update as appropriate
eqhi._bkgtrans = "113519" # update as appropriate
eqhi._sensitivityfilename = "/SNS/EQSANS/shared/NeXusFiles/EQSANS/2019B_mp/
Sensitivity_patched_thinPMMA_4m_108772.nxs"
```



- d. All parameter names are to be written in lowercase letters.

Disclaimer

The data reduction scripting method presented here was developed by Dr. Changwoo Do (doc1@ornl.gov). Responsibility for its use, bug fixes and further development lie solely with the EQ-SANS team. All questions and concerns should be directed to your local contact, who will either help debug your reduction script or provide feedback to the Research Software Engineering group about bugs in the drtsans package that performs the reduction.

3. EQSANS Data Reduction with drtsans—Quick Reference for Working in MantidWorkbench

Editors: Changwoo Do, Gergely Nagy, William Heller

Date: 07/16/2020

Video tutorial: <https://www.youtube.com/watch?v=g04A2DwE4Mc&feature=youtu.be>

3.1 Introduction

EQ-SANS data reduction is typically performed through two equivalent means:

- via scripts run in the terminal window or
- via MantidWorkbench.

The present document details the latter method. Your local contact will work with you to configure the reduction for the various instrument configurations that you use during your experiment.

Below is a step by step description of the procedure.

3.2 Data Reduction Using MantidWorkbench and Scripts

3.2.1 Visit analysis.sns.gov

- a. Data reduction can be performed both from inside and outside of ORNL
- b. Log in with your ucams ID and password
- c. The same credentials can be used for easy file transfer to personal computer via e.g. WinSCP

3.3 Populate the Shared Directory and Activating the Reduction Environment

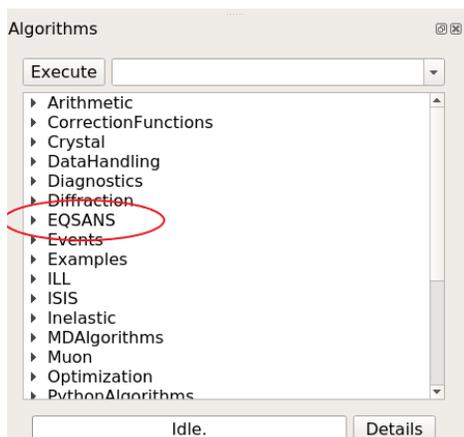
Populate the shared directory of your IPTS with the required reduction tools and activate the reduction environment.

- a. open a terminal
- b. go to the shared folder of your IPTS
 - i. `cd /SNS/EQSANS/IPTS-*****/shared`
- c. copy eqsans_setup.sh from /SNS/EQSANS/shared/usertools/
 - i. `cp /SNS/EQSANS/shared/usertools/* ./`
- d. run eqsans_setup.sh by typing
 - i. `./eqsans_setup.sh`
- e. run eqsans_activatedrtsans.sh by typing
 - i. `source ./eqsans_activatedrtsans.sh`

3.4 Start mantidworkbenchnightly

- a. In the terminal, type `mantidworkbenchnightly` and press Enter.
- b. When running the software for the first time you will not see EQSANS in the algorithm list

- i. To make it available go to File -> Manage user directories -> Python Script Directories Tab -> Browse to Directory and select the following directory: /SNS/EQSANS/shared/script/MantidAlgorithms and Open it.
- ii. Close mantidworkbench and restart it as shown in Step 3.a.
- iii. You will now see EQSANS listed in the algorithm browser window, shown below.



- c. Under File, open reduce_template_mantid.py script that was created during the actions of Step 3.3.
- d. The template is very similar to the reduce_template.py described in the partner document. The main differences are summarized below.
 - i. The “from drtsans.stitch import stitch_profiles” is removed
 - ii. The line “from eqsans_drtsans_script import *” has been changed to “from eqsans_drtsans_script_mantid import *”
 - iii. The command “reduceNow” has been changed to the command “mreduceNow”
- e. To run the reduction, click the green arrow above the script.

3.5 Example of Writing and Running a Script for a Single Configuration Reduction

Information about how to write a data reduction script for reducing data collected with a single instrument configuration is provided in the partner document. The process does not change.

3.6 Stitching of Individual Runs

Information about how to stitch data collected using two different configurations into a single profile is provided in the partner document. The process does not change.

3.7 Reducing and Stitching Two Configurations in a Single Script

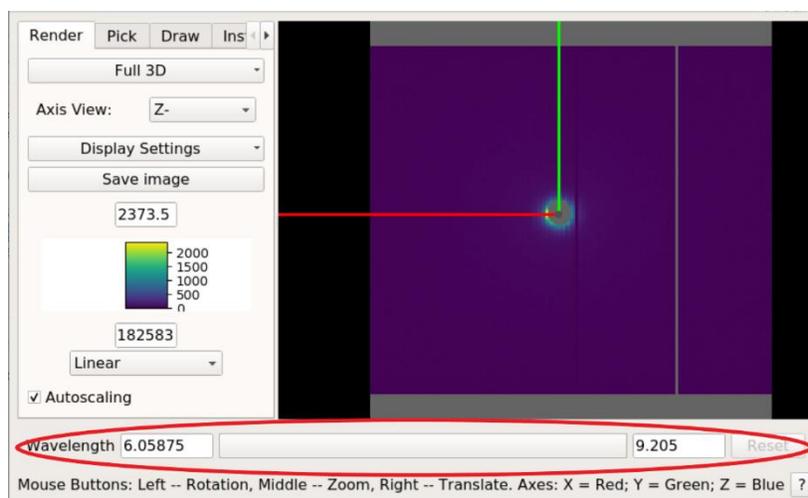
The integration of data reduction of multiple configurations with automated data stitching into a single provide is provided in the partner document. The process does not change.

3.8 Data Reduction with Added Flexibility

Information about how to access the flexibility provided by drtsans for data reduction is provided in the partner document. The method does not change. Users are encouraged to discuss their needs with their local contact.

3.9 Displaying the Obtained Results

- a. The reduced 1D data files, which are simple ASCII text, can be loaded via the Load button
 - i. Note that in the Load Dialogue the proper unit of the data files for the x-axis has to be selected i.e. Energy or Momentum transfer etc. When plotting I(q) files for EQSANS always use Momentum transfer as unit.
 - ii. Files loaded into the workspaces window can be plotted
 1. Right click on the desired workspace.
 2. Select plot spectrum with errors
 3. Within the plot, axis can be changed by right click and choosing desired axis combination.
- b. The detector-efficiency calibrated, masked 2D data, which have file names that end in “.nxs”, can be also loaded into the workspaces window by the Load button of the interface.
 - i. Once loaded and visible in the workspaces window, right click on the workspace and select “show instrument”.
 - ii. The data can be displayed as a function of the considered wavelength band, via the bar at the bottom of the pop-up window



3.9.1 Data reduction using MantidWorkbench and a data catalog

An alternative method for reducing data is to use an algorithm that allows necessary information to be entered in a spreadsheet. The actual data reduction software remains drtsans, so the use of the different approach does not impact the final results.

3.10 Visit analysis.sns.gov

- a. Data reduction can be performed both from inside and outside of ORNL
- b. Log in with your ucams ID and password
- c. The same credentials can be used for easy file transfer to personal computer via e.g. WinSCP

3.11 Creating a Catalog of the Measurement Parameters

- a. A catalog of the runs collected up to that point in time during the experiment can be created with the EQSANSCreateCatalog algorithm. You must supply the IPTS number of the experiment.
 - i. Simple catalogues – containing total counts, duration, sample-to-detector distance and wavelength information can be created via checking SimpleCatalog box. Such catalogs are useful when working with the scripting described in the partner document.
 - ii. For data reduction purposes leave the SimpleCatalog box option unchecked
 - iii. If the catalog file already exists under the same name, it will be overwritten only if the “Overwrite” box is checked. Otherwise, the catalog will not be created.
- b. The resulting catalog is saved in .xlsx format which can be viewed using spreadsheet software. The file format is native to Excel, but can also be read on the Linux computers (analysis.sns.gov or the instrument data reduction computers) using gnumeric or Calc. Table file can also be opened by using the opentable algorithm from the EQSANS algorithm list.
 - i. The top of the table contains reduction configuration parameters, which can be used here, or in support of customizing the script based reduction.
 - ii. If good practice was used when naming scattering and transmission runs, the table will also show a guess at the transmission run numbers with their corresponding scattering run numbers.
 1. It is a good practice to verify that that the association of scattering and transmission runs is correct before reducing data.

3.12 Catalogue-based Data Reduction

- a. Your catalog must have been created with the SimpleCatalog option left unchecked.
- b. Column A in the catalog is used to specify how information on that line is treated. There are 3 options. Leaving the column blank means that the row is not processed.
 - i. y – for reduction
 - ii. s – for stitching
 - iii. v – for changing variablesAn explanation of the options is also provided on the top three lines of the catalog.
- c. To reduce data listed in a specific row complete columns D to G with relevant information
 - i. Reduction can be performed without subtracting a background. To do so, leave columns E and F empty
- d. Sample thickness, output name and number of Q bins in the output intensity data set can also be specified independently for each row. The absolute scale factor that is specified in column J should come from a measurement and analysis of the standard sample, which your local contact will help you with. Filenames will be created with the “_suffix” parameter specified at the top of the table along other parameters.
- e. If specific configuration information needs to be provided for each different instrument configuration employed, it can be provided using the “Config name” parameter. Your local contact can be of assistance.
 - i. Config name is the same variable that is used to define the EQVar class object. For example, in the script method, reduction variable object can be defined as
 1. eq = EQVar(‘2020A’) or by specifying json file such as eq=EQVar(‘4m10a.json’)
 2. Those configuration json files are created and provided by the instrument scientists.

- f. To stitch data from different configurations together, create new rows in the table and flag them with “s”, as described above. The rows for stitching will not interfere with the data reduction process. Additionally, creating extra rows in the table and copying another line to use as a template for performing an operation does not interfere with the data reduction processes specified in the catalog.
 - i. Note that during stitching, the “ref-to” option defines the data set in the list to which the other scattering data will be scaled. Unlike in script mode, in the catalogue based reduction 1 means that the data will be stitched to the first data set in the list.
 - ii. As is done in the script-based reduction, provide the desired name for the stitched data file and the overlapping momentum transfer ranges to use for stitching and calculating the relative scale factor.
 - iii. By default, the output format for stitching will be ASCII text, and the file extension will be “.txt”.

| | | | | | | | | | | | | | |
|----|-------------------|---------------|----------------------|--------|--------|-----------------|--------|------|------|---------------|-----|-----|------|
| 42 | | 113458 | S-empty beam 4m 2.5A | 113454 | | | | | 1 | 1 | 120 | | True |
| 43 | | 113459 | S-empty cell 4m 2.5A | 113455 | | | | | 1 | 1 | 120 | | True |
| 44 | y | 113460 | S-porsil 4m 2.5A | 113456 | 113459 | 113455 | 113454 | | 1 | porsil_4m2o5a | 1 | 120 | True |
| 45 | | 113461 | S-agbe 4m 2.5A | 113457 | | | | | 1 | | 1 | 120 | True |
| 46 | | 113462 | T-empty beam 4m 10a | | | | | | | | | | |
| 47 | | 113463 | T-empty cell 4m 10a | | | | | | | | | | |
| 48 | | 113464 | T-porsil 4m 10a | | | | | | | | | | |
| 49 | | 113465 | S-empty beam 4m 10a | 113462 | | | | | 1 | 1 | 120 | | True |
| 50 | | 113466 | S-empty cell 4m 10a | 113463 | | | | | 1 | 1 | 120 | | True |
| 51 | y | 113467 | S-porsil 4m 10a | 113464 | 113466 | 113463 | 113462 | | 1 | porsil_4m10a | 1 | 120 | True |
| 52 | Stitch (stitch/s) | conf1 | conf2 | conf3 | ref-to | savename | q1l | q1f | q2l | q2f | | | |
| 53 | s | porsil_4m2o5a | porsil_4m10a | | | 1_porsil_stitch | | 0.06 | 0.07 | | | | |

- g. After filling all of the desired rows, save the file and close the catalogue.
- h. To reduce the data, chose the EQSAMSTableDRT algorithm from the list in MantidWorkbench and select the catalog that you have created.
- i. Execute the algorithm
- j. The reduced data can be displayed as described in paragraph 3.9.

Disclaimer

The data reduction scripting method presented here was developed by Dr. Changwoo Do (doc1@ornl.gov). Responsibility for its use, bug fixes and further development lie solely with the EQ-SANS team. All questions and concerns should be directed to your local contact, who will either help debug your reduction script or provide feedback to the Research Software Engineering group about bugs in the drtsans package that performs the reduction.

4. Bio-SANS Data Reduction with drtsans—Quick Reference for the Data Reduction Parameters

The various parameters required by drtsans are listed below with a brief description of their meaning, the acceptable values, and appropriate format for the information. Additional information can be obtained through your local contact. An example is shown here.

Below is the same configuration file expanded into a more readable format.

```
{"schemaStamp": "2020-04-15T21:09:52.745905",
"instrumentName": "BIOSANS",
"iptsNumber": 25816,
"dataDirectories": null,
"sample": {"runNumber": "6679",
"thickness": 0.1,
"transmission": {"runNumber": "6679", "value": null}},
"background": {"runNumber": "6649, 6659",
"transmission": {"runNumber": "6649, 6659", "value": null}},
"emptyTransmission": {"runNumber": "6641", "value": null},
"beamCenter": {"runNumber": "5896"},
"outputFileName": "test_data",

"configuration": {
"outputDir": "/SNS/users/q3n/reduce2020/etcetc",
"wavelength": 6.0,
"wavelengthSpread": 0.132,
"useTimeSlice": false,
"timeSliceInterval": 7200.0,
"useLogSlice": false,
"logSliceName": "CG3:SE:PolyScience:TempRead",
"logSliceInterval": 0.01,
"sampleOffset": null,
"sampleApertureSize": null,
"sampleDetectorDistance": null,
"sampleToSi": null,
"sourceApertureDiameter": null,
"usePixelCalibration": false,
"maskFileName": null,
"useDefaultMask": true,
"defaultMask": [{"Pixel": "1-14,242-256"}, {"Bank": "21-24,45-48"}]},
"useMaskBackTubes": false,
"darkMainFileName": "CG3_5884.nxs.h5",
"darkWingFileName": "CG3_5884.nxs.h5",
"normalization": "Monitor",
"sensitivityMainFileName":
"/SNS/users/q3n/reduce2020/sensitivity487/CG3_sens_main5904sac_tdc7m.nxs",
"sensitivityWingFileName":
"/SNS/users/q3n/reduce2020/sensitivity487/CG3_sens_wing5946sac_tdc3.2d.nxs",
"useSolidAngleCorrection": true,
"blockedBeamRunNumber": null,
"useThetaDepTransCorrection": true,
"DBScalingBeamRadius": 40.0,
"mmRadiusForTransmission": null,
"absoluteScaleMethod": "standard",
"StandardAbsoluteScale": 4.71e-11,
"numMainQxQyBins": 100,
"numWingQxQyBins": 100,
"1DQbinType": "scalar",
```

```

"QbinType": "log",
"numMainQBins": null,
"numWingQBins": null,
"LogQBinsPerDecadeMain": 30,
"LogQBinsPerDecadeWing": 30,
"useLogQBinsDecadeCenter": false,
"useLogQBinsEvenDecade": true,
"WedgeMinAngles": [-45.0, 165.0],
"WedgeMaxAngles": [45.0, 190.0],
"autoWedgeQmin": 0.003,
"autoWedgeQmax": 0.04,
"autoWedgeQdelta": 0.01,
"autoWedgeAzimuthalDelta": 1.0,
"autoWedgePeakWidth": 0.25,
"autoWedgeBackgroundWidth": 1.5,
"autoWedgeSignalToNoiseMin": 2.0,
"AnnularAngleBin": 1.0,
"useErrorWeighting": false,
"smearingPixelSizeX": null,
"smearingPixelSizeY": null,
"useSubpixels": false,
"subpixelsX": null,
"subpixelsY": null,
"QminMain": 0.0067,
"QmaxMain": 0.1,
"QminWing": 0.07,
"QmaxWing": 0.6,
"overlapStitchQmin": [0.075],
"overlapStitchQmax": [0.095],
"wedge1QminMain": 0.02,
"wedge1QmaxMain": 0.09,
"wedge1QminWing": 0.08,
"wedge1QmaxWing": 0.09,
"wedge1overlapStitchQmin": 0.0825,
"wedge1overlapStitchQmax": 0.0875,
"wedge2QminMain": 0.02,
"wedge2QmaxMain": 0.125,
"wedge2QminWing": 0.06,
"wedge2QmaxWing": 1.0,
"wedge2overlapStitchQmin": 0.075,
"wedge2overlapStitchQmax": 0.095,
"wedges": [[-45.0, 45.0], [165.0, 190.0]],
"symmetric_wedges": true},
"logslice_data": {}
}

```

4.1 Parameter Descriptions

Note that all key:value pairs use quotes around both the key and value unless the value is null or a mathematical constant. Also note that the file has a hierarchical structure, where {} are used to denote groupings. The descriptions of the parameters below reflect the structure of the hierarchy.

1. "schemaStamp": "2020-04-15T21:09:52.745905"
This particular parameter is autogenerated by the scripting method for reducing data. It should not be changed if you can access it, even when hand-modifying the contents of the configuration file.

2. "instrumentName": "BIOSANS"
The instrument name is used by drtsans to know how to use some of the specified parameters. It must be consistent with the instrument used for the data collection (i.e. do not try to reduce data from BIOSANS if this parameter is set to "GPSANS"). Note that there is no dash in the name of the instrument in the drtsans parameter file.
3. "iptsNumber": "25816"
The proposal number for the experiment allows drtsans to quickly find the data to be reduced, rather than using tools to find the data based solely on the run number. It can be left blank (i.e. "").
4. "sample":
This is the first parameter that contains a set of parameters grouped using {}. The various parameters in the group follow.
 - a. "runNumber": "6679"
This is the run number for the sample scattering to be reduced. It can be found via OnCat. It is possible to specify a set of scattering runs for a single sample that are to be summed together into a single data set for reduction. To do so, use the following format, which uses a single pair of quotes to enclose the list.
 - i. "runNumber":{"run1, run2"}
 - b. "thickness": 0.1
This parameter specifies the sample thickness in centimeter. Note that the value is not enclosed in quotes.
 - c. "transmission":
This is the start of another level of the hierarchical structure. Of the two key:value pairs in this grouping, only one can have an actual value: either the run number or the value of the transmission to use for the reduction. One rarely specifies a simple value for the transmission for EQ-SANS data because the transmission is wavelength-dependent.
 - i. "runNumber": "6679"
This is the run number of the transmission for the sample. At Bio-SANS, we are using a semi-transparent beam stop for 6Å neutron so that the transmission is taken while measuring the scattering. The run number in this case will be the same as the sample run number. But for other wavelengths, the run number will be different. There can only be a single run number specified here.
 - ii. "value": ""
This would be a numerical value for the transmission to use for the reduction, which would normally only be done for quick qualitative checks if the data needs to be viewed prior to the completion of the transmission measurement for a sample. Note that the value must be enclosed in quotes ("").

5. "background":
The set of parameters that follow specify information required to identify the background to use for the reduction. It is possible to reduce data without a background by leaving the run numbers in this set of parameters empty (i.e. "").
 - a. "runNumber": "6649, 6659",
The run number(s) of the background data to subtract from the sample scattering. In this case, two runs are used.
 - b. "transmission":
The following set of parameters are used to specify either the run number for the background's transmission measurement or to specify a value for the transmission of the background.
 - i. "runNumber": "6649, 6659"
 - ii. The run number for the background's transmission measurement. If no background is specified, then this run number should not be specified (i.e. set to "").
 - iii. "value": ""
 - iv. This would be a numerical value for the transmission to use for the reduction, which would normally only be done for quick qualitative checks if the data needs to be viewed prior to the completion of the transmission measurement for a sample. Note that the value must be enclosed in quotes ("").

6. "emptyTransmission":
This grouping of parameters is used to specify the reference measurement (usually an empty position in the sample holder), or value, used to calculate the transmission from the other specified measurements or values. If the transmissions are specified as values, the value specified here should be "1.0".
 - a. "runNumber": "6641"
The run number for the background's transmission measurement.
 - b. "value": null
A value can be specified for the reference transmission. If used, it should be "1.0", if not specify it as null, as shown above.

7. "beamCenter":
The beam center is specified by providing a run number for an empty beam's transmission measurement to calculate the beam center from.
 - a. "runNumber": "5896"
This is the run number of an empty beam's transmission measurement without a beam stop in front of detector. It cannot be left blank.

8. "outputFileName": " **test_data** "
This is the prefix used to construct all of the file names that result from the data reduction process. In this example, all of the associated files will be named "**test_data***.*". The filename can be any valid string that is acceptable for filenames for a unix operating system.

9. "configuration":
A large number of parameters are specified within this hierarchical grouping, most of which directly impact the reduction process and results produced. Many of these parameters will be provided by your local contact and should not be changed without discussion with the local contact. In the jupyter notebook, some of these parameters may or may not be presented to you. If they are not presented to you in either the scripts that your local contact helps set up for you, then you do not need to provide them directly.
 - a. "outputDir": "/SNS/users/q3n/reduce2020/etcetc",
The directory to write the data reduction result to is listed here. Normally, it would be the shared directory for the particular proposal, which allows other team members and the local contact to view the results. However, it is also possible to specify a location in a user's home directory. It is left to the discretion of the user.

 - b. "wavelength": 6.0,
Wavelength in Angstrom, it is can be specified or leave as null, in which the meta data value in the raw data file will be used.

 - c. "wavelengthSpread": 0.132
Wavelength spread in decimal, it is can be specified or leave as null, in which the meta data value in the raw data file will be used.

 - d. "useTimeSlice": false
If the user wishes to parse the event stream contained in the run specified in the "sample:" parameter set, then set this value to true. If this value is true, then the parameter "useLogSlice", below, must be false.

 - e. "timeSliceInterval": 7200.0
This is the interval in seconds to use for the time slicing of the event stream. The event stream will be cut into as many consecutive portions of the event stream as exist in the file, with a final bin that contains as much time as remains in the stream. In this case, the various slices are for the following intervals: $0 \leq t < 7200$ seconds, $7200 \leq t < 14400$ seconds, etc. Note that the value is not contained in quotation marks.

 - f. "useLogSlice": false,
It is possible to divide an event stream into bins that derive from another parameter that is saved by EPICS in the NeXus file, such as temperature, pressure, magnetic field, or even a motor that continuously moves during data collection. If a user wishes to do so, set the value to true. Note that useLogSlice and useTimeSlice cannot both be true. Discuss the use of log slicing with your local contact.

- g. "logSliceName": "CG3:SE:PolyScience:TempRead"
This is the name of the instrument log to use for log slicing. If useLogSlice is true, change this to the name of the EPICS parameter that you wish to employ. Discuss the use of log slicing with your local contact.
- h. "logSliceInterval": 0.01
This parameter sets the interval of the instrument log specified in logSliceName to use. It must be in the units of the device, be it degrees, millimeters, Celcius, etc. Discuss the use of log slicing with your local contact. Note that the value is not enclosed in quotation marks.
- i. "sampleOffset": null
This parameter is not used by HFIR SANS instruments (Bio-SANS and GPSANS). Please ignore.
- j. "sampleApertureSize": null
This parameter specifies the diameter of the sample aperture used in millimeters. While it is possible to specify the diameter of this aperture during data acquisition, specifying a different value here allows you to over-write the incorrect value saved in the data files in case it is needed. The sampleApertureSize impacts the calculation of the resolution information for the instrument (i.e. the uncertainty in Q), which is required to accurately analyze your data. Note that the value is enclosed in quotation marks.
- k. "sampleDetectorDistance": null,
This parameter overwrites the meta data "**sample-to-detector-distance**" from the raw data in case there is an error. It is the full sample to detector distance in in the unit of meter. Don't change it without consultation with your local contact.
- l. "sampleToSi": null,
This parameter overwrites the meta data the distance between the sample to Bio-SANS detector tank Si window from the raw data in case there is an error. The unit is mm. Don't change it without consultation with your local contact.
- m. "sourceApertureDiameter": null
This can be used to specify the diameter of the source aperture in millimeters used for a measurement. Normally, this parameter is pulled from data file meta data. If you feel that you need to change this value, which you would specify as a number enclosed in quotation marks, consult your instrument scientist.
- n. "usePixelCalibration": false
This parameter is using a pixel map that takes into account the center of pixel on the detector along with its corresponding width and height. This calibration takes into account the nonlinearity of the detector tubes. Please consult the local contact before changing this option.
- o. "maskFileName": null
This is the name of a hand-drawn mask. Currently it is not used at Bio-SANS since no detector bank shows abnormality.

- p. "useDefaultMask": true
This is to use additional mask is applied in addition to the user-specified mask from the maskFileName parameter. If the value is set to true, any mask specified with the "defaultMask" parameter, below, will be applied.
- q. "defaultMask": [{"Pixel": "1-14,242-256"}, {"Bank": "21-24,45-48"}]
This parameter is used to select certain tube banks not used. At Bio-SANS, it is usually used to mask the shadowed tubes or the edge pixels that are distorted. Don't change the value without consulting your local contact.
- r. "useMaskBackTubes": false
The Bio-SANS detector, like the EQ-SANS and GP-SANS detectors, consists of an array of linear position sensitive detectors that are arranged in two planes that are offset to ensure complete coverage across the area of the detector. When this parameter is set to true, the back plane of tubes, being those furthest away from the sample, are all masked. Typically, this is only done when the detector is positioned close to the sample.
- s. "darkMainFileName": "CG3_5884.nxs.h5",
"darkWingFileName": "CG3_5884.nxs.h5",
They specify the names of the files that contains the "dark current" measurement for main and wing detectors, respectively. At Bio-SANS, it is normally a measurement performed during regular calibrations with the facility running but the instrument shutter closed. It is a measure of cosmic radiation and detector electronic noise. Your local contact will provide the correct file to use.
- t. "normalization": "Monitor"
The data can either be normalized by the measurement time ("Time") or the beam monitor ("Monitor"). The normal method for normalizing Bio-SANS data is "Monitor". "Time" is less accurate and reserved for the rare monitor malfunction event.
- u. "sensitivityMainFileName":
"/SNS/users/q3n/reduce2020/sensitivity487/CG3_sens_main5904sac_tdc7m.nxs",
"sensitivityWingFileName":
"/SNS/users/q3n/reduce2020/sensitivity487/CG3_sens_wing5946sac_tdc3.2d.nxs",
The file names of the pre-processed relative pixel response of the detector is specified with the parameters. These calibration files are measured during instrument commissioning each cycle and are prepared by staff for use in data reduction. Consult your local contact for the correct file to use.
- "useSolidAngleCorrection": true
This parameter specifies whether or not to correct the data for the solid angle subtended by each pixel, which can be a considerable effect for configurations with the detector positioned close to the sample. It is recommended to leave this parameter set to true.
- v. "blockedBeamRunNumber": null,
This is the option to use the blocked beam as dark background correction. It is not used at Bio-SANS as the instrument background is low.

- w. "useThetaDepTransCorrection": true
When set to true, the data reduction will correct the data in each pixel for the actual distance that the neutrons travel through the sample when performing the correction for the transmission. The effect increases with scattering angle and can be considerable when the detector is positioned near the sample. It is recommended to leave this parameter set to true.
- x. "DBScalingBeamRadius": 40.0,
This value is to set the beam radius that is used by empty beam scaling which is not deployed at the Bio-SANS. In the current implementation, the empty beam scaling is disabled.
- y. "mmRadiusForTransmission": null
This parameter allows the user to specify the radius in millimeters to use when integrating the attenuated direct beam measurements for calculating the transmissions. At Bio-SANS, this value is optimally determined in the drtsans, and is not required. Consult your local contact if you feel that another value may be required.
- z. "absoluteScaleMethod": "standard"
At present, the method available for scaling data collected on Bio-SANS into absolute units of 1/cm is by using a calibrated standard. Do not change the value of this parameter. Presently, the standard is well-characterized sample of porous silica or H₂O that your local contact will provide to you during your experiment. A measurement of the standard is used to derive the absolute scale factor, which is specified with the StandardAbsoluteScale parameter, described below.
- aa. "StandardAbsoluteScale": "4.71e-11"
This is the scale factor that must be applied to the data to place it into absolute units of 1/cm. Your local contact can help you derive it from a measurement of a standard.
- bb. "numMainQxQyBins": 100,
"numWingQxQyBins": 100,
This parameter specifies the number of Q-bins in the 2D reduced data, which is always part of the output by drtsans. Note that only a single value may be provided, which implies that the 2D reduced data is on a regular, square grid that covers the Q-range in 2D measured by the detectors. The beam center is not necessarily in the center of the output data. The grid in Q-space is always linear.
- cc. "1DQbinType": "scalar"
Three options exist for the kind of 1D data that are output by drtsans. Possible values are "scalar", which is used for 1D azimuthally averaged data that most people are familiar with; "wedge" makes it possible to define wedges to perform scalar binning within, as one might do for anisotropic data and utilize the WedgeMinAngles, WedgeMaxAngles and the various autoWedge parameters described below, although automatic wedge determination is not enabled for EQ-SANS at this point in time. The "annular" binning makes it possible to visualize how data varies around the beam center within a Q-range specified by the user and requires that the parameters AnnularAngleBin, Qmin and Qmax, described below, be provided.

dd. "QbinType": "log"

This parameter dictates whether the Q-spacing of the intensity profiles calculated when performing scalar or wedge binning is logarithmic or linear. The possible values of this parameter are "log" and "linear". The choice of binning determines how the numQBins, LogQBinsPerDecade and useLogQBinsEvenDecade parameters work.

ee. "numMainQBins": null,
"numWingQBins": null,

This parameter must be set to an integer value if QbinType is "linear", but can also be used if it is "log". The value is the number of Q-values that are in the 1D data that is binned as "scalar" or "wedge" and their spacing is determined by the value of QbinType. This parameter must be null if LogQBinsPerDecade is set to an integer value. Note that the value is enclosed in quotation marks.

ff. "LogQBinsPerDecadeMain": 30,
"LogQBinsPerDecadeWing": 30,

This parameter only works when QbinType is "log". The value specified here will be the number of Q-bins that are present within each decade between the minimum and maximum Q values that the reduced data contain. For example, if the value is "30", then there are 30 Q-bins between 0.01 \AA^{-1} and 0.10 \AA^{-1} and 30 Q-bins between 0.10 \AA^{-1} and 1.0 \AA^{-1} or any other decade in Q that are present in the reduced data. The parameter useLogQBinsEvenDecade must be set to true to enable this option and numQBins must be null.

gg. "useLogQBinsDecadeCenter": false

At present, this option is no longer enabled. The Q-values when using an even number of Q-bins per decade by setting useLogQBinsEvenDecade to true and providing a value for logQBinsPerDecade to a non-zero, positive integer always have a bin centered on 0.001 \AA^{-1} , 0.010 \AA^{-1} , 0.100 \AA^{-1} , etc.

hh. "useLogQBinsEvenDecade": true

This parameter tells drtsans to use a fixed number of Q-bins per decade when binning the result. The logQBinsPerDecade parameter must have a non-zero integer value and numQBins must be null.

ii. "WedgeMinAngles": [-45, 165]

"WedgeMaxAngles": [45, 190]

The WedgeMinAngles and WedgeMaxAngles are only used when QbinType is set to "wedge". The arrays provide a matched set of angles, specified in degrees and indexed from the Qx axis, within which to perform 1D Q-binning. In this particular example, 1D Q-binning will be performed in two wedges: from -45° to 45° and from 165° to 190° . The angles need not be the same size and need not be symmetric. It is also possible for the angles to overlap, should the user desire it. The only requirement is that both arrays have the same number of elements and that the minimum angle for a wedge be lower than the maximum value for that wedge.

Parameters shown in points kk through qq, zz and ccc, below, are required for the drtsans methods for automatically determining the correct wedges to use for binning reduced data

into 1D. Development of these routines was driven by the Bio-SANS instrument team. At present, automatic wedge determination is not available for data collected using EQ-SANS.

jj. "autoWedgeQmin":

"autoWedgeQmax": null

"autoWedgeQdelta": null

"autoWedgeAzimuthalDelta": null

These parameters are used to convert the Qy vs Qx 2d-image into a series of curves, Intensity vs. Phi (azimuthal angle) for different fixed Q-values. The Q-range of the main detector determines Qmin ('kk') and Qmax ('ll'). The Q bin size is determined by Qdelta ('mm'); an optimal setting of Qdelta would be to result in ~10 Q-bins in the range- Qmin to Qmax. The choice of Qdelta is a delicate balance between small Qdelta (weak signal to resolve the wedge angles) and large Qdelta (smeared anisotropy in the data). The Phi bin size is determined by 'nn'; a good estimate is between 1° to 5°.

kk. "autoWedgePeakWidth": null

"autoWedgeBackgroundWidth": null

"autoWedgeSignalToNoiseMin": 2.0

These parameters are used to determine wedge angles by performing peak fitting to the curves produced above (kk). The angular range of the wedge(s) associated to the enhanced scattering peak is set by the peak width parameter ('oo'). This number is a ratio of the peak's full-width-half-maximum (FWHM); typical values are between 0.25 to 1.0, i.e., from 1/4th FWHM to one FWHM. Similarly, the angular range of the wedge(s) associated to the background scattering (flat background scattering) is set by the background width parameter ('pp'); typical values are between 1.0 to 2.0. The last term is used to detect the presence of enhanced scattering peaks. If the process of detecting a peak has failed due to weak scattering signal, one option is to reduce signal-to-noise min value progressively until 1.25. Note, a value of 1.0 implies that the signal and noise are of equal magnitude, which is not recommended.

ll. "AnnularAngleBin": 1.0,

When the 1DQbinType parameter is set to "annular" this parameter specifies the size of the bins in degrees that are to be used for binning. Annular binning takes the data in a ring of Q-values and creates a profile as a function of angle around the beam center. Annular binning also requires that Qmin and Qmax, described below, be specified.

mm. "useErrorWeighting": false,

If weighting by the experimental uncertainty is desired when binning the reduced data and propagating the corresponding uncertainties, set the value of this parameter to true.

nn. "smearingPixelSizeX": null,

"smearingPixelSizeY": null,

The detectors used in the SANS instruments at ORNL are gas detectors. The pixel sizes are determined from parameters supplied to the hardware that determines where a neutron is detected and can be varied by changing said parameters. In actuality, there is intrinsic uncertainty in the position of the event along the tube. Further, the arrangements of the tubes in the detector makes it possible to have a neutron in the region of overlap between a tube in the front panel and a tube in the back panel be detected in either, which also creates

uncertainty in the position in which an event is encoded. The `smearingPixelSizeX` and `smearingPixelSizeY` parameters make it possible to account for this uncertainty when calculating the uncertainty in Q . The effect is small for most Q -values, but can impact data analysis when sharp features are present. Your local contact can provide suitable values for the parameters. Note that specifying values for these two parameters does not change the calculation of the value of Q or the intensity profile that results after reduction. It only alters the uncertainty in Q (ΔQ) of the result.

oo. `"useSubpixels": null`

In cases where there are sharp features in the data, or a need to use as much data near the beam stop as possible, it is possible to divide the pixels defined on the detector into sub pixels to improve the quality of the results from the 1D binning process. Subpixels, if specified, will also be used in the 2D binning. To enable this feature, set `useSubpixels` to true and set `subpixelsX` and `subpixelsY`, described below, to positive integers.

pp. `"subpixelsX": null,`
`"subpixelsY": null,`

Set these two parameters to a non-zero, positive integer to use subpixels when binning the data. The real pixels will then be divided into subpixels for the binning in the data reduction. If `subpixelsX` is set to 2 and `subpixelsY` is set to 3, then each pixel will be divided into a 2 by 3 grid for the binning process.

qq. `"QminMain": 0.0067,`
`"QmaxMain": 0.1,`
`"QminWing": 0.07,`
`"QmaxWing": 0.6,`

When performing annular binning this is the minimum and maximum Q -values, specified in \AA^{-1} , to use during the binning. These values are used at Bio-SANS to create a clear cut-off for both main and wing detector in both scalar and annular binning.

rr. `"overlapStitchQmin": [0.075],`
`"overlapStitchQmax": [0.095],`

This pair of parameters are to set the overlap range for stitching 1D data from two instrument configurations to produce a single curve. This is in addition to the merged curve from two detectors at one single configuration. The range is usually determined during the calibration, please consult your local contact if any change is desired.

ss. `"wedge1QminMain": 0.02,`
`"wedge1QmaxMain": 0.09,`
`"wedge1QminWing": 0.08,`
`"wedge1QmaxWing": 0.09,`
`"wedge1overlapStitchQmin": 0.0825,`
`"wedge1overlapStitchQmax": 0.0875,`

These parameters help cleanly present the data from the main detector, wing detector and based on the overlap region defined, the stitched data for wedge1. These parameters are only enabled when wedge reduction is chosen (auto or manual).

tt. "wedge2QminMain": 0.02,
"wedge2QmaxMain": 0.125,
"wedge2QminWing": 0.06,
"wedge2QmaxWing": 1.0,
"wedge2overlapStitchQmin": 0.075,
"wedge2overlapStitchQmax": 0.095,

These parameters help cleanly present the data from the main detector, wing detector and based on the overlap region defined, the stitched data for wedge2. These parameters are only enabled when wedge reduction is chosen (auto or manual).

uu. "wedges": [[-45.0, 45.0], [165.0, 190.0]],

There is no need to change this. This is part of some output parameters, not input for reduction. They are used in plotting. If you specify the `WedgeMinAngles` and `WedgeMaxAngles`, or if you use automatic wedge detection, this "wedges" entry will be populated to give you easier access to plot with those parameters.

vv. "symmetric_wedges": true,

This parameter is associated with the auto-wedge process. If the scattering has 2-fold symmetry ('true'), the wedges on diametrically opposite directions are set to be identical. If 4-fold symmetry ('false'), then all the four wedges are considered to have independent angular ranges. Default is 'true'.

ww. "logslice_data": {}

There is no need to change this. This is part of some output parameters, not input for reduction. This contains information about the splitting. For example, if you use temperature metadata as a function of to slice data, this will provide metadata reference to the temperature.

5. Bio-SANS Data Process Guide—Quick Reference for using Jupyter Notebook to Reduce Data

Video tutorial: <https://www.youtube.com/watch?v=DniWKMSIX0&feature=youtu.be>

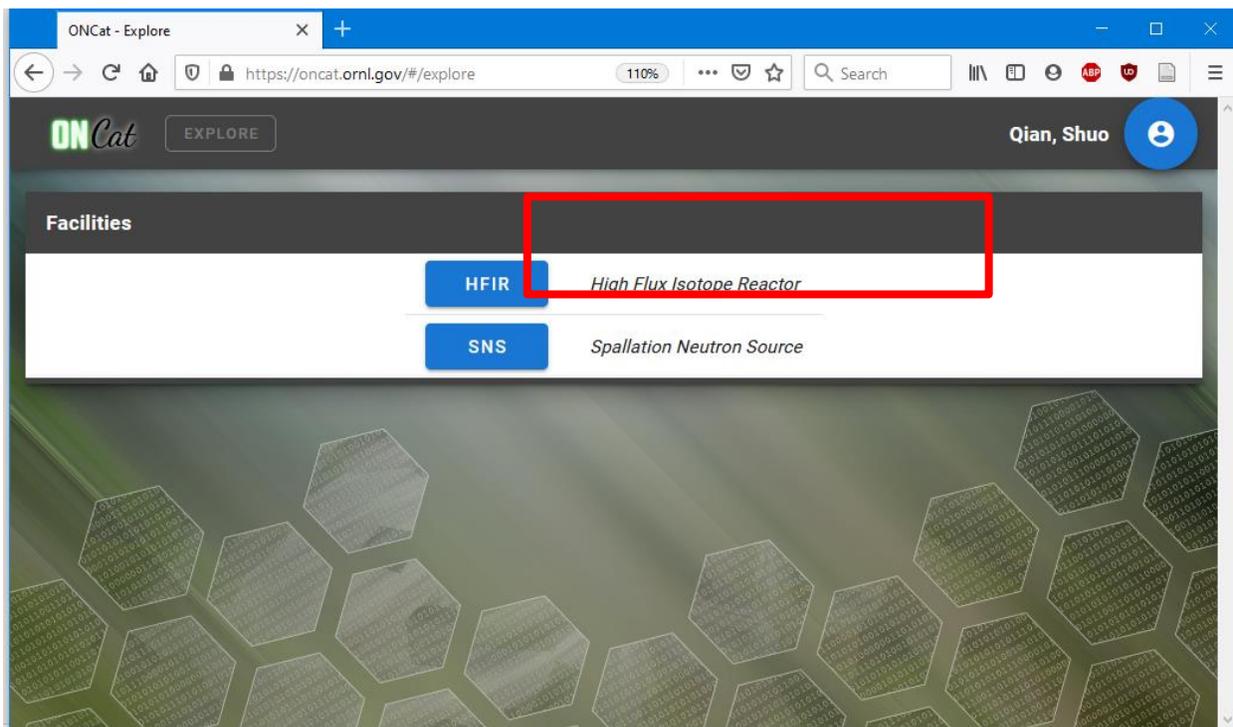
Note:

- This is a quick reference to guide you through using data reduction for Bio-SANS. It won't replace the function of your instrument local contact, who is the first and foremost the best person for instrument related questions. **Please work with her/him to setup and understand the data reduction process before using the guide.**
- Various on-line systems will be used for this process, you should have your ORNL GUEST Portal login and password handy. They are accessible both inside and outside ORNL.
 - <https://oncat.ornl.gov> <data catalogue, Demo: oncat.ornl.gov/videos/demo.mp4>
 - <https://jupyter.sns.gov> <data reduction notebook script interface>
 - <https://analysis.sns.gov/> <data analysis cluster, where all data are located>

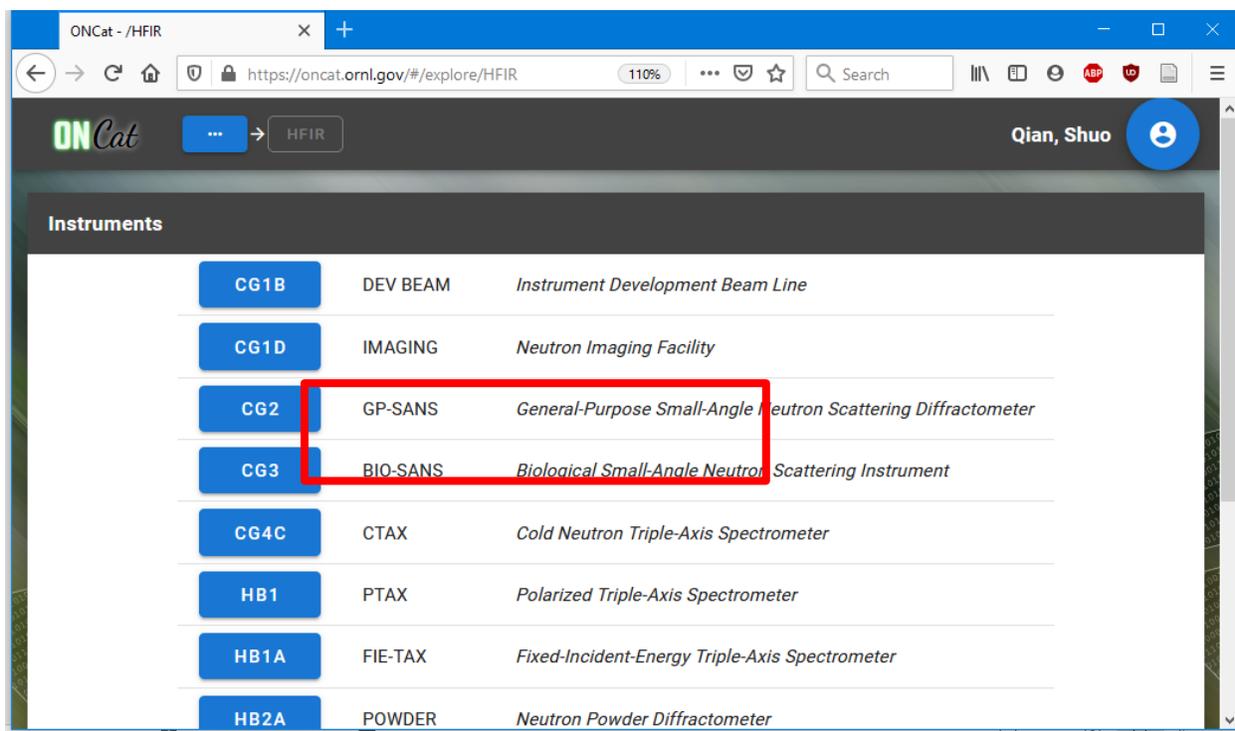
5.1 Identify the Run Numbers for the Data in ONCat.ornl.gov

All data are saved in sequential number (Run #) with all metadata information such as title, time and other user specified information. The run number is used in the reduction to call the data. Identifying the run number for the data to be reduced in the data catalogue is the first step in the process.

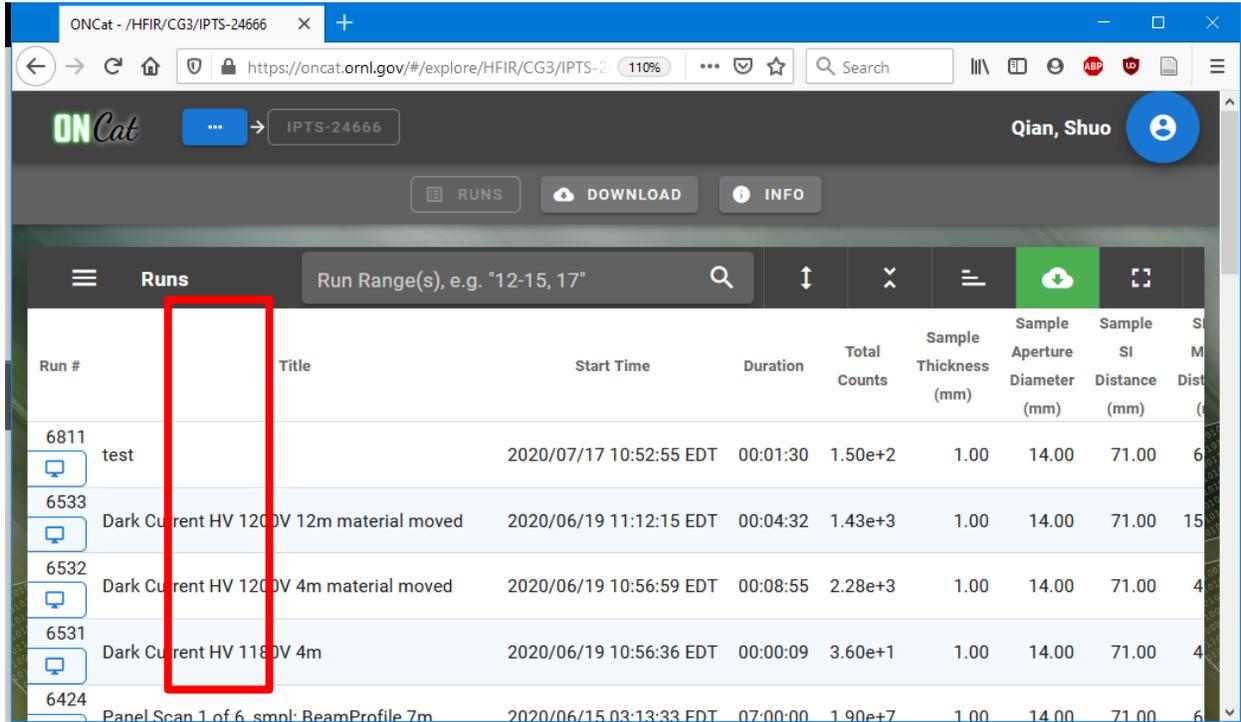
5.1.1 Login into oncat.ornl.gov.



5.1.2 Click into HFIR > CG3, then find your experiment IPTS.



5.1.3 The run number is the very first column in the list, along with other useful information to identify data.



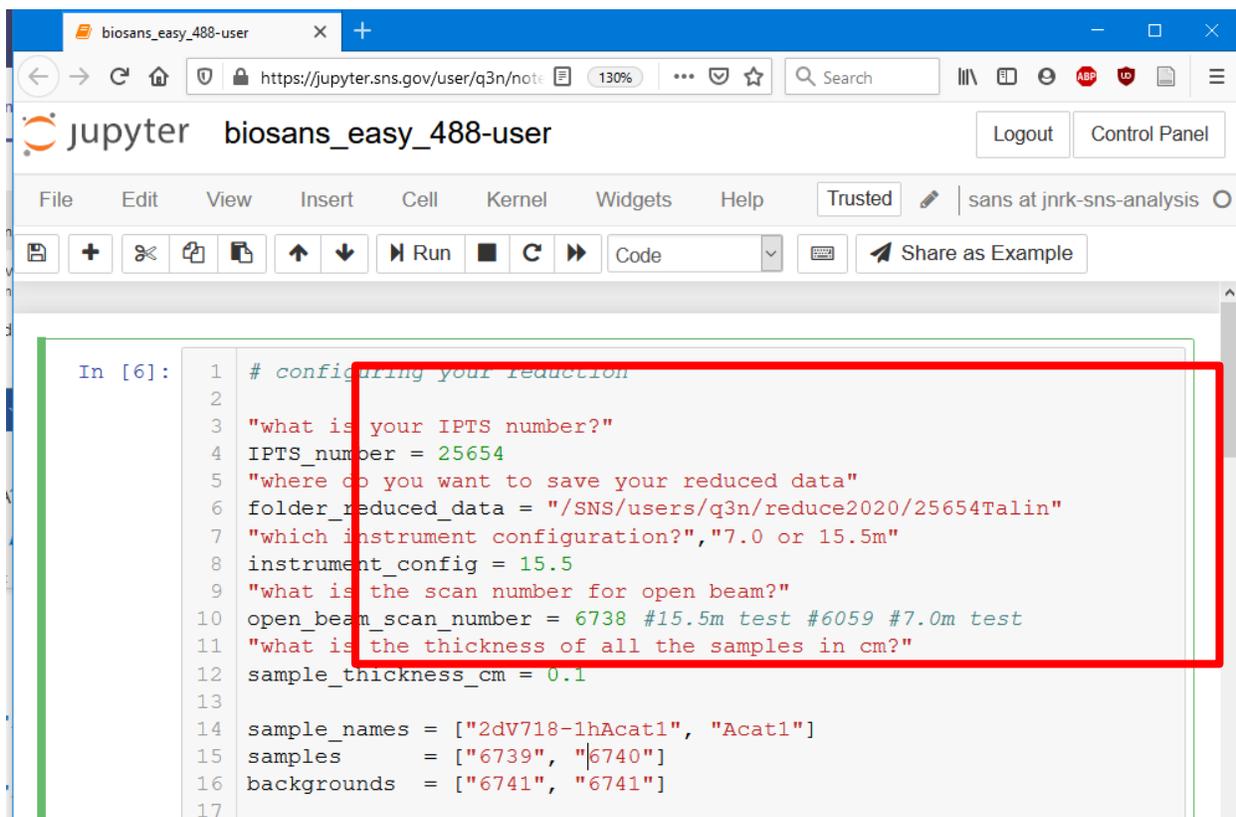
The screenshot shows the ONCat web interface for experiment IPTS-24666. The 'Runs' section is active, displaying a table of experimental runs. A red box highlights the 'Run #' column. The table includes columns for Run #, Title, Start Time, Duration, Total Counts, Sample Thickness (mm), Sample Aperture Diameter (mm), and Sample SI Distance (mm).

| Run # | Title | Start Time | Duration | Total Counts | Sample Thickness (mm) | Sample Aperture Diameter (mm) | Sample SI Distance (mm) | Dist |
|-------|--|-------------------------|----------|--------------|-----------------------|-------------------------------|-------------------------|------|
| 6811 | test | 2020/07/17 10:52:55 EDT | 00:01:30 | 1.50e+2 | 1.00 | 14.00 | 71.00 | 6 |
| 6533 | Dark Current HV 1200V 12m material moved | 2020/06/19 11:12:15 EDT | 00:04:32 | 1.43e+3 | 1.00 | 14.00 | 71.00 | 15 |
| 6532 | Dark Current HV 1200V 4m material moved | 2020/06/19 10:56:59 EDT | 00:08:55 | 2.28e+3 | 1.00 | 14.00 | 71.00 | 4 |
| 6531 | Dark Current HV 1180V 4m | 2020/06/19 10:56:36 EDT | 00:00:09 | 3.60e+1 | 1.00 | 14.00 | 71.00 | 4 |
| 6424 | Panel Scan 1 of 6. smpl: BeamProfile 7m | 2020/06/15 03:13:33 EDT | 07:00:00 | 1.90e+7 | 1.00 | 14.00 | 71.00 | 6 |

5.2 Data Reduction with Jupyter Notebook, jupyter.sns.gov

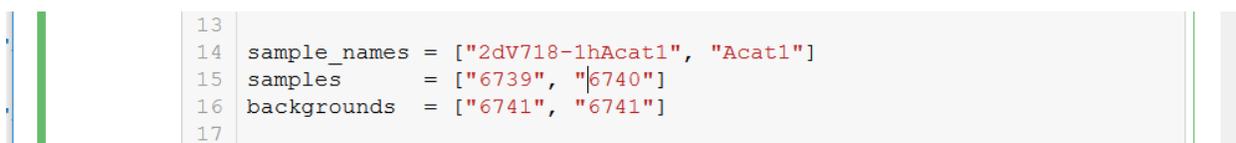
Login to jupyter.sns.gov and have a Jupyter Notebook setup for your experiment with your local contact.

5.2.1 As instructed by your local contact, input the IPTS number, the folder to save the reduced data, and other necessary information, usually at the top of the script.



```
In [6]: 1 # configuring your reduction
2
3 "what is your IPTS number?"
4 IPTS_number = 25654
5 "where do you want to save your reduced data"
6 folder_reduced_data = "/SNS/users/q3n/reduce2020/25654Talin"
7 "which instrument configuration?", "7.0 or 15.5m"
8 instrument_config = 15.5
9 "what is the scan number for open beam?"
10 open_beam_scan_number = 6738 #15.5m test #6059 #7.0m test
11 "what is the thickness of all the samples in cm?"
12 sample_thickness_cm = 0.1
13
14 sample_names = ["2dV718-1hAcat1", "Acat1"]
15 samples      = ["6739", "6740"]
16 backgrounds  = ["6741", "6741"]
17
```

5.2.2 At the Bio-SANS, data is reduced in a batch mode; build the lists of sample names, sample run numbers, and associated background run numbers into the reduction script.



```
13
14 sample_names = ["2dV718-1hAcat1", "Acat1"]
15 samples      = ["6739", "6740"]
16 backgrounds  = ["6741", "6741"]
17
```

- *Sample_names*: Enter text that describes the reduced sample; this name will be used to name the reduced output data as prefix.
- *Sample run numbers*: Enter a list of run numbers in 'double quotes (")' individually for samples. For samples with multiple run numbers, list them separated by comma (,) or dash (-, for continuous runs) within a single double quote (").
- *Backgrounds run numbers*: Enter a list of background run numbers, individually or multiple run numbers as the same as 'sample run numbers'
- The number of items in the 3 lists must be the same as they are in one-to-one correspondence during the reduction loop.

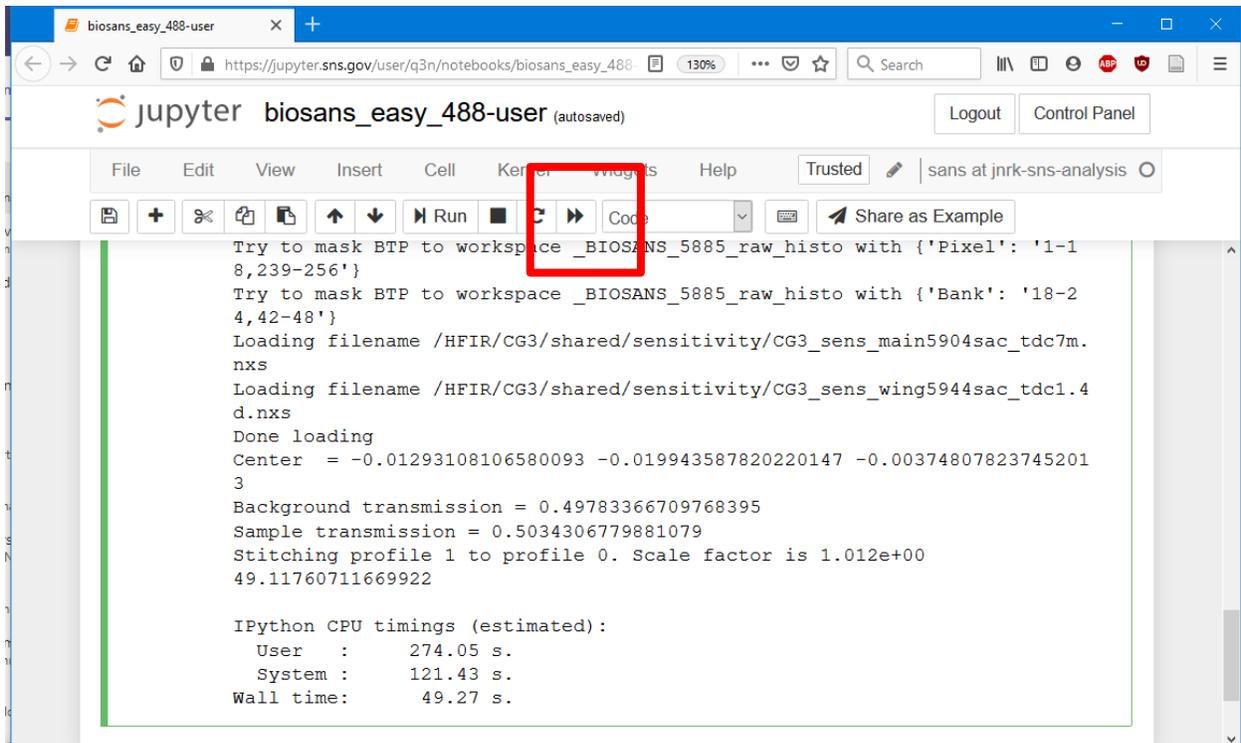
For example:

```
27
28 sample_names = ["name1", "name2", "name3", "name4"]
29 samples      = ["run#1", "run#2", "run#3", "run#4"]
30 backgrounds  = ["bg#1", "bg#2", "bg#3", "bg#4"]
31
```

Note:

- Each run number at the Bio-SANS contains data collected by both main and wing detectors. The reduction process independently reduces to 1D data from the two detectors, scales the wing detector curve to match the main detector curve prior to stitching them together.
- For single configuration measurements- scattering and transmission data are measured simultaneously and saved in the same run number.
- For two configuration measurements- your local contact will provide you with a script that will contain additional lists such as lists of run numbers for sample and background transmissions, additional configuration, and an additional stitching of data from the two configurations.

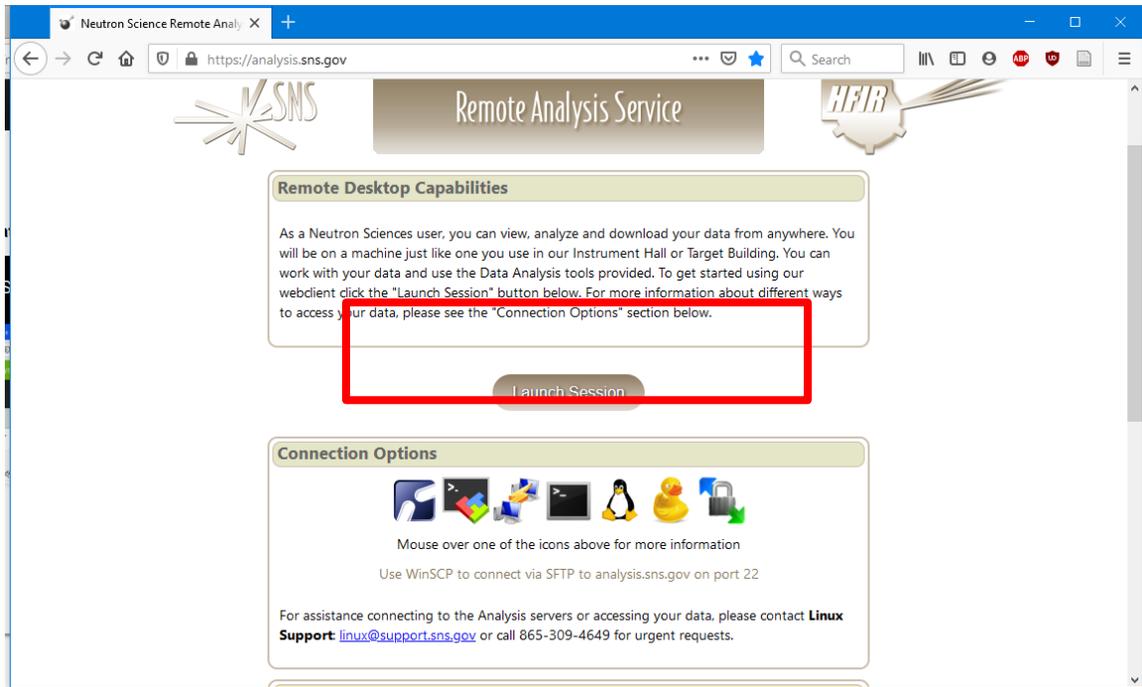
5.2.3 Once the lists of run numbers are completed, click the 'Run' button under the notebook menu. The data will be reduced in the order of the list. Some useful information will be displayed, e.g., the progress, the transmissions etc. The information is also saved.



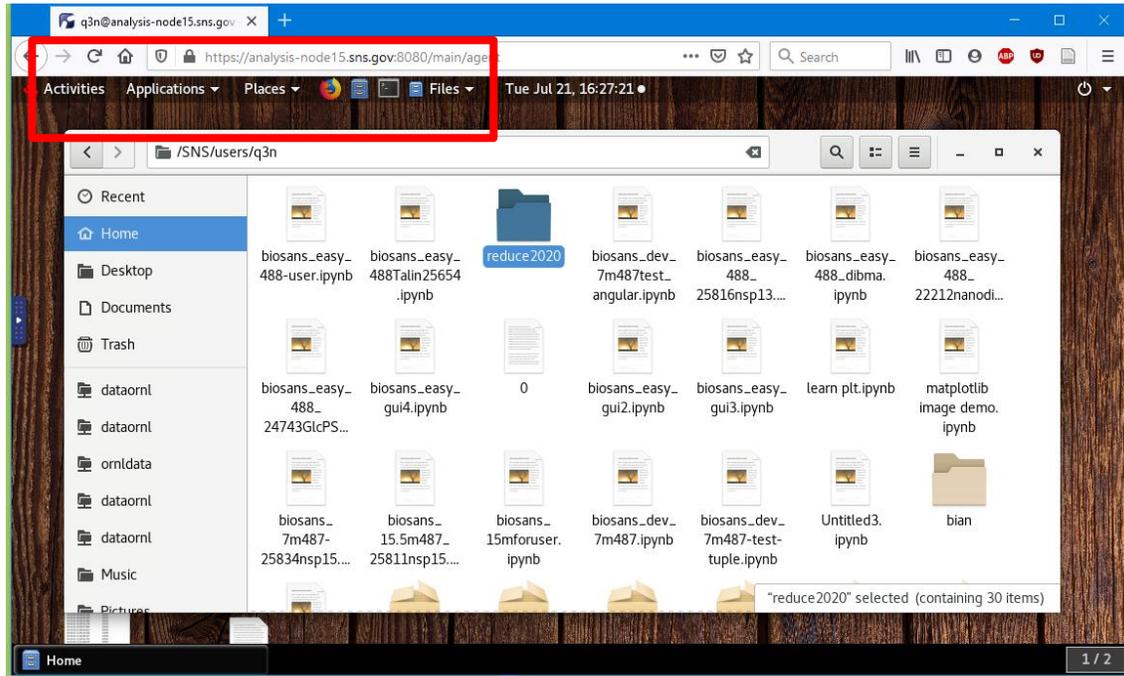
5.3 Accessing Reduced Data from analysis.sns.gov

Reduced data can be downloaded and viewed from analysis.sns.gov in the designated output folder as specified in the reduction script. The server provides various connection options to access and download data as shown below in the front page of the analysis cluster.

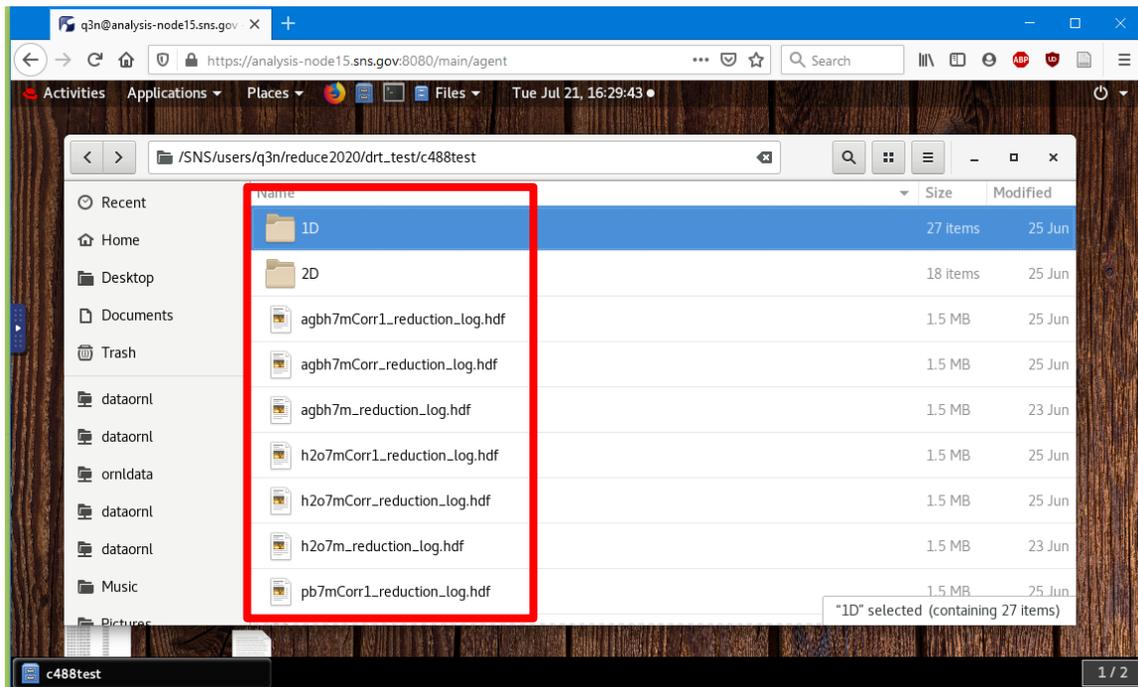
Alternatively, one can launch **Remote Desktop** and located these files. As shown below, go to <https://analysis.sns.gov> and launch remote desktop by clicking the “Launch Session” button.



5.3.1 Once logged-in, use the file browser to locate the reduced files.



5.3.2 Reduced files are saved into 1D folder (1D curves) and 2D folder (reduced as in QxQy coordinates). The HDF files have all the raw and reduction metadata, as well as the reduced data. Please consult your local contact on how to utilize them.



5.3.3 Typical isotropic data in 1D format (4 columns- Q, I, ΔI , ΔQ) are saved in the 1D folder with the reduced 1D curves from main detector, wing detector and both (main/wing curves stitched). Once the files are downloaded, you can view them in the SANS analysis software of your choice.

```

1 # I(Q)
2 #Q (1/A)      I (1/cm)      dI (1/cm)     dQ (1/A)
3 6.852634E-03  2.047596E+00  9.199905E-02  2.047426E-03
4 7.168412E-03  1.882514E+00  7.491347E-02  2.050290E-03
5 7.498741E-03  1.591331E+00  7.075505E-02  2.053905E-03
6 7.844292E-03  1.408008E+00  6.088258E-02  2.057404E-03
7 8.205767E-03  1.272576E+00  5.190825E-02  2.061867E-03
8 8.583899E-03  1.131054E+00  4.968454E-02  2.066313E-03
9 8.979456E-03  1.049385E+00  4.276573E-02  2.071048E-03
10 9.393241E-03  9.010178E-01  3.939873E-02  2.076481E-03
11 9.826093E-03  8.704374E-01  3.607811E-02  2.082255E-03
12 1.027889E-02  7.485104E-01  3.132184E-02  2.088380E-03
13 1.075256E-02  6.183244E-01  2.774788E-02  2.095345E-03
14 1.124805E-02  6.034584E-01  2.544007E-02  2.102947E-03
15 1.176637E-02  5.397191E-01  2.274883E-02  2.111479E-03
16 1.230858E-02  5.265366E-01  2.158992E-02  2.120459E-03
17 1.287578E-02  4.851290E-01  2.015130E-02  2.130264E-03
18 1.346911E-02  4.591927E-01  1.790173E-02  2.140907E-03
19 1.408978E-02  4.625635E-01  1.741104E-02  2.152525E-03
20 1.473906E-02  4.510110E-01  1.628214E-02  2.164990E-03
21 1.541825E-02  4.297651E-01  1.470034E-02  2.178989E-03
22 1.612874E-02  4.250320E-01  1.495176E-02  2.193464E-03
23 1.687197E-02  4.153823E-01  1.319730E-02  2.209413E-03
24 1.764946E-02  4.026304E-01  1.233939E-02  2.227686E-03
25 1.846277E-02  3.828347E-01  1.176615E-02  2.246864E-03
26 1.931355E-02  3.899373E-01  1.125195E-02  2.267334E-03
27 2.020355E-02  3.723523E-01  1.039217E-02  2.289898E-03

```

6. GP-SANS Data Reduction With drtSANS – Quick Reference for the Data Reduction Parameters

Editors: Lisa DeBeer-Schmitt, Lilin He, Ken Littrell

Date: 07/22/2020

6.1 Introduction

The various parameters required by drtsans are listed below with a brief description of their meaning, the acceptable values, and appropriate format for the information. An example is shown here.

```
{"schemaStamp": "2020-04-15T21:09:52.745905", "instrumentName": "GPSANS",
"iptsNumber": 25849, "dataDirectories": null, "sample": {"runNumber": "11038",
"thickness": 0.1, "transmission": {"runNumber": "11028", "value": null}}, "background":
{"runNumber": "11001", "transmission": {"runNumber": "10991", "value": null}},
"emptyTransmission": {"runNumber": "10991", "value": null}, "beamCenter":
{"runNumber": "10991"}, "outputFileName": "s16high_q", "configuration": {"outputDir":
"/HFIR/CG2/IPTS-25849/shared/LDS/", "wavelength": null, "wavelengthSpread": null,
"useTimeSlice": false, "timeSliceInterval": null, "useLogSlice": false, "logSliceName":
null, "logSliceInterval": null, "sampleOffset": null, "useDetectorOffset": true,
"detectorOffset": 0.0, "sampleDetectorDistance": null, "sampleToSi": null,
"sampleApertureSize": null, "sourceApertureDiameter": null, "usePixelCalibration": false,
"maskFileName":
"/HFIR/CG2/IPTS-25849/shared/high_q_mask.nxs",
"useDefaultMask": true, "defaultMask": [{"Pixel": "1-10,247-256"}],
"useMaskBackTubes": true, "darkFileName": null, "normalization": "Monitor",
"sensitivityFileName":
"/HFIR/CG2/shared/drt_sensitivity/sens_c487_bar.nxs",
"useSolidAngleCorrection": true, "blockedBeamRunNumber": "11054",
"useThetaDepTransCorrection": true, "DBScalingBeamRadius": 80.0,
"mmRadiusForTransmission": 80.0, "absoluteScaleMethod": "direct_beam",
"StandardAbsoluteScale": 1.0, "numQxQyBins": 160, "1DQbinType": "scalar",
"QbinType": "log", "numQBins": null, "LogQBinsPerDecade": 33,
"useLogQBinsDecadeCenter": true, "useLogQBinsEvenDecade": true,
"WedgeMinAngles": null, "WedgeMaxAngles": null, "autoWedgeQmin": 0.003,
"autoWedgeQmax": 0.04, "autoWedgeQdelta": 0.01, "autoWedgeAzimuthalDelta": 1.0,
"autoWedgePeakWidth": 0.25, "autoWedgeBackgroundWidth": 1.5,
"autoWedgeSignalToNoiseMin": 2.0, "AnnularAngleBin": 1.0, "Qmin": null, "Qmax":
null, "useErrorWeighting": false, "smearingPixelSizeX": null, "smearingPixelSizeY": null,
"useSubpixels": true, "subpixelsX": 5, "subpixelsY": 5, "wedges": null,
"symmetric_wedges": true}, "logslice_data": {}}
```

Below is the same configuration file expanded into a more readable format.

```
{
"schemaStamp": "2020-04-15T21:09:52.745905",
"instrumentName": "GPSANS",
"iptsNumber": 25849,
"dataDirectories": null,
"sample": {
"runNumber": "11038",
"thickness": 0.1,
"transmission": {
```

```

        "runNumber": "11028",
        "value": null}},
"background": {
  "runNumber": "11001",
  "transmission": {
    "runNumber": "10991",
    "value": null}},
"emptyTransmission": {
  "runNumber": "10991",
  "value": null},
"beamCenter": {
  "runNumber": "10991"},
"outputFileName": "s16high_q",
"configuration": {
  "outputDir": "/HFIR/CG2/IPTS-25849/shared/LDS/",
  "wavelength": null,
  "wavelengthSpread": null,
  "useTimeSlice": false,
  "timeSliceInterval": null,
  "useLogSlice": false,
  "logSliceName": null,
  "logSliceInterval": null,
  "sampleOffset": null,
  "useDetectorOffset": true,
  "detectorOffset": 0.0,
  "sampleDetectorDistance": null,
  "sampleToSi": null,
  "sampleApertureSize": null,
  "sourceApertureDiameter": null,
  "usePixelCalibration": false,
  "maskFileName": "/HFIR/CG2/IPTS-25849/shared/high_q_mask.nxs",
  "useDefaultMask": true,
  "defaultMask": [
    {"Pixel": "1-10,247-256"}],
  "useMaskBackTubes": true,
  "darkFileName": null,
  "normalization": "Monitor",
  "sensitivityFileName": "/HFIR/CG2/shared/drt_sensitivity/sens_c487_bar.nxs",
  "useSolidAngleCorrection": true,
  "blockedBeamRunNumber": "11054",
  "useThetaDepTransCorrection": true,
  "DBScalingBeamRadius": 80.0,
  "mmRadiusForTransmission": 80.0,
  "absoluteScaleMethod": "direct_beam",
  "StandardAbsoluteScale": 1.0,
  "numQxQyBins": 256,
  "1DQbinType": "scalar",
  "QbinType": "log",
  "numQBins": null,
  "LogQBinsPerDecade": 33,
  "useLogQBinsDecadeCenter": true,
  "useLogQBinsEvenDecade": true,
  "WedgeMinAngles": null,
  "WedgeMaxAngles": null,
  "autoWedgeQmin": 0.003,
  "autoWedgeQmax": 0.04,
  "autoWedgeQdelta": 0.01,
  "autoWedgeAzimuthalDelta": 1.0,
  "autoWedgePeakWidth": 0.25,
  "autoWedgeBackgroundWidth": 1.5,
  "autoWedgeSignalToNoiseMin": 2.0,
  "AnnularAngleBin": 1.0,
  "Qmin": null,
  "Qmax": null,
  "useErrorWeighting": false,
  "smearingPixelSizeX": null,
  "smearingPixelSizeY": null,
  "useSubpixels": true,
  "subpixelsX": 5,
  "subpixelsY": 5,

```

```
"wedges": null,  
"symmetric_wedges": true},  
"logslice_data": {}  
}
```

6.2 Parameter Descriptions

Note that all key:value pairs use quotes around both the key and value unless the value is null or a mathematical constant. Also note that the file has a hierarchical structure, where {} are used to denote groupings. The descriptions of the parameters below reflect the structure of the hierarchy. The jupyter notebook reduction scripts used by GP-SANS convert these schemas into python dictionaries. This means that true/false must be changed to True/False and null to None otherwise the script will throw errors.

1. "schemaStamp": "2020-05-26T22:28:16.336908"

This particular parameter is autogenerated by the scripting method for reducing data and when using MantidWorkbench. It should not be changed, even when hand-modifying the contents of the configuration file.

2. "instrumentName": "GPSANS"

The instrument name is used by drtsans to know how to use some of the specified parameters. It must be consistent with the instrument used for the data collection (i.e. do not try to reduce data from EQ-SANS if this parameter is set to "BIOSANS"). Note that there is no dash in the name of the instrument in the drtsans parameter file.

3. "iptsNumber": "25849"

The proposal number for the experiment allows drtsans to quickly find the data to be reduced, rather than using tools to find the data based solely on the run number. It can be left blank (i.e. "").

4. "sample":

This is the first parameter that contains a set of parameters grouped using {}. The various parameters in the group follow.

- a. "runNumber": "11038"

This is the run number for the sample scattering to be reduced. It can be found via OnCat or using the catalog in MantidWorkbench. It is possible to specify a set of scattering runs for a single sample that are to be summed together into a single data set for reduction. To do so, use the following format, which uses a single pair of quotes to enclose the list.

- i. "runNumber":{"XXXXXX, YYYYYY"}

b. "thickness": 0.1

This parameter specifies the sample thickness in centimeters. Note that the value is not enclosed in quotes.

c. "transmission":

This is the start of another level of the hierarchical structure. Of the two key:value pairs in this grouping, only one can have an actual value: either the run number or the value of the transmission to use for the reduction.

i. "runNumber": "11028"

This is the run number of the transmission for the sample. There can only be a single run number specified here.

ii. "value": ""

This would be a numerical value for the transmission to use for the reduction, which would normally only be done for quick qualitative checks if the data needs to be viewed prior to the completion of the transmission measurement for a sample. Note that the value must be enclosed in quotes ("").

5. "background":

The set of parameters that follow specify information required to identify the background to use for the reduction. It is possible to reduce data without a background by leaving the run numbers in this set of parameters empty (i.e. "").

a. "runNumber": "11001",

The run number of the background data to subtract from the sample scattering.

b. "transmission":

The following set of parameters are used to specify either the run number for the background's transmission measurement or to specify a value for the transmission of the background.

i. "runNumber": "10991"

ii. The run number for the background's transmission measurement. If no background is specified, then this run number should not be specified (i.e. set to "").

iii. "value": ""

iv. This would be a numerical value for the transmission to use for the reduction, which would normally only be done for quick qualitative checks if the data needs to

be viewed prior to the completion of the transmission measurement for a sample. Note that the value must be enclosed in quotes ("").

6. "emptyTransmission":

This grouping of parameters is used to specify the reference measurement, or value, used to calculate the transmission from the other specified measurements or values. If the transmissions are specified as values, the value specified here should be "1.0".

a. "runNumber": "10991"

The run number for the background's transmission measurement.

b. "value": null

A value can be specified for the reference transmission. If used, it should be "1.0", if not specify it as null, as shown above.

7. "beamCenter":

The beam center is specified by providing a run number for an empty beam or a transmission measurement to calculate the beam center from. This data is also used to calculate the absolute scaling on GP-SANS when the direct beam method is selected in "absoluteScaleMethod": "direct_beam"

a. "runNumber": "10991"

This is the run number of an empty beam or a transmission measurement. It cannot be left blank.

8. "outputFileName": "s16high_q"

This is the base used to construct all of the file names that result from the data reduction process. In this example, all of the files will be named "s16high_q *.*". The filename can be any valid string that is acceptable for filenames for a Linux operating system.

9. "configuration":

A large number of parameters are specified within this hierarchical grouping, most of which directly impact the reduction process and results produced. Many of these parameters will be provided by your local contact and should not be changed without discussing the reasons for the change with him or her. When using the jupyter notebook for data reduction, some of these parameters may not be presented to you.

a. "outputDir": "/HFIR/CG2/IPTS-25849/shared/LDS"

The directory to write the data reduction result to is listed here. Normally, it would be the shared directory for the particular proposal, which allows other team members and

the local contact to view the results. However, it is also possible to specify a location in a user's home directory. It is left to the discretion of the user.

b. "wavelength":null

This is a place where if the wavelength saved to the metadata needs to be overwritten. This should only be done with your local contact

c. "wavelength_spread":null

This is a place where if the wavelength spread saved to the metadata needs to be overwritten. This should only be done with your local contact.

d. "useTimeSlice": false

If the user wishes to parse the event stream contained in the run specified in the "sample:" parameter set, then set this value to true. If this value is true, then the parameter "useLogSlice", below, must be false.

e. "timeSliceInterval": 300

This is the interval in seconds to use for the time slicing of the event stream. The event stream will be cut into as many consecutive portions of the event stream as exist in the file, with a final bin that contains as much time as remains in the stream. In this case, the various slices are for the following intervals: $0 \leq t < 300$ seconds, $300 \leq t < 600$ seconds, etc. Note that the value is not contained in quotation marks.

f. "useLogSlice": false,

It is possible to divide an event stream into bins that derive from another parameter that is saved by EPICS in the NeXus file, such as temperature, pressure, magnetic field, or even a motor that continuously moves during data collection. If a user wishes to do so, set the value to true. Note that useLogSlice and useTimeSlice cannot both be true. Discuss the use of log slicing with your local contact.

g. "logSliceName": null

This is the name of the instrument log to use for log slicing. If useLogSlice is true, change this to the name of the EPICS parameter that you wish to employ. Discuss the use of log slicing with your local contact.

h. "logSliceInterval": 10

This parameter sets the interval of the instrument log specified in logSliceName to use. It must be in the units of the device, be it degrees, millimeters, Celcius, etc. Discuss the use of log slicing with your local contact. Note that the value is not enclosed in quotation marks.

- i. "sampleOffset": null

This parameter specifies the distance, in mm, that the actual sample position differs from the central axis of the large sample environment flange that can be seen on the ceiling of the downstairs sample environment enclosure of EQ-SANS. A positive number means that the sample position is offset from this axis in the direction of the detector, while a negative number means that it is offset towards the SNS target. Your local contact has either determined this number for the sample environment that you are using for your experiment, or they will work with you to determine the correct value. Note that this value is contained in quotation marks.

- j. "useDetectorOffset": true

This parameter is an expert parameter and should not be changed without consulting your local contact. If you have any questions, ask your local contact.

- k. "detectorOffset": 0.0

This parameter is an expert parameter and should not be changed without consulting your local contact. If you have any questions, ask your local contact. Note that this value is not enclosed in quotation marks.

- l. "sampleDetectorDistance": null,

This parameter is to overwrite the sample to detector distance saved in the metadata in case it is incorrect. This number should not be changed without the help of your local contact.

- m. "sampleToSi": null,

This parameter is to overwrite the sample to silicone window distance saved in the metadata in case it is incorrect. This number is usually set at the beginning of your experiment after your sample environment is installed and the distance from the sample to the front of the detector is known. This number should not be changed without the help of your local contact.

- n. "sampleApertureSize": null

This parameter specifies the diameter of the sample aperture used in millimeters. While it is possible to specify the diameter of this aperture during data acquisition, specifying a different value here allows you to over-write the incorrect value saved in the data files. The sampleApertureSize impacts the calculation of the resolution information for the instrument (i.e. the uncertainty in Q), which is required to accurately analyze your data. Note that the value is enclosed in quotation marks.

- o. "sourceApertureDiameter": null

This can be used to specify the diameter of the source aperture in millimeters used for a measurement. Normally, this parameter is taken position of the aperture in the

collimator boxes. It is usually in the box after the last guide in the beam. For maximum resolution on GP-SANS, there is 20 mm source diameter that can be used in box 1 otherwise this number is usually 40 mm for all other settings.

p. "usePixelCalibration": true

This parameter is using a pixel map that takes into account the center of pixel on the detector along with its corresponding width and height. This calibration takes into account the nonlinearity of the detector tubes.

q. "maskFileName": "/HFIR/CG2/IPTS-25849/shared/high_q_mask.nxs"

This is the name of a hand-drawn mask. Your local contact can help you prepare a mask for your specific experiment.

r. "useDefaultMask": true

On GP-SANS, the instrument applies a default mask that will remove the top and bottom 10 pixels of the detector since these are not truly active regions of the detector.

s. "defaultMask": [

```
{"Pixel": "1-10,247-256"}],
```

This how the default top and bottom pixels are masked. If more are needed, discuss this with your local contact.

t. "useMaskBackTubes": false

The GP-SANS detector, like the Bio-SANS and EQ-SANS detectors, consists of an array of linear position sensitive detectors that are arranged in two planes that are offset to ensure complete coverage across the area of the detector. When this parameter is set to true, the back plane of tubes, being those furthest away from the sample, are all masked. Typically, this is only done when the detector is positioned close to the sample <2 m.

u. "darkFileName": null

This parameter specifies the name of the file that contains the "dark current" measurement, which for GP-SANS is normally a measurement performed either during regular calibrations with the facility running but the instrument shutter closed or during your experiment in case non-standard instrument configurations is used. It is a measure of cosmic radiation and detector electronic noise. Your local contact will help you find the correct file to use.

v. "normalization": "Monitor"

The data can either be normalized by the measurement time ("Time") or the beam monitor ("Monitor"). The normal method for normalizing GP-SANS data is "Monitor" so

that the constant increase of the flux from the reactor can be taken into account. "Time" can be used but only if the data is being compared is within 2 to 3 days of each other.

- w. "sensitivityFileName": "/HFIR/CG2/shared/drt_sensitivity/sens_c487_bar.nxs"

The file name of the pre-processed relative pixel response of the detector is specified with this parameter. These calibration files are measured during instrument commissioning each cycle and are prepared by staff for use in data reduction. Consult your local contact for the correct file to use.

- x. "useSolidAngleCorrection": true

This parameter specifies whether or not to correct the data for the solid angle subtended by each pixel, which can be a considerable effect for configurations with the detector positioned close to the sample. It is recommended to leave this parameter set to true.

- y. "useThetaDepTransCorrection": true

When set to true, the data reduction will correct the data in each pixel for the actual distance that the neutrons travel through the sample when performing the correction for the transmission. The effect increases with scattering angle and can be considerable when the detector is positioned near the sample. It is recommended to leave this parameter set to true.

- z. "DBScalingBeamRadius": 40.0,

This parameter allows users to specify the radius in millimeters to use when integrating the attenuated beam center data for calculating the scaling factor for putting the data on an absolute scale (See bb). The instrument team has found 40 mm to perform well under most circumstances, but it is possible that certain sample environments or instrument configurations may benefit from the use of a different value. Consult your local contact if you feel that another value may be required.

- aa. "mmRadiusForTransmission": "40"

This parameter allows the user to specify the radius in millimeters to use when integrating the attenuated direct beam measurements for calculating the transmissions. The instrument team has found 40 mm to perform well under most circumstances, but it is possible that certain sample environments or instrument configurations may benefit from the use of a different value. Consult your local contact if you feel that another value may be required.

- bb. "absoluteScaleMethod": "direct_beam"

There are two methods available for scaling data collected on GP-SANS into absolute units of 1/cm. The first is by the "direct_beam" method which takes attenuated beam center data specified earlier and calculates the total intensity at the beam center by

taking into account the known attenuation rates of the attenuator. This number is then used by the reduction script to divide the intensity to put it on an absolute scale. The other method is “standard” which uses a calibrated standard. Do not change the value of this parameter. Presently, the standard is a well-characterized sample of porous silica that your local contact will provide to you during your experiment if needed. A measurement of the standard is used to derive the absolute scale factor, which is specified with the StandardAbsoluteScale parameter, described below. GP-SANS uses the direct beam by default since large sample environments that cannot always allow for measurement of the standard are used.

cc. "StandardAbsoluteScale": "1.0"

This is the scale factor that must be applied to the data to place it into absolute units of 1/cm. Your local contact can help you derive it from a measurement of a standard. If using “direct_beam” method, this number is ignored but it is always safe to leave it at 1.0

dd. "numQxQyBins": "160"

This parameter specifies the number of Q-bins in the 2D reduced data, which is always output by drtsans. Note that only a single value may be provided, which implies that the 2D reduced data is on a regular, square grid that covers the Q-range in 2D measured by the detector. The beam center is not necessarily in the center of the output data. The grid in Q-space is always linear.

ee. "1DQbinType": "scalar"

Three options exist for the kind of 1D data that are output by drtsans. Possible values are “scalar”, which is used for 1D azimuthally averaged data that most people are familiar with; “wedge” makes it possible to define wedges to perform scalar binning within, as one might do for anisotropic data and utilize the WedgeMinAngles, WedgeMaxAngles and the various autoWedge parameters described below, although automatic wedge determination is not enabled for GP-SANS at this point in time. The “annular” binning makes it possible to visualize how data varies around the beam center within a Q-range specified by the user and requires that the parameters AnnularAngleBin, Qmin and Qmax, described below, be provided.

ff. "QbinType": "log"

This parameter dictates whether the Q-spacing of the intensity profiles calculated when performing scalar or wedge binning is logarithmic or linear. The possible values of this parameter are “log” and “linear”. The choice of binning determines how the numQBins, LogQBinsPerDecade and useLogQBinsEvenDecade parameters work.

gg. "numQBins": null

This parameter must be set to an integer value if QbinType is “linear”, but can also be used if it is “log”. The value is the number of Q-values that are in the 1D data that is binned as “scalar” or “wedge” and their spacing is determined by the value of QbinType.

This parameter must be null if LogQBinsPerDecade is set to an integer value. Note that the value is enclosed in quotation marks.

hh. "LogQBinsPerDecade": 33

This parameter only works when QbinType is "log". The value specified here will be the number of Q-bins that are present within each decade between the minimum and maximum Q values that the reduced data contain. For example, if the value is "25", then there are 25 Q-bins between 0.01 \AA^{-1} and 0.10 \AA^{-1} and 25 Q-bins between 0.10 \AA^{-1} and 1.0 \AA^{-1} or any other decade in Q that are present in the reduced data. The parameter useLogQBinsEvenDecade must be set to true to enable this option and numQBins must be null.

ii. "useLogQBinsDecadeCenter": false

At present, this option is no longer enabled. The Q-values when using an even number of Q-bins per decade by setting useLogQBinsEvenDecade to true and providing a value for logQBinsPerDecade to a non-zero, positive integer always have a bin centered on 0.001 \AA^{-1} , 0.010 \AA^{-1} , 0.100 \AA^{-1} , etc.

jj. "useLogQBinsEvenDecade": false

This parameter tells drtsans to use a fixed number of Q-bins per decade when binning the result. The logQBinsPerDecade parameter must have a non-zero integer value and numQBins must be null.

kk. "WedgeMinAngles": "-30, 60"

ll. "WedgeMaxAngles": "30, 120"

The WedgeMinAngles and WedgeMaxAngles are only used when QbinType is set to "wedge". The arrays provide a matched set of angles, specified in degrees and indexed from the Qx axis, within which to perform 1D Q-binning. In this particular example, 1D Q-binning will be performed in two wedges: from -30° to 30° and from 60° to 120° . The angles need not be the same size and need not be symmetric. It is also possible for the angles to overlap, should the user desire it. The only requirement is that both arrays have the same number of elements and that the minimum angle for a wedge be lower than the maximum value for that wedge.

Parameters shown in points nn through tt, below, are required for the drtsans methods for automatically determining the correct wedges to use for binning reduced data into 1D. Development of these routines was driven by the Bio-SANS instrument team. At present, automatic wedge determination is not available for data collected using GP-SANS.

mm. "autoWedgeQmin": null

nn. "autoWedgeQmax": null

oo. "autoWedgeQdelta": null

pp. "autoWedgeAzimuthalDelta": null

qq. "autoWedgePeakWidth": null

rr. "autoWedgeBackgroundWidth": null

ss. "autoWedgeSignalToNoiseMin": 2.0

tt. "AnnularAngleBin": 1.0

When the 1DQbinType parameter is set to "annular" this parameter specifies the size of the bins in degrees that are to be used for binning. Annular binning takes the data in a ring of Q-values and creates a profile as a function of angle around the beam center. Annular binning also requires that Qmin and Qmax, described below, be specified.

uu. "Qmin": null

vv. "Qmax": null

When performing annular binning this is the minimum and maximum Q-values, specified in \AA^{-1} , to use during the binning. These parameters are only used when 1DQbinType is set to "annular".

ww. "useErrorWeighting": false

If weighting by the experimental uncertainty is desired when binning the reduced data and propagating the corresponding uncertainties, set the value of this parameter to true.

xx. "smearingPixelSizeX": null

yy. "smearingPixelSizeY": null

The detectors used in the SANS instruments at ORNL are gas detectors. The pixel sizes are determined from parameters supplied to the hardware that determines where a neutron is detected and can be varied by changing said parameters. In actuality, there is intrinsic uncertainty in the position of the event along the tube. Further, the arrangements of the tubes in the detector makes it possible to have a neutron in the region of overlap between a tube in the front panel and a tube in the back panel be detected in either, which also creates uncertainty in the position in which an event is encoded. The smearingPixelSizeX and smearingPixelSizeY parameters make it possible to account for this uncertainty when calculating the uncertainty in Q. The effect is small for most Q-values, but can impact data analysis when sharp features are present. Your local contact can provide suitable values for the parameters. Note that specifying values for these two parameters does not change the calculation of the value of Q or the intensity profile that results after reduction. It only alters the uncertainty in Q of the result.

zz. "useSubpixels": true

In cases where there are sharp features in the data, or a need to use as much data near the beamstop as possible, it is possible to divide the pixels defined on the detector into sub pixels to improve the quality of the results from the 1D binning process. Subpixels, if specified, will also be used in the 2D binning. To enable this feature, set useSubpixels to true and set subpixelsX and subpixelsY, described below, to positive integers.

aaa. "subpixelsX": 5

bbb. "subpixelsY": 5

Set these two parameters to a non-zero, positive integer to use subpixels when binning the data. The real pixels will then be divided into subpixels for the binning in the data reduction. If subpixelsX is set to 2 and subpixelsY is set to 3, then each pixel will be divided into a 2 by 3 grid for the binning process.

ccc. "wedges": null

This is the output of automatic wedges. It shows the wedges used by the function.

7. GP-SANS Data Process Guide—Quick Reference for Using Jupyter Notebook to Reduce Data

Video tutorial_1config:

https://www.dropbox.com/s/eq057xd3kh880gm/GP_SANS_1config_tutorial.mkv?dl=0

Video tutorial_multi config:

https://www.dropbox.com/s/lbn5chda9pbyamt/GP_SANS_multi_config_tutorial.mkv?dl=0

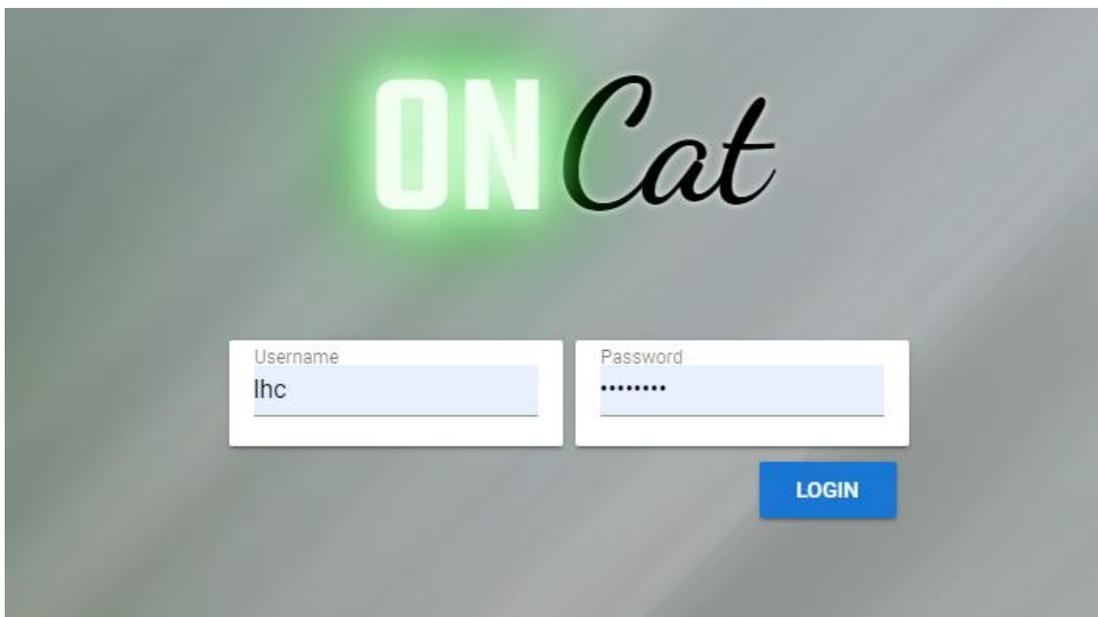
Note:

- This is a quick reference to guide you through using data reduction for GP-SANS. It will not replace the function of your instrument local contact, who is the primary resource for the instrument related questions. **Please work with her/him to setup and understand the data reduction process before using the guide.**
- Various on-line systems will be used for this process, you should have your ORNL GUEST Portal login and password handy. They are accessible both inside and outside ORNL.
 - <https://oncat.ornl.gov> <data catalogue, Demo: oncat.ornl.gov/videos/demo.mp4>
 - <https://jupyter.sns.gov> <data reduction notebook script interface>
 - <https://analysis.sns.gov/> <data analysis cluster, where all data are located>

7.1 Identify the Run Numbers for the Data in ONCat.ornl.gov

All data are saved in sequential number (Run #) with all metadata information such as title, time and other user specified information. The run number is used in the reduction to call the data. Identifying the run number for the data to be reduced in the data catalogue is the first step in the process.

7.1.1 Login into oncat.ornl.gov.



The image shows a login interface for ONCat. At the top, the logo "ONCat" is displayed, with "ON" in a glowing green font and "Cat" in a black script font. Below the logo, there are two input fields: "Username" with the text "lhc" and "Password" with a masked password "*****". A blue "LOGIN" button is positioned to the right of the password field.

7.1.2 Click into HFIR > CG2, then find your experiment IPTS and click on the blue button. This will take you to the runs tab.

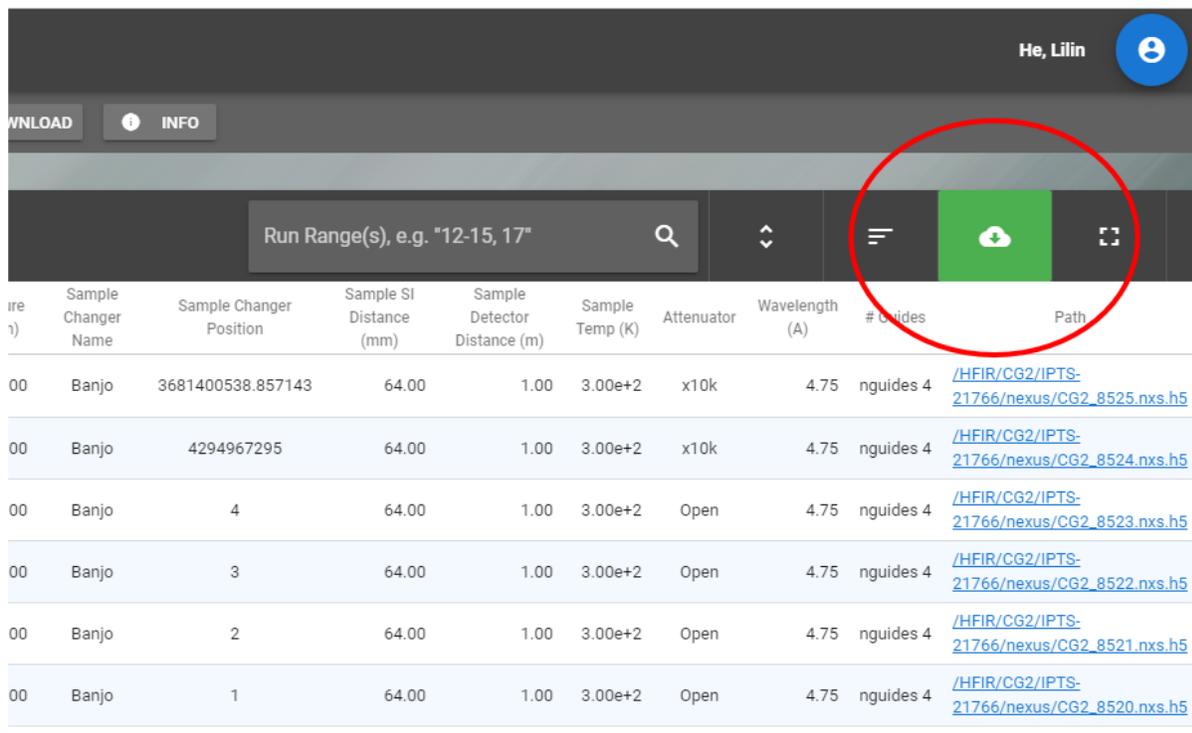
The screenshot shows a web browser at the URL `oncat.ornl.gov/#/explore/HFIR/CG2`. The navigation bar includes 'ONCat', 'EXPLORE', 'HFIR', and 'CG2'. The main content area displays a list of experiments with the following details:

| IPTS ID | EXP ID | Description |
|----------------------------|--|--|
| IPTS-23801 | | Commissioning new collimators and EPICS/CSS on GP-SANS |
| IPTS-22474 | | In-situ Precipitation kinetics in novel TRIP steel alloys |
| IPTS-22279 | | Characterization of Nanoprecipitates in NiCoFeCr-3Cu High Entropy Alloy |
| IPTS-22031 | | Discerning the Coalescence of He Bubbles in Tritiated Stainless Steels |
| IPTS-21978 | | Interface Magnetism of a Coordination Network Heterostructure |
| IPTS-21799 | | Structure of RTIL aggregates for f-block element separation |
| IPTS-21766 | | Elucidation of Ligand Arrangement on Nanoparticle Surfaces |
| IPTS-21674 | EXP342 | SANS investigation to perform in-situ dynamics measurements of skyrmion lattice in FeGd thin films. |
| IPTS-21564 | EXP325 | Explore and optimize macrocycle-derived gel systems with multidimensional porosity for selective gas separa |
| IPTS-21553 | EXP319 EXP321 | SANS study on the molecular relaxation and structural evolution of multi-functional 3D-printing lignin based c |
| IPTS-21537 | EXP320 | NX School: Pore Structure of Silica Studied by Contrast-Matching Small Angle Neutron Scattering |
| IPTS-21519 | EXP317 | SANS investigation into the stability of the ambient condition skyrmion lattice in FeGd thin films. |
| IPTS-21467 | EXP310 | Identification of thin film SANS in Mag-G (11 T superconductor magnet) |
| IPTS-21406 | EXP309 EXP327 | Effects of strain on flux lattice lines for application to SRF Nb cavities |
| IPTS-21368 | EXP334 | The effect of crosslinking on the morphology of phase separation in Anion Exchange Membrane for use in ele |

7.1.3 The run number is the very first column in the list, along with other useful information to identify data as seen in figure below.

| Run # | Title | Start Time | Duration | Total Counts | Sample Thickness (mm) | Sample Aperture Diameter (mm) | Sample Changer Name |
|-------|---------------------------------------|-------------------------|----------|--------------|-----------------------|-------------------------------|---------------------|
| 11845 | bkd test 12m | 2020/06/19 10:37:39 EDT | 00:05:37 | 9.09e+2 | 1.00 | 6.00 | Peltier |
| 11844 | bkd test 6m | 2020/06/19 10:27:11 EDT | 00:07:50 | 2.45e+4 | 1.00 | 6.00 | Peltier |
| 11843 | bkd test | 2020/06/19 10:18:03 EDT | 00:05:09 | 3.12e+3 | 1.00 | 6.00 | Peltier |
| 11306 | Prestart Checklist Cycle 488 | 2020/06/03 15:02:12 EDT | 00:09:31 | 1.02e+3 | 1.00 | 2.00 | Flat |
| 11305 | Drive the collimators to nguides 7 | 2020/06/03 14:30:21 EDT | 00:00:03 | - | 1.00 | 2.00 | Flat |
| 11304 | Drive the collimators to nguides 4 | 2020/06/03 14:28:49 EDT | 00:00:03 | - | 1.00 | 2.00 | Flat |
| 11303 | Drive the collimators to nguides 0 | 2020/06/03 14:27:18 EDT | 00:00:03 | - | 1.00 | 2.00 | Flat |
| 11302 | Drive the collimators to nguides -1 | 2020/06/03 14:26:29 EDT | 00:00:03 | - | 1.00 | 2.00 | Flat |
| 11301 | Drive attenuator to open | 2020/06/03 14:24:55 EDT | 00:00:05 | - | 1.00 | 2.00 | Flat |
| 11300 | Drive attenuator to close | 2020/06/03 14:24:19 EDT | 00:00:05 | - | 1.00 | 2.00 | Flat |
| 11298 | checking bar offset 545 | 2020/05/23 10:48:40 EDT | 00:00:48 | 2.06e+4 | 1.00 | 2.00 | Banjo |
| 11297 | checking bar offset 555 | 2020/05/23 10:47:47 EDT | 00:00:17 | 6.34e+3 | 1.00 | 2.00 | Banjo |
| 11296 | checking bar offset 550 | 2020/05/23 10:46:29 EDT | 00:00:54 | 2.29e+4 | 1.00 | 2.00 | Banjo |
| 11295 | checking bar offset 550 | 2020/05/23 10:46:03 EDT | 00:00:04 | 1.60e+1 | 1.00 | 2.00 | Banjo |
| 10904 | Panel Scan 24 of 24, smpl: MT air | 2020/05/17 02:31:50 EDT | 01:00:00 | 1.23e+4 | 1.00 | 10.00 | Flat |
| 10903 | Panel Scan 23 of 24, smpl: H2O | 2020/05/17 02:16:36 EDT | 00:15:00 | 3.09e+3 | 1.00 | 10.00 | Flat |
| 10902 | Panel Scan 22 of 24, smpl: Porasil C3 | 2020/05/17 02:01:23 EDT | 00:15:00 | 3.10e+3 | 1.00 | 10.00 | Flat |
| 10901 | Panel Scan 21 of 24, smpl: Cadmium | 2020/05/17 02:01:09 EDT | 00:00:00 | - | 1.00 | 10.00 | Flat |
| 10900 | Panel Scan 20 of 24, smpl: Al4 | 2020/05/17 01:45:56 EDT | 00:15:00 | 3.13e+3 | 1.00 | 10.00 | Flat |
| 10899 | Panel Scan 19 of 24, smpl: Ag Beh | 2020/05/17 01:30:42 EDT | 00:15:00 | 3.13e+3 | 1.00 | 10.00 | Flat |
| 10898 | Panel Scan 18 of 24, smpl: D2O | 2020/05/17 00:30:29 EDT | 01:00:00 | 1.28e+4 | 1.00 | 10.00 | Flat |
| 10897 | Panel Scan 17 of 24, smpl: MT helima | 2020/05/16 23:30:15 EDT | 01:00:00 | 1.26e+4 | 1.00 | 10.00 | Flat |

7.1.4 You can click “download CSV” in the upper right corner of the runs tab to get a tab delimited list of your data along with pertinent metadata.

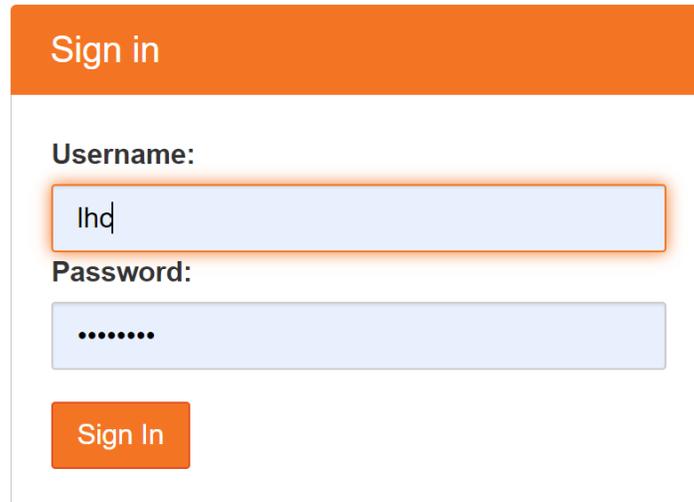


7.1.5 The table below is a good way of organizing run data for samples and configurations on GP-SANS. Use the run numbers and information from OnCat to populate table for your experiment with local contact’s help. This table will help you fill out the different sections of the jupyter notebook for data reduction.

| Sample | 19m12A scatt+trans | 8m4.75A scatt | 8m4.75A trans | 2m4.75A scatt | 2m4.75A center |
|-----------|-----------------------|------------------|------------------|------------------|-------------------|
| Porasil B | 10597 | 10605 | 10613 | 10621 | 10634 |
| Ag Beh | 10598 | 10606 | 10614 | 10622 | |
| H2O | 10599 | 10607 | 10615 | 10623 | |
| Al4 | 10600 | 10608 | 10616 | 10624 | |
| D2O | 10601 | 10609 | 10617 | 10625 | |
| MT cell | 10602 | 10610 | 10618 | 10626 | |
| Mt air | 10637 | 10638 | 10639 | 10640 | 10641 |
| | sample_config_1 | sample_config_2 | | sample_config_3 | bc_config_3 |

7.2 Data Reduction with Jupyter Notebook, jupyter.sns.gov

7.2.1 Log into jupyter.sns.gov.



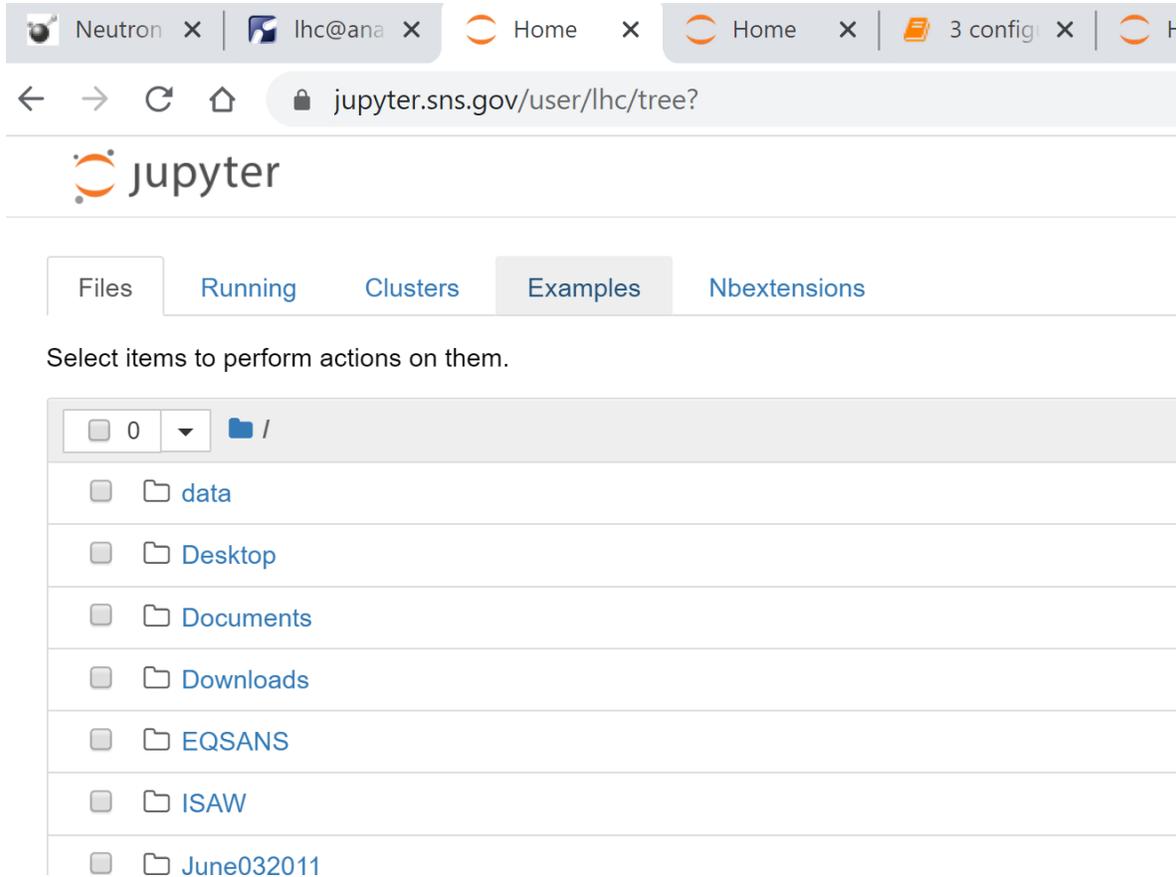
Sign in

Username:
lhq

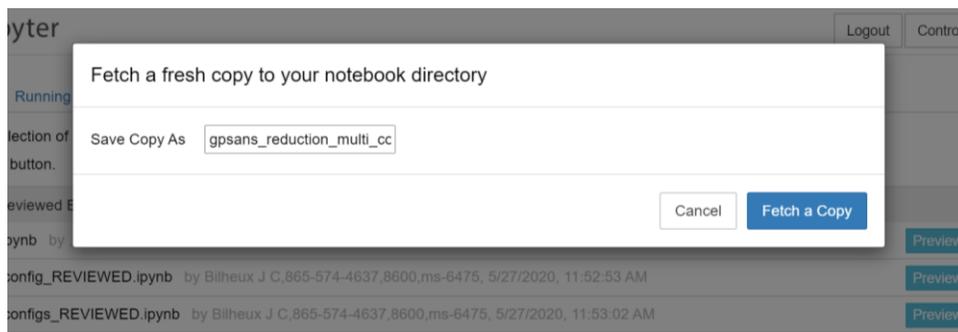
Password:
.....

Sign In

7.2.2 Your local contact will direct you to the best example for your experiment. These examples can be found on the examples tab. For this guide use `gpsans_reduction_multi_config.ipynb`.



7.2.3 Click “Use” and fetch a copy to your home directory on the analysis cluster.



7.2.4 The first cell is for setting up your data. This is where the table you created in 6.1.5 will come in handy.

The screenshot shows a Jupyter Notebook with the following content:

```

1 1 ipts_number      = 23801
2 2 output_directory = "/HFIR/CG2/IPTS-{}/shared/LDS_tutorial/".format(ipts_number)
3
4
5 sample_names      = ["Porasil", "AgBeh", "H2O", "A14", "D20"] # sample names in quotes separated by a comma
6 sample_thick      = ['0.1']*len(sample_names) # units in cm * number of samples to run
7
8 # q range 1
9 sample_1          = ['10597', '10598', '10599', '10600', '10601']
10 sample_trans_1    = ['10597', '10598', '10599', '10600', '10601']
11 bkgd_1            = ['10602']*len(sample_names) # empty cell scattering
12 bkgd_trans_1      = ['10602']*len(sample_names) # empty cell transmission
13 beam_center_1     = 10637 # don't change
14 empty_trans_1     = beam_center_1 # don't change
15
16 # q range 2
17 sample_2          = ['10605', '10606', '10607', '10608', '10609']
18 sample_trans_2    = ['10613', '10614', '10615', '10616', '10617']
19 bkgd_2            = ['10610']*len(sample_names) # empty cell scattering
20 bkgd_trans_2      = ['10618']*len(sample_names) # empty cell transmission
21 beam_center_2     = 10639 # don't change
22 empty_trans_2     = beam_center_2
23
24 # q range 3
25 sample_3          = ['10621', '10622', '10623', '10624', '10625']
26 sample_trans_3    = sample_trans_2 #
27 bkgd_3            = ['10626']*len(sample_names)
28 bkgd_trans_3      = bkgd_trans_2
29 beam_center_3     = 10641
30 empty_trans_3     = empty_trans_2
31
32 # q range 4
33 sample_4          = ['10621', '10622', '10623', '10624', '10625']
34 sample_trans_4    = sample_trans_2 #
35 bkgd_4            = ['10626']*len(sample_names)
36 bkgd_trans_4      = bkgd_trans_2
37 beam_center_4     = 10641
38 empty_trans_4     = empty_trans_2
39
40 # stitching overlaps
41 stitching_q_1_2    = [0.008, 0.016]
42 stitching_q_2_3    = [0.066, 0.1]
43 stitching_q_3_4    = [0.08, 0.12]

```

2 USER INPUT

```

In [1]:

```

3 STAFF INPUT

```

In [3]:
1 config_num      = 3 # 2, 3 or 4
2
3 # q range 1 masks and dark/blackbed beam scan

```

Sample_names: the reduced data will be saved with the text as prefix

Samples_config_1: run numbers for the data to be reduced, multiple run numbers can be use with comma (,) or dash (-, a range of run numbers) for a specific configuration.

Samples_config_2, samples_config_3 and samples_config_4 are for the run numbers for the other configurations in your run table.

Bkg_1: run numbers for the background to be subtracted for a specific configuration.

Bkgd_config_2, Bkgd_config_3, Bkgd_config_4 are the backgrounds for the other configurations in your run table

The number of items in the multiple configurations lists must be the same as they are in one-to-one correspondence during the reduction loop.

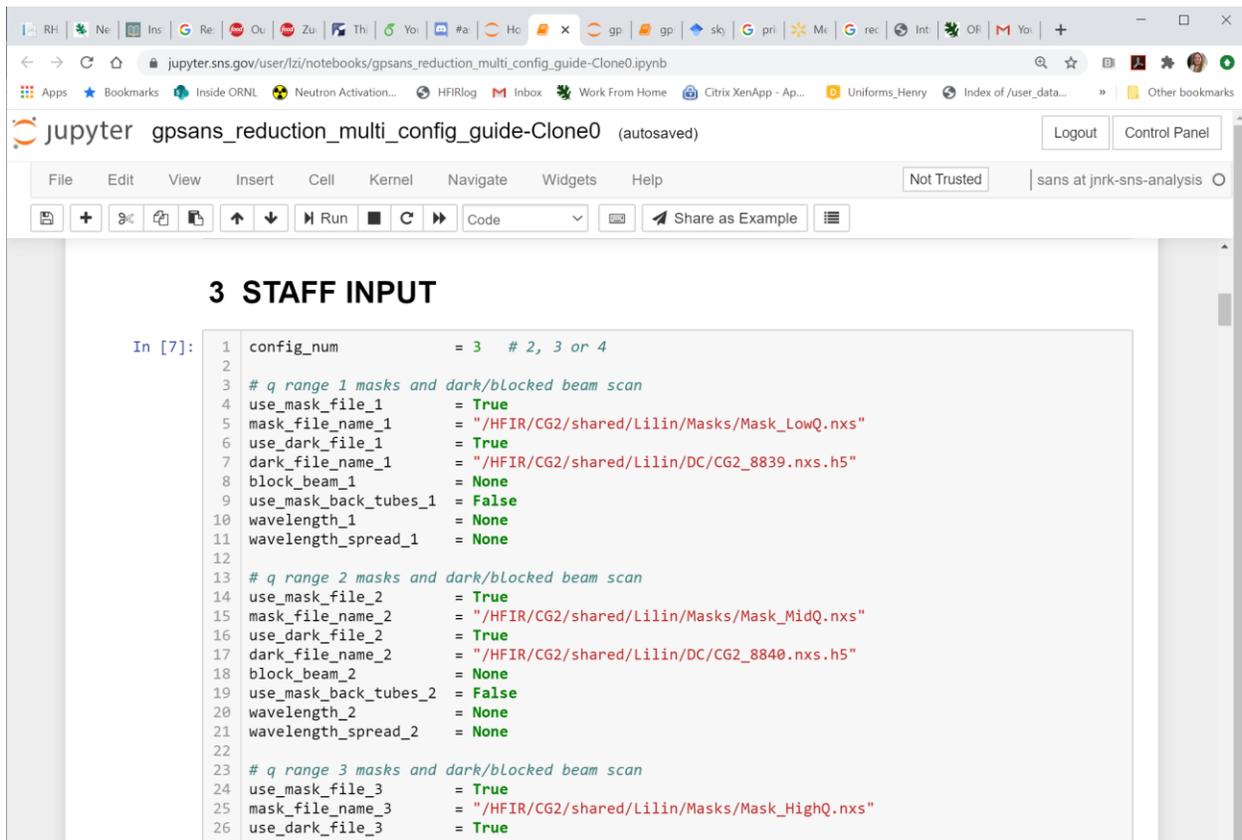
For example:

```
27
28 sample_names = ["name1", "name2", "name3", "name4"]
29 samples      = ["run#1", "run#2", "run#3", "run#4"]
30 backgrounds  = ["bg#1", "bg#2", "bg#3", "bg#4"]
31
```

Note:

- Sometimes for the lowest q setting, the scattering and transmission will be the same data file. Please use the same list for example: sample_config_1 and sample_trans_config_1.
- For the config_3, the transmission usually but not always comes from config_2 as long as the wavelength, collimation, and sample aperture remains the same between configurations.
- The merging and scaling process are handled by the reduction process.

7.2.5 The second cell labeled “Staff Input” will be filled out by your local contact and contain specific settings for the instrument, i.e. detector sensitivity correction. Once the run numbers are inputted and the local contact has filled out the staff section, click the Run button at the top of the page to run the entire notebook. Another way to run the notebook is to hit ctrl+Enter in each cell to run them individually.



The screenshot shows a Jupyter Notebook interface in a web browser. The browser address bar shows the URL: `jupyter.sns.gov/user/lzi/notebooks/gpsans_reduction_multi_config_guide-Clone0.ipynb`. The Jupyter interface includes a menu bar (File, Edit, View, Insert, Cell, Kernel, Navigate, Widgets, Help), a toolbar with icons for file operations and execution, and a status bar indicating "Not Trusted" and "sats at jnrk-sns-analysis".

The main content of the notebook is a code cell titled "3 STAFF INPUT". The code in the cell is as follows:

```
In [7]: 1 config_num          = 3 # 2, 3 or 4
2
3 # q range 1 masks and dark/blocked beam scan
4 use_mask_file_1     = True
5 mask_file_name_1   = "/HFIR/CG2/shared/Lilin/Masks/Mask_LowQ.nxs"
6 use_dark_file_1    = True
7 dark_file_name_1   = "/HFIR/CG2/shared/Lilin/DC/CG2_8839.nxs.h5"
8 block_beam_1       = None
9 use_mask_back_tubes_1 = False
10 wavelength_1      = None
11 wavelength_spread_1 = None
12
13 # q range 2 masks and dark/blocked beam scan
14 use_mask_file_2     = True
15 mask_file_name_2   = "/HFIR/CG2/shared/Lilin/Masks/Mask_MidQ.nxs"
16 use_dark_file_2    = True
17 dark_file_name_2   = "/HFIR/CG2/shared/Lilin/DC/CG2_8840.nxs.h5"
18 block_beam_2       = None
19 use_mask_back_tubes_2 = False
20 wavelength_2      = None
21 wavelength_spread_2 = None
22
23 # q range 3 masks and dark/blocked beam scan
24 use_mask_file_3     = True
25 mask_file_name_3   = "/HFIR/CG2/shared/Lilin/Masks/Mask_HighQ.nxs"
26 use_dark_file_3    = True
27 dark_file_name_3   = "/HFIR/CG2/shared/Lilin/DC/CG2_8844.nxs.h5"
```

The data will be reduced in the order of the list. Some useful information will be displayed, e.g., the progress, the transmissions etc. The information is also saved into a `reduction_log.hdf5` file that will appear in the output directory you specified in User Input section.

```

221         overlaps=[stitching_q_s_4[0], stitching_q_s_4[1]],
222         target_profile_index=0)
223     plot_IQmod([merged_profile], None, loglog=True, backend='mpl')
224
225     filename = output_directory + '/1D/' + sample_names[sample_idx] + '_merged.txt'
226
227     save_ascii_binned_1D(filename, "I(Q)", merged_profile)
228
229     end_time = time.time()
230     print('Total run time: {}'.format(end_time - start_time))

```

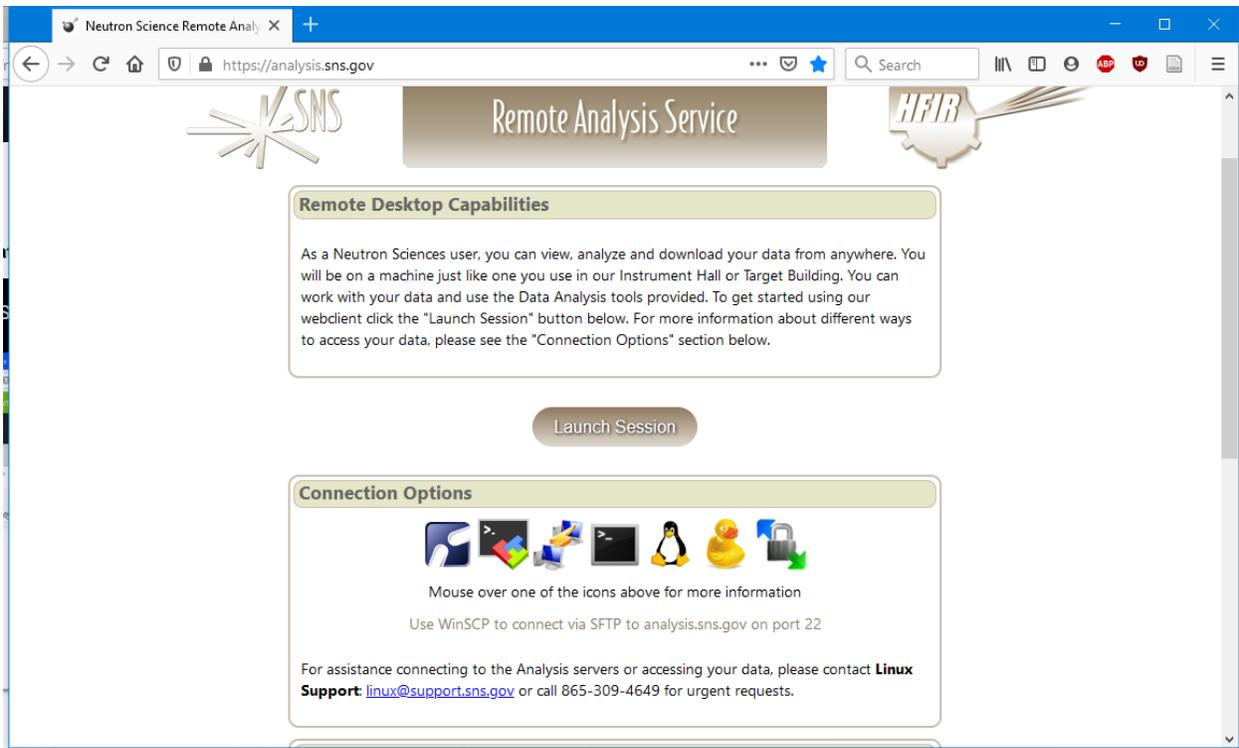
```

Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10597.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10597.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10637.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10637.nxs.h5" exists
Loading filename /HFIR/CG2/IPTS-23801/nexus/CG2_10597.nxs.h5
Try to mask BTP to workspace _GPSANS_10597_raw_histo with {'Pixel': '1-10,247-256'}
Loading filename /HFIR/CG2/IPTS-23801/nexus/CG2_10637.nxs.h5
Try to mask BTP to workspace _GPSANS_10637_raw_histo with {'Pixel': '1-10,247-256'}
Loading filename /HFIR/CG2/shared/LiIn/DC/CG2_8839.nxs.h5
Try to mask BTP to workspace _GPSANS_8839_raw_histo with {'Pixel': '1-10,247-256'}
Loading filename /HFIR/CG2/shared/drt_sensitivity/sens_c486_LDS.nxs
Loading filename /HFIR/CG2/IPTS-23801/shared/LDS_tutorial/mask_1.nxs
Center = 0.0037282018731741268 -0.04754813278056688
Sample transmission = 0.8562637718668116
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10605.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10613.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10639.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10639.nxs.h5" exists
Loading filename /HFIR/CG2/IPTS-23801/nexus/CG2_10605.nxs.h5
Center = 0.00654860632713965 -0.0213271161722356
Sample transmission = 0.9150419624213681
Stitching profile 0 to profile 1. Scale factor is 1.258e+00
Stitching profile 1 to profile 0. Scale factor is 9.707e-01
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10598.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10598.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10637.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10637.nxs.h5" exists
Loading filename /HFIR/CG2/IPTS-23801/nexus/CG2_10598.nxs.h5
Try to mask BTP to workspace _GPSANS_10598_raw_histo with {'Pixel': '1-10,247-256'}
Loading filename /HFIR/CG2/IPTS-23801/nexus/CG2_10637.nxs.h5
Try to mask BTP to workspace _GPSANS_10637_raw_histo with {'Pixel': '1-10,247-256'}
Loading filename /HFIR/CG2/shared/LiIn/DC/CG2_8839.nxs.h5
Try to mask BTP to workspace _GPSANS_8839_raw_histo with {'Pixel': '1-10,247-256'}
Loading filename /HFIR/CG2/shared/drt_sensitivity/sens_c486_LDS.nxs
Loading filename /HFIR/CG2/IPTS-23801/shared/LDS_tutorial/mask_1.nxs
Center = 0.0037282018731741268 -0.04754813278056688
Sample transmission = 0.4343047612451629
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10606.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10614.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10639.nxs.h5" exists
Seeing if "/HFIR/CG2/IPTS-23801/nexus/CG2_10639.nxs.h5" exists

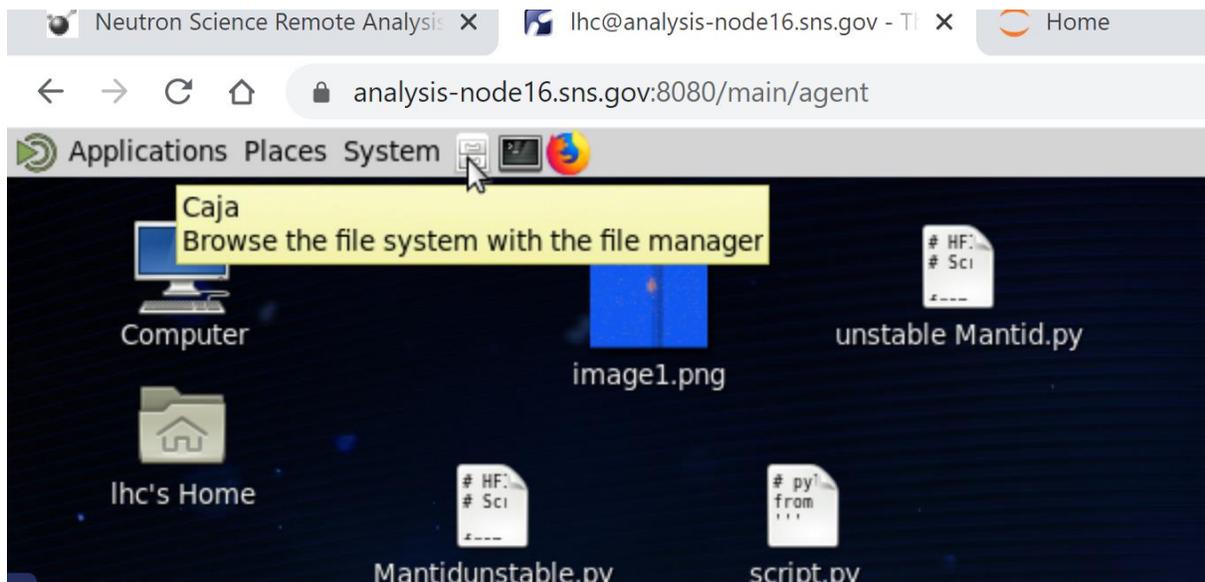
```

7.3 Download and View the Data from analysis.sns.gov

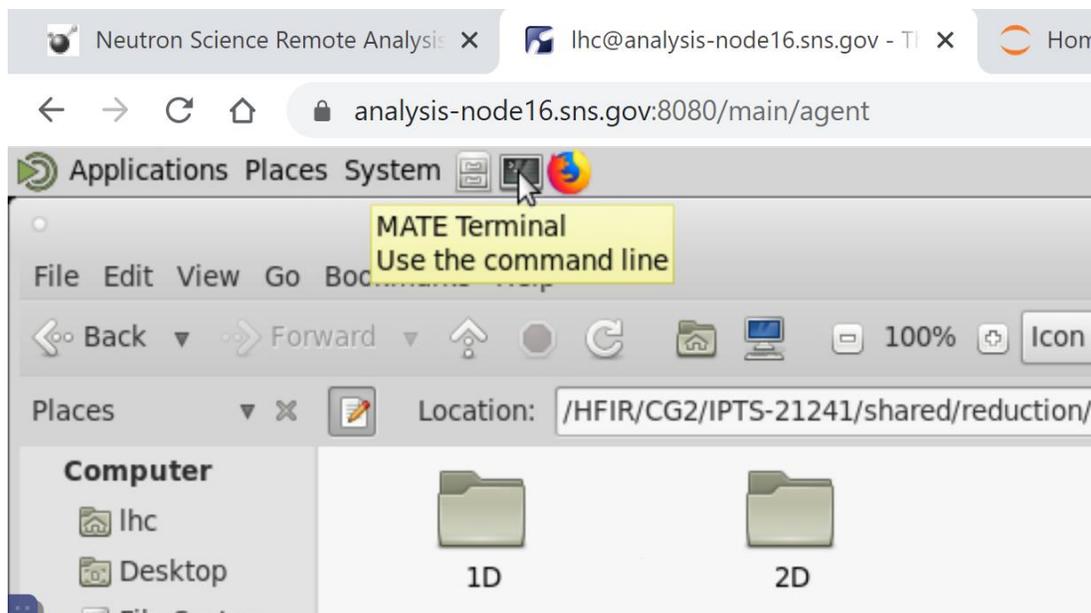
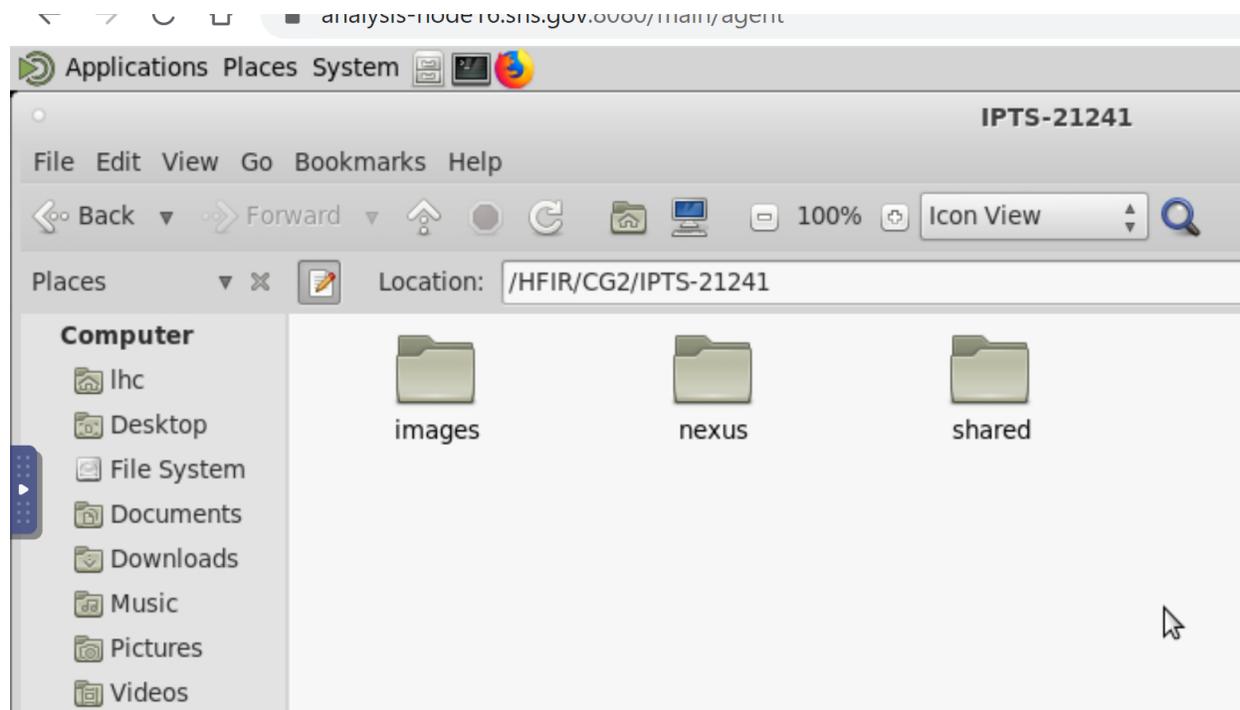
The reduced data and metadata are all saved in the folder designated by users on `analysis.sns.gov`. The server provides various connection options to download the data, with support from linux@support.sns.gov. Here, we will show you how to locate the folder and files with the Remote Desktop, which can be launched from any browser by click “Launch Session”



7.3.1 Once logged in, it is a full functional remote desktop. You can use the file browser to locate the files reduced.

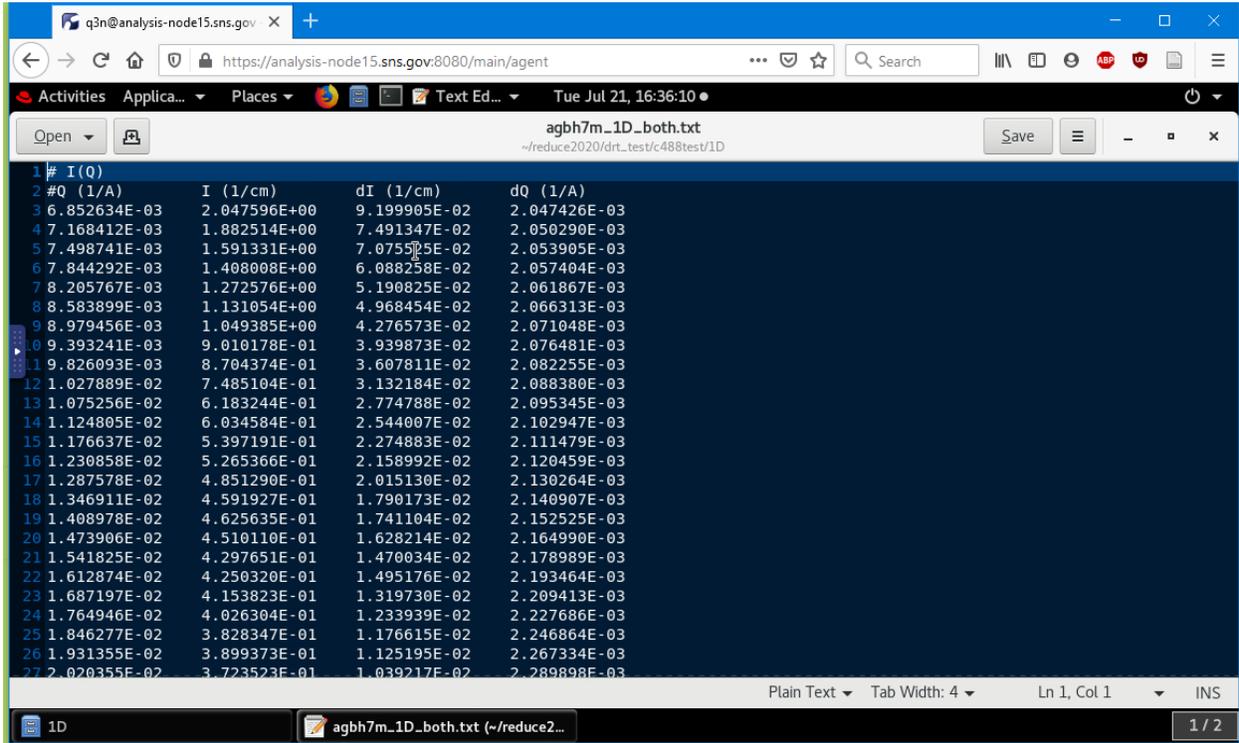


7.3.2 Reduced files are saved into 1D folder (1D curves) and 2D folder (reduced in Qx-Qy plane). The HDF files have all the raw and reduction meta data, as well as the reduced data. Please consult your local contact on how to utilize them.



7.3.3 The typical isotropic data in 1D format are saved in the 1D folder with merged data if multiple configurations are used. They are typical SANS data format of 4 columns: Q, I,

ΔI , ΔQ . You can download them and view them in the SANS analysis software of your choice.



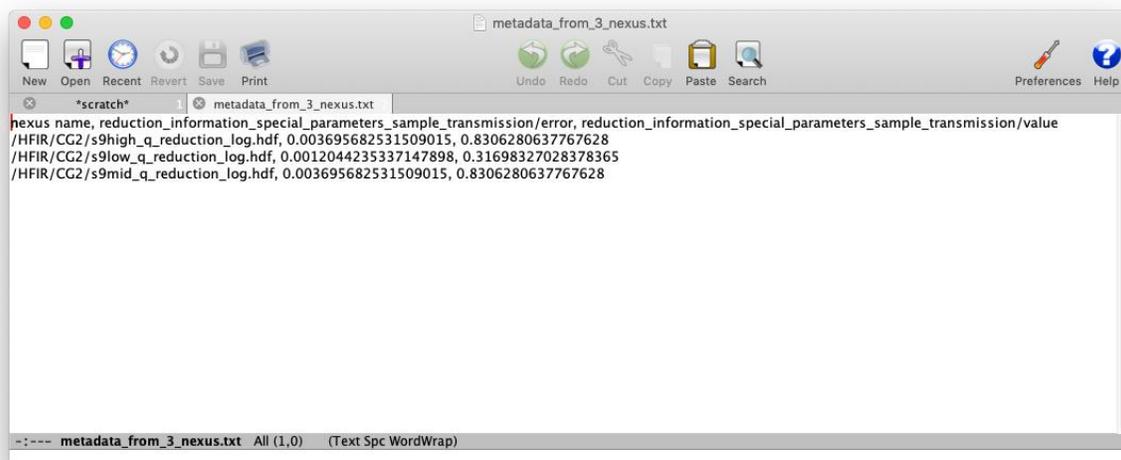
```
1 # I (Q)
2 #0 (1/A)      I (1/cm)      dI (1/cm)     dQ (1/A)
3 6.852634E-03  2.047596E+00  9.199905E-02  2.047426E-03
4 7.168412E-03  1.882514E+00  7.491347E-02  2.050290E-03
5 7.498741E-03  1.591331E+00  7.075525E-02  2.053905E-03
6 7.844292E-03  1.408008E+00  6.088258E-02  2.057404E-03
7 8.205767E-03  1.272576E+00  5.190825E-02  2.061867E-03
8 8.583899E-03  1.131054E+00  4.968454E-02  2.066313E-03
9 8.979456E-03  1.049385E+00  4.276573E-02  2.071048E-03
10 9.393241E-03  9.010178E-01  3.939873E-02  2.076481E-03
11 9.826093E-03  8.704374E-01  3.607811E-02  2.082255E-03
12 1.027889E-02  7.485104E-01  3.132184E-02  2.088380E-03
13 1.075256E-02  6.183244E-01  2.774788E-02  2.095345E-03
14 1.124805E-02  6.034584E-01  2.544007E-02  2.102947E-03
15 1.176637E-02  5.397191E-01  2.274883E-02  2.111479E-03
16 1.230858E-02  5.265366E-01  2.158992E-02  2.120459E-03
17 1.287578E-02  4.851290E-01  2.015130E-02  2.130264E-03
18 1.346911E-02  4.591927E-01  1.790173E-02  2.140907E-03
19 1.408978E-02  4.625635E-01  1.741104E-02  2.152525E-03
20 1.473906E-02  4.510110E-01  1.628214E-02  2.164990E-03
21 1.541825E-02  4.297651E-01  1.470034E-02  2.178989E-03
22 1.612874E-02  4.250320E-01  1.495176E-02  2.193464E-03
23 1.687197E-02  4.153823E-01  1.319730E-02  2.209413E-03
24 1.764946E-02  4.026304E-01  1.233939E-02  2.227686E-03
25 1.846277E-02  3.828347E-01  1.176615E-02  2.246864E-03
26 1.931355E-02  3.899373E-01  1.125195E-02  2.267334E-03
27 2.020355E-02  3.723523E-01  1.039217E-02  2.289898E-03
```

8. Neutron Imaging—Extract Metadata from SANS ReductionLog

[Step by Step demo](#)

8.1 Description

This notebook creates an ASCII file of any of the metadata selected in the ReductionLog file. This file is created at the end of each reduction and contains a lot of information about the reduction process. Metadata from all ReductionLog files are listed side-by-side in a comma separated format as shown here.



```
hexus name, reduction_information_special_parameters_sample_transmission/error, reduction_information_special_parameters_sample_transmission/value
/HFIR/CG2/s9high_q_reduction_log.hdf, 0.003695682531509015, 0.8306280637767628
/HFIR/CG2/s9low_q_reduction_log.hdf, 0.0012044235337147898, 0.31698327028378365
/HFIR/CG2/s9mid_q_reduction_log.hdf, 0.003695682531509015, 0.8306280637767628
```

In this format, all the metadata selected for a given input file are on the same row.

8.2 Select Your Instrument

Select your HFIR SANS instrument. This will allow the program to start directly from the instrument folder.

Select your instrument

| |
|----------------|
| GP-SANS (CG2) |
| BIO-SANS (CG3) |

8.3 Select the ReductionLog files

Using the folder selection tool, select all the ReductionLog files (*.hdf) you want to extract metadata from.

Once you selected those files, the notebook will automatically display all the metadata you can extract. This list of metadata has been provided by the instrument team. This allows you to only display the metadata of interest and hides most of the ones you don't really need.

8.4 Select List of Metadata to Extract

Use a combination of **CLICK**, **SHIFT + CLICK** and/or **CTRL + CLICK** to make sure you selected all the metadata.

Select the output folder.

Using the folder selection tool, select the output folder where you want to create the ASCII file.