ORNL/TM-2025/4160

User Guide for Sample Reduction at GP-SANS

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January 2026

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ORNL/TM-2025/4160

Neutron Science Directorate
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USER GUIDE FOR DATA REDUCTION AT GP-SANS

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Prepared by
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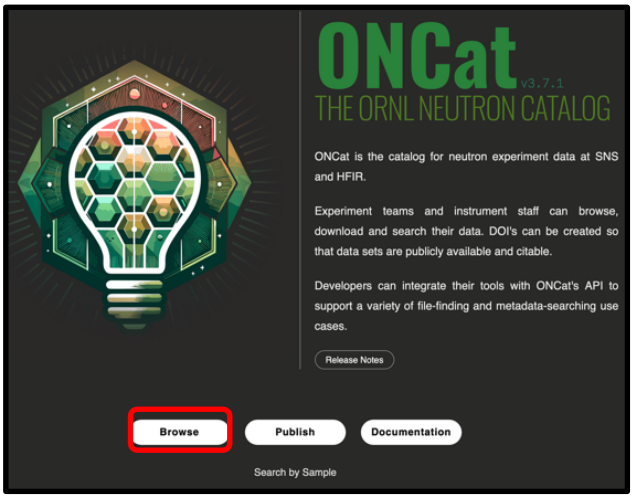
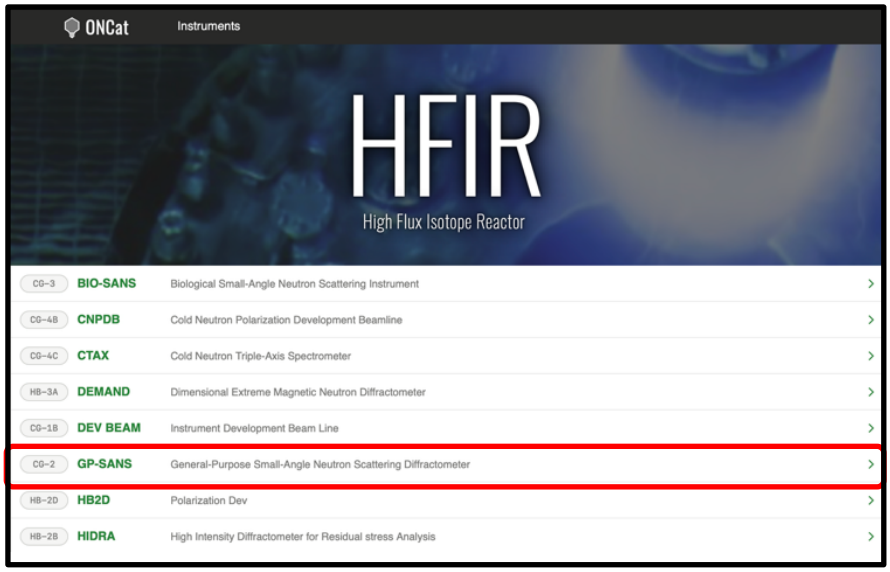
Oak Ridge, TN 37831
managed by
UT-BATTELLE LLC
for the
US DEPARTMENT OF ENERGY
under contract DE-AC05-00OR22725

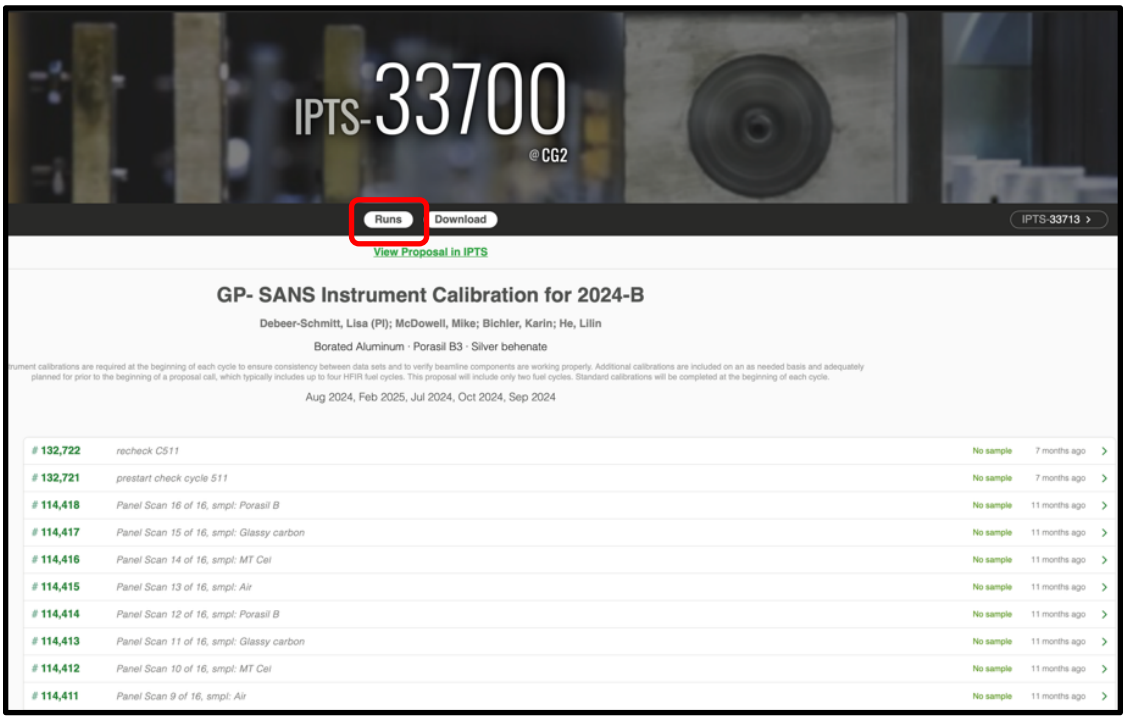
This manual is intended as a quick guide for data reduction of GP-SANS data. It includes all necessary steps to do the data reduction based on absolute calibration using the **open beam method** and how to transfer the reduced data to the personal computer system. If any errors are coming up so that the reduction script is not functioning as intended, please contact the instrument scientist.

1. Download Run Numbers from OnCat

On OnCat webpage (**oncat.ornl.gov**), download .csv table from all the runs of the experiment **Login → Browse → at HFIR select CG-2 GP SANS → go into your IPTS number → Runs →** **Download as CSV** (upper right corner)



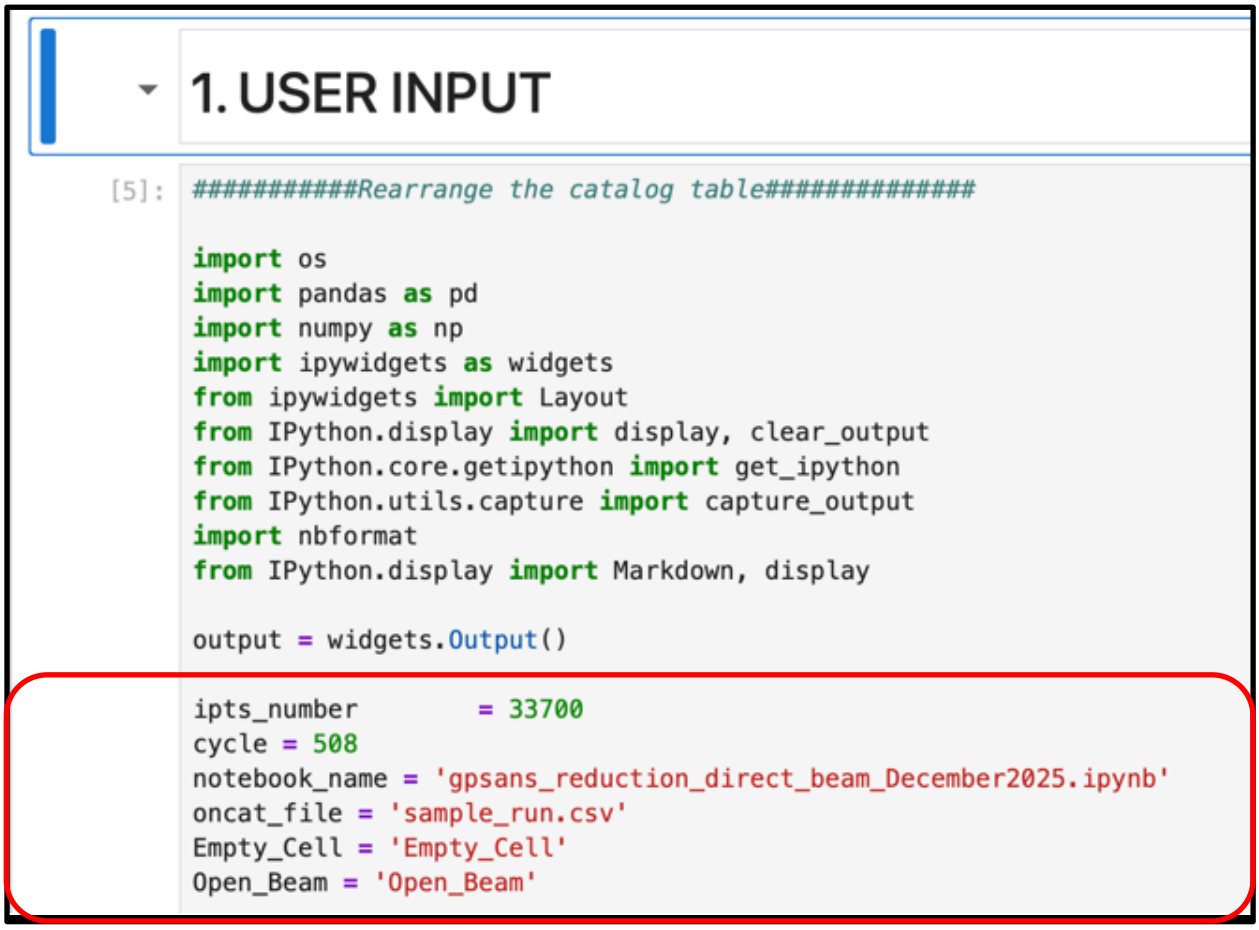




2. Upload OnCat file to Jupyter Notebook

Import to: **Jupyter.sns.gov** into your IPTS shared folder

3. User Input in Script



From the downloaded OnCat table, several information is **taken automatically**:

- Scattering and Transmission run number
- Thickness of the samples
- Sample names

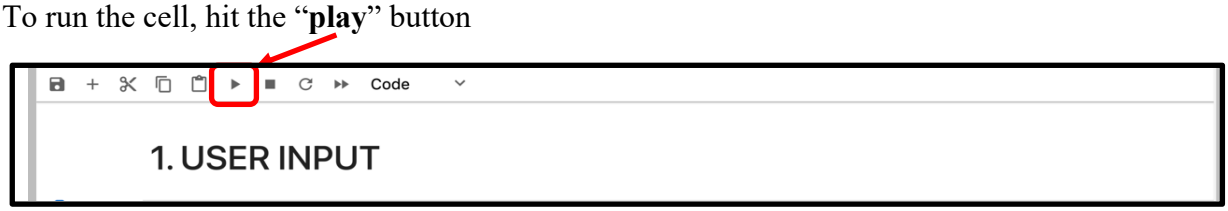
Adjust the following entries are required:

- IPTS-Number (user experiment number)
- Cycle
- Notebook_name (must match Jupyter notebook name)
- Oncat_file (must match name of .cvs table)
- Adjust Name of: Empty_Cell and Open_Beam

After adjusting the entries, run the first cell. (Please see **Step 4: Running First Cell**)

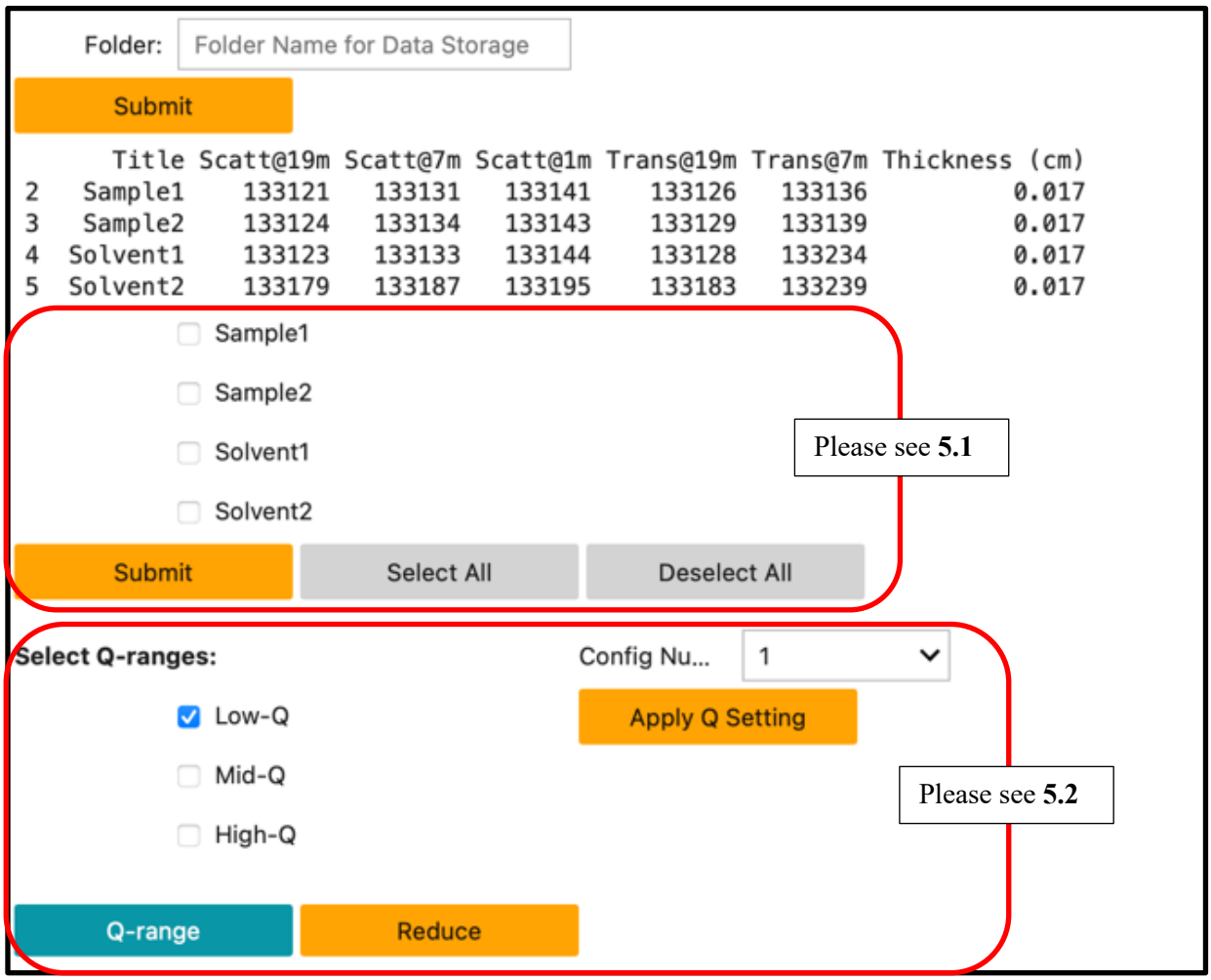
4. Running First Cell

To run the cell, hit the "**play**" button



Running the first cell opens a pop-up field with following **information** included (as shown below):

1. Sample Title
2. Scattering and Transmission runs at different detector distances
    a. Scattering and transmission runs are **automatically sorted in a descending order**, with scattering runs first, followed by transmission runs.
3. Sample Thickness



In this step, the user needs to specify the folder for saving the reduced data. This is done by including the folder name into the field "**Folder: Folder Name for Data Storage**" and clicking on the "**Submit"** button

After specifying the folder for data storage, the directory is set for further data processing.
(Please see **Step 5: Adjusting the Q-Range for Data Merging (Part I)**)

5. Adjusting the Q-Range for Data Merging (Part I)

After setting the folder and the directory (**Step 4**), the selection of the Q -range for merging the data from different detector settings is next.

This involves the adjustment of the different Q -ranges from the different detector distances. These defined regions are used for merging the data and for defining the stitching ranges, leading to the full Q -range selected for the experiment.

The determined Q-ranges and stitching regions are saved in its own .csv file – *Q-values-direct-beam.csv* – in the user IPTS folder per default. Those ranges are further used for reducing all samples from the experiment until a new Q-range selection is done.

5.1 Sample selection:
For starting this step, you need to select **one** sample where the Q-ranges and stitching ranges will be adjusted on. Sample selection is done by setting the tick accordingly and click the "**Submit"** button. This confirms the sample selection. Any sample can be taken for this step.

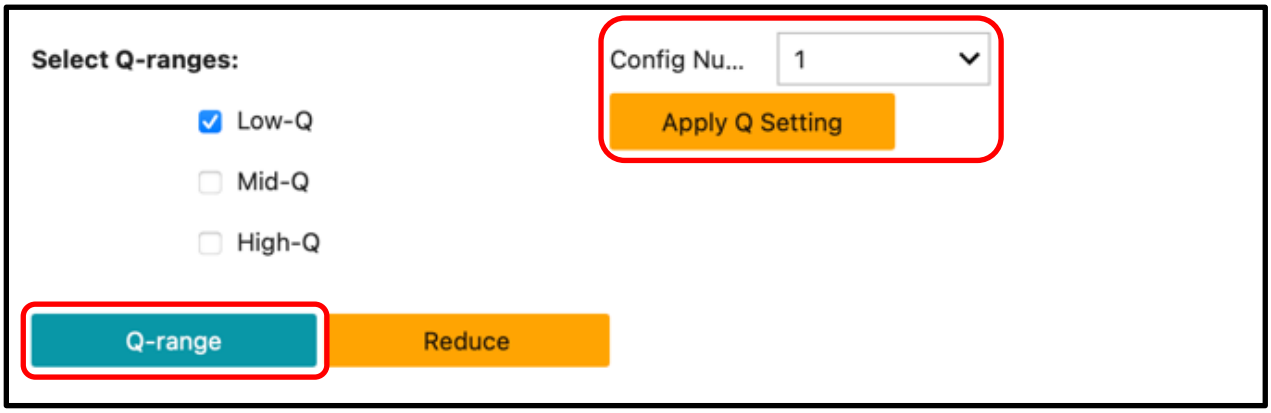
5.2 *Q – setting and Q – range adjustment:*

Before starting the ***Q*-range adjustment,** the desired Q - setting needs to be selected. It can be any configuration between 1 and 3 detector distances as selected by the drop-down menu. Based on the configuration number the Q ranges need to be ticked.

Note: *Config. Num. 1:* Low Q or Mid Q or High Q (only **one** tick is possible)
Config. Num. 2: Low Q and Mid Q, or Low Q and High Q, or Mid Q and High Q (only **two** ticks are possible)
Config. Num. 3: Low Q, Mid Q, and High Q (**three** ticks are set per default)

After selecting the right Q - setting, click the button "**Apply *Q* Setting**"

The next step is to **start the *Q*-range adjustment** by clicking the "***Q*-range"** button.

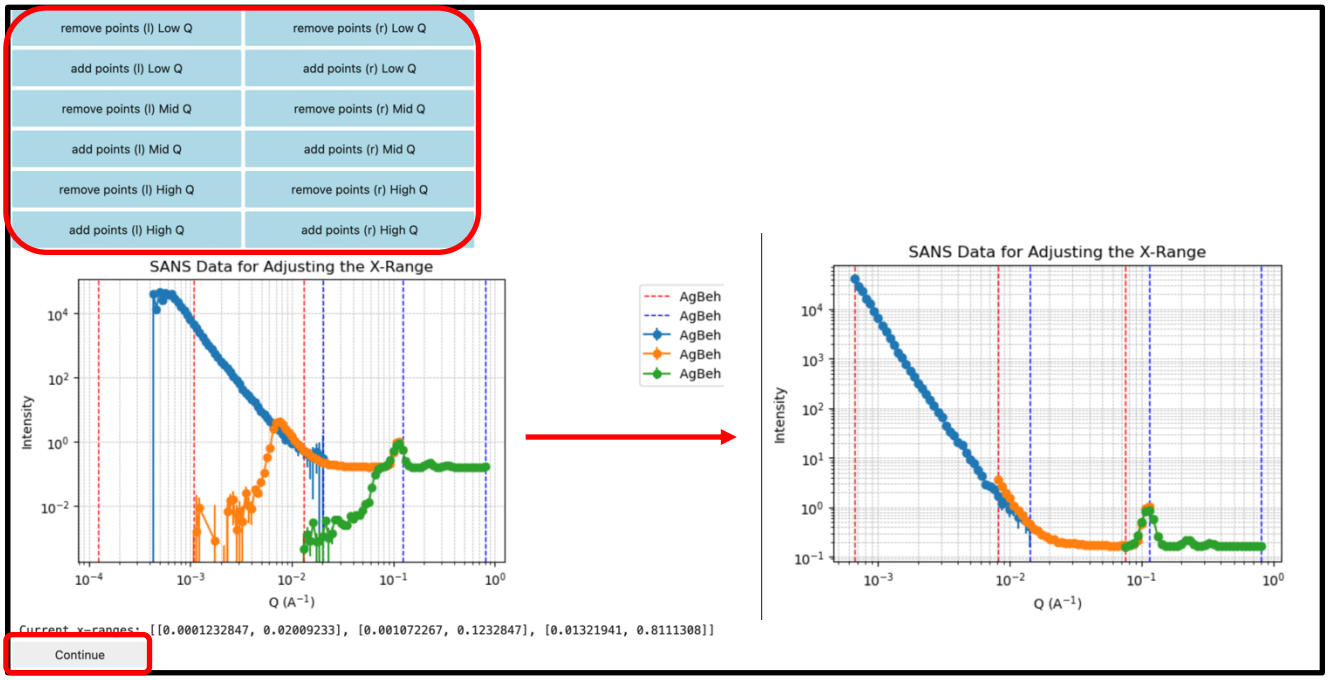


Please see **Step 6: Adjusting the *Q*-Range for Data Merging (Part II)**

6. Adjusting the Q-Range for Data Merging (Part II)

The data reduction for one specific sample that is used for adjusting the Q-range is running and stops once each single Q-range is reduced.

At this time, you have the option to adjust/change the Q- and stitching ranges for further data reduction. That option is provided with the buttons "**removing or adding points**" for each Q-range. Changes are applied and visible immediately leading to cleaned Q-ranges.



Once satisfied with the adjusted Q- and stitching ranges, click the "**Continue**" button. This starts the further data reduction including merging the Q-ranges together.

This step is only required once and provides the Q- and stitching ranges for all the other samples.

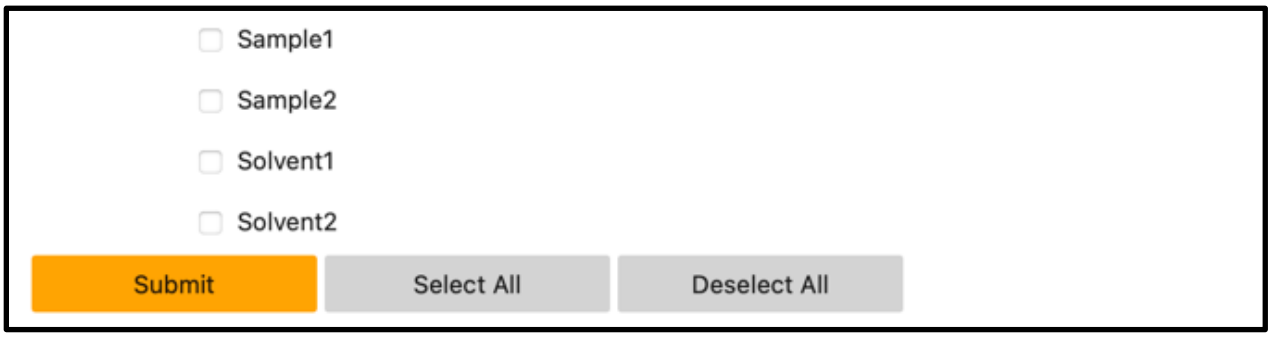
Next step is reducing the actual samples from the experiment.

Please see **Step 7: Sample Reduction**

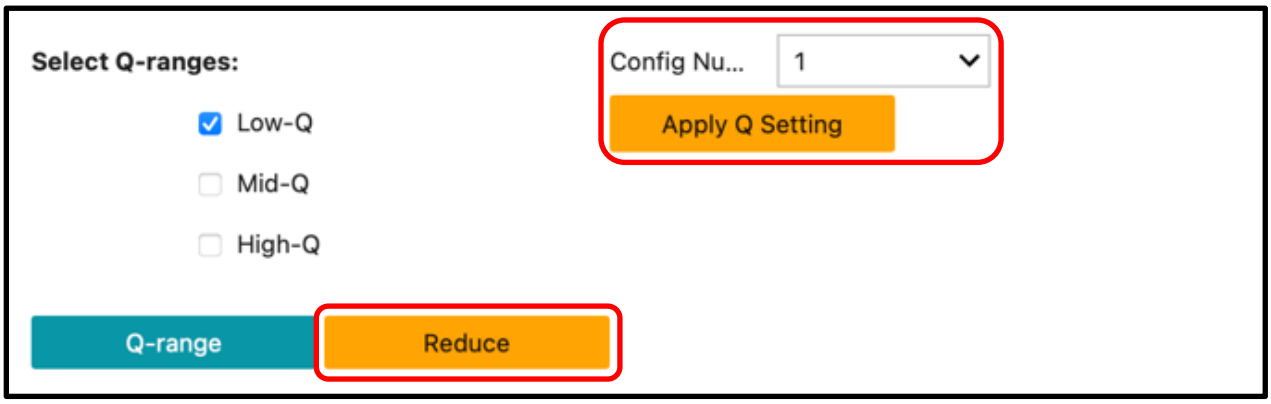
7. Sample Reduction

Starting the sample reduction requires to go back to **Step 4** (**skipping Step 5 and Step 6**) and set the directory for saving the reduced sample data and click "**Submit**".

As a next step you can either select specific samples by selecting them followed by clicking "**Submit**" or you can click "**Select All**" which takes every sample in the list for data reduction.



Independently on the sample selection, the next step is clicking the "**Apply Q Setting**" button again followed by clicking the button "**Reduce**"



This starts the data reduction for the selected samples based on the previously adjusted Q- and stitching regions.

Data reduction is running

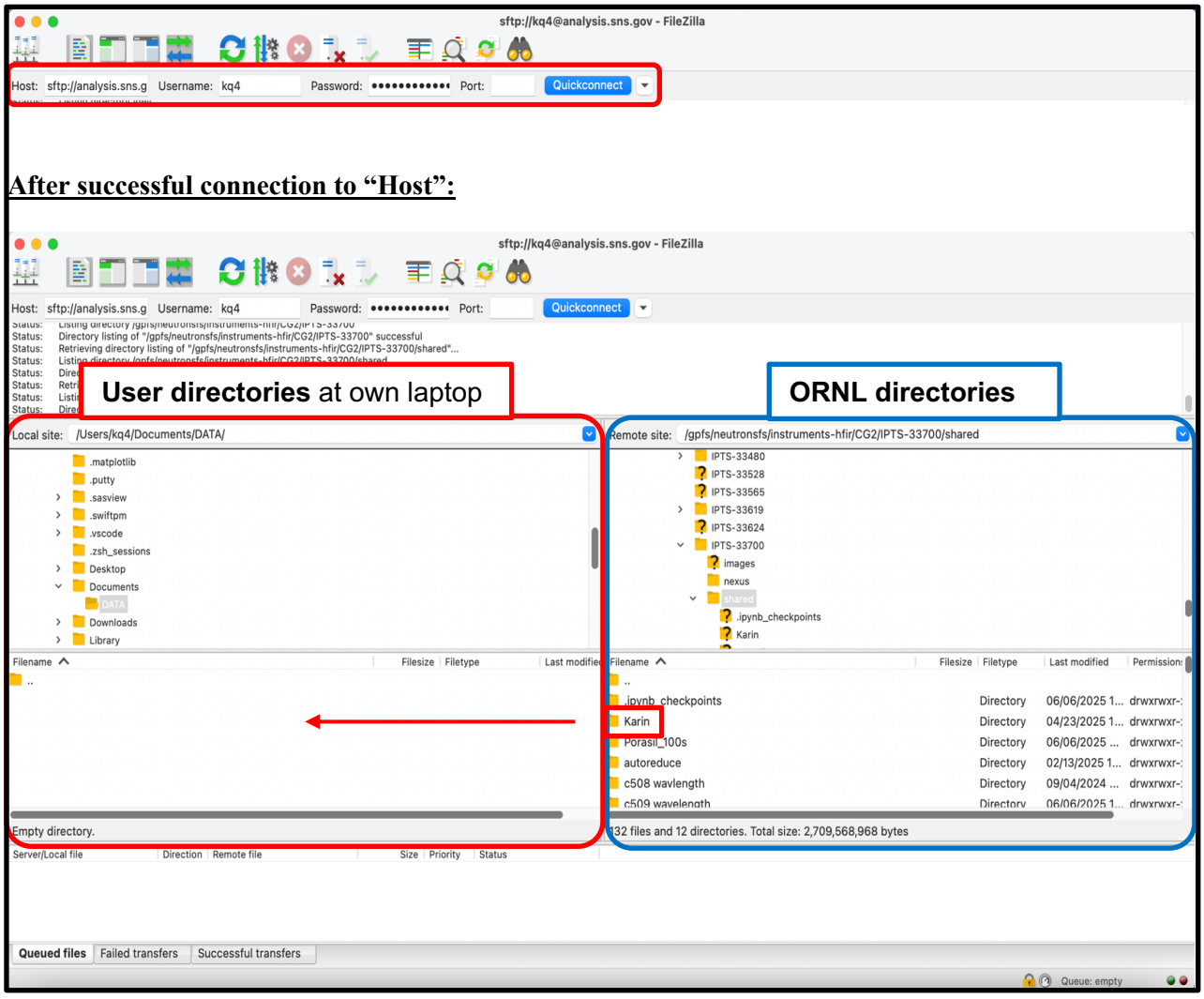
When data reduction is done, 1D and 2D data for each single Q-range together with the merged data are saved in the specified directory. Also, transmission values for each sample and Q-range are extracted and saved in an own .csv file.

8. Exporting Data to Personal Laptop

Use any client for data transfer. This guide uses "FileZilla", an open-source FTP (File Transport Protocol) client.
(FileZilla: https://filezilla-project.org/download.php?type=client)

Log in to FileZilla using:

- **Host:** analysis.sns.gov
- **Username and password:** The same as used for the user portal
- **Port:** 22



After successful connection to "Host":

- In the ORNL directories, go to the **"shared"** folder in **YOUR experiment IPTS:**

  /gpfs/neutronsfs/instruments-hfir/CG2/IPTS-…/shared

- Select the data to transfer and **drag and drop** them into the desired "user directory" on your personal system