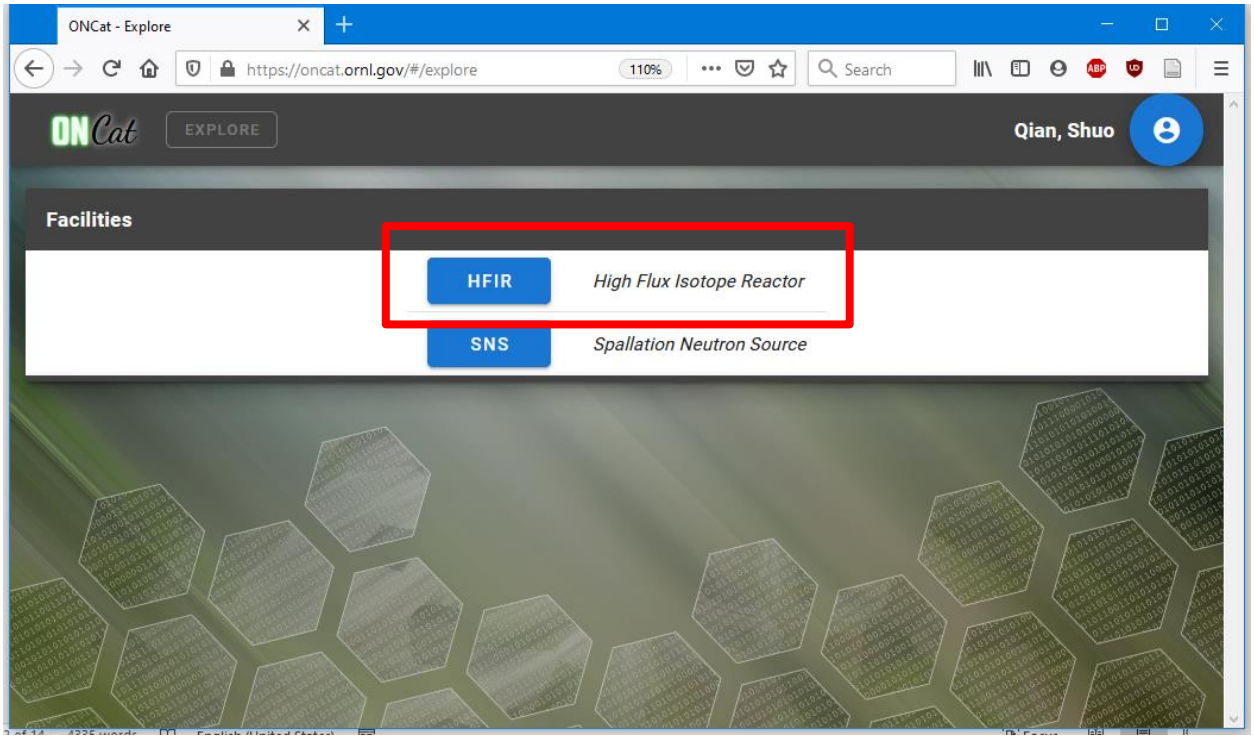
Bio-SANS Data Process Guide

Quick Reference for using jupyter notebook to reduce data

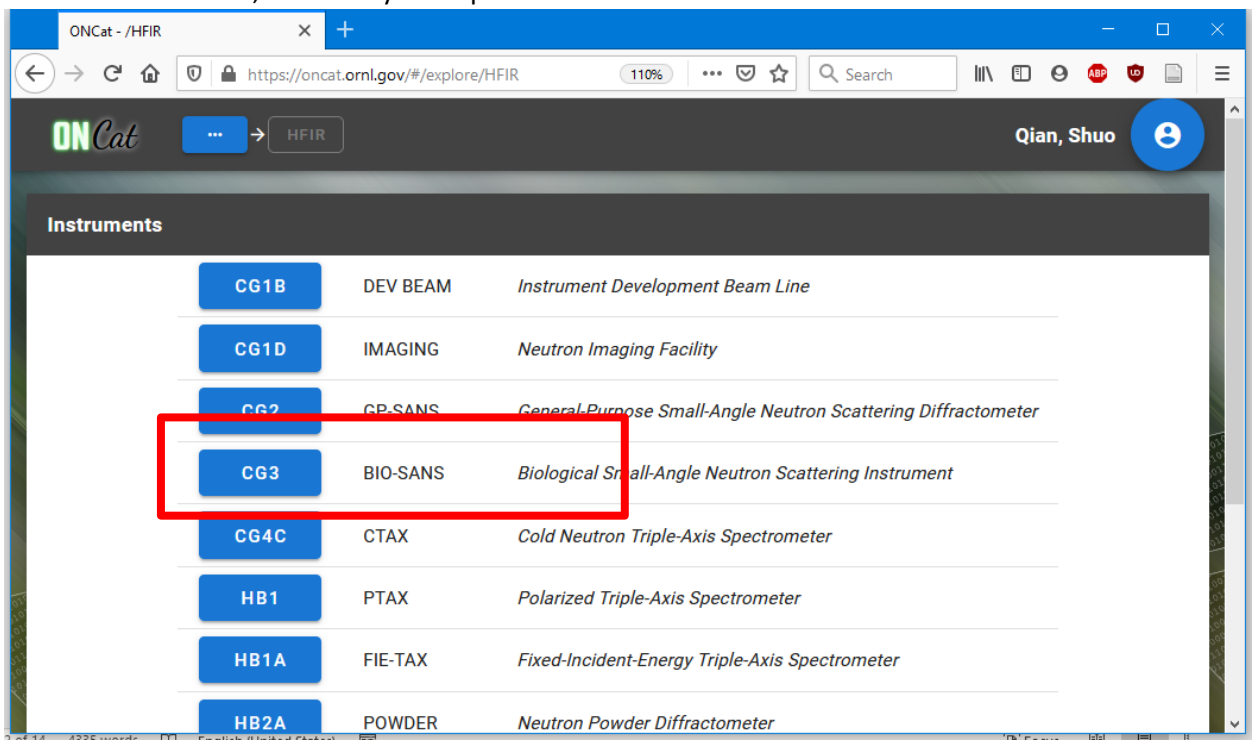
Note:

- 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>
- A companion video tutorial can be found in YouTube: https://youtu.be/_DniWKMSIX0

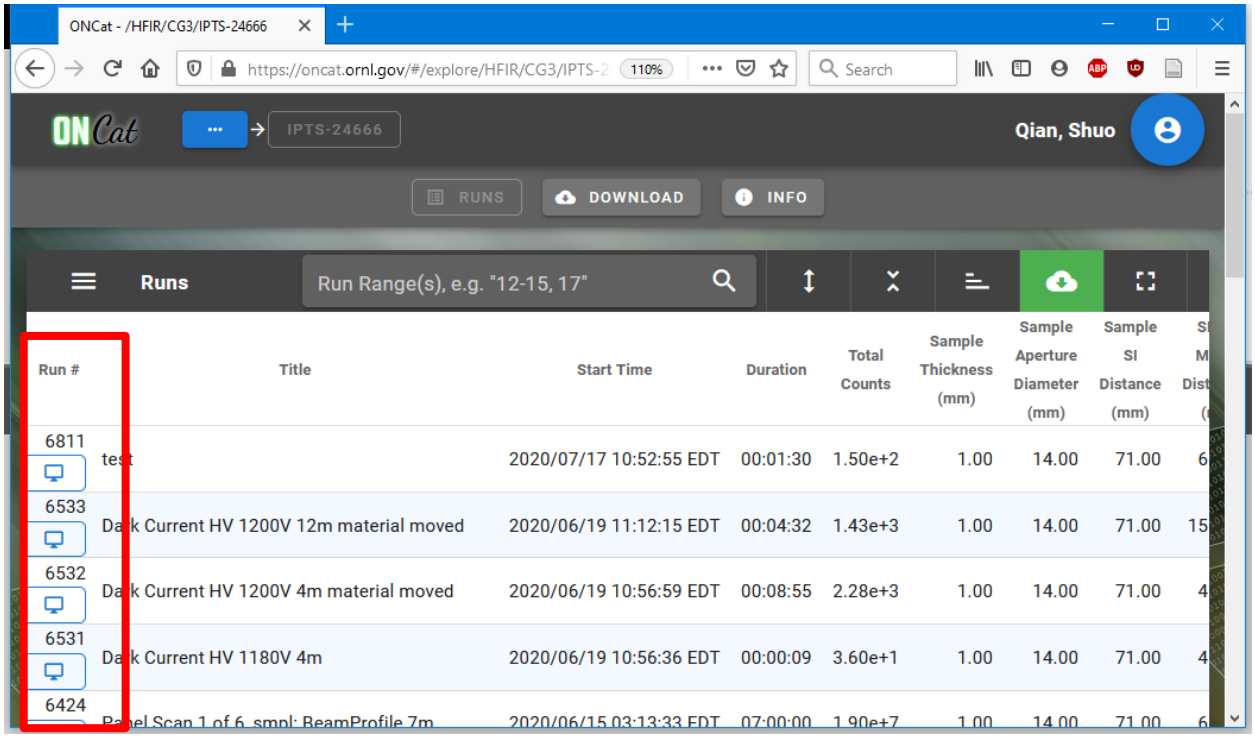
1. **Identify the run numbers for the data in ONCat.ornl.gov**
   All data are saved in sequential number (Run #) with all metadata information such as title, time and other user specified information. The run number is used in the reduction to call the data. Identifying the run number for the data to be reduced in the data catalogue is the first step in the process.
   1.1 Login into oncat.ornl.gov



1.2 Click into **HFIR** > CG3, then find your experiment IPTS



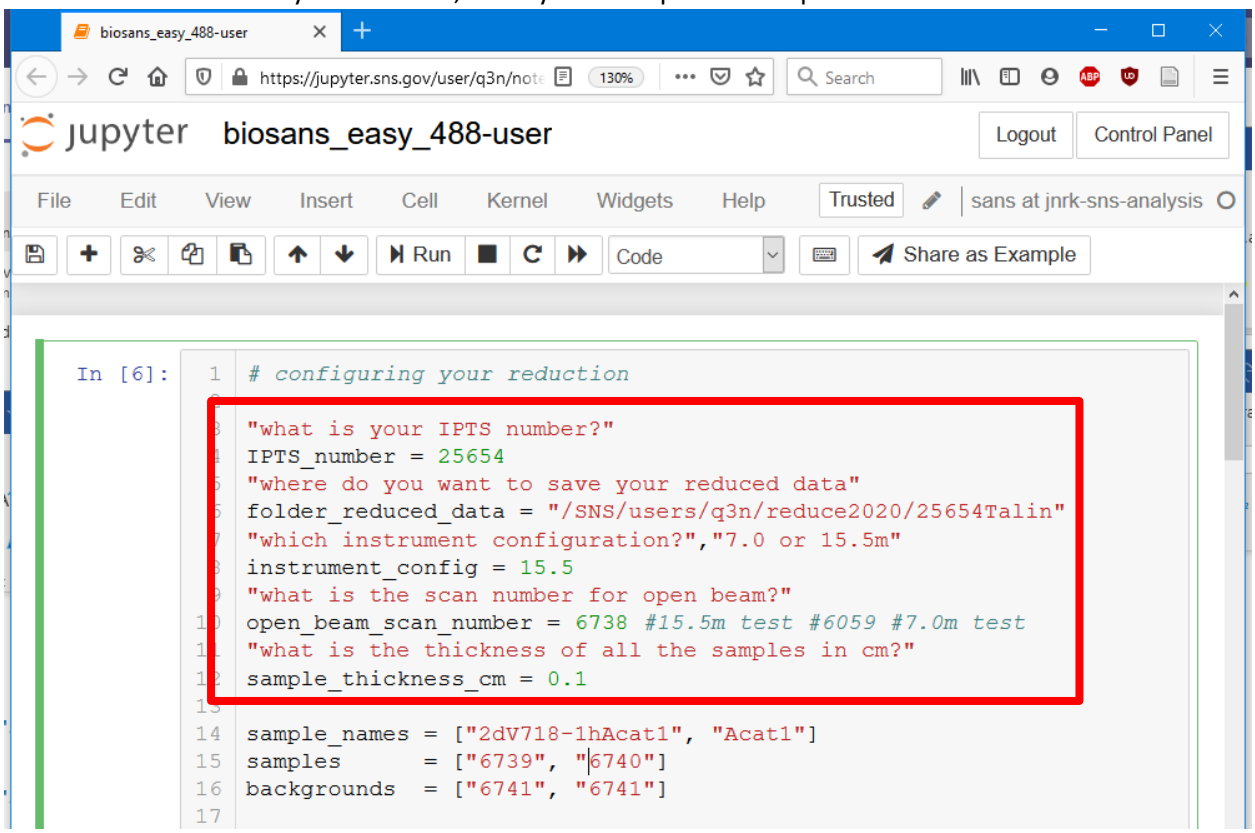
1.3 The Run number is the very first column in the list, along with other useful information to identify data



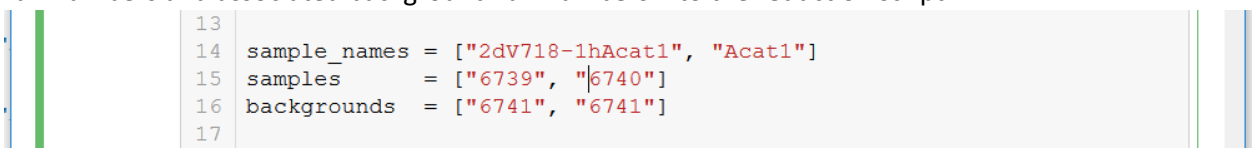
2. Data reduction with jupyter notebook, jupyter.sns.gov

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

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.



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.



- *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.

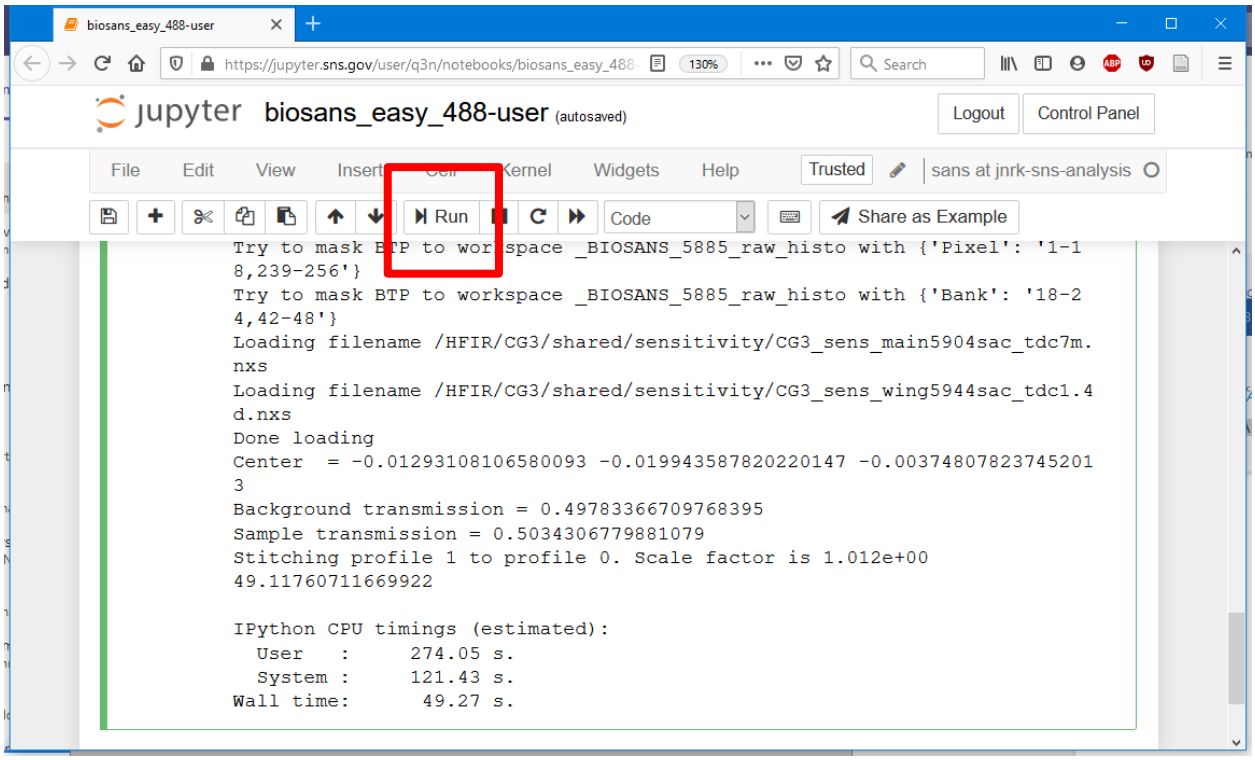
For example:

```
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.

2.3 Once the lists of run number are completed and click '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.

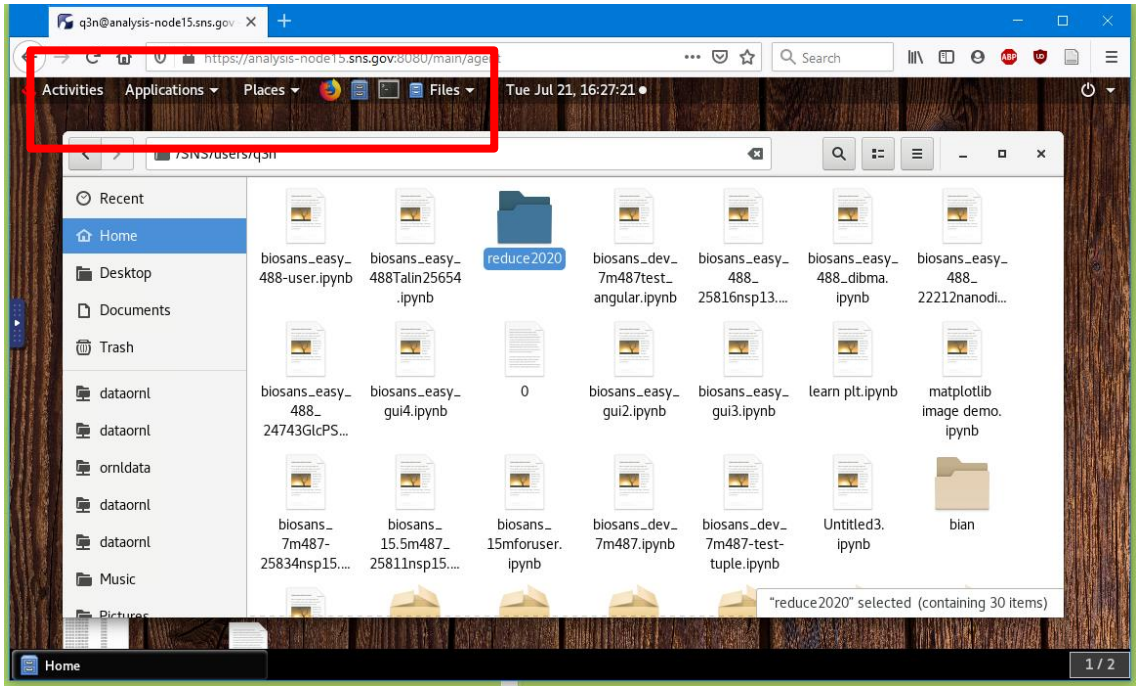


3. **Accessing reduced data from analysis.sns.gov**

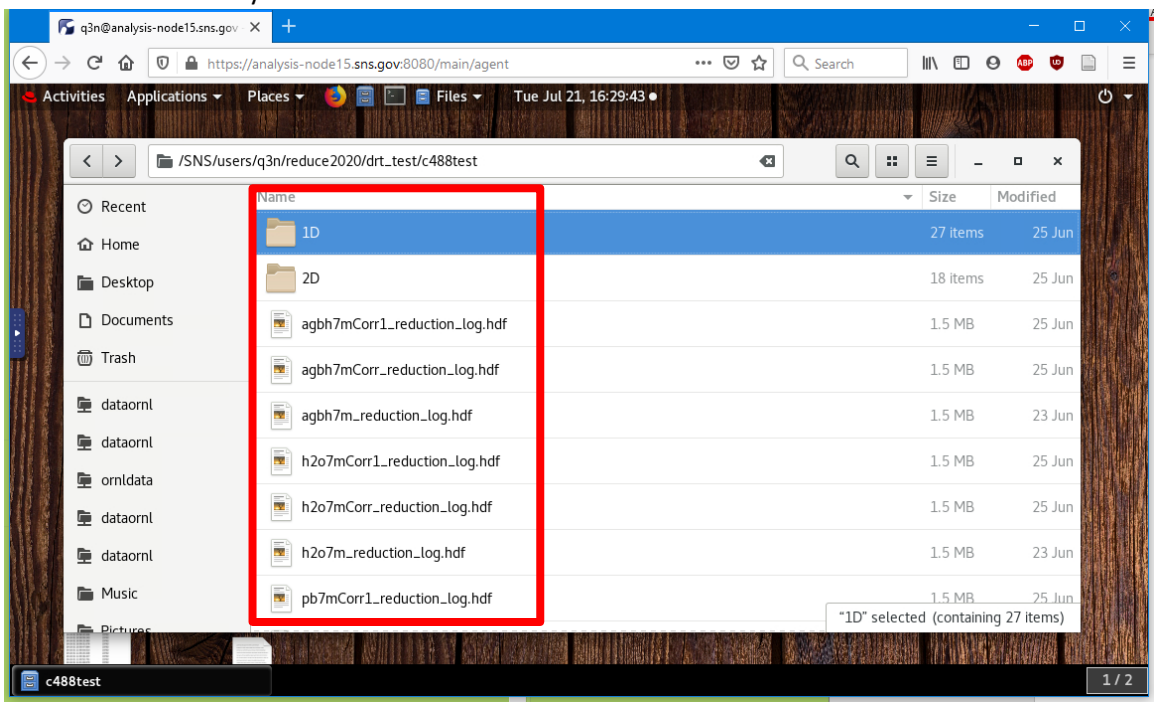
Reduced data can be downloaded and viewed from analysis.sns.gov in the designated output folder as specified in the reduction script. The server provides various connection options to access and download data as shown below in the front page of the analysis cluster.

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.

3.1 Once logged-in, use the file broswer to locate the reduced files.



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.



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.