EQSANS Data Reduction with drtsans – Quick Reference for Script Mode

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Introduction

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

- via scripts run in the terminal window,
- via mantidworkbench or
- via jupyter notebooks

The present document details the first method. Your local contact will work with you to configure the reduction for the various instrument configurations that you use during your experiment.
The content of the document is also explained through several tutorial video linked within the text below.
Below please find the step-by-step description of the procedure.

1. **Visit analysis.sns.gov**
    a. Data reduction can be performed both from inside and outside of ORNL
    b. Log in with your xcams ID and password (IPTS system username and password)
        i. The same credentials are needed to transfer files to your personal computer via e.g. WinSCP
2. **Set up the conda environment**
    a. Video tutorial: https://youtu.be/L4xBdUX80e8
    b. for the activation type one of the following commands into the terminal
        i. source /opt/anaconda/bin/activate sans
        ii. source /SNS/EQSANS/shared/software/testing/bashrc_conda_new
        conda activate sans
    c. check with the *which conda* command if the activation was successful
        i. also if the activation was successful you will see the environment ("sans") before the prompt
    d. If none of the methods was successful, please contact the Linux team on rt-linux@support.sns.gov
3. **Populate the shared directory of your IPTS with the required reduction tools and activate the reduction environment**
    a. Video tutorial: https://youtu.be/O7DwtdnficI
    b. open a terminal
    c. go to the shared folder of your IPTS
        i. cd /SNS/EQSANS/IPTS-*****/shared
    d. copy eqsans_setup.sh from /SNS/EQSANS/shared/usertools/
        i. cp /SNS/EQSANS/shared/usertools/* .
        ii. run eqsans_setup.sh by typing
            1. ./eqsans_setup.sh
        iii. or one can directly run the shell script by typing /SNS/EQSANS/shared/usertools/eqsans_setup.sh and enter.
4. **Edit the template reduction script, which is written in python 3**
    a. Use any of your preferred text editors e.g. gedit or pluma to edit reduce_template.py
        i. gedit reduce_template.py &
        ii. pluma reduce_template.py &

b. The script contains examples for reduction of data from 2 configurations in a single script

5. Example of writing and running a script for reduction

a. Update output directory

```
###################################
# USER INPUT BEGINS HERE
# CHANGE THIS TOP FOLDER AS NEEDED
###################################

ipts_number          = 25961
output_directory     =f"/SNS/EQSANS/IPTS-{ipts_number}/shared/output/"
```

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 run numbers and names for individual scattering and transmission runs corresponding to the standard measurements of porous silica

```
#low-q
samscatt_1      = [120068]
samtrans_1      = [120067]
bkgscatt_1       = [120095] * len(samscatt_1)
bkgtrans_1       = [120089] * len(samscatt_1)
emptybeam_1      = 120066

#high-q
samscatt_2      = [120071]
samtrans_2      = [120070]
bkgscatt_2       = [120107] * len(samscatt_2)
bkgtrans_2       = [120101] * len(samscatt_2)
emptybeam_2      = 120069

overlap = [0.056, 0.065]
sample_thick    = [1] * len(samscatt_1)
sample_names    = ['porsil_25961']
print('Sample number =',len(samscatt_1))
print('Sample name number =',len(sample_names))
```

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

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

```
##################################
# USER INPUT 2 BEGINS HERE
# CHANGE THIS TOP FOLDER AS NEEDED
# COMMENT-OUT UNUSED USER INPUT BLOCKS IF NEEDED
##################################
# SILICON WAFER SAMPLES
ipts_number          = 25961
output_directory     =f"/SNS/EQSANS/IPTS-{ipts_number}/shared/output/"

#low-q
samscatt_1      = [120077, 120078, 120079, 120080]
samtrans_1      = [120073, 120074, 120075, 120076]
# if no background subtraction is wanted, use below two lines
bkgscatt_1       = [''] * len(samscatt_1)
bkgtrans_1       = [''] * len(samscatt_1)
# if using the A1 as background use below two lines
# bkgscatt_1       = [120077] * len(samscatt_1)
# bkgtrans_1       = [120073] * len(samscatt_1)

emptybeam_1      = 120066

samscatt_2      = [120085, 120086, 120087, 120088]
samtrans_2      = [120081, 120082, 120083, 120084]
# bkgscatt_2       = [120085] * len(samscatt_2)
# bkgtrans_2       = [120081] * len(samscatt_2)
bkgscatt_2       = [''] * len(samscatt_2)
bkgtrans_2       = [''] * len(samscatt_2)
emptybeam_2      = 120069


overlap = [0.056, 0.065]
sample_thick   = [1] * len(samscatt_1)
sample_names   = ['A1', 'A2', 'A3', 'A4']
print('Sample number =',len(samscatt_1))
print('Sample name number =',len(sample_names))
```

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. 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

f. Save the file and run the reduction script from the terminal. For the example file shown in the video, which was saved as reduce_test.py, 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.

g. 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.
    ii. I(q) files can be also displayed via launching eqsans_rungui.sh created in paragraph 3, clicking on the “Display IQ” button and select the data of interest.

iii. Analysis cluster has 'sasview' software, which can also display and perform fittings. To launch sasview, open a terminal and type the following.

1. sasview

6. 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, MergBC_max, …]", having 2·(Num_Configurations -1) pairs of minimum and maximum Q-values for the merge regions.

```
overlap = [0.056, 0.065]
```

b. The stitching ranges are generally determined by examining the data files. Feel free to ask your local contact or another instrument scientist for advice.

c. The stitching ranges have to be listed in order of increasing momentum transfer (from low-Q to high-Q)

d. 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.**

e. The applied scale factor will be displayed in the terminal window during script execution.

f. Unless another name is provided for the merged_fn variable in the save_iqmod command, the stitched file will have an ending of _merged_*nameOfTheSample*_Iq.txt. In the example presented in the video, the output file for the stitched data is "merged_porasil_25961_Iq.txt".

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 prettyjason.sh script that is created during the steps described in section 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, custom time-of-flight values are defined for limiting the range of neutrons of interest.

```
print('..... config 2')
eq = EQVar('2020B/2o5m.json')
eq._outputdir = output_directory
eq._ipts = ipts_number
eq._standardabsolutescale = 1
eq._sampleaperturesize = 10
eq._maskfilename = "/SNS/EQSANS/shared/NeXusFiles/EQSANS/2020B_mp/mask_4m_20201106.nxs"
eq._numqbins = 80
eq._qbintype = "log"
eq._showjson = False
eq._cuttofmin = 500 # custom tof
eq._cuttofmax = 12000 # custom tof
eq._empty = emptybeam_2
eq._thickness = sample_thick[i]
eq._bkgscatt = str(bkgscatt_2[i])
eq._bkgtrans = str(bkgtrans_2[i])
eq._samscatt = str(samscatt_2[i])
eq._samtrans = str(samtrans_2[i])
eq._filename = str(sample_names[i])+'_conf2'
iqname2 = eq._filename
reduceNow(eq)
print('......reduction complete.')
```

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.