POWGEN User Manual for Data Access

This document contains a detailed description of how to access POWGEN data offsite. Data may be reduced using our analysis machines, either on-site via powgen (powgen.sns.gov) and powgen2 (powgen2.sns.gov), or outside ORNL via the analysis cluster (analysis.sns.gov).

1) Go to the user portal and create an XCAMS ORNL Resource account (if you don't already have an account). This is the same as your account for the IPTS system.

https://user.ornl.gov/Account/Login.aspx

If you have forgotten your password, use the "Forgot your password?" link to retrieve it.

- 2) To connect to the analysis cluster, go to https://analysis.sns.gov/ (Figure 1).
 - To use the web-based client in your browser, click the "Launch Session" button. You may also go directly to https://analysis.sns.gov:8080. Login with your XCAMS username and password.
 - Alternatively, you can install the Thinlinc client on your machine. Click on the Thinlinc button and follow the steps to install and configure the client (Figure 2). Login credentials will be the same as XCAMS.



Figure 1. Access the analysis cluster by going to http://analysis.sns.gov and either clicking "Launch Session" or installing the Thinlinc client.



Figure 2. Thinlinc client installation instructions are available at https://analysis.sns.gov/instructions/.

3) Once you login, under your home directory you will see the following folder structure: /data/SNS/PG3/IPTS-#/, where # is your IPTS proposal number. If you fail to see the IPTS-# folder, then try /SNS/PG3/IPTS-#/shared/autoreduce. This is the real location of the file whereas the first one is a symlink or shortcut. All the run numbers will appear for your data.

Data are automatically reduced to GSAS, FullProf and Topas formats using the default parameters. Those data can be found in the /shared/autoreduce folder. You can of course re-reduce data with other binning values using mantidplot.

Extension **.gsa** for GSAS: Files are numbered with banks which correspond to the wavelength used. Please use the corresponding bank number from the parameter files for refinements.

Extension .dat for FullProf: The data file names themselves tell you which bank they are and the same bank IRF file should be used.

Extension .xye for Topas: Again, the data file names themselves tell you which bank they are. For example, PG3_24759-2.xye is run number 24759 collected with bank 2.

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 Secure ftp or secure shell will allow you to get the data onto your local drive. Two such programs can be downloaded from http://cyberduck.io/ or http://filezillaproject.org. Enter the following information to connect to the analysis computers:

Host: analysis.sns.gov XCAMS username and password Port: 22

5) Parameter files for GSAS and IRF files for FullProf can be downloaded from the table titled "Data Reduction and Analysis by Run Cycle" on the Powgen website. There is also a Topas template file with the appropriate parameters. Be sure to pick the correct cycle.

http://neutrons.ornl.gov/powgen/users

These files are also stored on the analysis computer in the following folder, where cycle is year_1 (for cycle A) or year_2 (for cycle B)

/SNS/PG3/shared/CALIBRATION/cycle_11A_CAL.

The parameter and IRF file names contain HR or HI to denote whether High Resolution (HR) or High Intensity (HI) mode, respectively, was used for data collection. If the guide value is approximately -54 in your summary file (see below), then the data were collected using HR, while if the value is approximately +163, then the data were collected using HI guide.

6) A summary file called PG3_IPTS-#_runsummary.csv, which is a csv file with all relevant information about the runs (e.g. wavelength, sample temperature, etc.), is available in the folder /SNS/PG3/IPTS-#/shared/autoreduce.