

# EQ-SANS Cheat Sheet — J.K. Zhao, zhaoj@ornl.gov

## Experiment Planning:

Use the "EQSANS calculation" from the "EQSANS post it" pad on the control PC to:

1. Estimate the covered Q-range as a function of detector location and selected wavelength band.
2. Determine the required slit size (Direction beam on detector should be << beam stop size).

## Data Collection (On Control PC):

1. Start 'NewPyDas'
2. Create a run script:
  - a. Click the '**ScriptEditor**' button at the lower right corner of *PyDas's ControlCenter*.
  - b. Select commands you need. Read command instructions if needed.
  - c. Save your script.
3. Run the script you just saved: Click the '**Run**' button

## Data Reduction & Analysis (On eqsans.sns.gov, outback.sns.gov, or outback2.sns.gov)

1. Computer access
  - a. Obtain account on eqsans.sns.gov, outback.sns.gov, or outback2.sns.gov
    - i. Goto <http://neutrons.ornl.gov/portal/>
    - ii. Click 'Computer Access Request' on right
    - iii. Click 'SNS user ( on-site and off-site )'
    - iv. Select 'EQ-SANS'
  - b. Access to eqsans.sns.gov, outback.sns.gov, or outback2.sns.gov
    - i. Goto <http://neutrons.ornl.gov/portal/>
    - ii. Click 'Portal Help' On right
    - iii. Click 'Nx' on left and follow the instructions.
2. Using **fatcat** and other programs on eqsans.sns.gov (and outback.sns.gov, or outback2.sns.gov):
  - a. Open a terminal window (shell, console, terminal etc)
  - b. Make a sub folder if you wish to:
    - i. `mkdir mydata`
    - ii. `cd mydata`
  - c. Type **fatcat** or **fatcats** (fatcats being the parallel version of fatcat). Read printed instructions.
  - d. Type **factcat -r 1234** (replace 1234 with your run number) to reduce the data.
    - i. An  $I(Q)$  v  $Q$  file **EQSANS\_1234.iq** is produced and saved.
    - ii. Type **saaf -log xy EQSANS\_1234.iq** to view or model the data.

Example of other **fatcats** options:

  - e. Type **fatcat -v 10 -h** for more instructions.
  - f. Use **factcat -r 1234:1240** to reduce all data between run 1234 and 1240.
  - g. Use **factcat -r 1234:1240 -sri** to print short run info for those runs.
  - h. Type **factcat -r 1234 -save lvxy** to save addition Intensity vs. (x,y) map.
    - i. Use **jzg -3m EQSANS\_1234.2d** to view the just produced 2d map. You can use the toolbar of **jzg** to zoom or display 2d cuts. Use RightClick to change scale etc.
    - ii. You can specify any number of output using valid "-save ????" switches to fatcat.
  - i. Type **factcats -r 1234 -save lvxyt0f** to save addition 3D-Intensity vs. (x,y,tof) map
  - ii. Use **jzg -3m EQSANS\_1234.3dt0f** to view the just produced 3d map. Use pageup & down key to flip through the pages. Press x,y, or z to turn the map to x vs y, y vs z or z vs x.
  - j. Note: **fatcat** use configurations files as well as command line inputs to control the data reduction. By default, an instrument-wide configuration file exists. Type **fatcat -H** (note the capital H) for instructions of how to create your own *eqsans\_configuration.ini* file in the current working folder. If you name you ini file differently, say to "my.ini", use fatcats -ini my.ini to load the your ini file.
3. Other programs (type each of the command for instructions)
  - a. **eqsans\_dataop** : Scale, add,sub,multiply, or divide  $I(Q)$  vs  $Q$  data sets (data format:  $Iq$   $Q$   $stddev\_Iq$ )
  - b. **eqsans\_respace**: Change the  $Q$ -spacing of  $I(Q)$  data by interpolation.
  - c. **guinier, rodguinier,diskguinier**: Guinier plots.
  - d. **saaf**: Command line data modeling program:
    - i. type **saaf -h** for help, or **saaf** to see available models
    - ii. **saaf -log xy EQSANS\_1234.iq EQSANS\_4567.iq** : Plot two data sets in log-log scale (use -log y or -log x for lin-log plots)
    - iii. **saaf -m sphere EQSANS\_1234.iq** : fit EQSANS\_1234.iq to a spherical model
    - iv. **saaf -m guinier -x .01 .02 EQSANS\_1234.iq** : Guinier fit to EQSANS\_1234.iq between x value ( $Q$ ) of 0.01 and 0.02
    - v. **saaf -em sphere** : print a short explanation of the sphere model
4. Use pythonfatcat for data reduction and analysis (Graphical UI for above programs)