XPCSGUI2 Analysis Procedure Documentation

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Modification history:

V1: January 04, 2018

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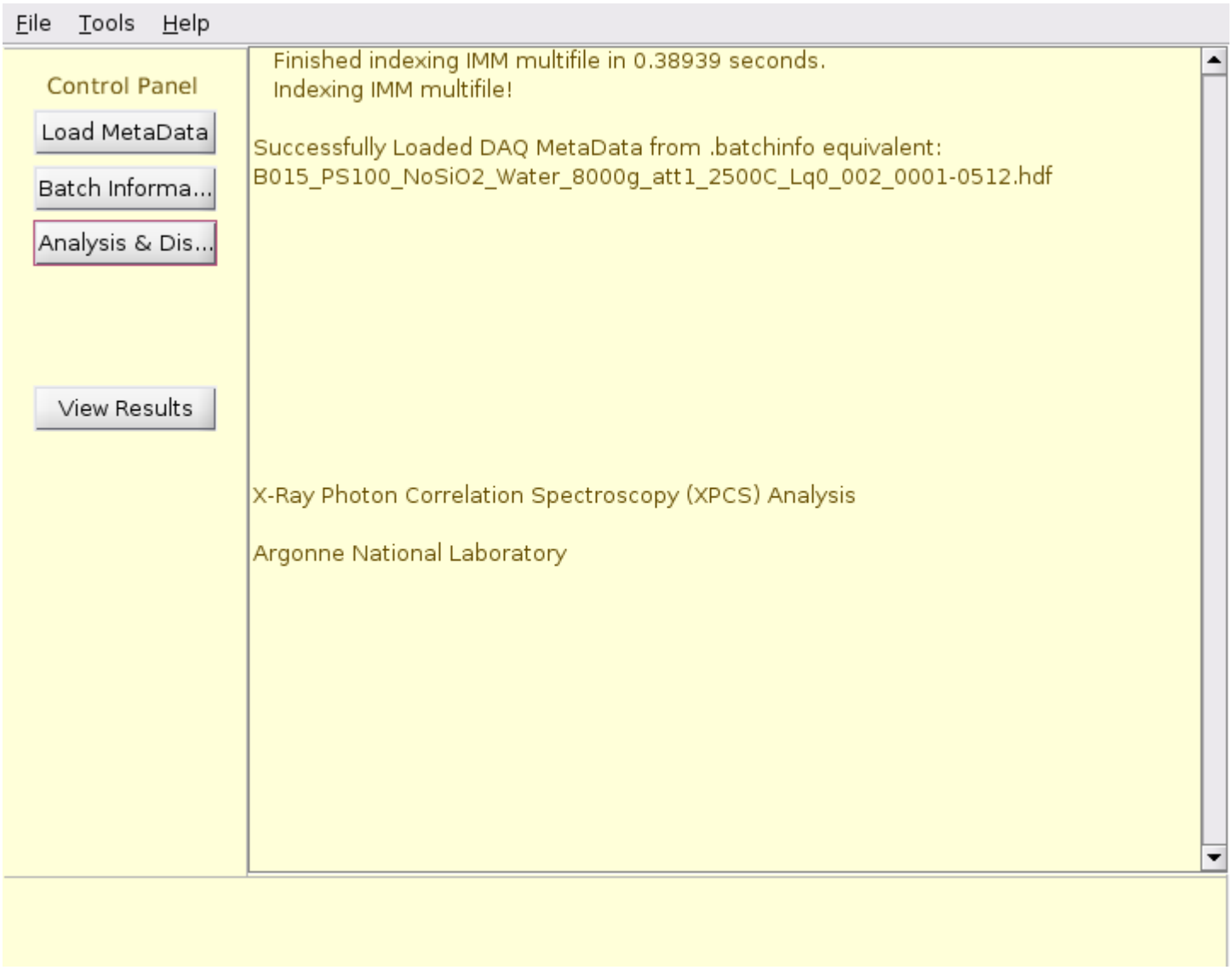

Directory structure of Software:

snow% cd /local/XPCSGUI2/

/local/XPCSGUI2

snow% ls

how_to_set_path.txt XPCS_DEVELOPMENT XPCS_LocalProcessing

keep.m XPCS_DisplayFiles XPCS_MetaDataFiles

readme.txt XPCS_FileReader XPCS_ProcessingTemplates

set_xpcsgui2_path.m XPCS_Geometry XPCS_ToBeDeleted

XPCS_ClusterProcessing XPCS_GUIFiles XPCS_Tools

XPCS_DetectorFiles XPCS_HDF5Files XPCS_TwoTimeG2

The file how_to_set_path.txt provides documentation on how to set the path for this software in matlab for your own computer.

Basically, it describes how to edit the file **set_xpcsgui2_path.m** and execute to add the above folders to the path.

The path has to be saved in matlab after this step so that it will remember after the next restart of matlab.

The description also involves editing the file **loadMetaData.m** in the sub-folder XPCS_MetaDataFiles to define some defaults for the user computer.

This is shown below for clarity.

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ccdimginfo.map_local_location = '/home/8-id-i/partitionMapLibrary/2017-2/';

ccdimginfo.combined_result_folder = 'cluster_results';

ccdimginfo.force_save_to_matfile=0; %1 will save result as .mat, 0 as .hdf

ccdimginfo.static_mean_window_size = 10; %makes this many parts of the time series for SAXS (stability

plot)

ccdimginfo.G2_Tensor_Save = 0; % setting to 1 will save the tensors, takes a lot of space

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```

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xpcsgui
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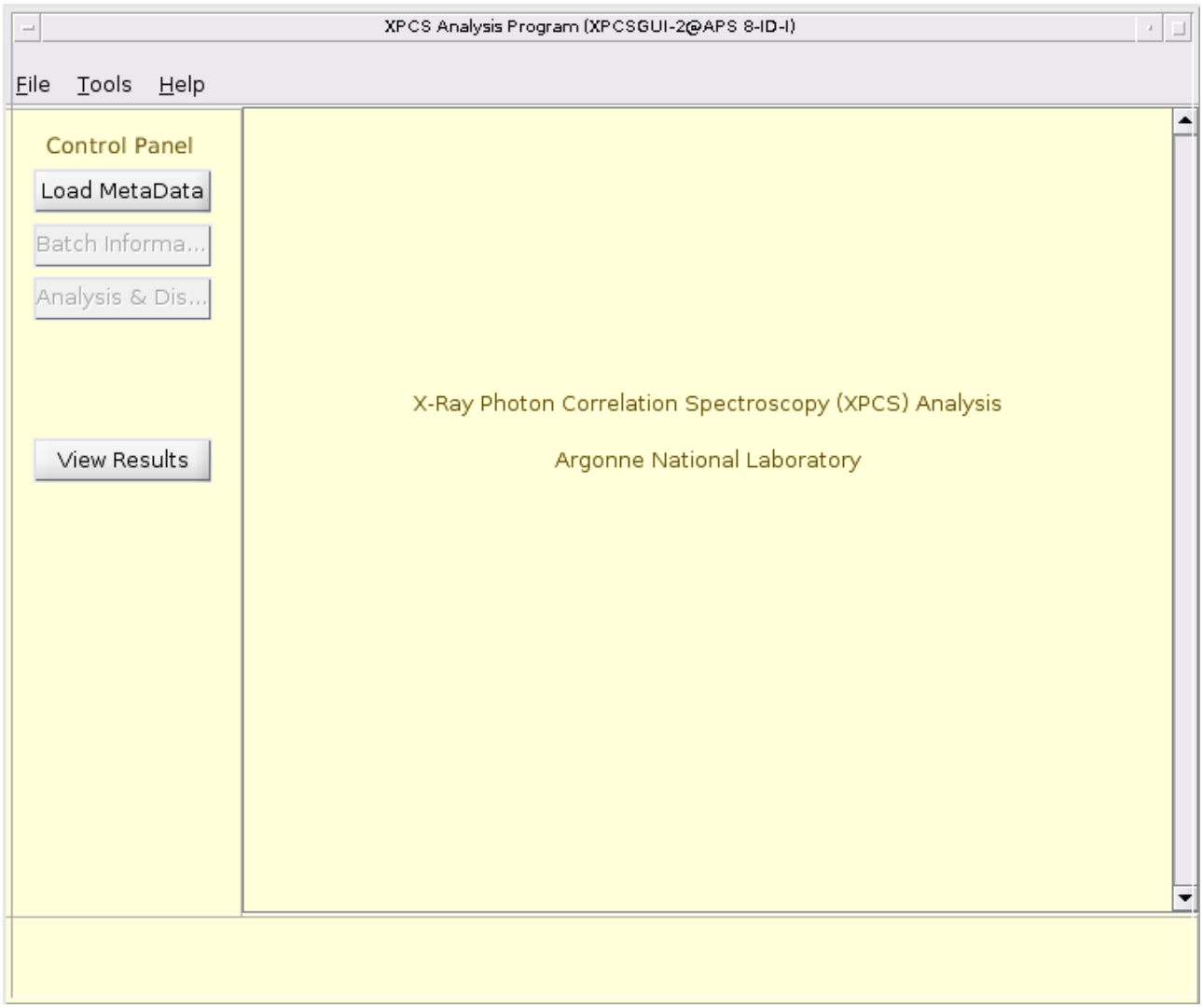
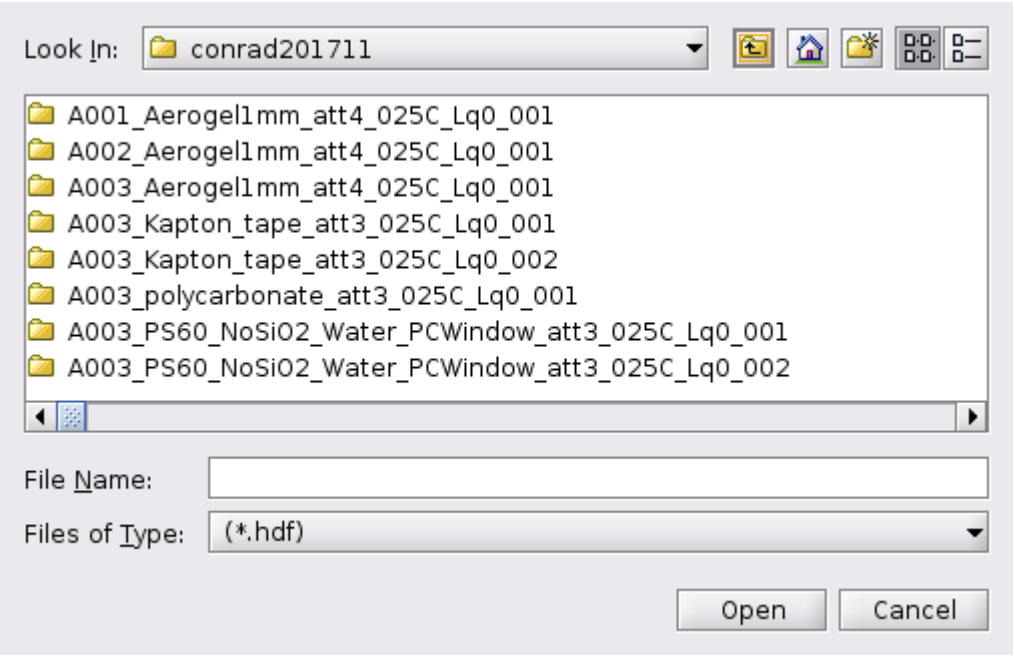


Click on **Load MetaData**

Traverse to the main user data folder (typically PIlastnameYYYYMM) - not the cluster_results folder

pick the desired folder and select the .hdf file (metadata in it, no raw data)

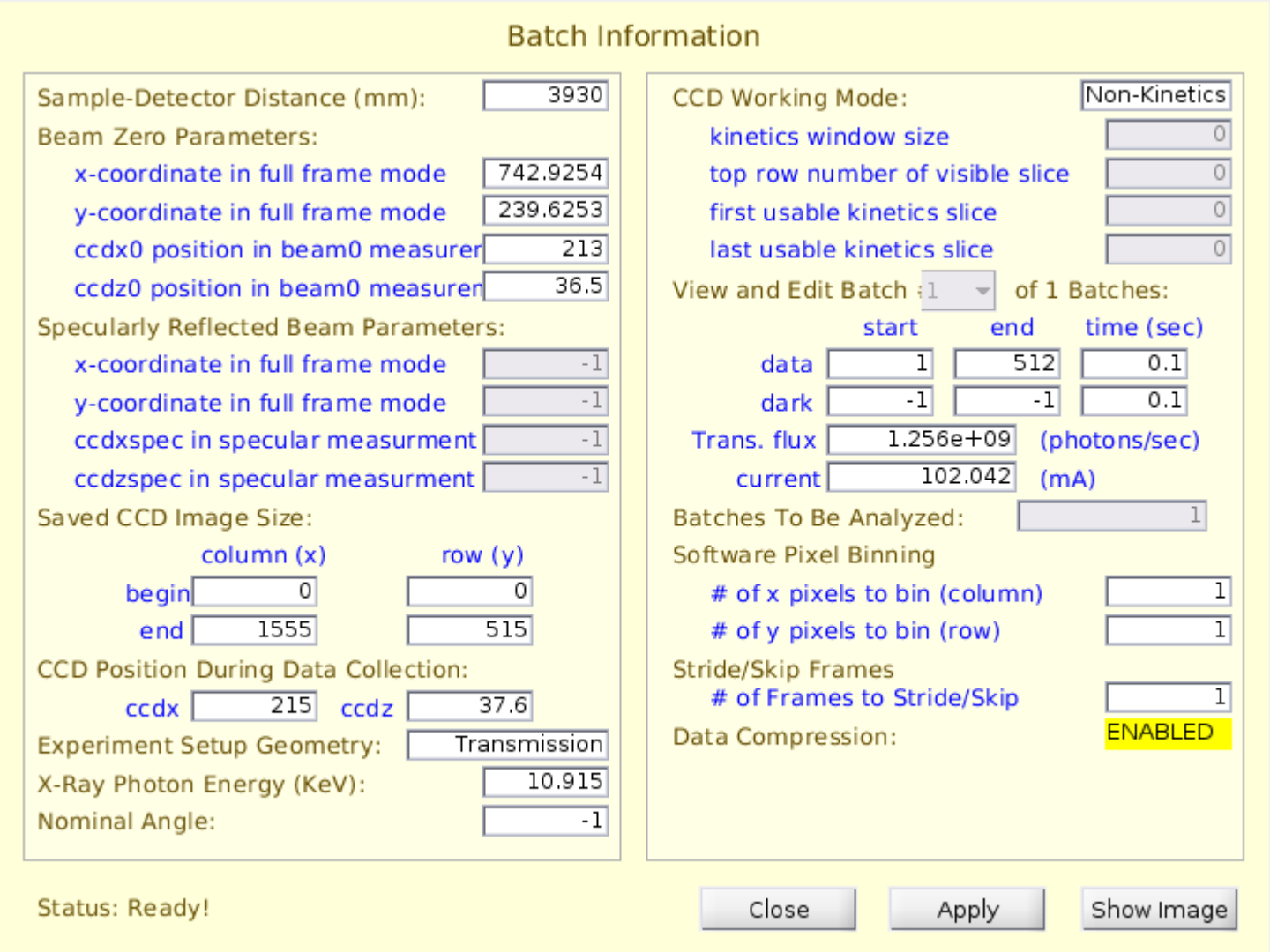


Click on **Batch Information** (usually not much to do in this GUI except for thin films reflection geometry)

In the reflection geometry, the specular direction can be corrected for small errors.

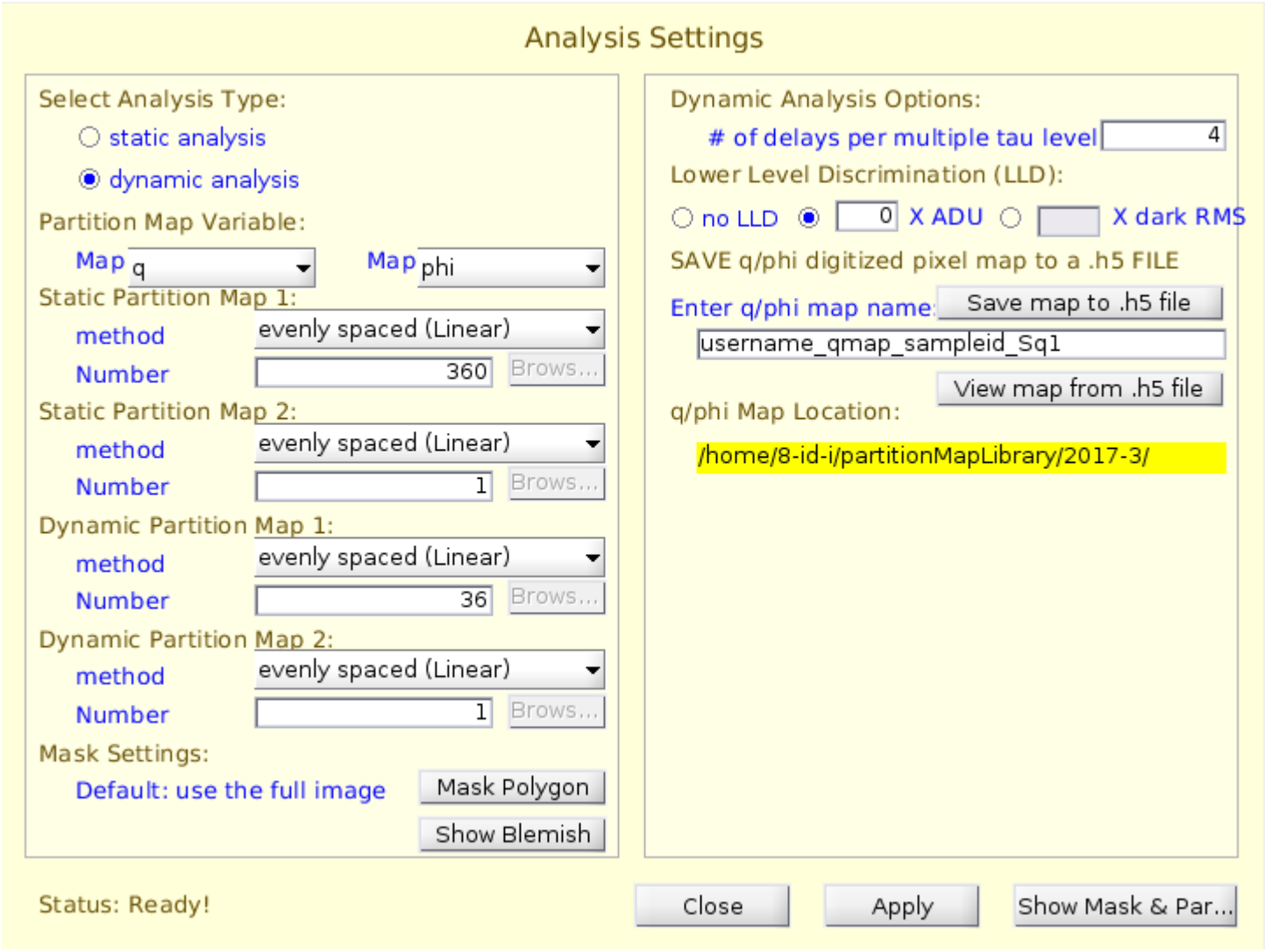
Click on **Show Image** to see a preview of the scattering (usually 100 or so images are averaged)

If any changes are made, click **Apply** and **Close**, else just simply **Close**

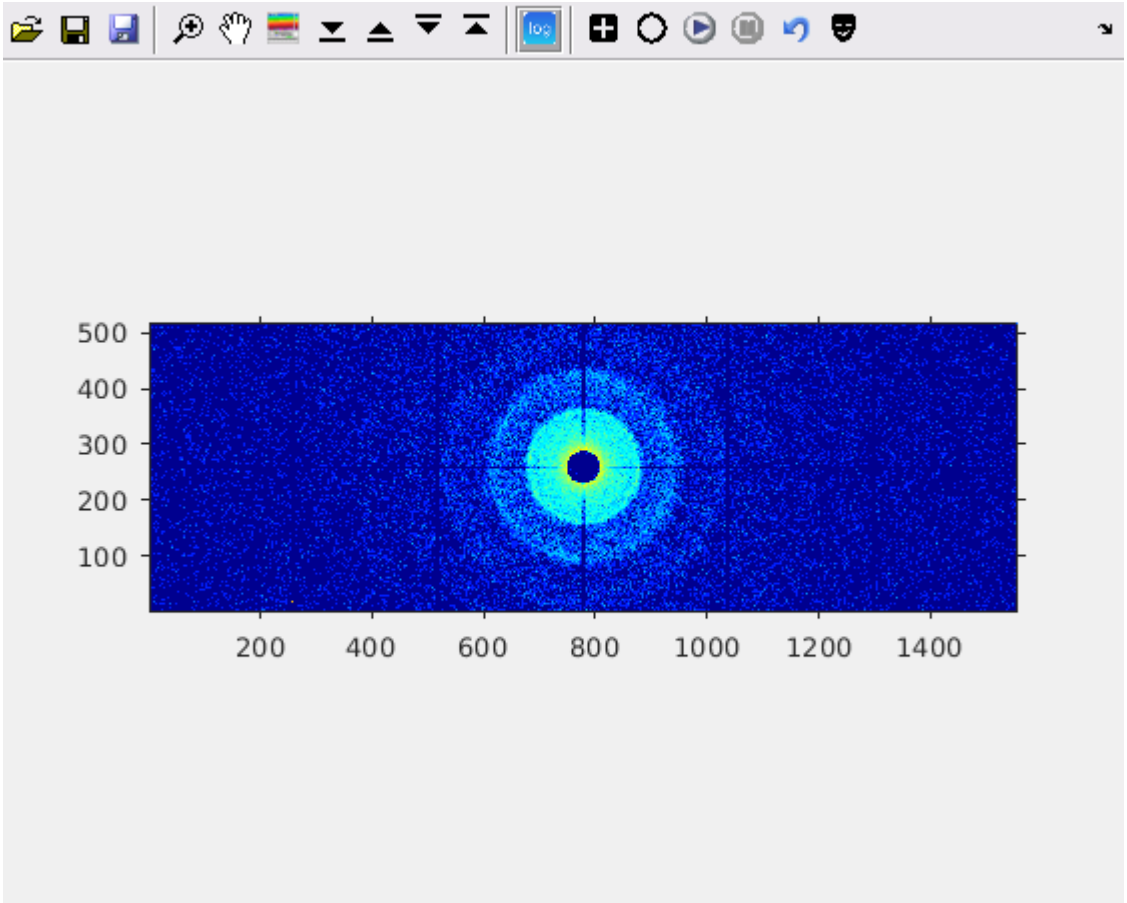


Click on **Analysis & Dis..** (Analysis & Display Settings)

This is the main part.



Click on **Mask Polygon** to select a mask (region) to analyze



There are a lot of features in the toolbar icons:

1. "log" will toggle the scale of the image between linear and log.
2. The "+" sign will toggle bewtween + and - which means to include/exclude the region within respectively.
3. The 4 arrow marks are as follows: 2 for raising/lowering the max scale, 2 for raising/lowering the min scale.
4. Or one could click on the colormap next to "Pan" to manually define the color scale for the image.
5. **Open** is to load an existing mask file (.mat), one could load an existing mask from a file and add or remove regions.This is convenient to remove streaks from the scattering that are more random on some sample spots.
6. **Circle** icon will let you draw a circle by clicking on 3 (min) or more points along a best guess circumference. This can be combined with the + and -.
7. Start masking by clicking on the **Play** button and end by clicking on **Pause.** You can continue to make contiguous or disjointed regions by combining **Play** and Pause after each block of clicks. Zoom can be combined with drawing mask to seek more clarity.
8. At any point, the **Clear** icon (2nd right) will erase and you can start over with no issue.
9. When finished, it is time to save the mask. This has 2 steps.
10. Left **Save** button saves the mask as a logical matrix to a .mat file with 1 for included pixels and 0 for excluded pixels. This step is optional but highly recommended.
11. Right **Save** button saves the mask matrix to the workspace and **this is a must else the mask will not be inlcuded in the qmap and the entire procedure is a waste**.
12. The **mask icon** at the right end shows the mask you have drawn and is good to check.

Show Blemish will display the known bad regions which come from the software database. This gets automatically included on top of the drawn mask.

Selecting Q/Phi Partitions for the Analysis:

This is not described exhautively below. I would rely on the staff describing the concepts rather than a bunch of lines describing it.

But, basically, there are 2 Maps, naively one is for Static and the other is for Dynamics.

For transmission, (q and phi) are the maps used.

For reflection, (qr and qz) or (qy and qz) are typically used.

It is a MUST to select the ratio of (# in Map 1 / # in Map 2) to be an integer for both Static and Dynamics.

Typical thumb rule is to pick this integer to be some where between 5 and 10.

Note: The spacing in q/phi can be selected to be linear/log as well, will help with coarser binning at higher q where signal is weaker.

Concept:

During correlation analysis, individual pixels are correlated with itself as a function of time. Let us call this as G2 and is of the size of the image array.

Then during the **first normalization step**, G2 from the pixels that belong to the Static partition (Map 1) are averaged together and normalized by the time averaged intensities

over the group of pixels in Map 1. Please note that each bin in Map 2 comprises of integral number of bins in Map 1. In the **second normalization step**, the sub-averages from the first step are further averaged to give you the final g2 as specified in Map 2.

Note: It is also possible and useful in some cases to pick q/phi anisotropic bins for Map 1 and isotropic q/phi=1 bins for Map 2. One example is a case where the structure might be anisotropic and the dynamics could be isotropic.

Saving Qmaps:

On the right side of the Analysis & Display Settings screen, a place to enter the qmap name is provided.

Users are encouraged to follow a standard as the qmaps are saved in a common location for all users.

Suggested template: PIlastname201801_qmap_******_Lq0_****

PI last name and year and cycle (which should be the main user data folder) and qmap is highly recommended.

The q location is another useful part to have in the name to quickly identify.

Users are welcome to add their sample details and other things as they find it to be helpful to them.

The location where it gets saved is shown below (highlighted in yellow) and this comes from software initialization (loadMetaData.m)

Click on Apply and then Click on "Save map to .h5 file" (which is a .hdf file)

Once it is done, you can click on "View map from .h5 file" to see the qmap.

Note: It is a good idea to view the map to make sure the mask was taken into consideration for example and to check for other aspects.

Running the job:

The GUI functionality stops here as the job running is handled by the scripts.

Typically, there are 3 files that handle the analysis of multitau and two time:

conrad201711_batchmode_XPCS_Job_Creation.m (multitau on the cluster)

Multitau_LocalProcessing_hdf_Template.m (multitau on the local machine)

Twotime_hdf_Template.m (two time on the local machine)