

New features, 2018-2 run

General

Our administrative assistant, Sheila Trznadel has been replaced by Kristin Ahrens, kahrens@anl.gov, Tel: (630)252-0662, Fax: (630)252-0667.

Sample automounter

Both the IDD and IDB beamlines are now equipped with 18-puck capacity automounters. Download the appropriate template if you are filling in the spreadsheet prior to your beamtime. Rigaku pucks are not accepted at this time.

Resuming a paused data collection

If the image collection with EIGER detector was paused in the Collect or Raster tabs, it can be resumed. The last frame of the initial collection will be moved to an .overwrite subdirectory of the collect directory.

If a collect or raster run is started from the beginning with an existing filename and directory, the existing images will be overwritten instead of moving to the .overwrite directory.

Spotfinders

Each of the spotfinder programs, DOZOR, DIALS and DISTL, have their own output, instead of a common, “standardized” results table. By their own defaults, DOZOR will output its score, DIALS – the ice ring-corrected spots total and DISTL – to Bragg candidates total. As a result, the Spotfinder graph and the raster heat map may vary, depending on which sportfiner program is being used.

Raster

Configuration for DIALS is implemented and that for DISTL is updated (simplified). There is a new Test button allowing to see the effects of changed configuration. DOZOR configuration cannot be changed at the moment.

If a non-zero angle is selected as “delta” in a raster run, the sample will rotate within selected delta for each row in a “helical”, shutterless mode. Center of each row will fall at the same omega angle. Shuttered raster is still available by disabling the shutterless mode in the control panel. In this case, each frame will have same start and end rotation angles.

One-click sample rotation by +/-90° is added to the raster tab

Viewing diffraction images

Preferred image server can be selected for automated image display in JBlulce. The choices are the SSRL server (old style) and Small Spots server.

In the image, displayed with the Small Spots option, scroll button of the mouse changes the zoom. The degree of binning in the small spot will vary with the zoom.

Data processing

Analysis beta was renamed AnalysisNG. The results for the Analysis pipelines are located under process/analysis/, while processing results for AnalysisNG pipelines are located at process/analysisNG/. The right-click context menu was largely duplicated at the bottom. The terminal button now can open a new Terminal to the directory where the viewing content is

located.

AnalysisNG has added the ability to recursively parse directories for images. As a result, gmcaproc, xia2, autoPROC can handle multiple crystal data processing.

A new pipeline KAMO, developed at Spring-8, was added. This pipeline manages processing of data from tens and 100s of crystals using XDS, DIALS and BLEND. This utility is only available through the reprocessing function (i.e. it must be launched manually).

Remote access

All NX servers changed their names from bIXwsY.gmca.aps.anl.gov to bIXwsY-gmca.aps.anl.gov. Any existing scripts and NX sessions must be updated accordingly. It is best to re-download the NX session files from Table-2 of <https://www.gmca.aps.anl.gov/remote/>

NX players version 5 have been discontinued and cannot be used for remote login. Either the Webplayer or NX player version-6 can be used. Use of the most recent NX player will be encouraged by a popup note.

NOMACHINE discontinued installation of NX players via Java. If the player-6 is going to be used for remote login, one can either download it from the NOMACHINE website (and install) or download a portable version-6 player from the GMCA website (and then unpack).

Reminder

The energy range of the IDD beamline is restricted to 9.36 – 18.4 KeV. Flux is similar to last run.

Important changes for the upcoming 2018-3 run cycle

Starting from the 2018-3 run cycle, the remote ssh access will be disabled by the APS. As a result, only Webplayer will be used for remote login, while Globus will have to be used for on-line data transfer as sftp/scp will no longer work.