

New features in data collection and beamline controls

As of June 1, 2013

General

- To streamline data backup, the default directory within JBluIce has changed from user home directory to a pre-set one. For example, the data collection date: /mnt/share1/username/23IDD_2013_07_31
- Directory fields now have two parts: default on the left (../) and user-defined in the middle and browse on the right.
- Hovering over “../” with mouse will show the explicit path and clicking on it will open that directory.
- All parameters of screening, raster, scanning, data collection and analysis will be stored in MySQL database.

Hutch tab:

Sample tab:

Screening tab/Sample automounter

- Non-editable current directory indicator is added under the directory selection field of the “Screening” tab.
- Stop button is added after auto-centering.

Raster tab:

- Diffraction images, corresponding to the selected raster cells can be displayed.
- Default high resolution limit for the spot search during rastering is now updated whenever relevant motor positions are changed. This resolution corresponds to the detector edge but can be manually overridden.
- The “Fix” button is added to prevent resolution updates.
- A PNG snapshot is saved automatically after completion of each raster job.
- A PNG snapshot can be saved manually as well from the right-click menu. If the dialogue is cancelled, the snapshot will be still saved with a defaults name – same as in previous bullet item.

Collect and Analysis tabs:

- A beta version of multi-crystal data collection is added. Best data collection angles for the current crystal will be calculated based on the available partial data. Currently this tool can utilize only XDS.
- Intermediate processing results (first 5 frame, first 10 frames etc) are saved in separate directories. “Image Set:” selection in the “Analysis” tab allows the data statistics table and the plots to be updated for specific data set.
- In-house wrapper for automated data processing is being developed and can be selected as GMCAProc from the Tools/Options menu.
- If GMCAProc is selected while processing “inverse beam” data, or data from multiple sites of the same crystal, the crystal orientation matrix for the first set is used as a reference for all subsequent sets.

- If another client becomes master by force, collection will be paused. To resume data collection, “become master by force” and then click “Collect”.
- JBluIce instance, currently collecting data, is not allowed to close, or to become “passive”
- If JBluIce crashed while collecting data, upon restart it will automatically become master and will pause data collection.

Scan tab:

- Previous scan files (BIP) can be loaded back in to JBluIce from the File pull-down menu.
- After completion of the edge scan, the f' and f'' values, along with energies, are printed on the image.