

## **New features in data collection and beamline controls As of June 4, 2012**

### **General**

- PSS panel and the search boxes have changed
- Cancel option was added to the JBluIce startup screen
- The file name and directory dialogs have changed
- The ring light will turn on when images are being collected and will turn off when collection is completed
- The “+” and “-“ buttons on the diffraction image viewer will display the “next” and “previous” images even if their numbers are not adjacent
- From the Options pull-down menu, BEST or MOSFLM can be selected for strategy

### **Hutch tab**

- Pull-down arrows replaced the “A” buttons for stopping the motors. They will be replaced later with stop signs

### **Screening tab**

- Has moved in front of the Collect tab

### **Sample tab**

- Point-and-click works only with left click
- Point and click move undo/redo menu option is added

### **Raster tab:**

- Resolution limit selection is added to both Interactive and Auto raster tabs
- In Auto mode, the search polygons can be set up automatically, or semi-automatically to match the mounted loop
- When the sample is unmounted, all raster-related information is deleted after a prompt. This can be turned on or off for the robot-unmounted samples from the menu option
- Once rastering job starts, the “Start” button changes into “Resume”
- Display option check boxes have been replaced by toggle buttons
- Site centering buttons have been replaced by an option in the right click menu
- Results from interactive raster runs can be added to the site list with right click
- The site naming convention has changed. For example, AF3O2 would mean that the site came from Auto mode, fine-step raster job number 3, 2<sup>nd</sup> hit from the run in orthogonal plane. Right click on the site explains the site name
- Collect runs can be created for specific raster sites from right-click menu
- Multiple raster sites can be selected for passing to the Collect tab by CTRL + right click
- “A” is added to file name prefix in the Auto mode
- Reliability of the Auto raster results has been improved
- Color map can be hidden in fluorescence raster
- Fluorescence raster log is now written, similar to diffraction raster

- Right click on the raster video allows the image to be saved, including the color maps and any other overlays

**Collect tab:**

- A raster site can be chosen in the 0 tab
- Beamstop distance has been removed from the Collect tab
- Beam size is added to the Collect tab. The values are constrained to actual achievable size (5 $\mu$ m minimum and  $\pm 3\sigma$  maximum)
- When the sample is unmounted, all raster- and vector-related information is deleted. This feature can be turned on or off for the robot-unmounted samples from the menu option
- Raster or vector sites can be double-clicked to center
- “Select all” and “Select none” buttons have been added to the vector site setup
- The “Export strategy to current run” button is added
- Run sequence filename column resizes to display the whole file name
- Diffraction images have finer contrast control at lower values

**Scan:**

- Fluorescence spectrum plot shows vertical bars based on the selected elements
- Colors are slightly varied for multiple edges of the same element
- “Show all” button will display the edges of all elemental listed under the plot
- For overlapping edges, the nearby edge can be identified by hovering over with the mouse
- Zooming in can be done by left click-and-drag
- Right click offers menu of options, including zoom out, print, etc
- Chooch selection can be changed by dragging the corresponding bars and restored by clicking the “Defaults” button

**Analysis tab:**

This is a new tab. When auto-processing is selected in the Collect tab, data will be processed with XDS, POINTLESS, SCALA and TRUNCATE. Results will be displayed in this tab. Full log files can be displayed by clicking appropriate buttons