

## **New features in data collection and beamline controls As of Feb 6, 2012**

### **Raster tab:**

- In auto mode, the list of found and centered sites is passed to collect tab

### **Collect tab:**

- Collect User Interface has been redesigned substantially
- Collect tab diffraction viewer resizes to fill available space
- Run sequence table can be expanded (and restored to original size) by clicking the double arrows
- The Distance column in the run sequence table is replaced by Site Number
- Strategy
  - All possible space groups in the Labelit solution are displayed in strategy window
  - By default only the space groups within highest point group are processed initially
  - Multiple space groups are processed in parallel to increase the speed
  - User can choose lower symmetry solution, JBluice will process and display strategy
- Vector and Raster modes
  - Raster mode is added
  - Inverse beam geometry and multiple wavelength data collection now work with Vector and Raster modes
  - In Vector or Raster modes of data collection, given swath of data with inverse beam geometry or with multiple wavelengths is always measured from same sites
- XDS
  - XDS checkbox is changed to a dropdown with three choices: None, Native, Anomalous
  - When a failure “INSUFFICIENT PERCENTAGE of spots” is encountered, XDS runs second time to complete the integration of data.
  - XDS can process Anomalous data

### **Scan:**

- Chooch plot display is integrated into JBluIce. PDF is still available by double-clicking the plot.
- Edge scan adaptive mode option is added to the menu

### **Other:**

- There is a new GUI for starting the MAR software remotely
- In the “Help” pull-down menu, Selecting “Crystallographic Software” opens the web browser and displays clickable list of available software
- In the “Help” pull-down menu, Selecting “Video Tutorials” opens the web browser and displays clickable list of available tutorials
- Operating system has been upgraded to CentOS 6.2
- When external hard disk is mounted, the device name is assigned differently, not as /media/removable\*#