Auto-Raster: Unattended Diffraction-Based Sample Centering at GM/CA

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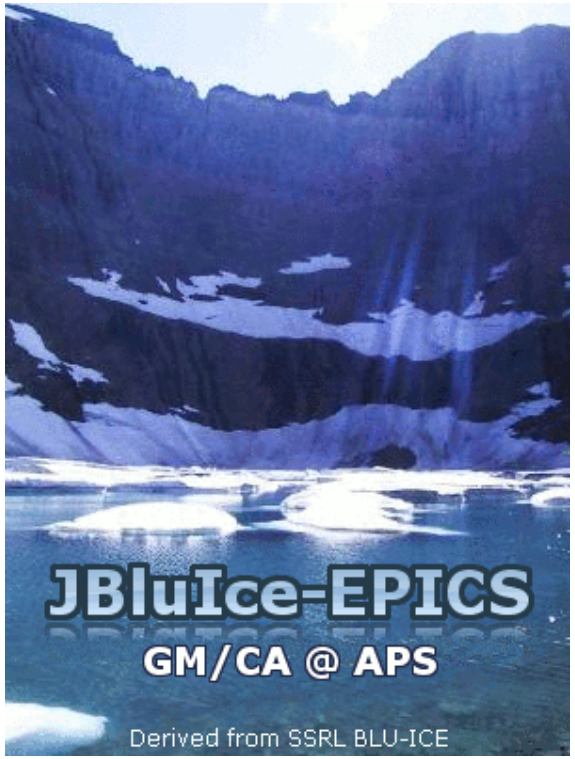
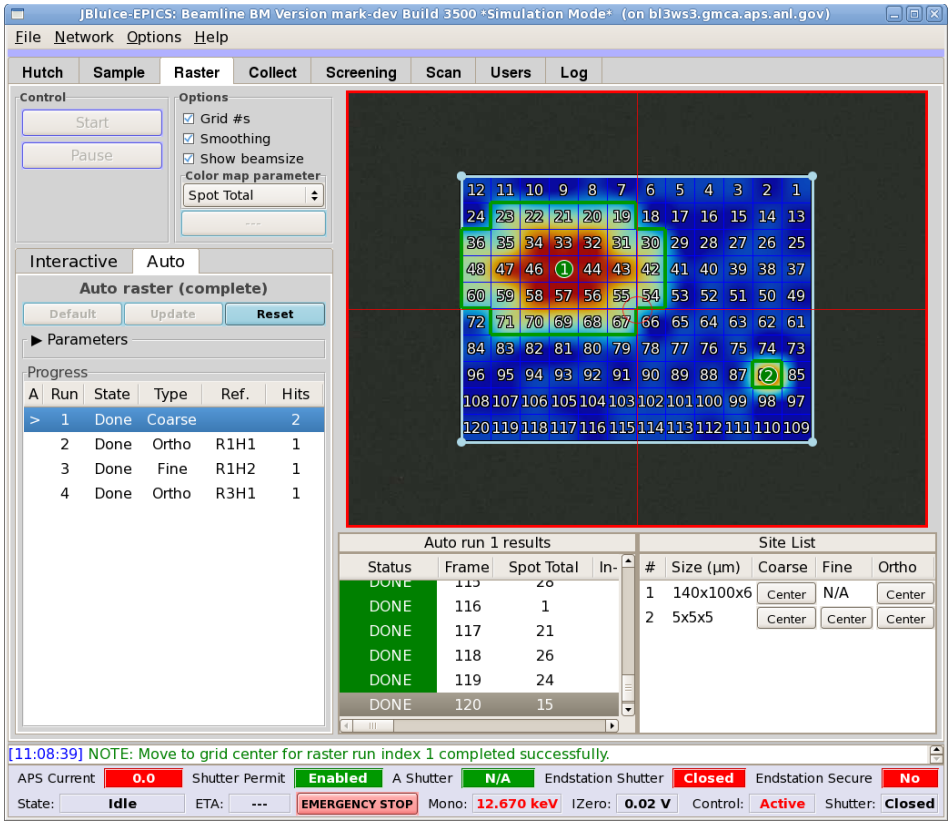
GM/CA@APS



Auto-Raster

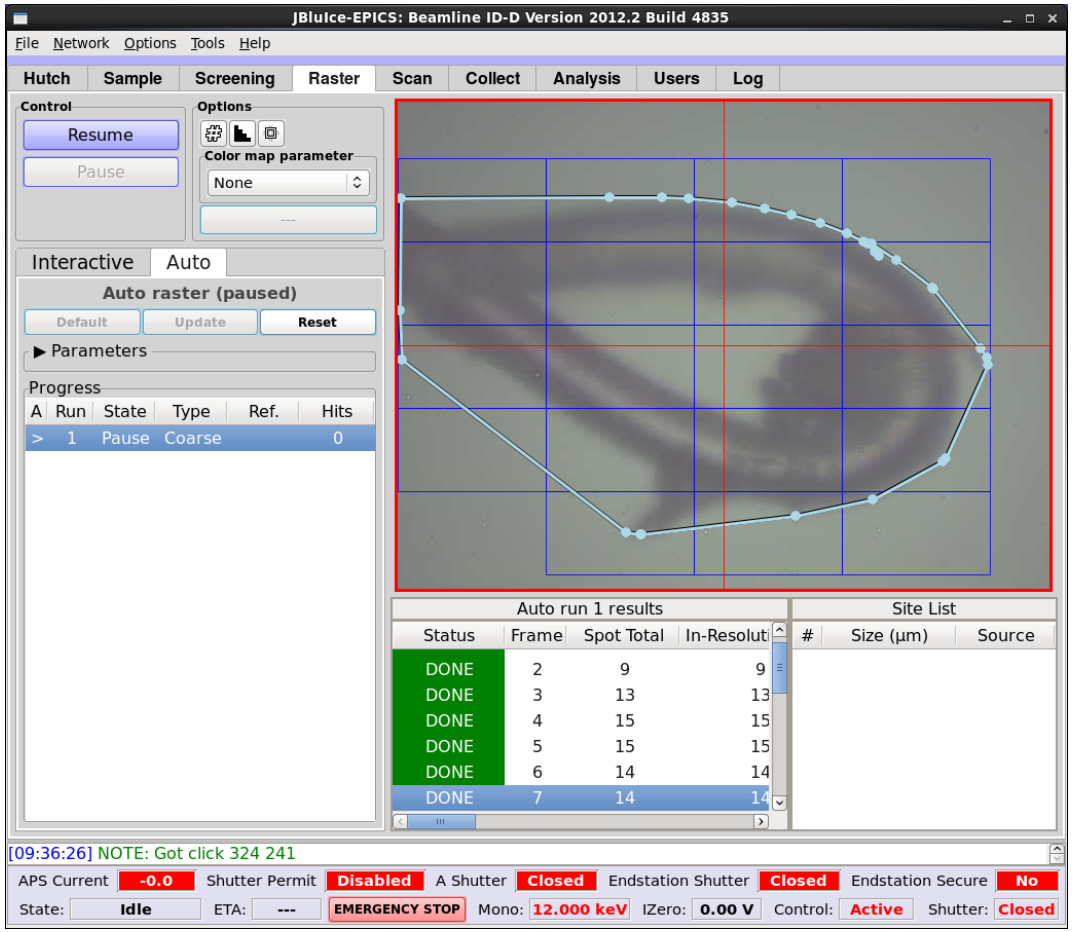
- Auto-Raster is a critical automation step, and also very difficult
  - Many different situations need to be handled
  - If full datasets are to be taken, the centering must be accurate so samples are not wasted
- Process:
  - Sample is **mounted** by a robot
  - Loop is optically **centered**
  - **Grid** is defined to cover the loop
  - **Diffraction** images taken at each cell
  - **Processing** results shown graphically
  - Algorithm sets up successive grid **searches**



Auto-Raster results in JBluIce-EPICS

Algorithm

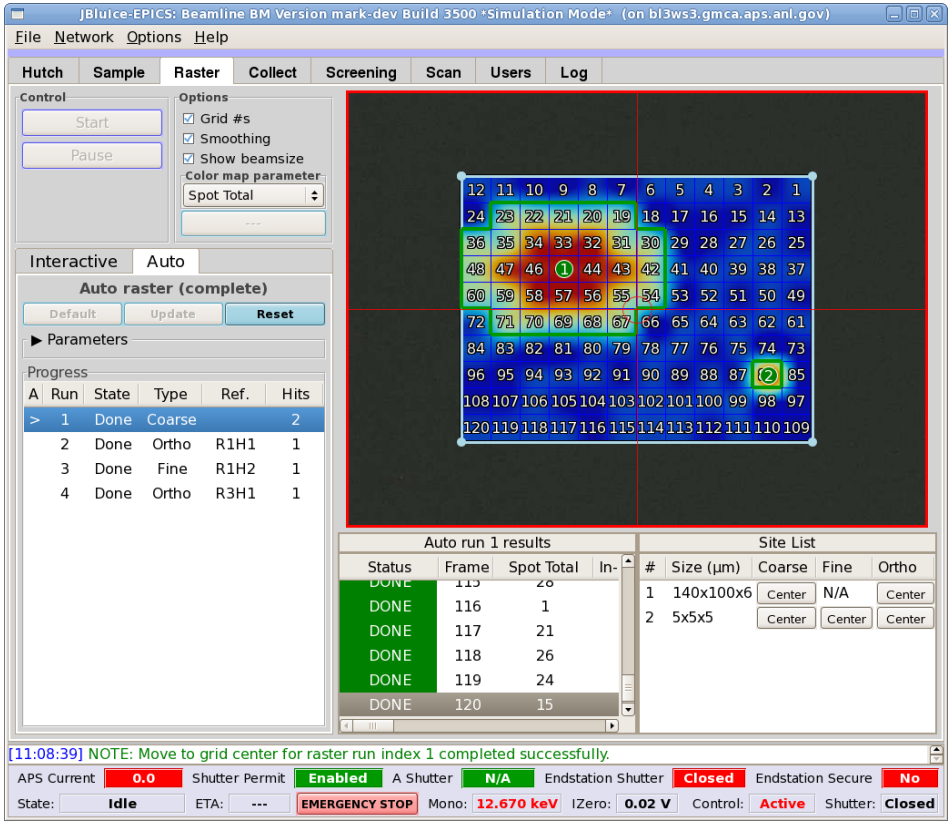
- Stage 1: AutoFind
  - XREC optically centers the loop in face-on orientation
  - XREC returns a polygon outline of the loop
- Stage 2: Coarse Grid
  - JBluIce fills the XREC-generated polygon with approximately 20 cells
  - An image is taken at each cell and processed with SpotFinder
  - Cells are ranked based on the number of potential Bragg candidates on that image minus a background number
  - Groups of cells are counted as a single "hit"



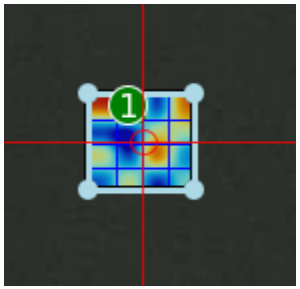
XREC-generated loop outline

Algorithm

- Stage 3: Fine Grid(s)
  - Individual cells from the coarse stage (those with no neighbors) are rastered with a fine beam of 5-20 microns
- Stage 4: Ortho Grid(s)
  - Hits from either the coarse or fine stage are then scanned in the orthogonal plane along a single column of cells
  - Hits from this stage generate 3D "sites" which can be passed to the collect tab
  - Multiple hits at this stage generate multiple sites, corresponding to the same cell from stages 2 or 3



Coarse grid: Two hits

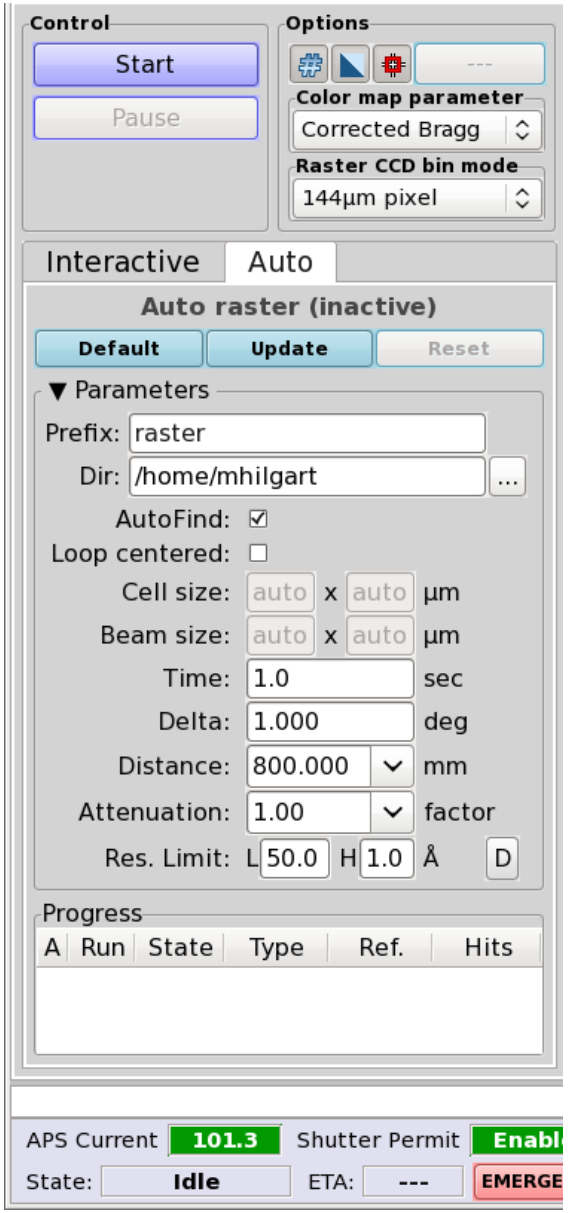


Fine grid: One hit

Ortho grid: One hit

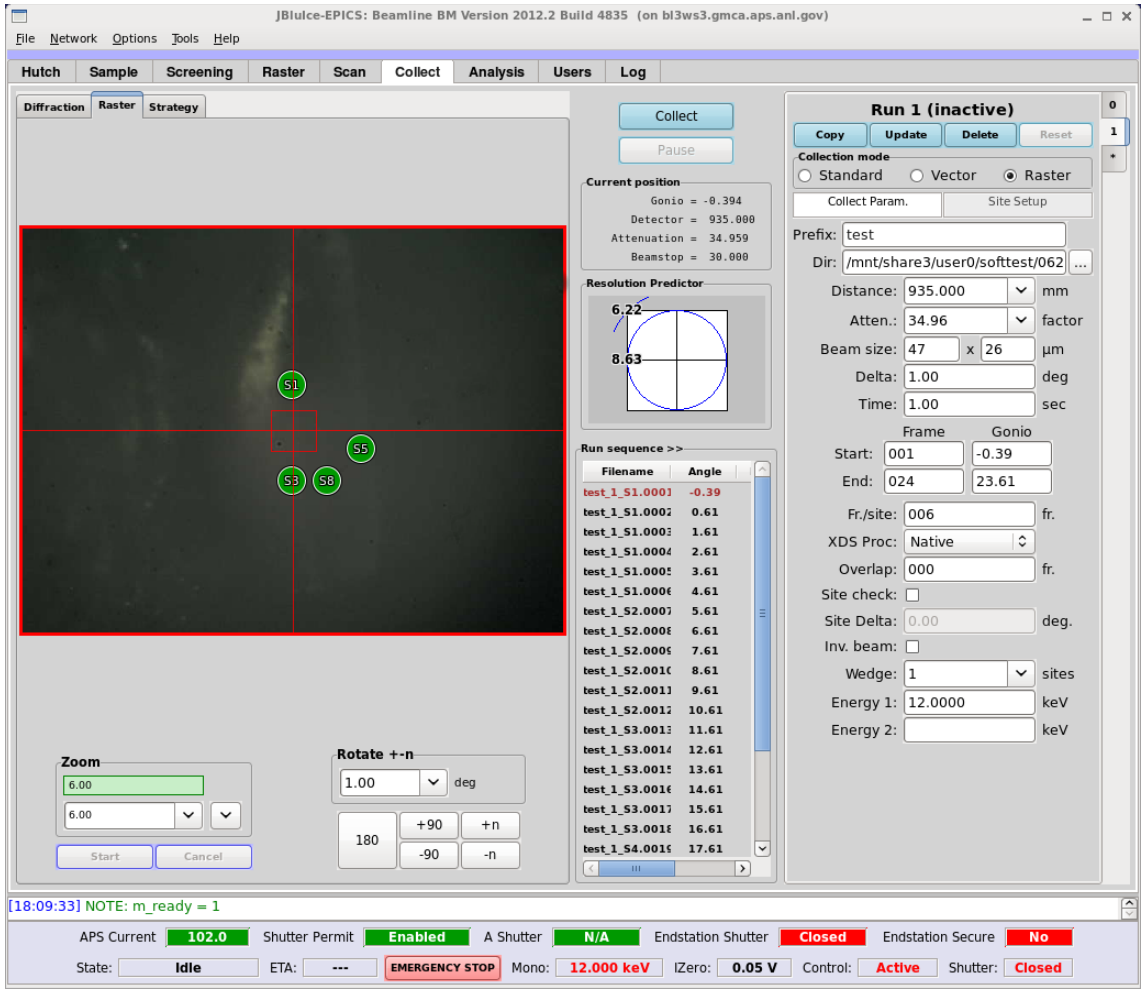
Auto-Raster GUI implementation

- One way to use Auto-Raster is to go directly to the Raster Tab and use the GUI shown at the right
- Auto-Raster is built on interactive raster
  - Interactive raster uses runs like in data collection
  - Runs each have their own collection parameters
  - Users set up each grid manually and then run a search
- Auto mode handles its own set of raster runs but simplifies this for the user
  - A single set of parameters is shown
  - There are some unique parameters to auto mode
    - AutoFind uses optical centering to find the loop and define the initial search outline
    - Resolution limits set the bounds for where to count spots
    - A progress tracker shows the history of grid searches and the results



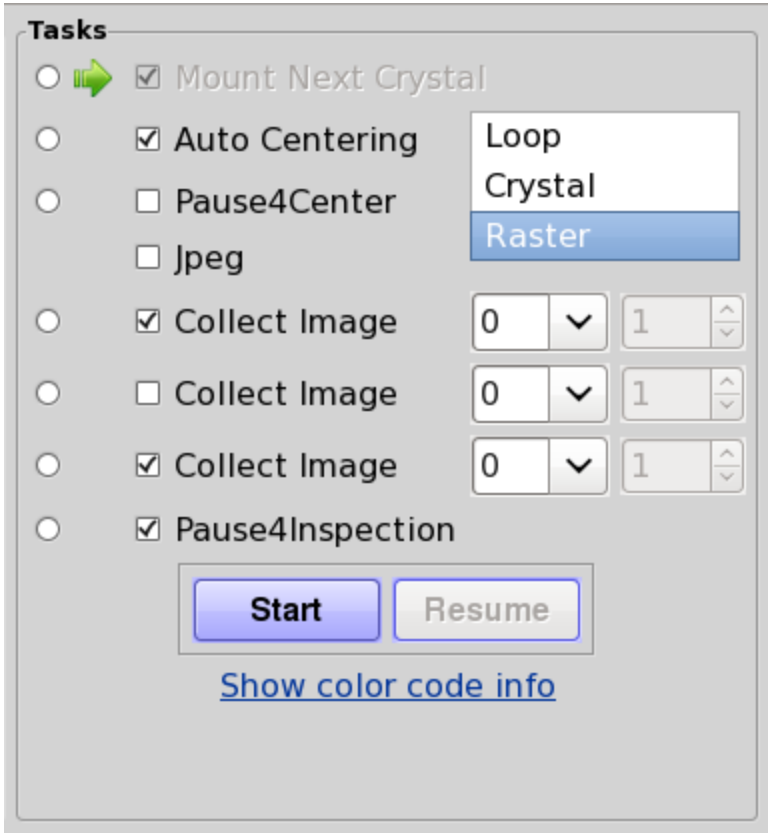
Auto-raster parameters

Auto-Raster GUI implementation



- Auto-Raster sites are sent automatically to the collect tab
  - Sites can be chosen for specific runs in each collect run tab

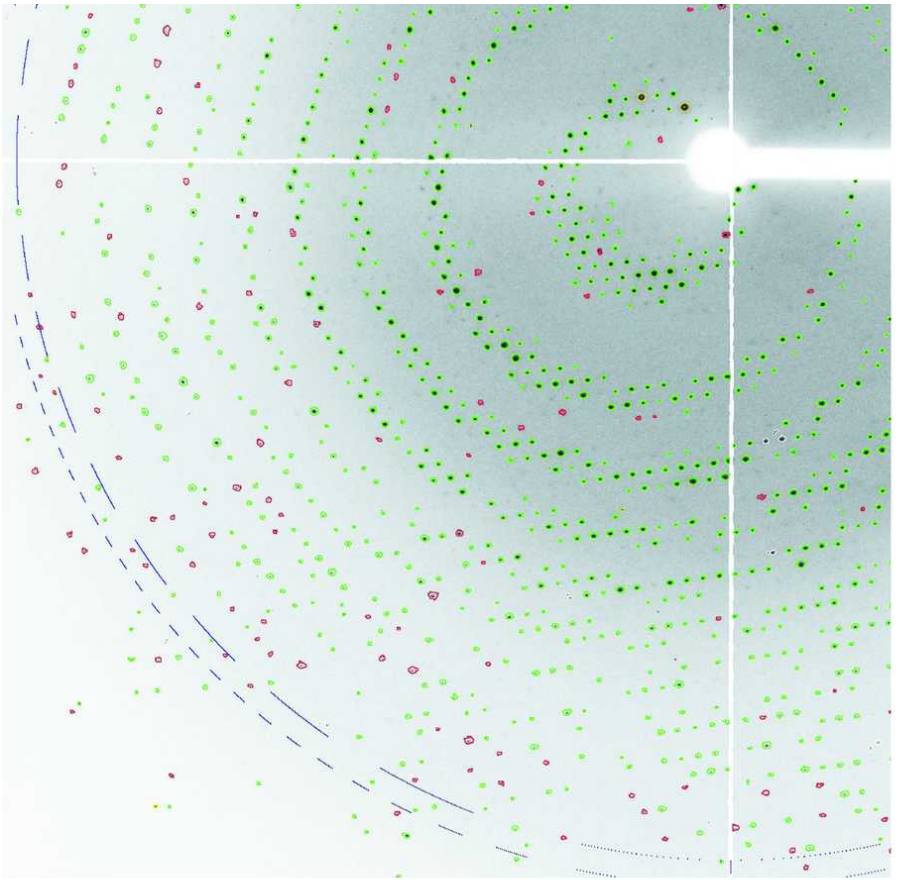
Auto-Raster GUI implementation



- Auto-Raster can be run as a centering method from the screening tab
  - Raster parameters are currently set in the raster tab, we may set defaults in the future
  - In unattended mode, data collection would follow directly after centering

Diffraction Image Analysis

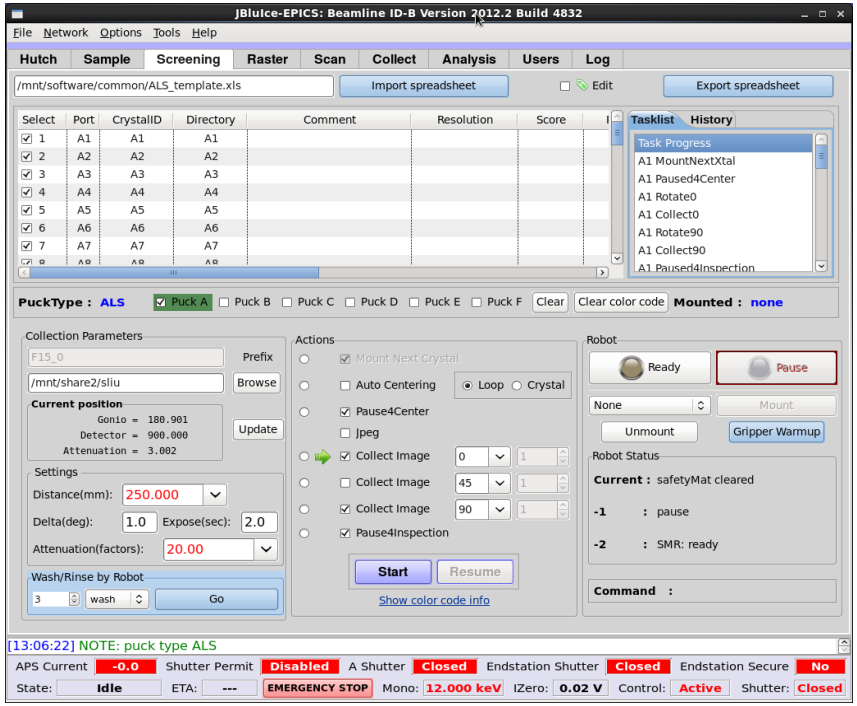
- Analysis is performed on single images, orthogonal image is not taken
- SpotFinder
  - Used at GM/CA, Diamond and SSRL for raster image analysis
  - Analyzes spots and detects ice rings
  - Claims to detect most crystal quality issues
  - Server processes images in parallel (200ms/ image)
- EDNA
  - Used by ESRF for raster image analysis
  - EDNA is a framework which pipelines MOSFLM, LabelIt, RADDOSE and BEST
  - Uses auto-indexing to detect when there are multiple lattices, a key advantage
  - Takes longer (5 seconds per image)



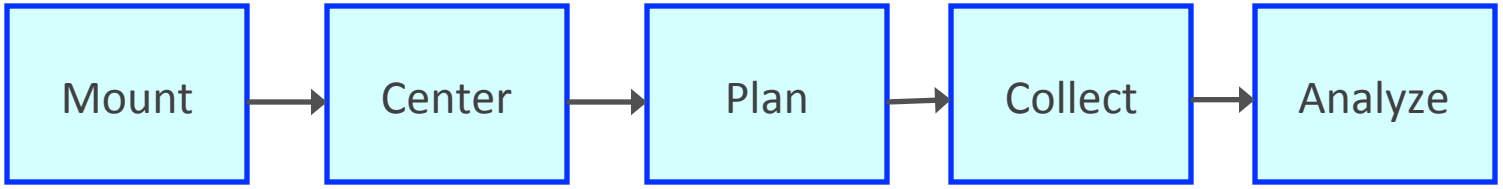
Example SpotFinder image:
Green: "good" quality
Red: multiple maxima

Lights-out Operation

- Goal: The user should interact with data acquisition only when necessary
- So we need to support
  - Zero interaction: all choices are made automatically
  - Up-front only interaction: Known parameters are entered before starting
  - Selective interaction: User intervenes only if they see something
  - Checkpoint interaction: Process stops at pre-determined tasks



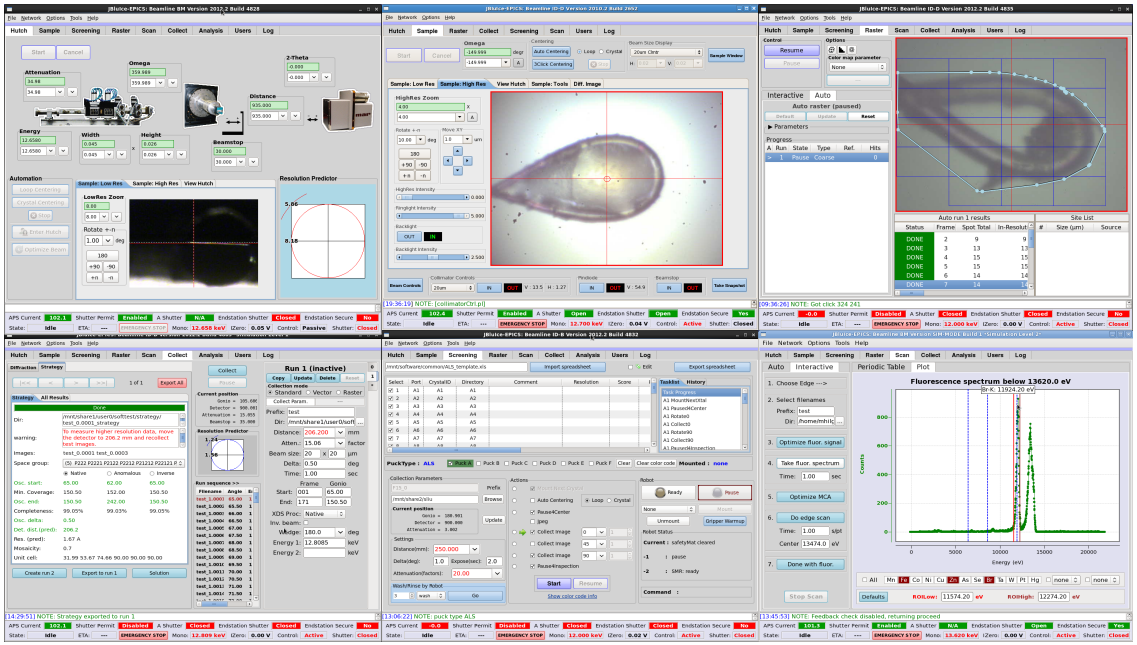
JBluIce Screening Tab: Central to lights-out mode



The data acquisition pipeline: All steps must be automated and linked

Conclusion

- Auto-Raster is a critical link in automation
- It is in the experimental phase now
  - Methods for image analysis are being evaluated for robustness
  - Whether indexing is necessary or not is an important question
- Data collection based on strategy also needs to be linked to screening
- With Auto-Raster and data collection as options on the screening tab, lights-out operation will become a supported mode for general use



JBluIce-EPICS

JBluIce Developers	EPICS Developers	Design Suggestions and Testing	Management
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