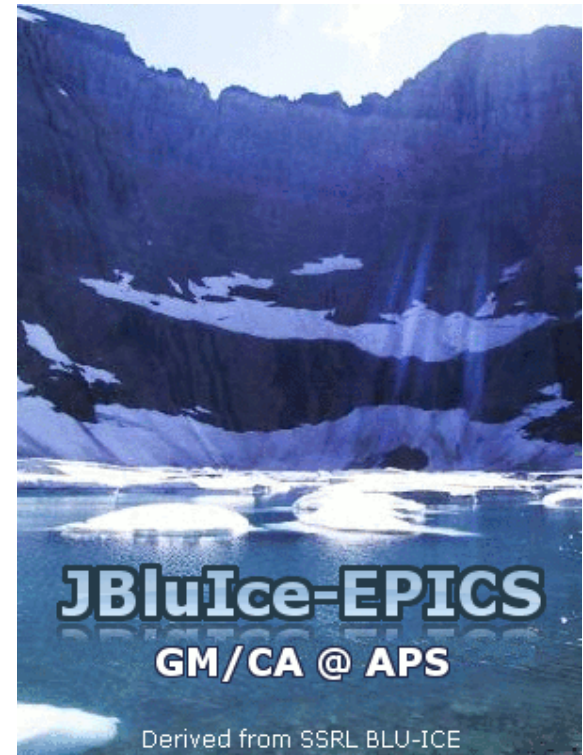


Auto-Raster: Unattended Diffraction-Based Sample Centering at GM/CA

Mark Hilgart, Ruslan Sanishvili, Sudhir Pothineni, Sergey Stepanov, Oleg Makarov, Nagarajan Venugopalan, Michael Becker, Craig Ogata and Robert F. Fischetti

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

The screenshot shows the JBlulce-EPICS software interface. The main window displays a 12x12 grid of data points with a color map. The grid is centered on a red spot, and the centering process is complete. The status bar shows 'EMERGENCY STOP' and 'Control: Active'.

A	Run	State	Type	Ref.	Hits
>	1	Done	Coarse		2
	2	Done	Ortho	R1H1	1
	3	Done	Fine	R1H2	1
	4	Done	Ortho	R3H1	1

Status	Frame	Spot Total	In-
DONE	115	20	
DONE	116	1	
DONE	117	21	
DONE	118	26	
DONE	119	24	
DONE	120	15	

#	Size (µm)	Coarse	Fine	Ortho
1	140x100x6	Center	N/A	Center
2	5x5x5	Center	Center	Center

[11:08:39] NOTE: Move to grid center for raster run index 1 completed successfully.

APS Current: 0.0 Shutter Permit: Enabled A Shutter: N/A Endstation Shutter: Closed Endstation Secure: No
 State: Idle ETA: --- EMERGENCY STOP Mono: 12.670 keV IZero: 0.02 V Control: Active Shutter: Closed

Auto-Raster results in JBlulce-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
 - JBlulce 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”

The screenshot shows the JBlulce-EPICS software interface. The main window displays a grayscale image of a sample with a blue polygon outline overlaid, representing the XREC-generated loop. The interface includes a menu bar (File, Network, Options, Tools, Help) and a toolbar with buttons for Resume, Pause, and Color map parameter. The Auto raster (paused) window is open, showing a grid of cells and a progress table.

Auto run 1 results					Site List		
Status	Frame	Spot Total	In-Resolut	#	Size (μm)	Source	
DONE	2	9	9				
DONE	3	13	13				
DONE	4	15	15				
DONE	5	15	15				
DONE	6	14	14				
DONE	7	14	14				

State: **Idle** APS Current: **-0.0** Shutter Permit: **Disabled** A Shutter: **Closed** Endstation Shutter: **Closed** Endstation Secure: **No** ETA: **---** **EMERGENCY STOP** Mono: **12.000 keV** IZero: **0.00 V** Control: **Active** Shutter: **Closed**

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

Auto raster (complete)

A	Run	State	Type	Ref.	Hits
>	1	Done	Coarse		2
	2	Done	Ortho	R1H1	1
	3	Done	Fine	R1H2	1
	4	Done	Ortho	R3H1	1

Auto run 1 results

Status	Frame	Spot Total	In-
DONE	115	20	
DONE	116	1	
DONE	117	21	
DONE	118	26	
DONE	119	24	
DONE	120	15	

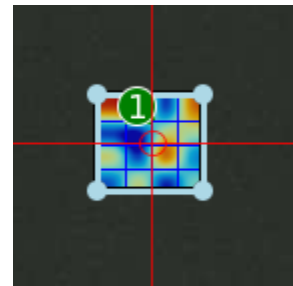
Site List

#	Size (µm)	Coarse	Fine	Ortho
1	140x100x6	Center	N/A	Center
2	5x5x5	Center	Center	Center

[11:08:39] NOTE: Move to grid center for raster run index 1 completed successfully.

APS Current: 0.0 Shutter Permit: Enabled A Shutter: N/A Endstation Shutter: Closed Endstation Secure: No
 State: Idle ETA: ... EMERGENCY STOP Mono: 12.670 keV IZero: 0.02 V Control: Active Shutter: Closed

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

The screenshot displays the Auto-Raster GUI interface. At the top left, there are 'Control' buttons for 'Start' and 'Pause'. To the right, the 'Options' section includes a 'Color map parameter' dropdown set to 'Corrected Bragg' and a 'Raster CCD bin mode' dropdown set to '144µm pixel'. Below these are tabs for 'Interactive' and 'Auto', with the 'Auto' tab selected. The main panel is titled 'Auto raster (inactive)' and contains sub-tabs for 'Default', 'Update', and 'Reset'. Under the 'Parameters' section, the following settings are visible: Prefix: raster; Dir: /home/mhilgart; AutoFind: checked; Loop centered: unchecked; Cell size: auto x auto µm; Beam size: auto x auto µm; Time: 1.0 sec; Delta: 1.000 deg; Distance: 800.000 mm; Attenuation: 1.00 factor; Res. Limit: L 50.0 H 1.0 Å D. A 'Progress' table is located below the parameters, with columns for A, Run, State, Type, Ref., and Hits. At the bottom of the GUI, there are status indicators: APS Current (101.3), Shutter Permit (Enabl), State (Idle), and ETA (---). A red 'EMERGE' button is also present.

Auto-raster parameters

Auto-Raster GUI implementation

The screenshot displays the JBIluce-EPICS Beamline BM Version 2012.2 GUI. The main window is titled "JBIluce-EPICS: Beamline BM Version 2012.2 Build 4835 (on bl3ws3.gmca.aps.anl.gov)". The menu bar includes File, Network, Options, Tools, and Help. The main toolbar contains buttons for Hutch, Sample, Screening, Raster, Scan, Collect, Analysis, Users, and Log. The "Raster" tab is active, showing a diffraction image with a red box highlighting a region. The "Run 1 (inactive)" panel on the right includes buttons for Collect, Pause, Copy, Update, Delete, and Reset. The "Collection mode" is set to Raster. The "Run sequence" table is visible, listing filenames and angles. The status bar at the bottom shows various system parameters and their states.

Filename	Angle
test_1_51.0001	-0.39
test_1_51.0002	0.61
test_1_51.0003	1.61
test_1_51.0004	2.61
test_1_51.0005	3.61
test_1_51.0006	4.61
test_1_52.0007	5.61
test_1_52.0008	6.61
test_1_52.0009	7.61
test_1_52.0010	8.61
test_1_52.0011	9.61
test_1_52.0012	10.61
test_1_53.0013	11.61
test_1_53.0014	12.61
test_1_53.0015	13.61
test_1_53.0016	14.61
test_1_53.0017	15.61
test_1_53.0018	16.61
test_1_54.0019	17.61

Current position:
Gonio = -0.394
Detector = 935.000
Attenuation = 34.959
Beamstop = 30.000

Resolution Predictor:
6.22
8.63

Run sequence >>>

Zoom: 6.00
Rotate +-n: 1.00 deg
180 +90 +n -90 -n

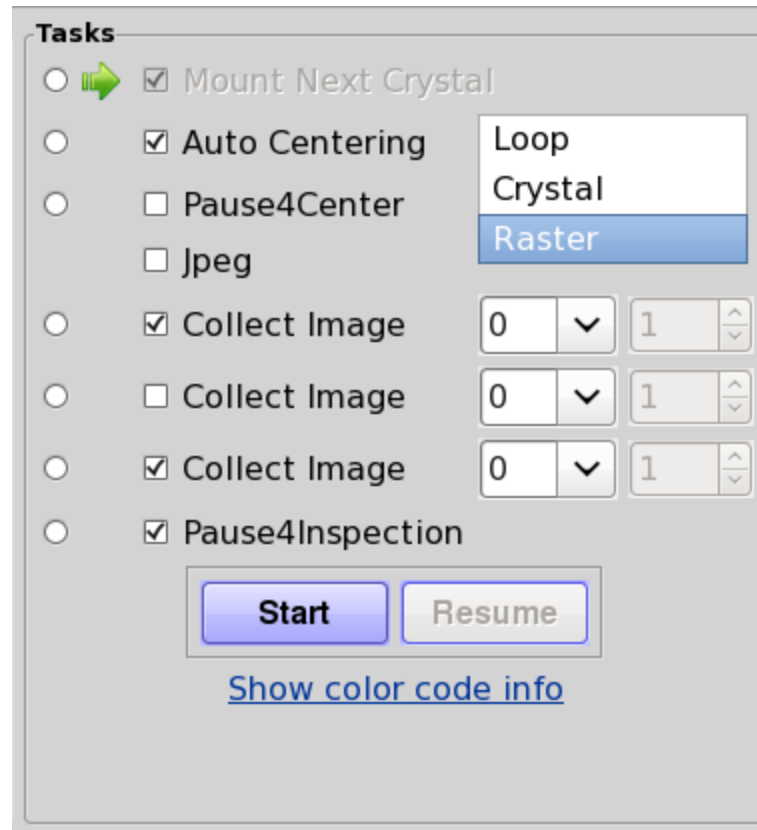
Run 1 (inactive)
Collection mode: Standard Vector Raster
Prefix: test
Dir: /mnt/share3/user0/softtest/062
Distance: 935.000 mm
Atten.: 34.96 factor
Beam size: 47 x 26 µm
Delta: 1.00 deg
Time: 1.00 sec
Start: 001 -0.39
End: 024 23.61
Fr./site: 006 fr.
XDS Proc: Native
Overlap: 000 fr.
Site check:
Site Delta: 0.00 deg.
Inv. beam:
Wedge: 1 sites
Energy 1: 12.0000 keV
Energy 2: keV

[18:09:33] NOTE: m_ready = 1

APS Current: 102.0 Shutter Permit: Enabled A Shutter: N/A Endstation Shutter: Closed Endstation Secure: No
State: Idle ETA: --- EMERGENCY STOP Mono: 12.000 keV IZero: 0.05 V Control: Active Shutter: Closed

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

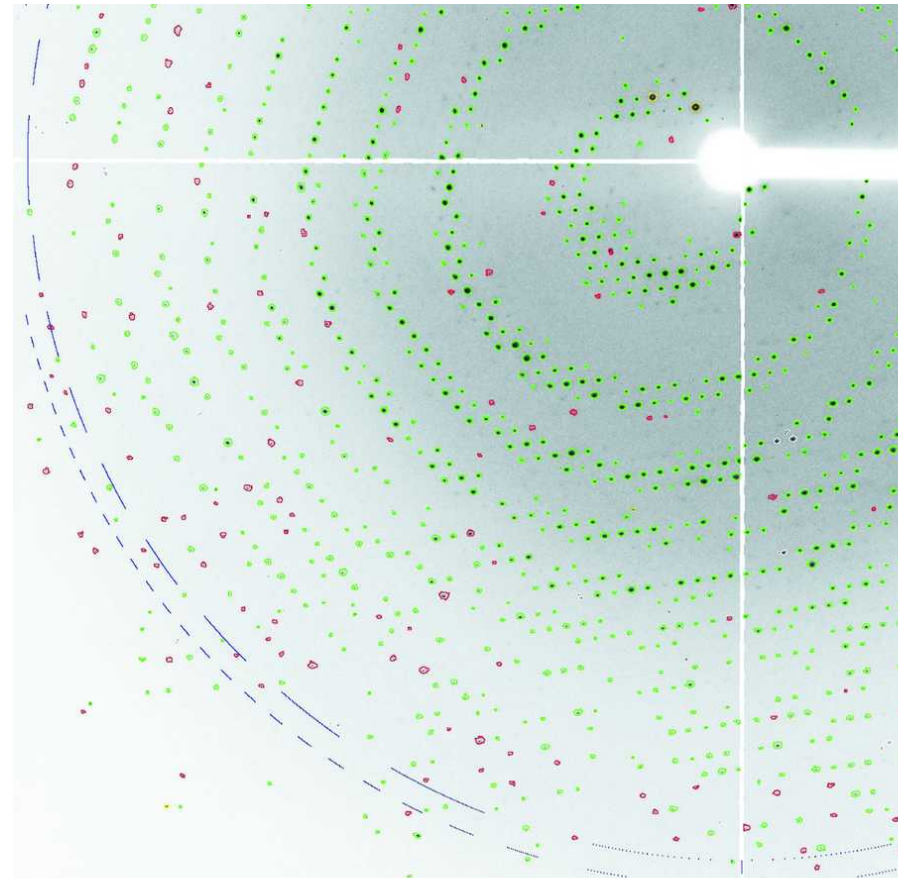
Auto-Raster GUI implementation



- 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

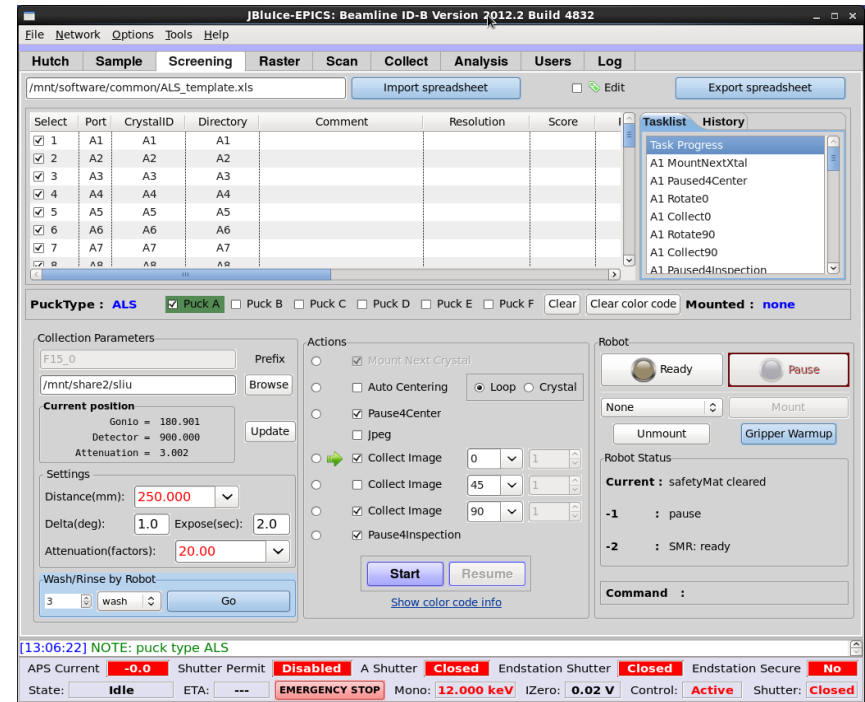
- Analysis is performed on single images, orthogonal image is not taken
- SpotFinder
 - Used at GM/CA, Diamond and SSRL for raster image analysis
 - Analyzes spots and detects ice rings
 - Claims to detect most crystal quality issues
 - Server processes images in parallel (200ms/image)
- EDNA
 - Used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



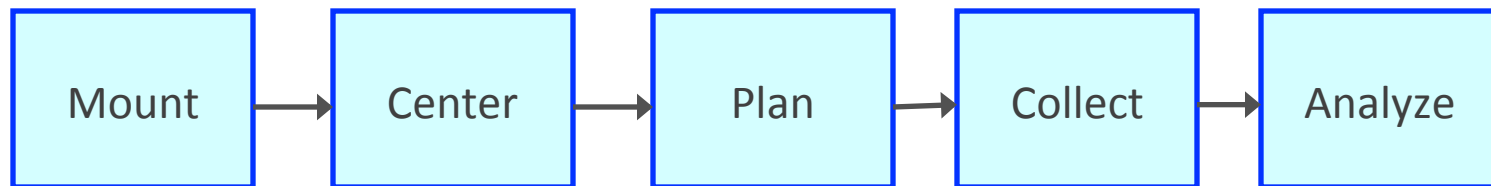
Example SpotFinder image:
Green: “good” quality
Red: multiple maxima

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



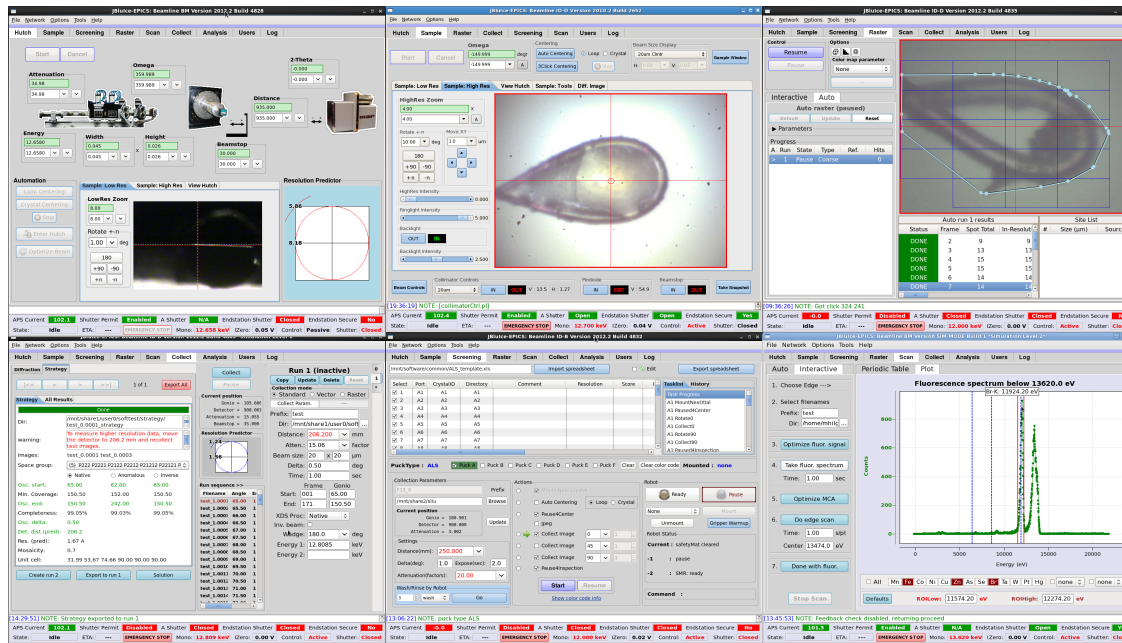
JBluice Screening Tab: Central to lights-out mode



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



JBlulce-EPICS

JBlulce Developers

EPICS Developers

Design Suggestions
and Testing

Management

Mark Hilgart
Sudhir Pothineni

Sergey Stepanov
Oleg Makarov

Craig Ogata
Ruslan Sanishvili
Michael Becker
Nagarajan Venugopalan

Janet Smith
Robert Fischetti