

PAUL SCHERRER INSTITUT



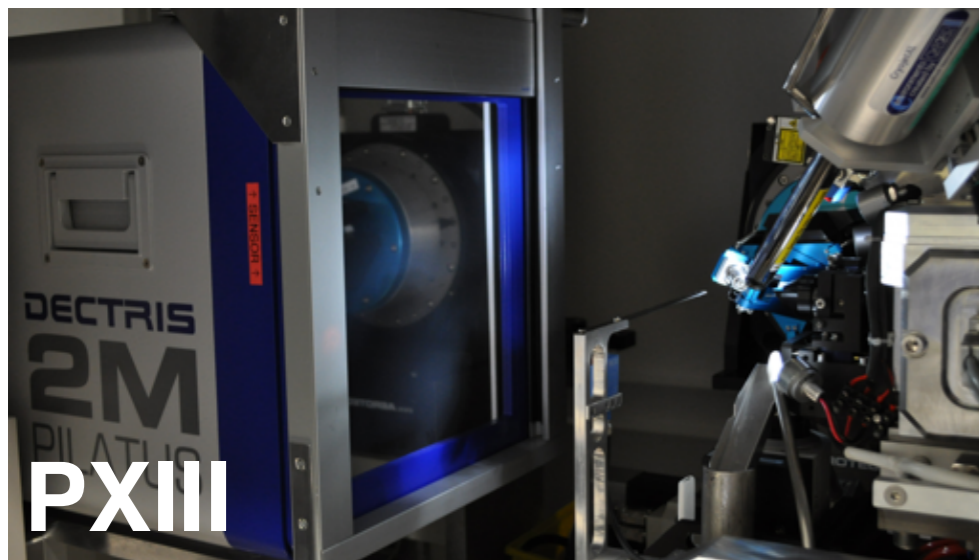
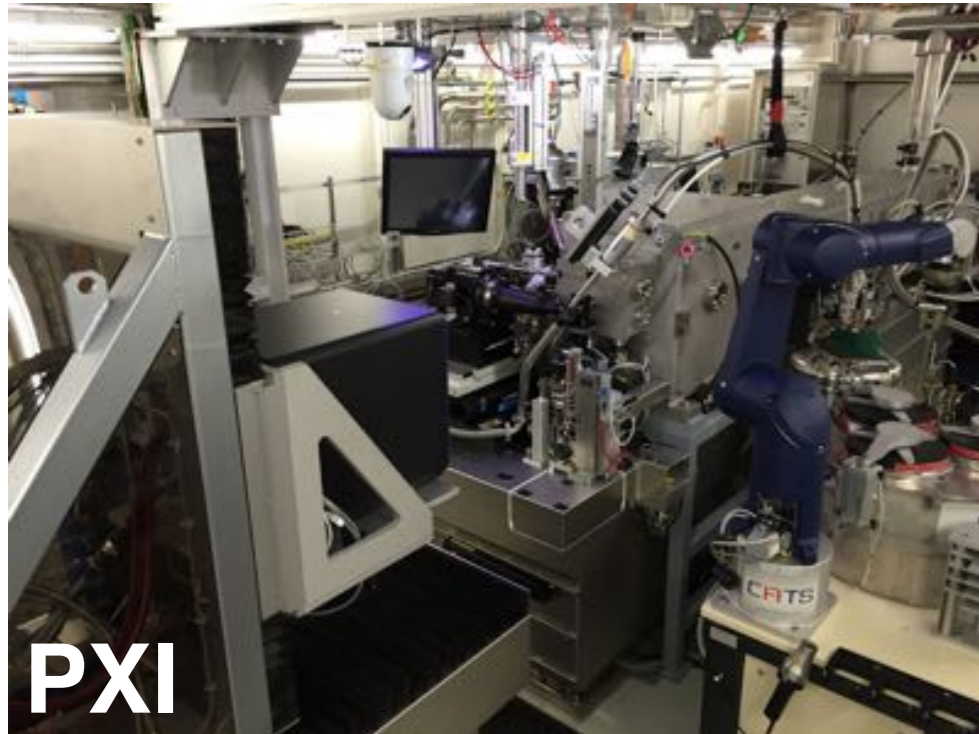
Justyna A. Wojdyla :: Beamline scientist :: Industry Liaison Scientist :: Paul Scherrer Institute

Data acquisition and analysis software at the SLS MX beamlines

MXCube/ISPyB meeting, 12th of March 2019, Lund, Sweden

SLS MX beamlines

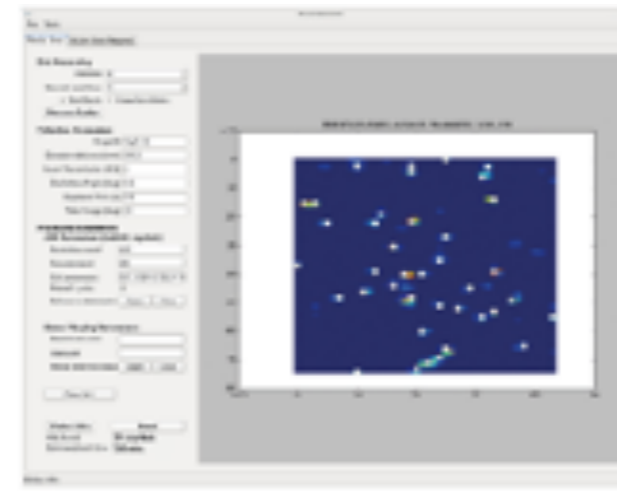
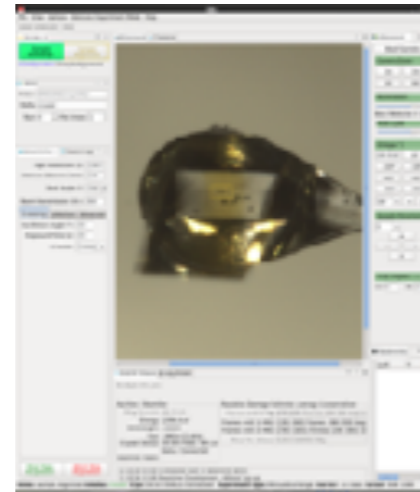
- 10 beamline partners & > 20 regular industry customers
- **6000 PDBs**



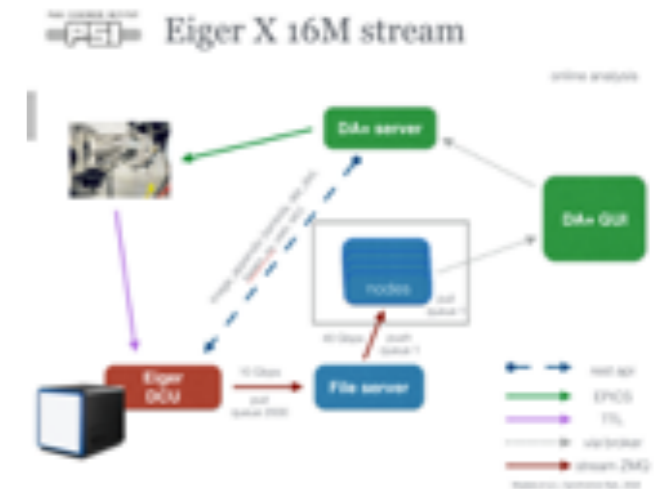
	PXI (X06SA)	PXII (X10SA)	PXIII (X06DA)
Wavelength range [Å]	0.7 - 2.2	0.62 - 2.07	0.71 - 2.07
Source	in-vacuum undulator	in-vacuum undulator	bending magnet
Spectral range	5.7 - 17.5	6.0 - 20.0	6.0 - 17.5
Flux at 12.4 keV [ph/s]	$> 2 \times 10^{12}$	$> 2 \times 10^{12}$	5×10^{11}
Focused spot size h x v [μm^2]	5 x 5 (2 x 1) -> 100 x 100	73 x 16	80 x 45
Detector	EIGER 16M	PILATUS 6M -> EIGER 16M	PILATUS 2M-F
Frame rates [Hz]	133 750 (4M ROI)	25	60
Goniometer	single-axis	single-axis	multi-axis PRIGo
Robot & pucks	TELL Unipucks	CATS Spinepucks	CATS Spinepucks

MX in-house software development

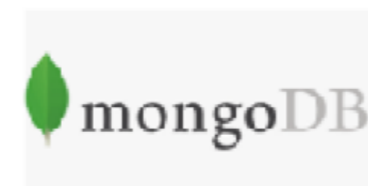
- robust, intuitive & user-friendly



- allows exploitation of latest instrumentation



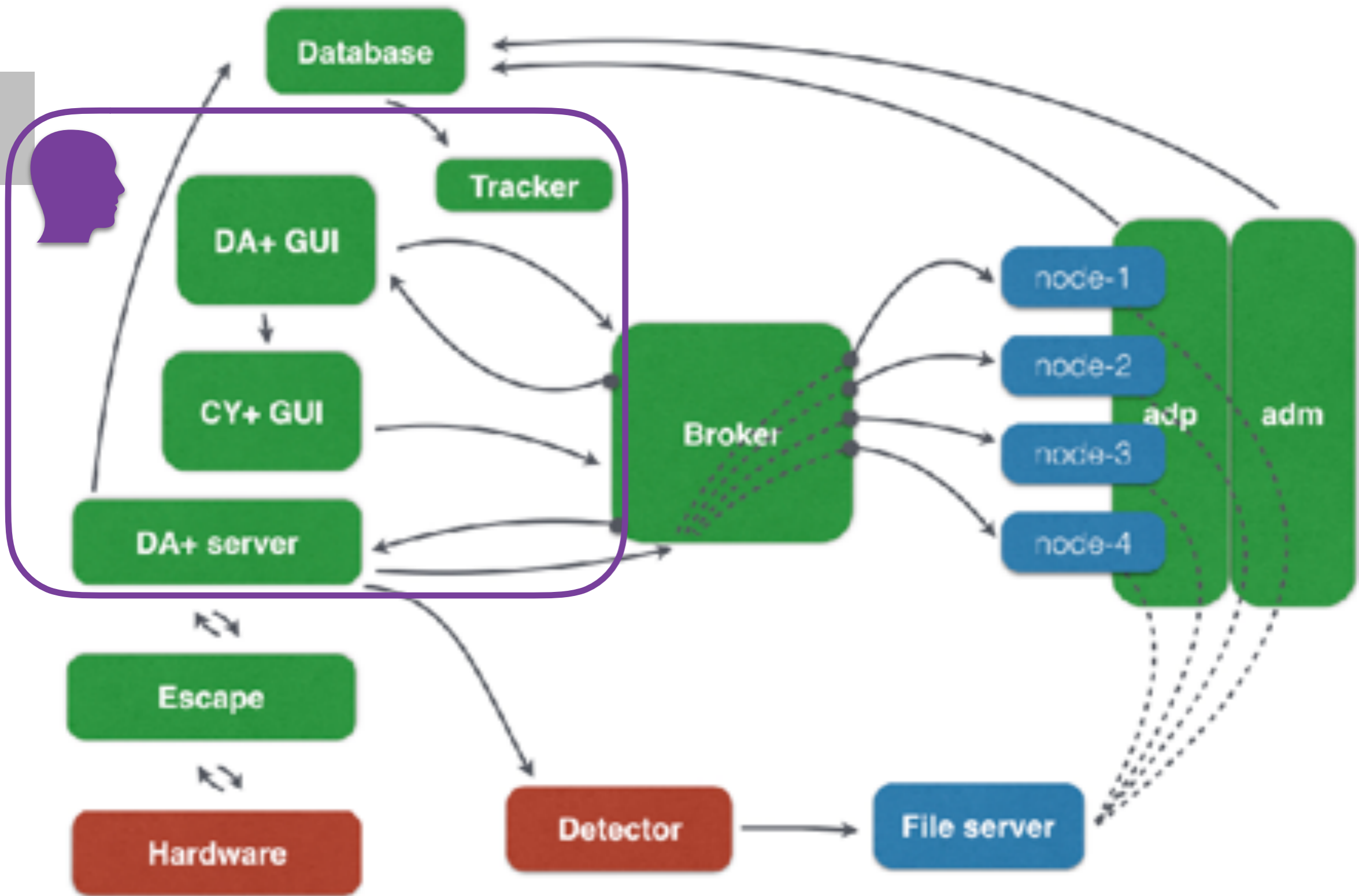
- utilises latest technology



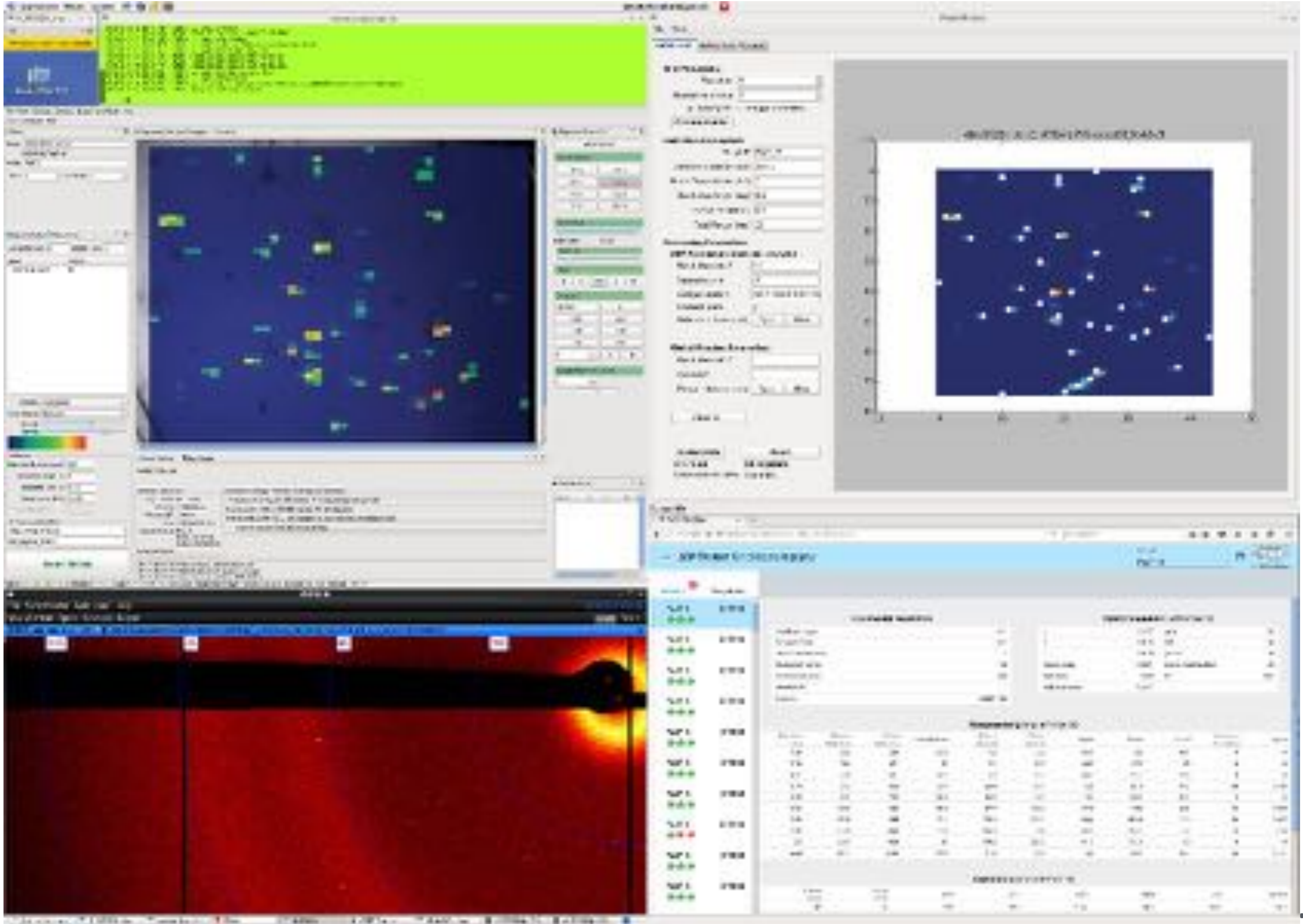
- provides expandable and sustainable solution supported by a small software team



Overall infrastructure



DA+
server



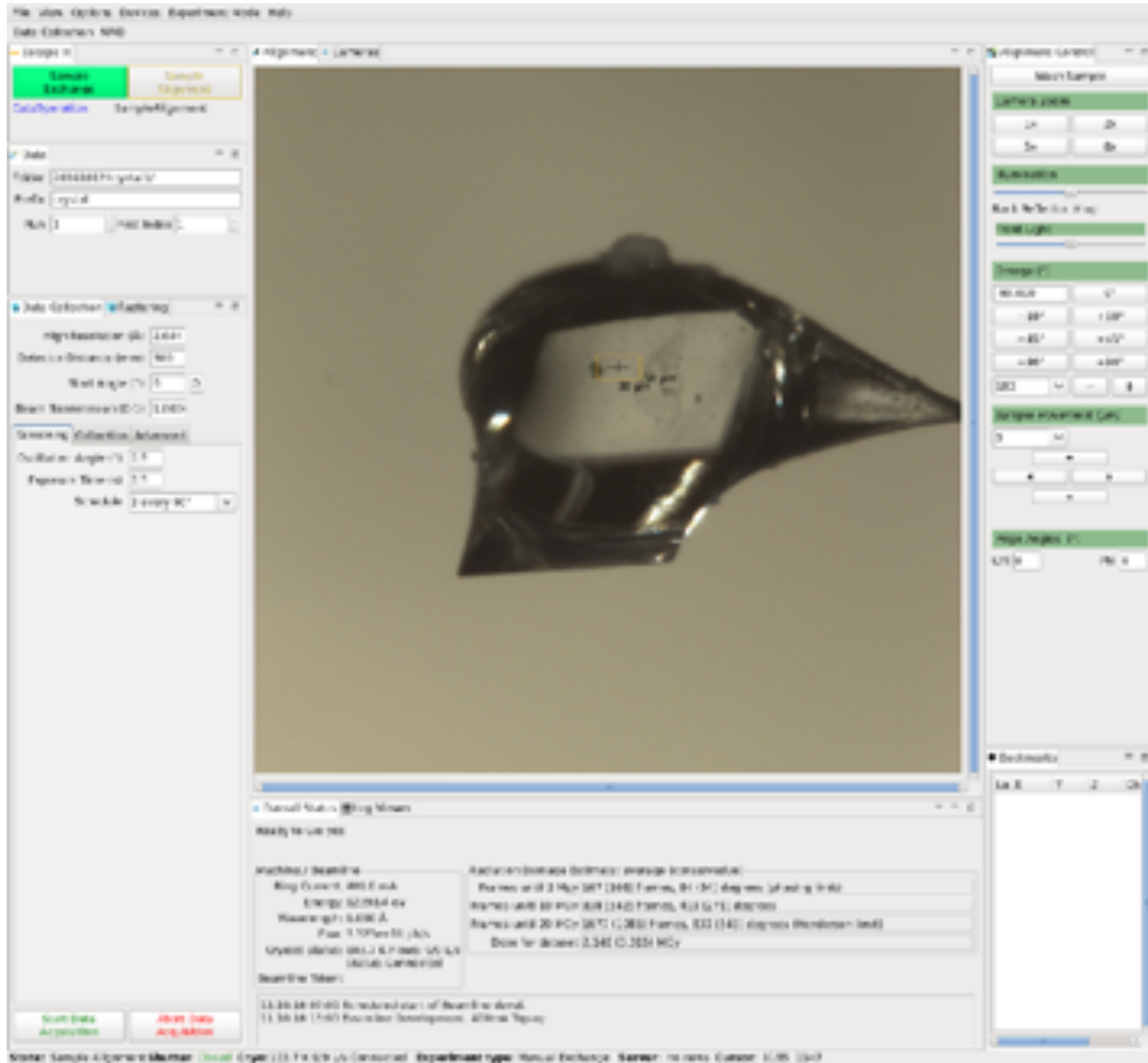
CY+
GUI

DA+
GUI

Albula

Tracker





Choose element



Change energy



Transmission search



Take spectrum

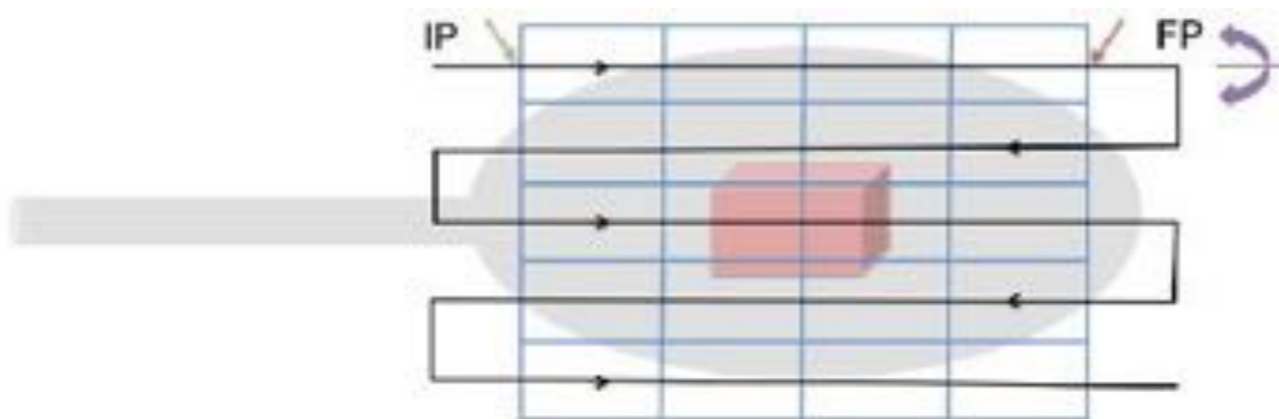
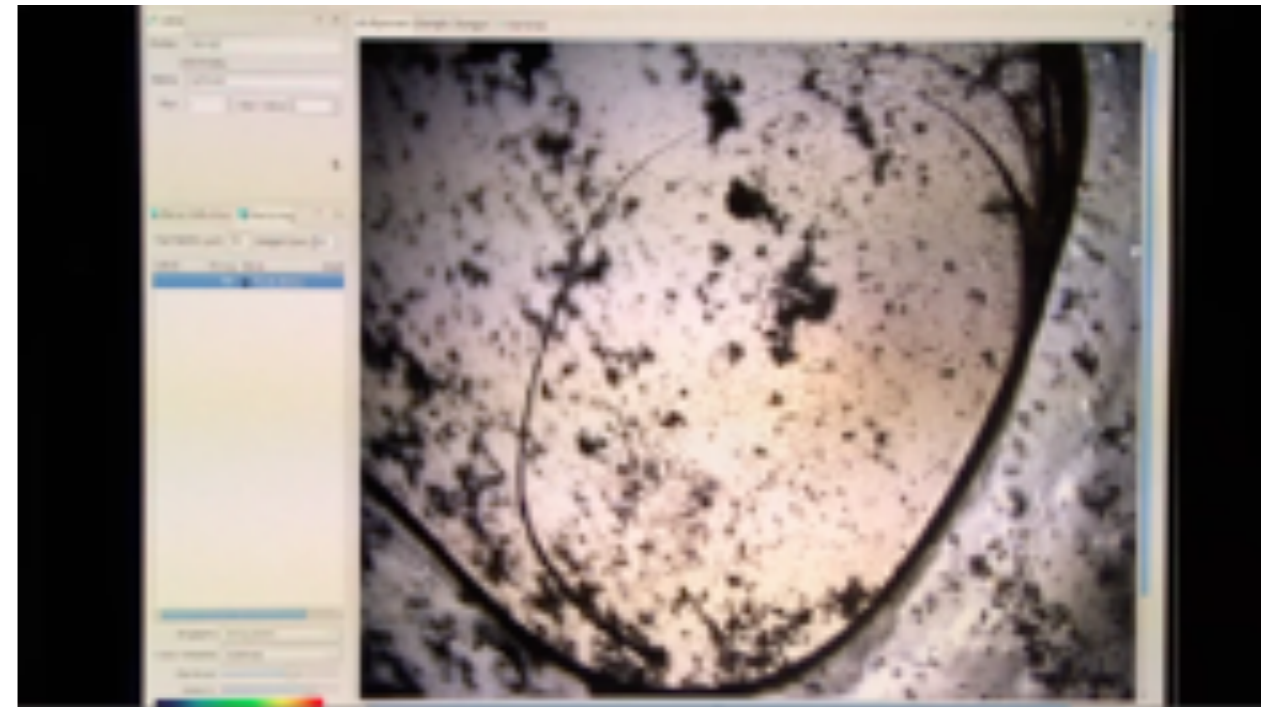


Scan edge



The screenshot displays the DA+ GUI interface. On the left, there are control panels for 'Select element & step', 'Set energy', 'Set beam transmission', 'Key fluorescence measurement', and 'Element edge scan'. On the right, there are two plots: 'Key Substance measurement' showing a peak at approximately 8477 eV, and 'Element edge scan' showing a derivative scan with a peak at approximately 8477 eV. The interface includes various input fields, buttons, and status indicators.

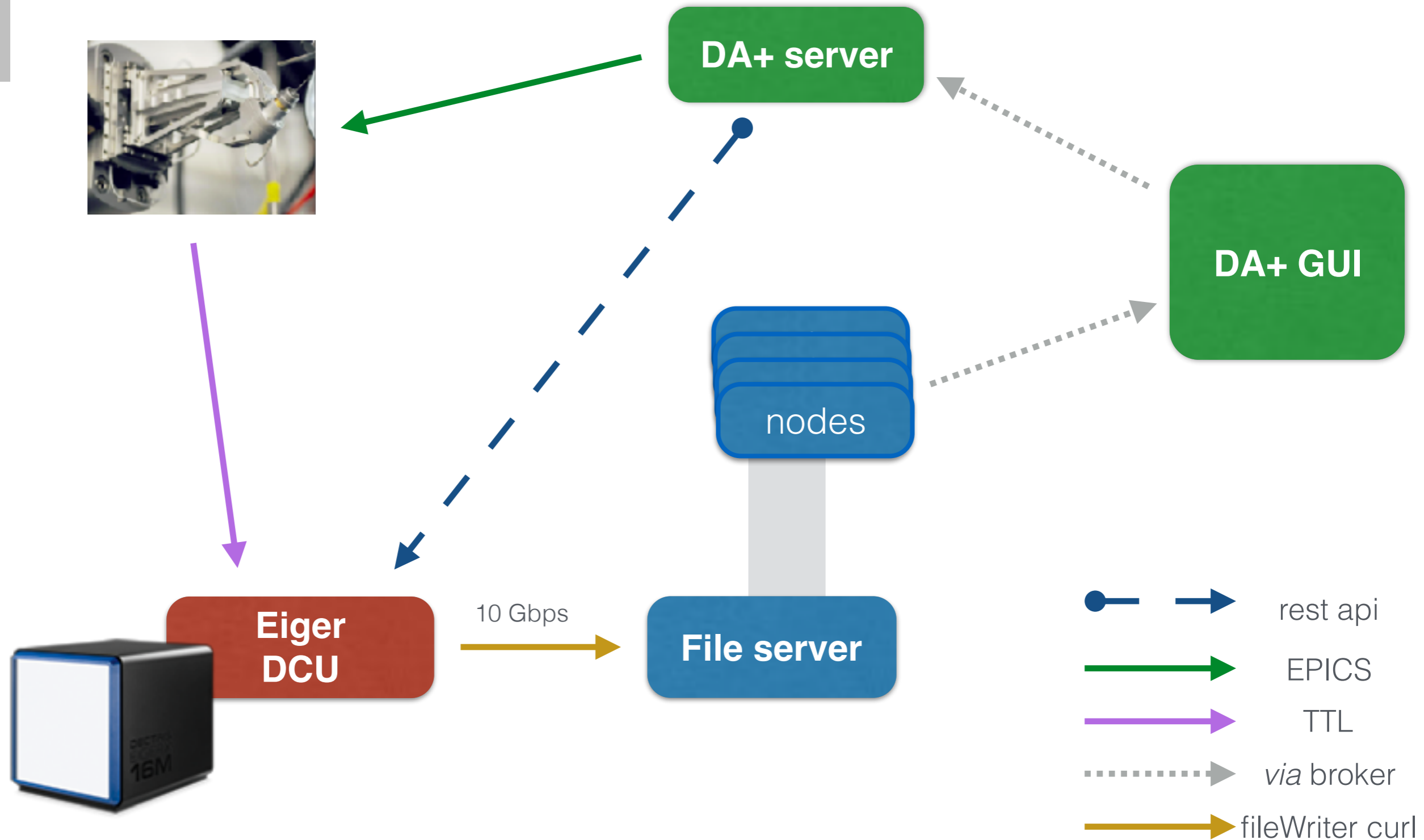
- Easily requested by user in the intuitive DA+ GUI
- Hardware (goniometer & detector) and software control allow for fast grid scanning
 - Eiger X 16M 4ROI at 50Hz
- PXI computer cluster with 16 nodes (576 cores) allow for immediate delivery of analysis (*labelit.distl* or Cheetah)
 - 288 workers (16 x 18)
 - Eiger X 16M 4ROI at 100Hz grid with 10.584 images








Wojdyla et al, J. Appl. Cryst., 2016

Eiger X 16M fileWriter

user inspection

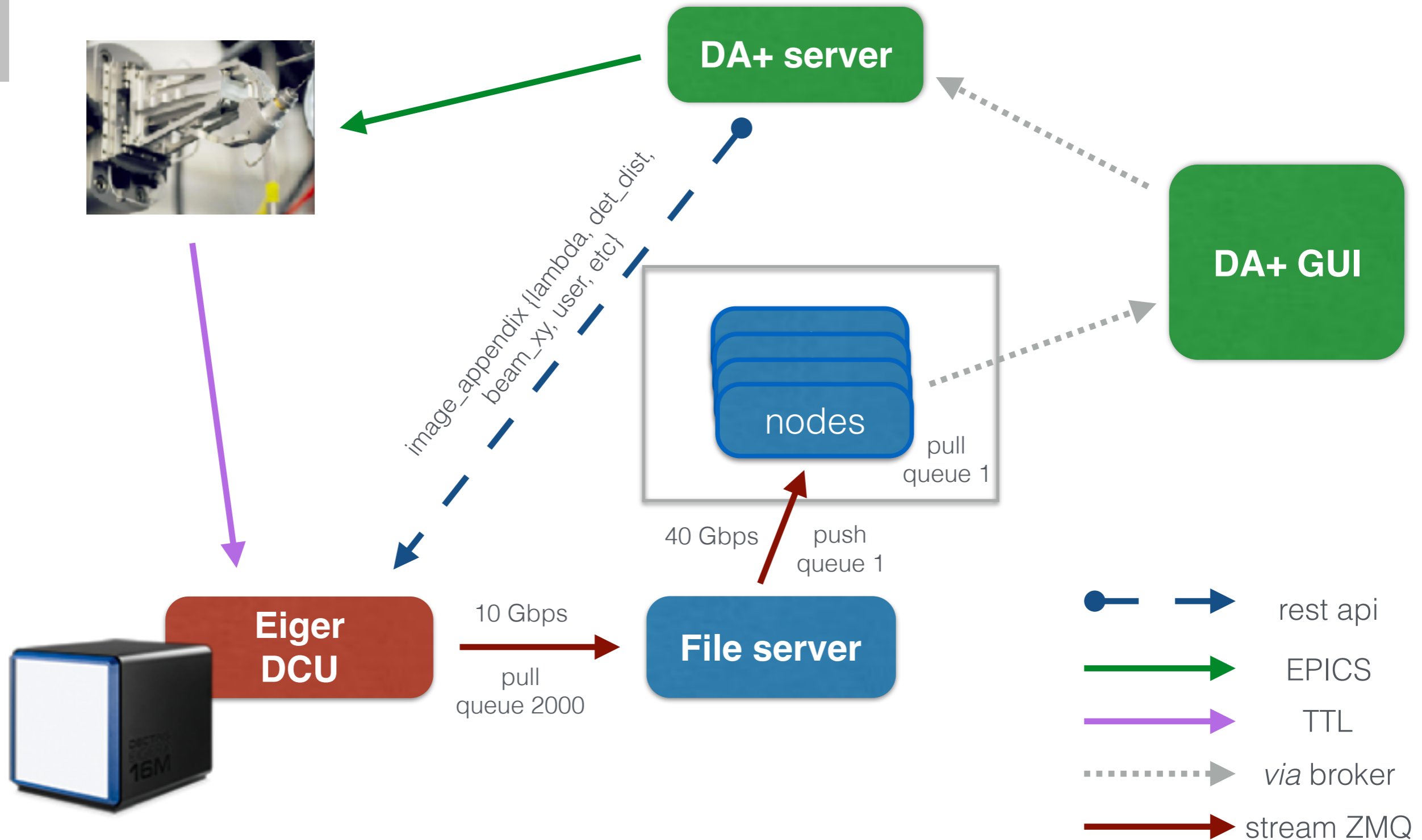


-  rest api
-  EPICS
-  TTL
-  via broker
-  fileWriter curl

Wojdyla et al, J. Synchrotron Rad., 2018

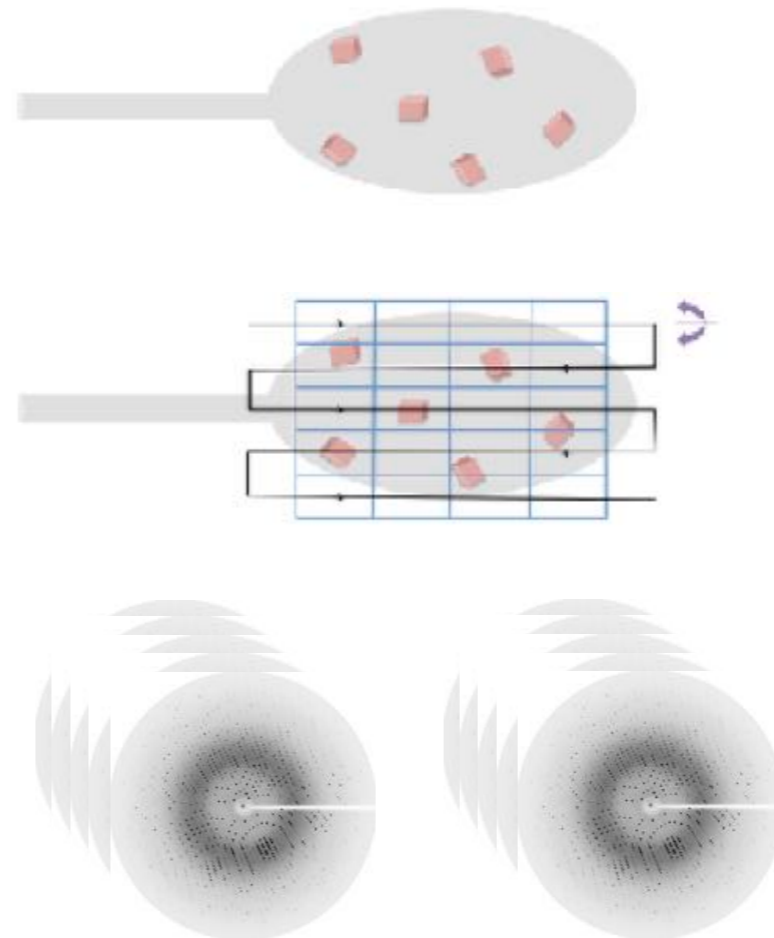
Eiger X 16M stream

online analysis



SSX data collection & analysis

- Load sample onto goniometer
- Locate well-diffracting crystals
- Collect datasets (so-called minisets)
- Process each miniset
- Merge minisets



DA+ GUI

DA+ GUI

CY+ GUI

adp

adm

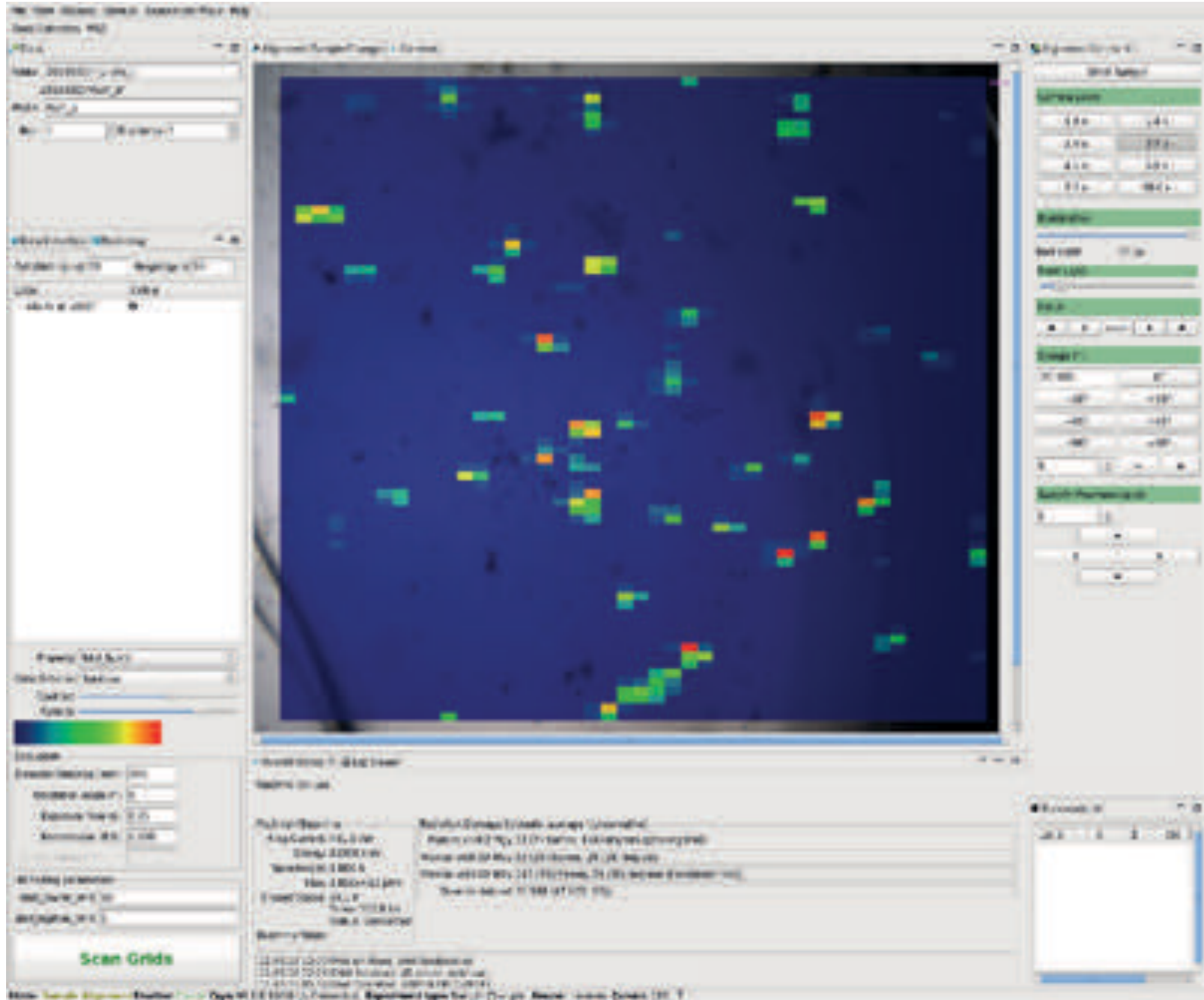
The screenshot displays the DA+ GUI interface for a grid scan. The central window shows a grayscale image of a grid with a yellow label '10µm 270°'. The interface includes several control panels:

- Left Panel:** Contains fields for 'Pencil', 'Beam', and 'Spot'. It also has a 'Table Extension' section with 'Cell Name' and 'Beam' fields, and a 'Color Scheme' dropdown set to 'Rainbow'. A 'Scan Grids' button is visible at the bottom.
- Right Panel:** Features an 'Auto Range' section with a 'Camera Zoom' list (1.0x to 16.0x). Below it are 'Position' controls for 'Back Sight' and 'Front Sight', and a 'Focus' section with 'Auto' and 'Manual' buttons. The 'Stage (°)' section includes angular controls for X, Y, and Z axes.
- Bottom Panel:** Displays 'Machine / Beamline' information (Ring Current: 400 mA, SHWR: 1236.8 Hz) and 'Position / Stage' data (X: 200.20, Y: 228.17, Z: 200.00). It also shows a 'Status' section with 'Status: Connected' and a 'Scan' button.

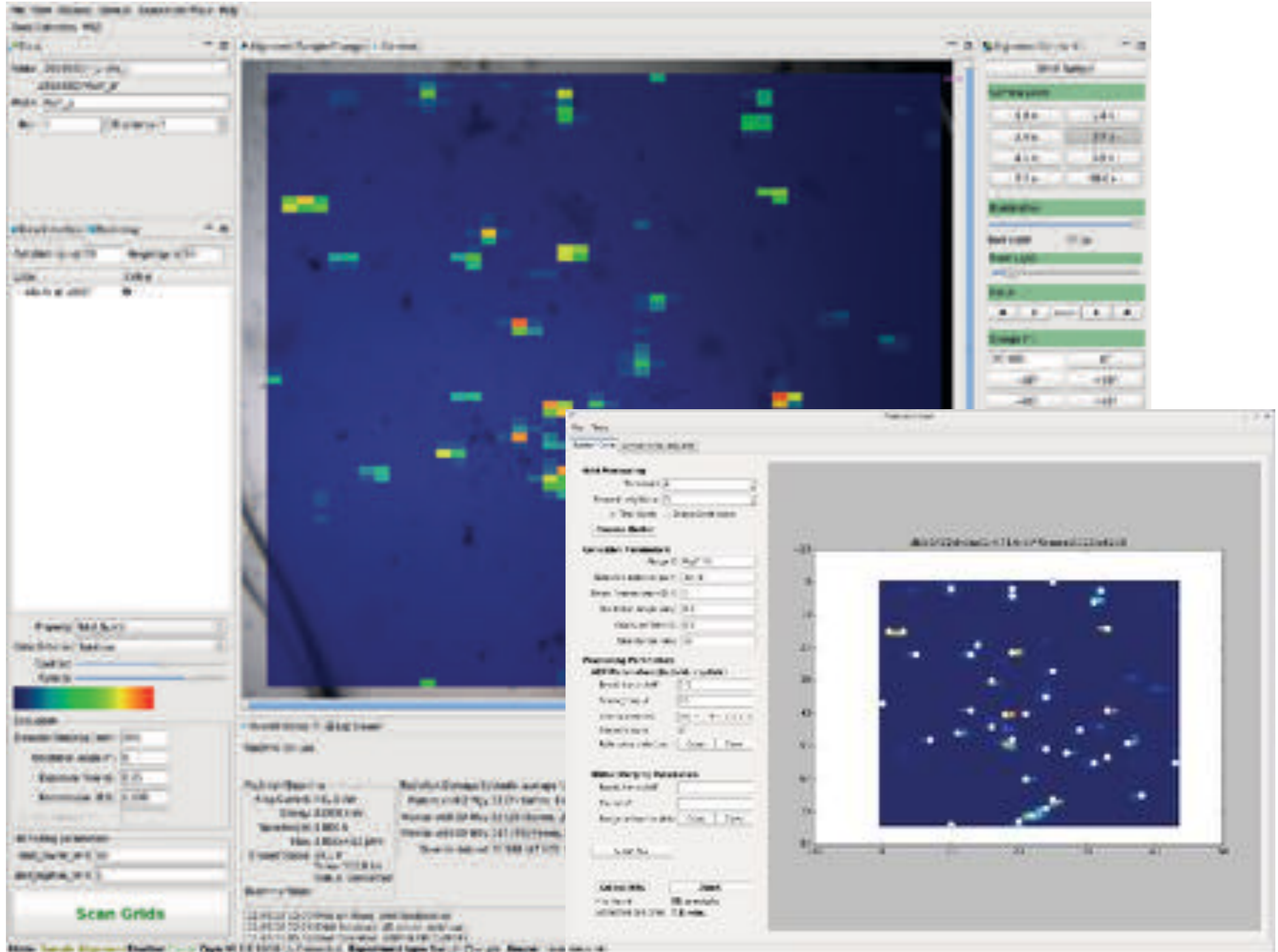
The screenshot displays the DA+ GUI interface. The central window shows a grayscale image of a sample with a red grid overlaid. The grid is composed of small squares, and the sample features several dark, irregular spots. The interface is divided into several panels:

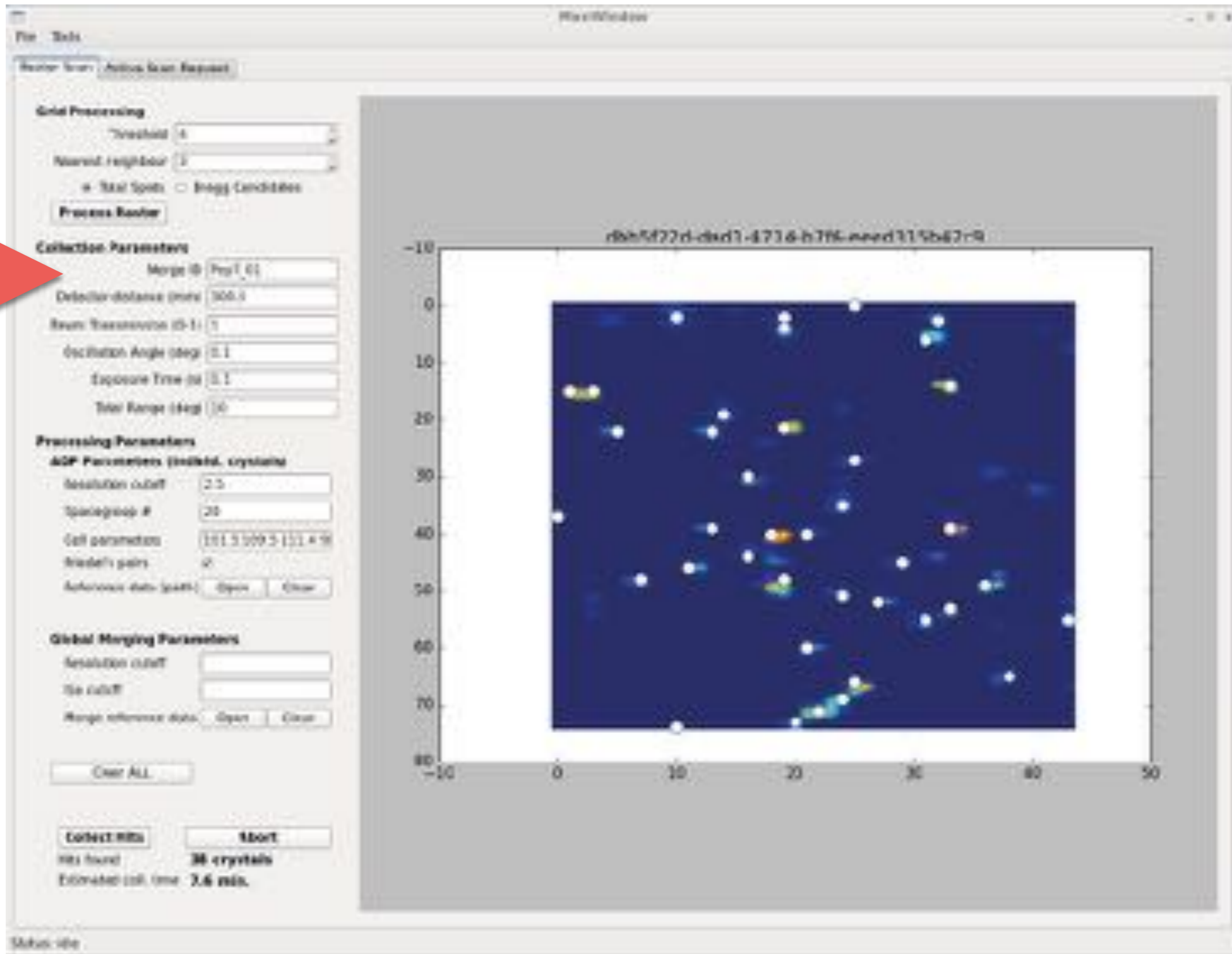
- Top Left:** Control panel for the 'Beam' and 'Sample' sections, including fields for 'Beam Size', 'Sample ID', and 'Beam Index'.
- Bottom Left:** 'Evaluation' section with fields for 'Detector Distance (mm)', 'Divergence Angle (°)', 'Exposure Time (s)', and 'Throttle (A)', along with a color calibration bar.
- Right Side:** 'Alignment Control' panel with buttons for 'Auto Range', 'Camera Zoom', 'Focus', and 'Stage Control'.
- Bottom Center:** 'Machine & Beamline' and 'Radiation Damage Estimate' sections, providing technical specifications and estimated damage levels.
- Bottom Right:** 'Bookmarks' section with a list of saved scan positions.

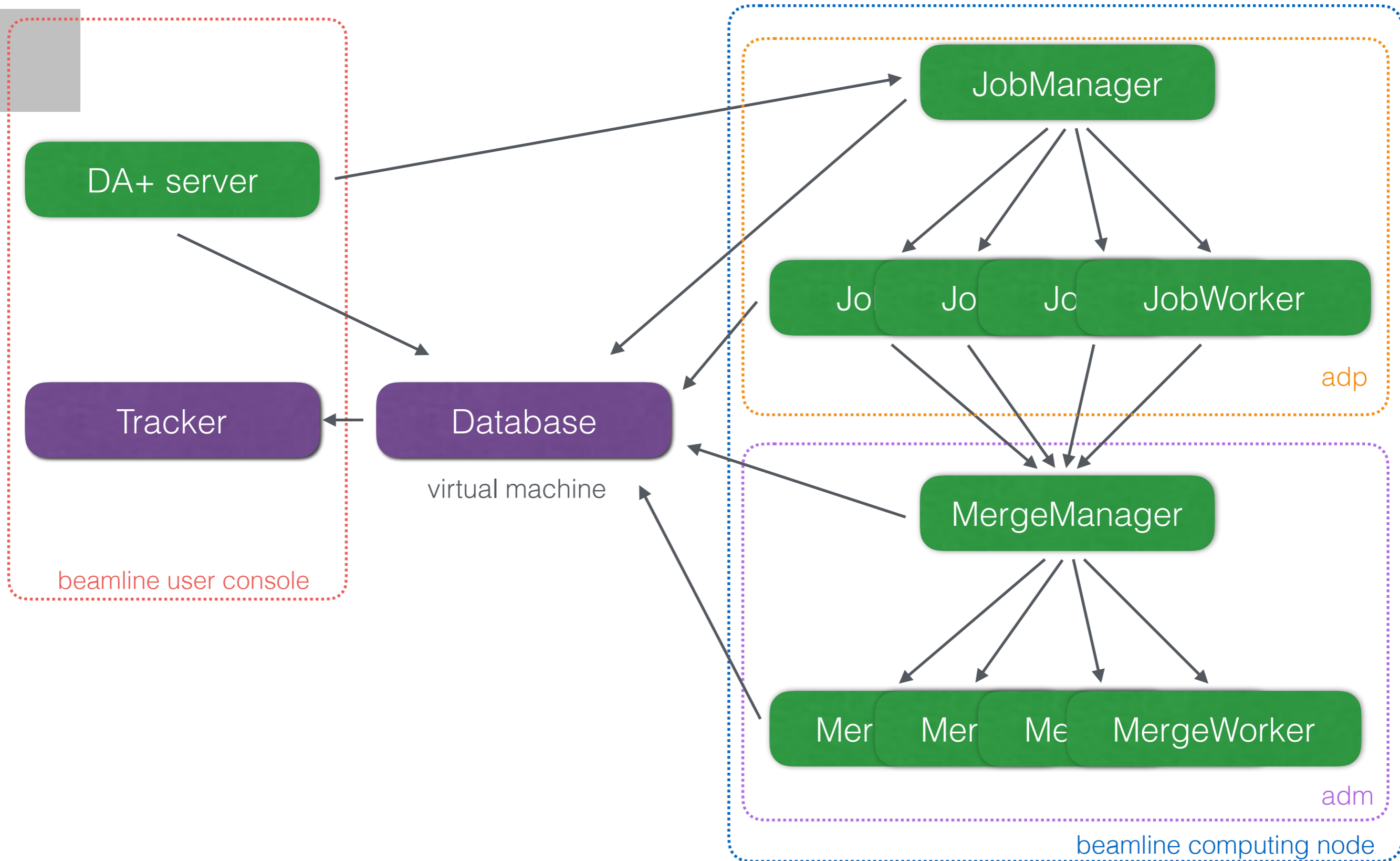
At the bottom of the window, a status bar displays the current scan parameters and coordinates.



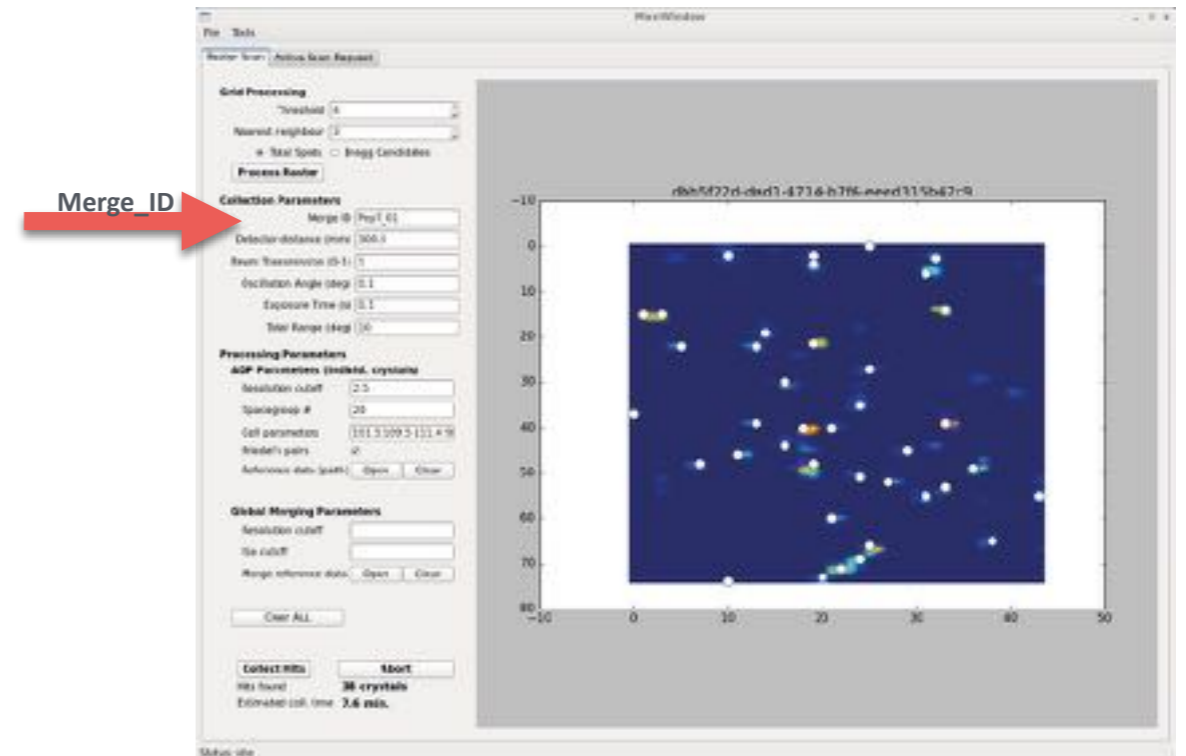
The image displays the CY+ GUI interface. The main window shows a grid scan visualization with a central plot area containing a grid of colored rectangles (green, yellow, orange, red) on a dark blue background. The left sidebar contains various control panels, including a color scale legend and a 'Scan Grids' button. The right sidebar shows a 'Grid Setup' panel with numerical input fields for grid dimensions and positions. An inset window in the foreground shows a 'Parameter' configuration panel with sections for 'Grid Planning', 'Collection Parameters', and 'Processing Parameters', each with multiple input fields and checkboxes. The bottom of the main window shows a status bar with technical details.

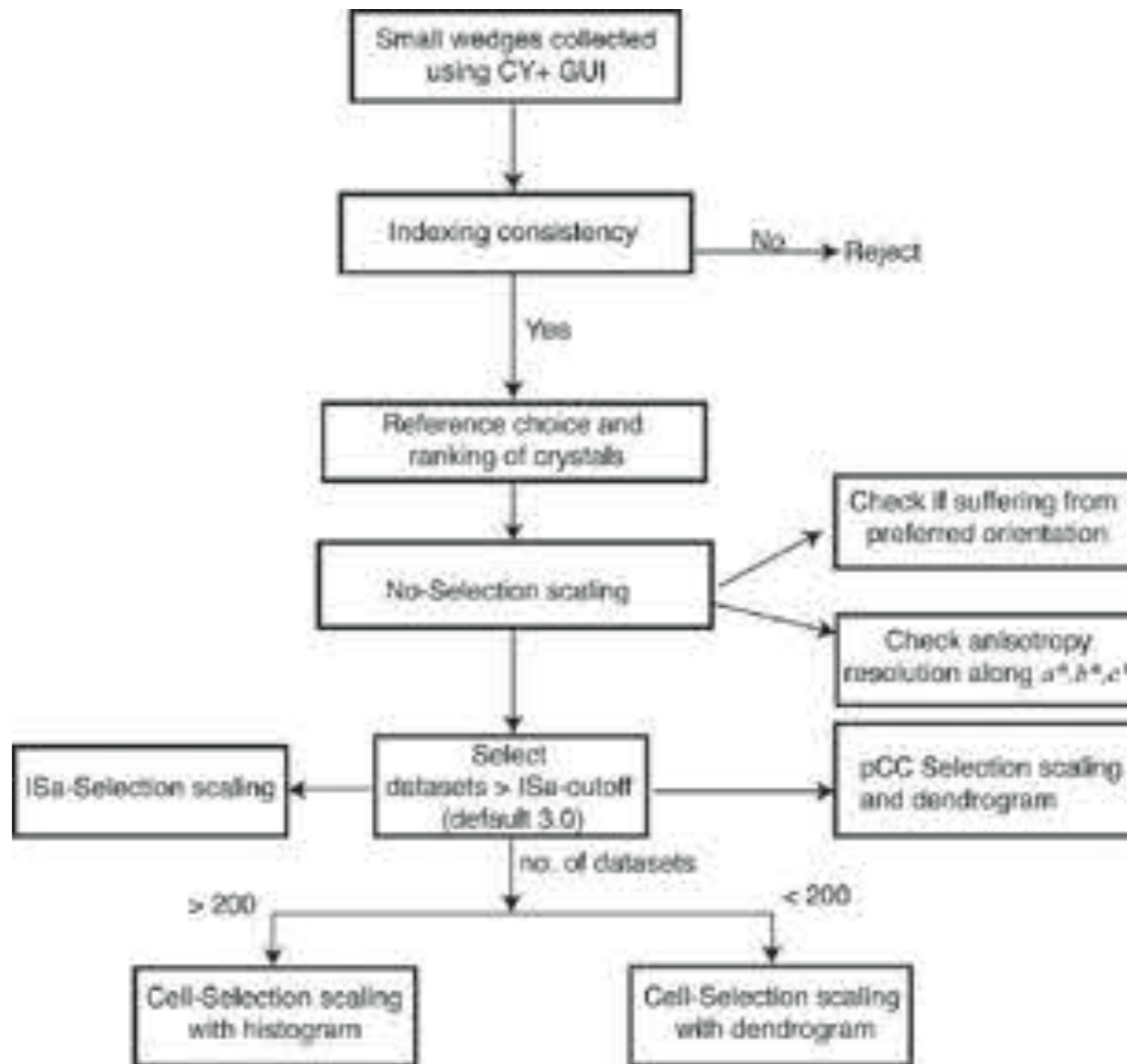


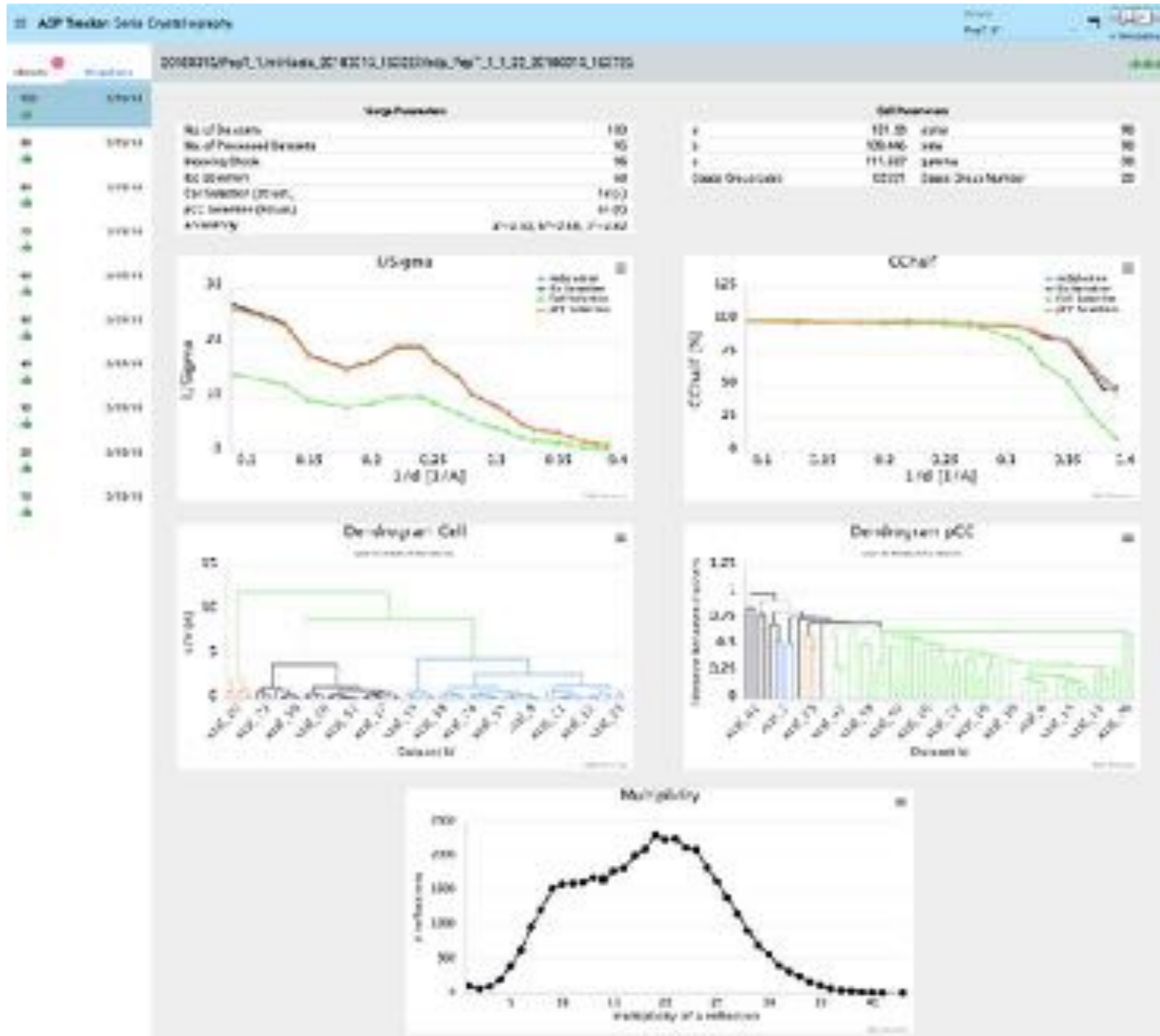




- projects identified based on the Merge_ID (defined by user in the CY+ GUI)
- adm module_1 counts all minisets collected for a given Merge_ID
- at predefined hardcoded intervals (10, 20, ..., 100, 120, ..., 200, 250, ..., 800) module_1 sends a merging request to module_2
- module_2 performs merging using SSX scaling and merging (sxdm) package (written by Shibom Basu) and sends results to the database







Summary

- extensive hardware and software developments in the SLS MX Group make SSX easily accessible to users
- in-house DAQ software supports standard and advanced data acquisition protocols
- grid scan and CY+ GUI allow fast location of well-diffracting microcrystals and automate collection of multiple small wedges of data
- on-the-fly automatic data processing and merging provide instant feedback

Acknowledgements

- Zac Panepucci
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- Simon Ebner
- Jose Gabadinho
- Shibom Basu
- Chia-Ying Huang
- MX team
- Controls
- IT support

Local contact persons



Shibom Basu
Post Doc
MX & serial crystallography, native IAD



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Beamline hardware, spectroscopy



Chia-Ying Huang
Post Doc
MX & serial crystallography



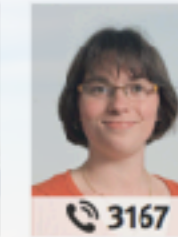
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<https://www.psi.ch/macromolecular-crystallography/>

Thank you

