



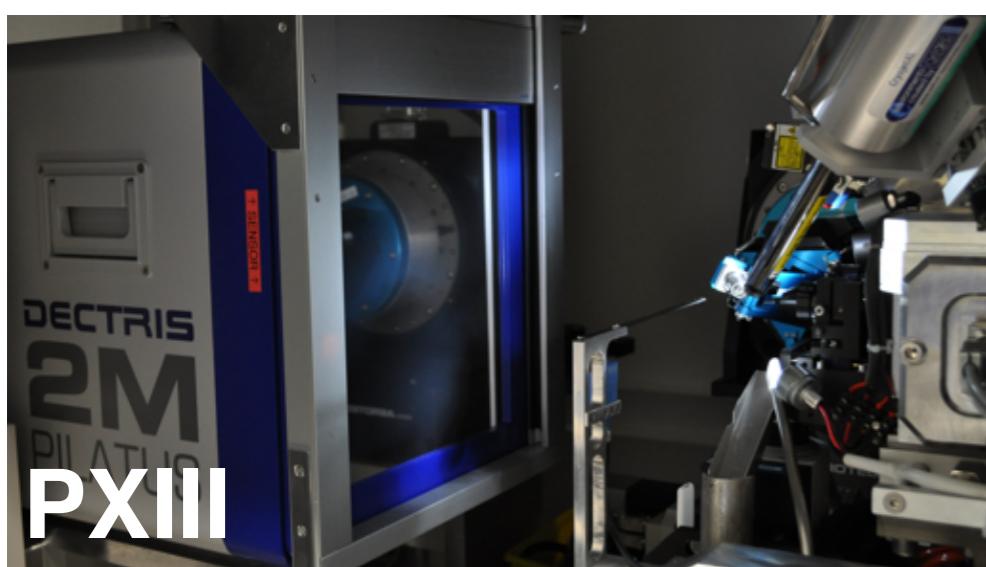
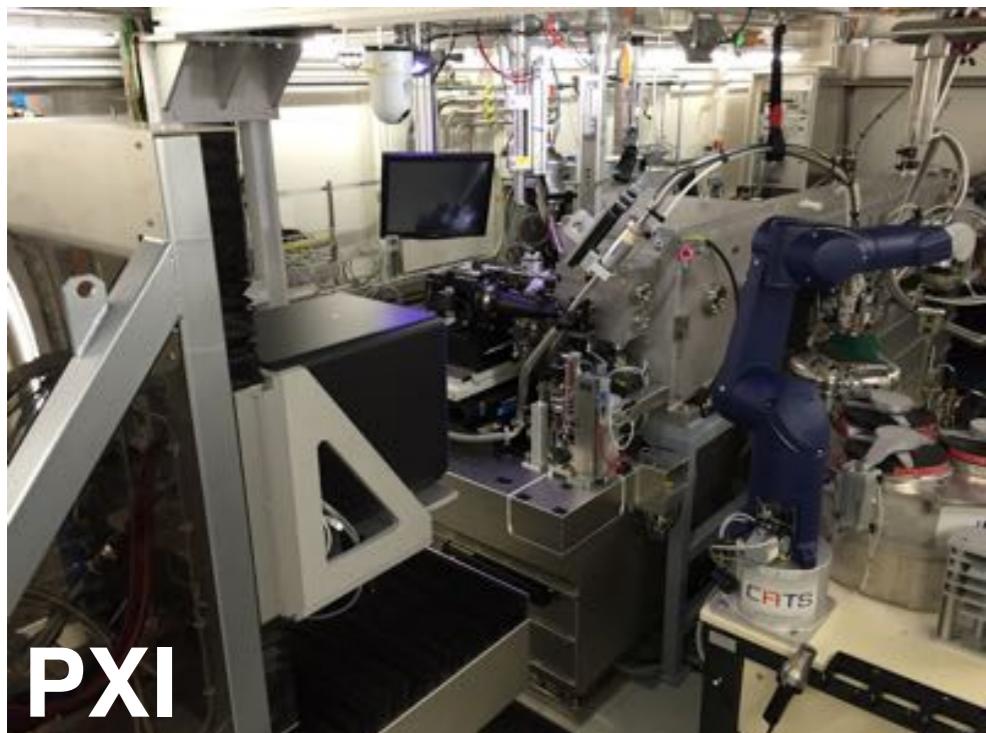
Justyna A. Wojdyla :: Beamlne scientist :: Industry Liaison Scientist :: Paul Scherrer Institute

Data acquisition and analysis software at the SLS MX beamlines

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

SLS MX beamlines

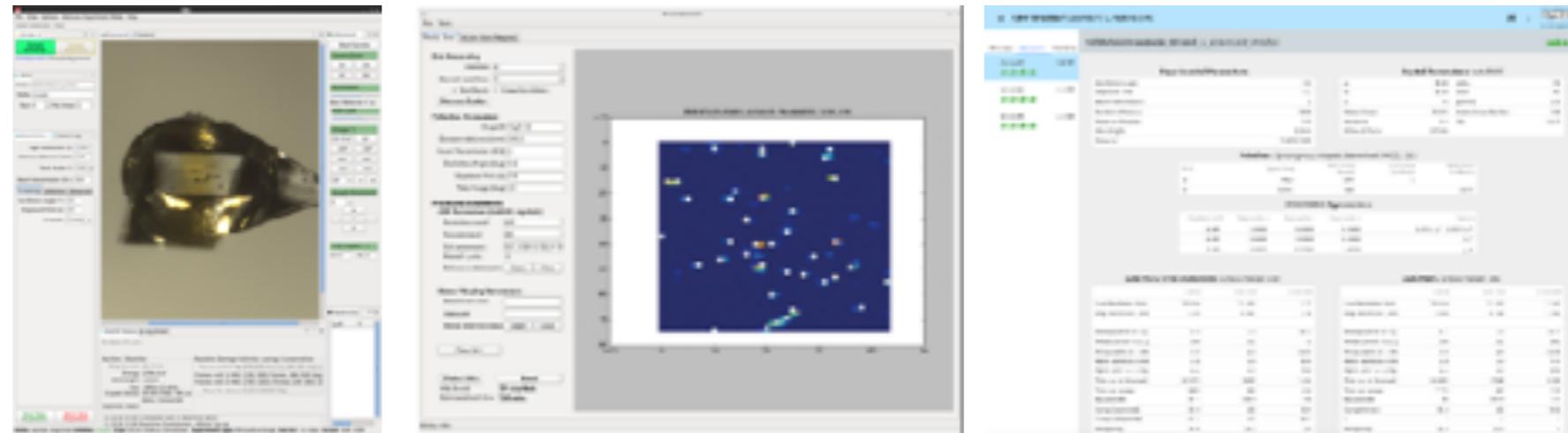
- 10 beamline partners & > 20 regular industry customers
- **6000 PDBs**



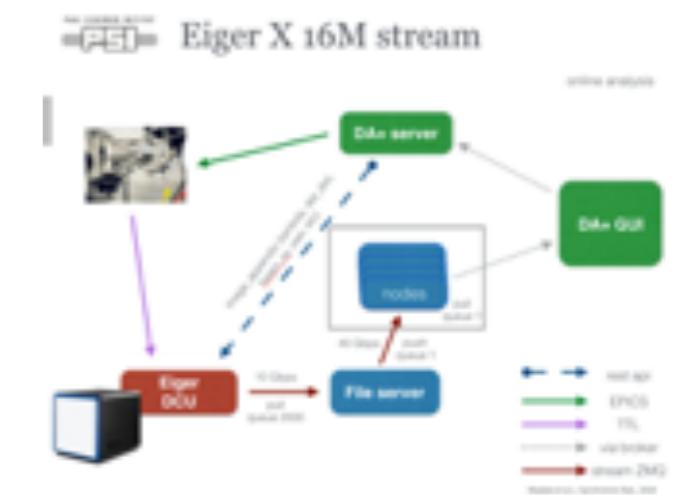
	PXI (X06SA)	PXII (X10SA)	PXIII (X06DA)
Wavelength range [Å]	0.7 - 2.2	0.62 - 2.07	0.71 - 2.07
Source	in-vacuum undulator	in-vacuum undulator	bending magnet
Spectral range	5.7 - 17.5	6.0 - 20.0	6.0 - 17.5
Flux at 12.4 keV [ph/s]	$> 2 \times 10^{12}$	$> 2 \times 10^{12}$	5×10^{11}
Focused spot size h x 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

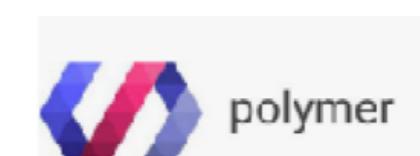
- robust, intuitive & user-friendly



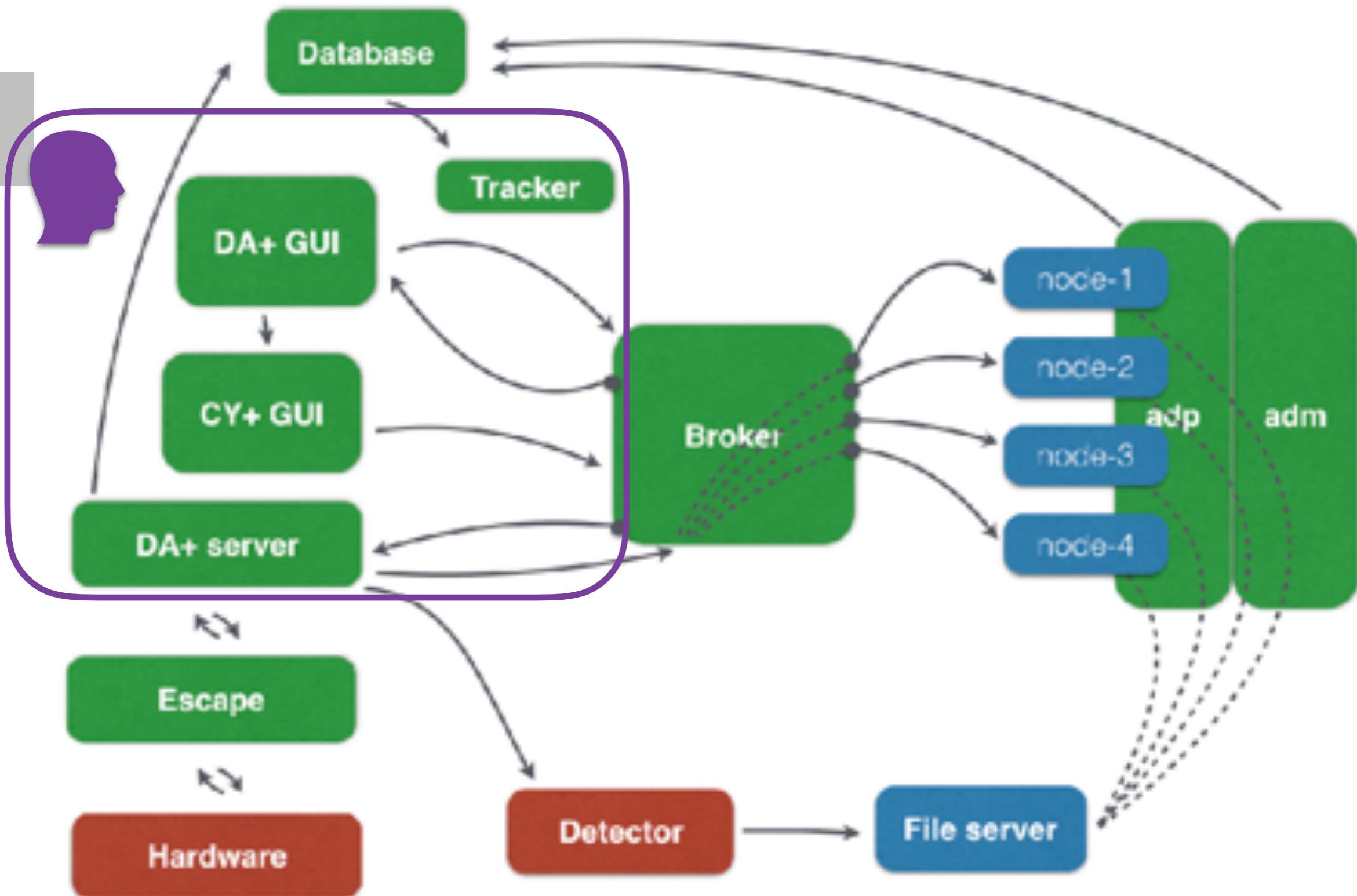
- allows exploitation of latest instrumentation
- utilises latest technology



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

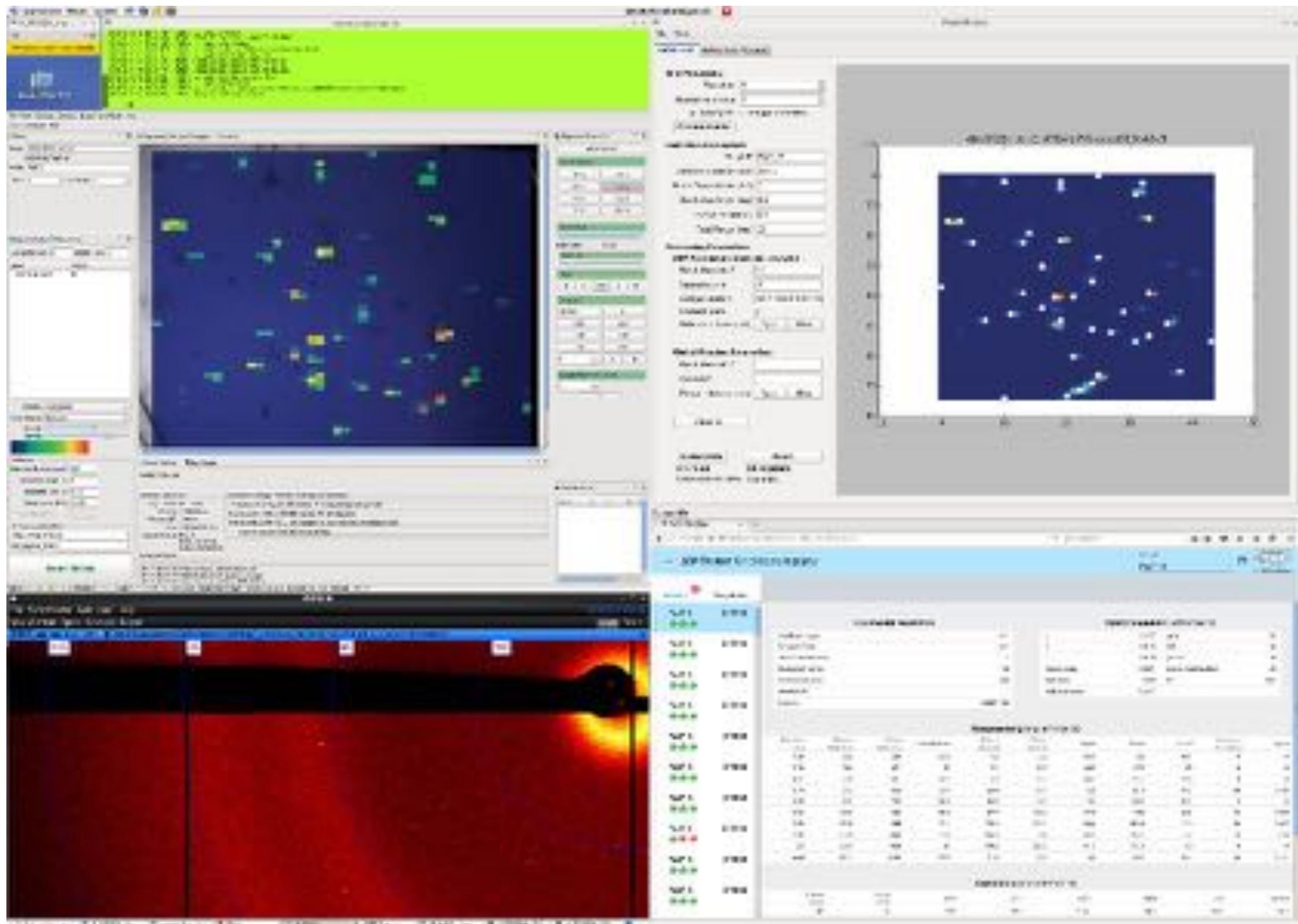


Overall infrastructure



DAQ from users' perspective 2018

DA+
server



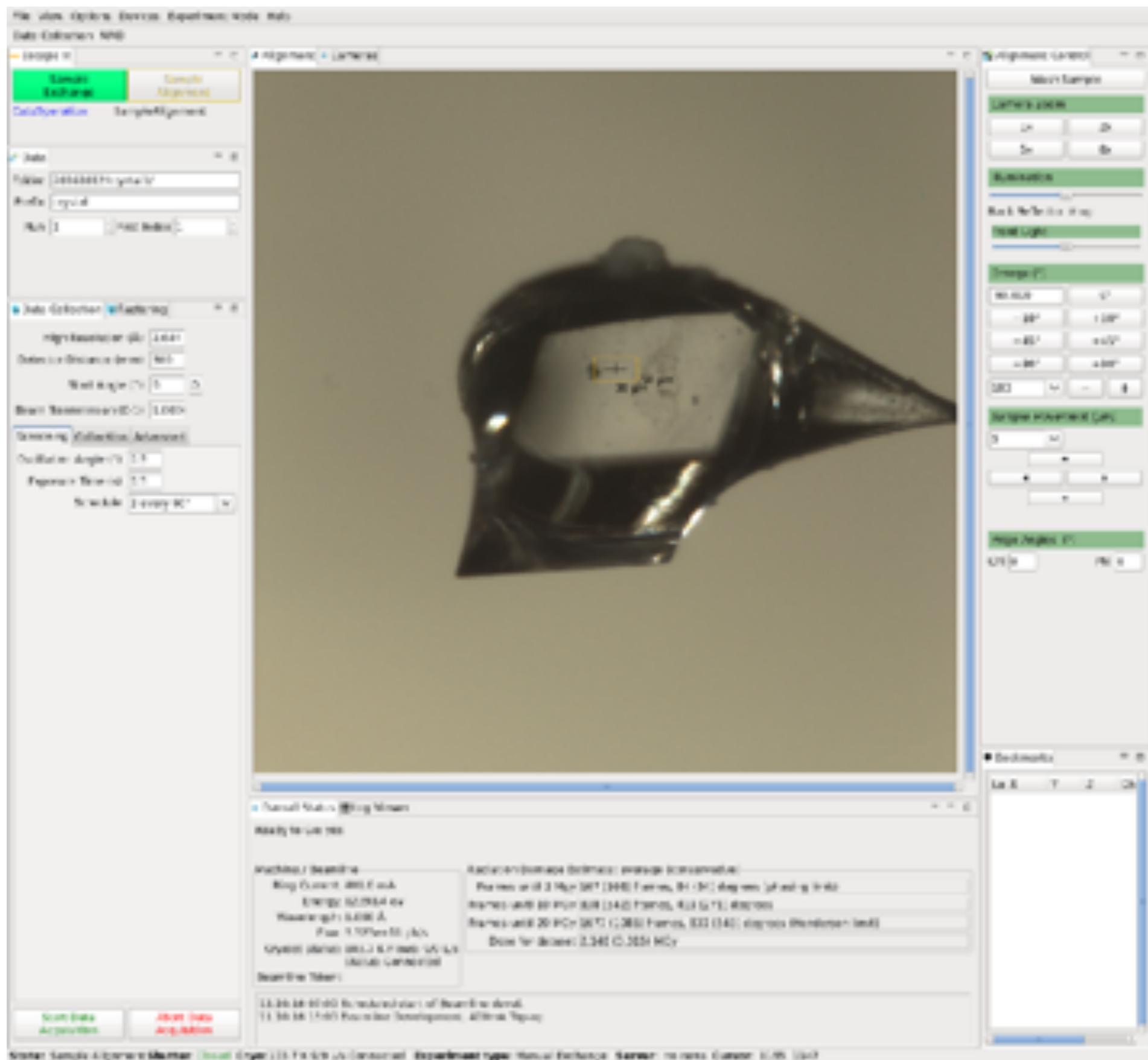
CY+
GUI

DA+
GUI

Tracker

Albulaa





Choose element

1

Change energy

2

Transmission search

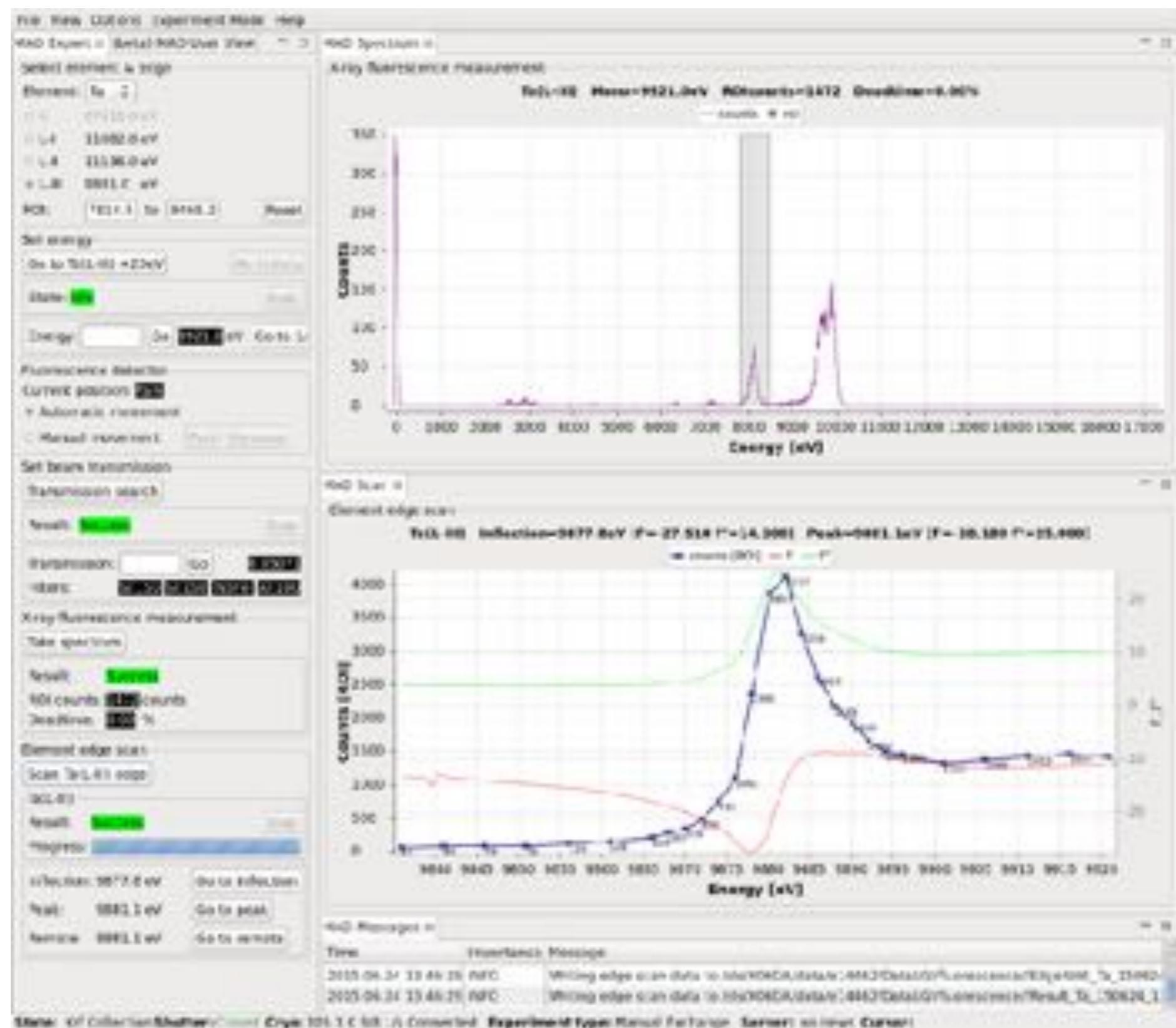
3

Take spectrum

4

Scan edge

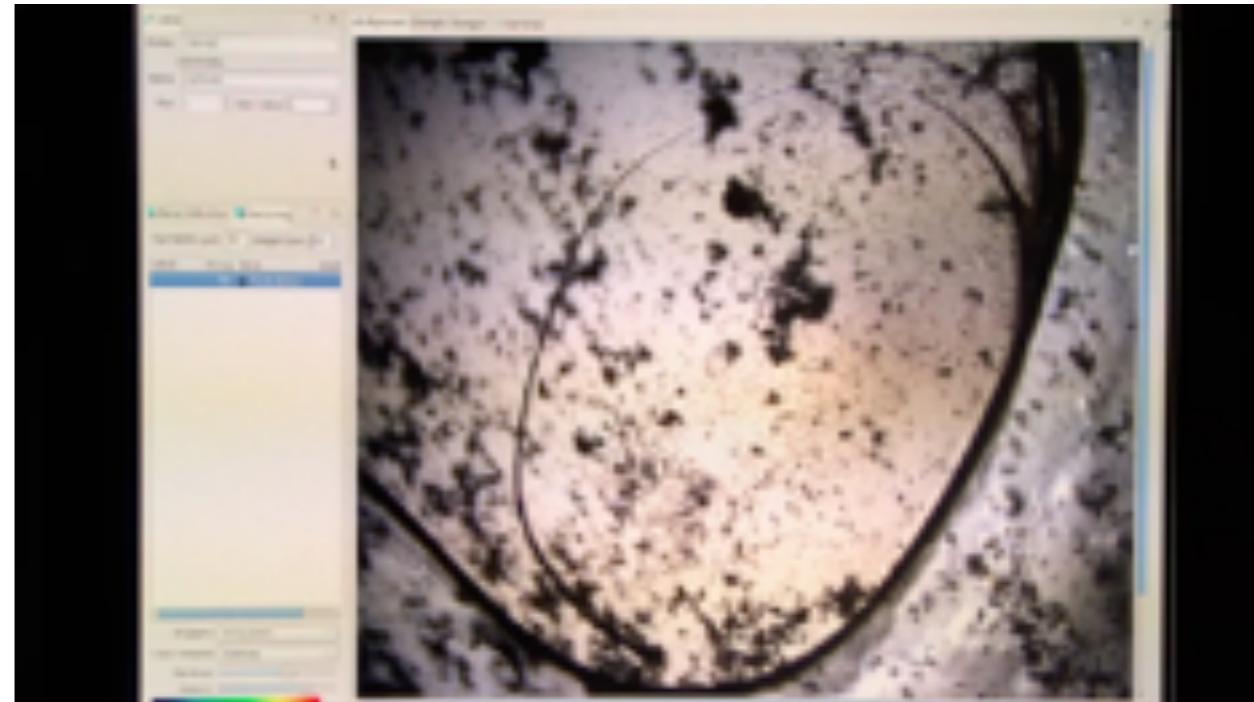
5



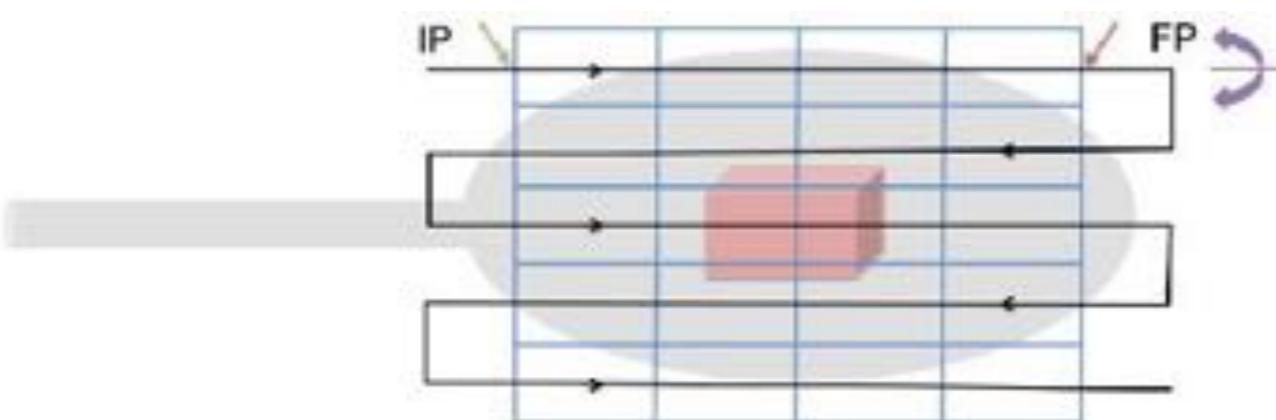
DA+ GUI grid scan

DA+ GUI

- 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)

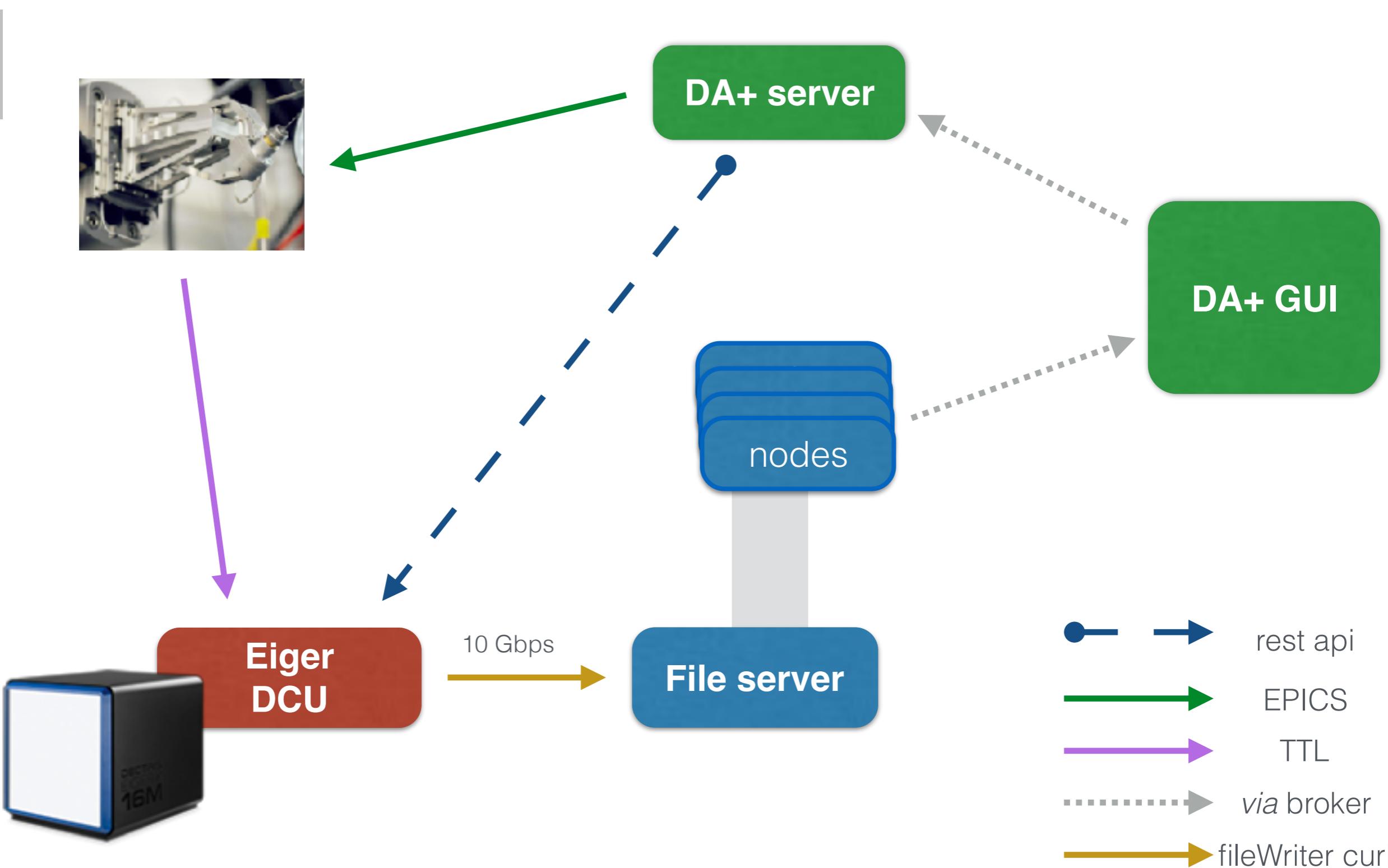


- 288 workers (16 x 18)
- Eiger X 16M 4ROI at 100Hz grid with 10.584 images



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

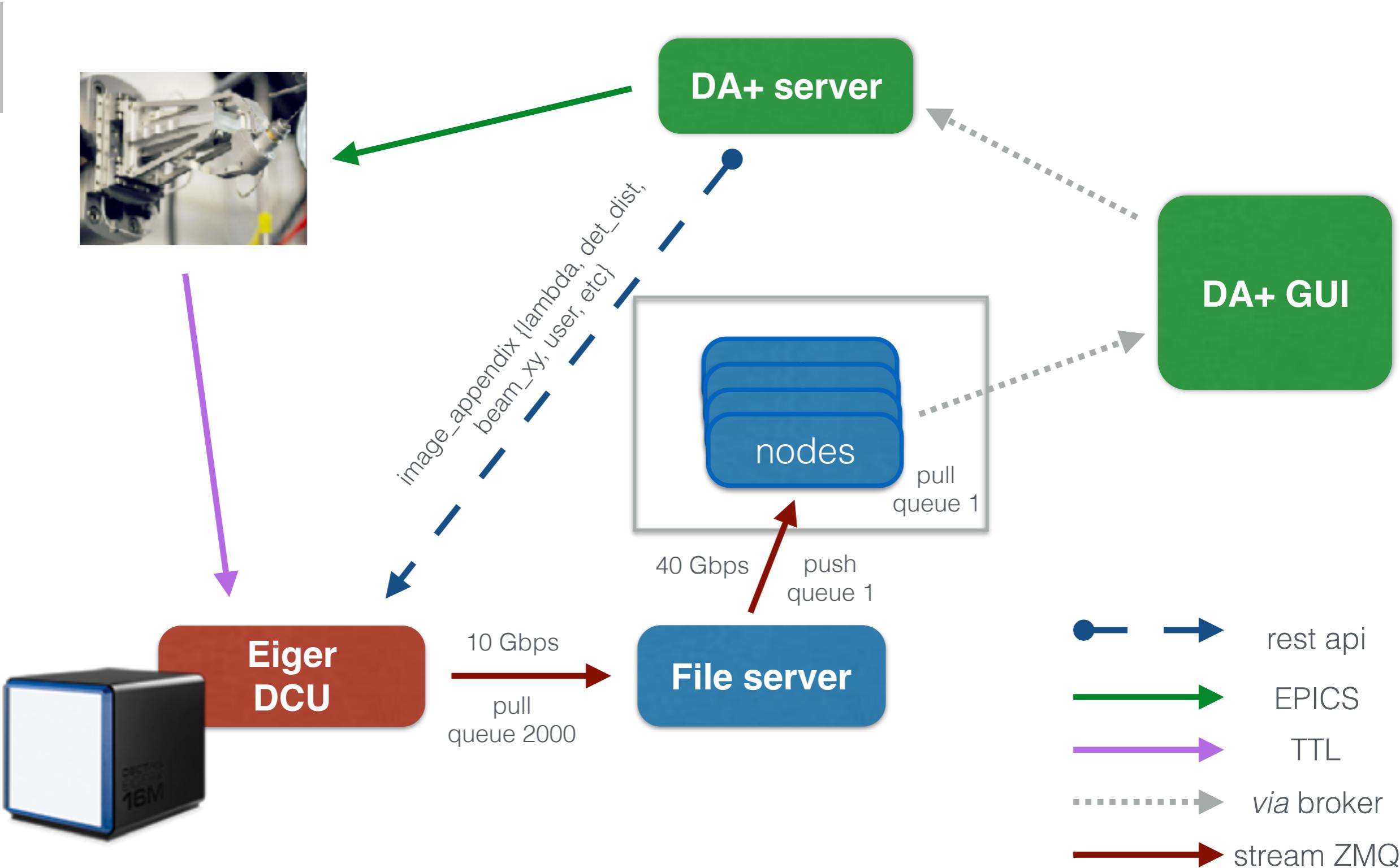
Eiger X 16M fileWriter



Wojdyla et al, J. Synchrotron Rad., 2018

Eiger X 16M stream

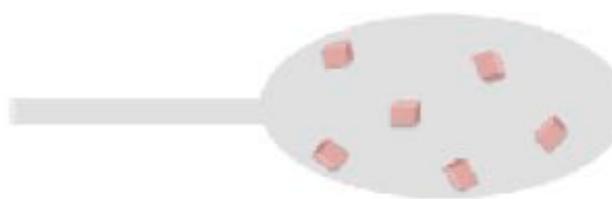
online analysis



Wojdyla et al, J. Synchrotron Rad., 2018

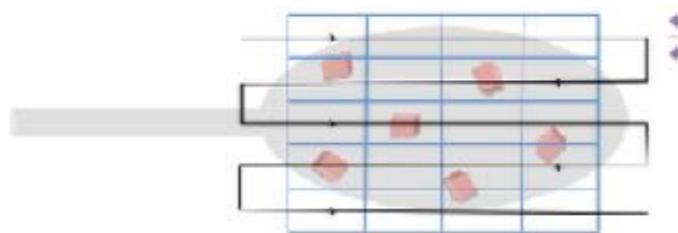
SSX data collection & analysis

- Load sample onto goniometer



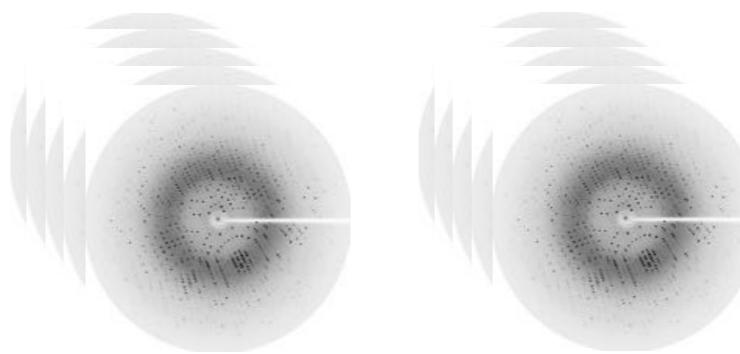
DA+ GUI

- Locate well-diffracting crystals



DA+ GUI

- Collect datasets (so-called minisets)



CY+ GUI

- Process each miniset

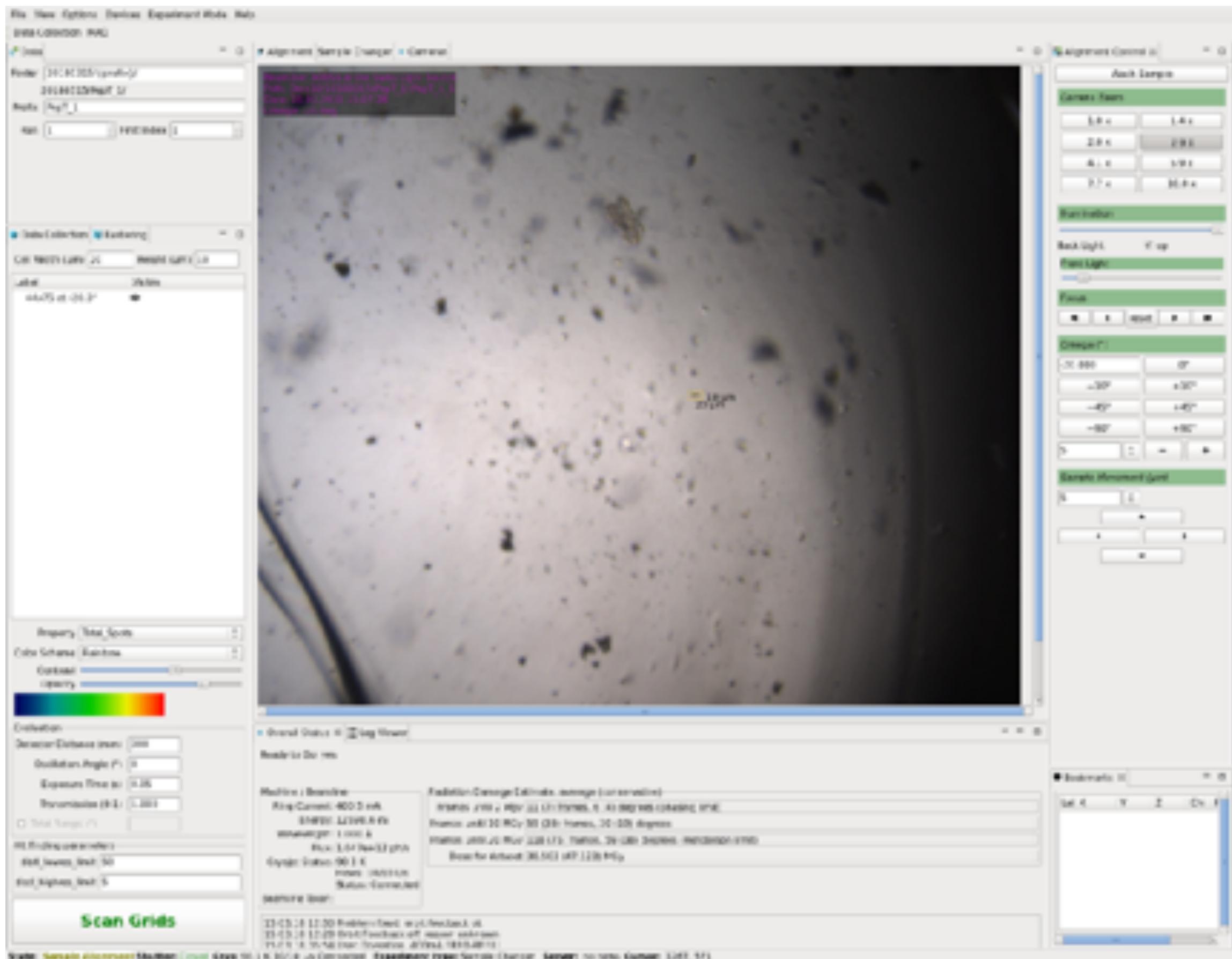
adp

- Merge minisets

adm

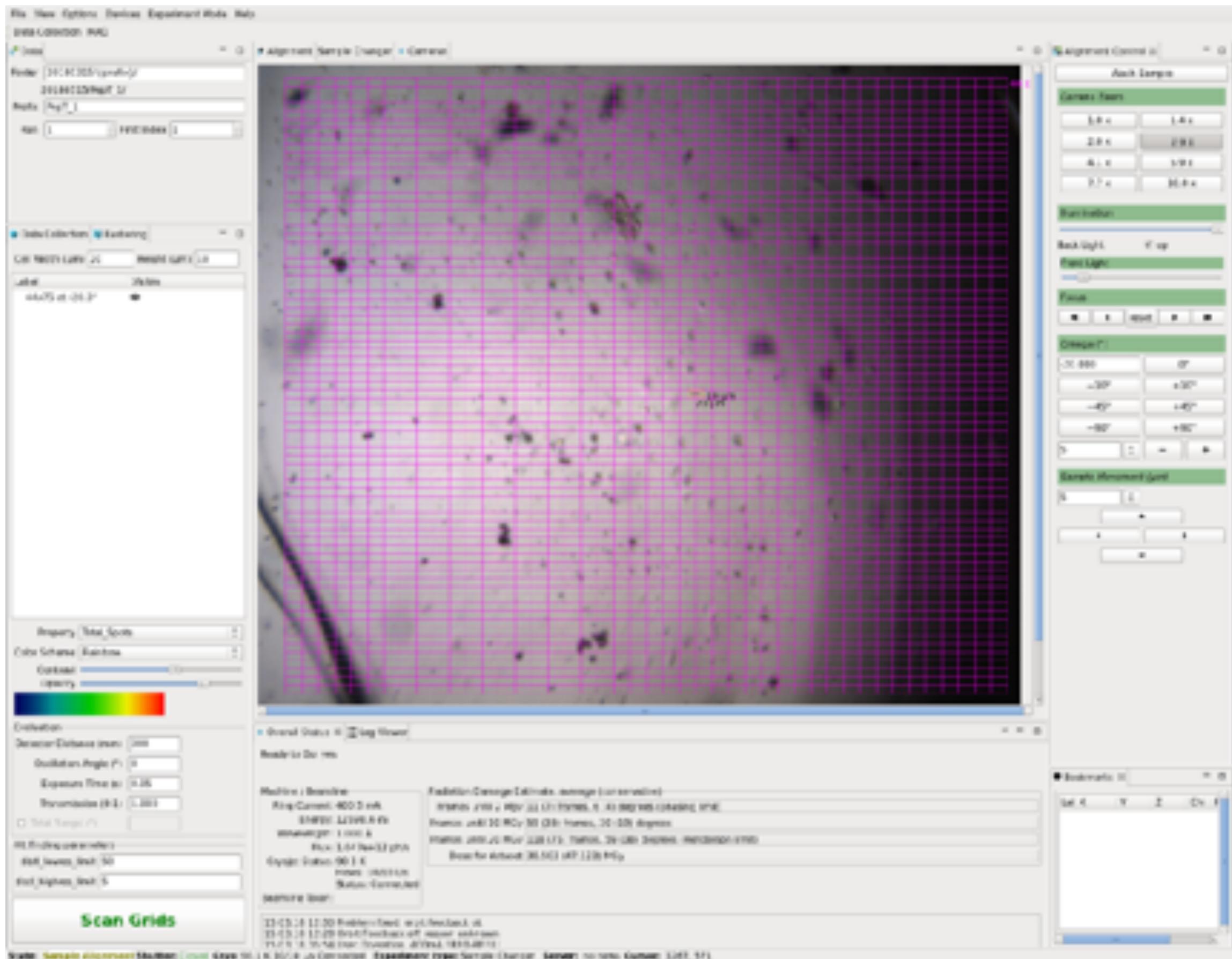
Grid scan & CY+ in sync

DA+ GUI

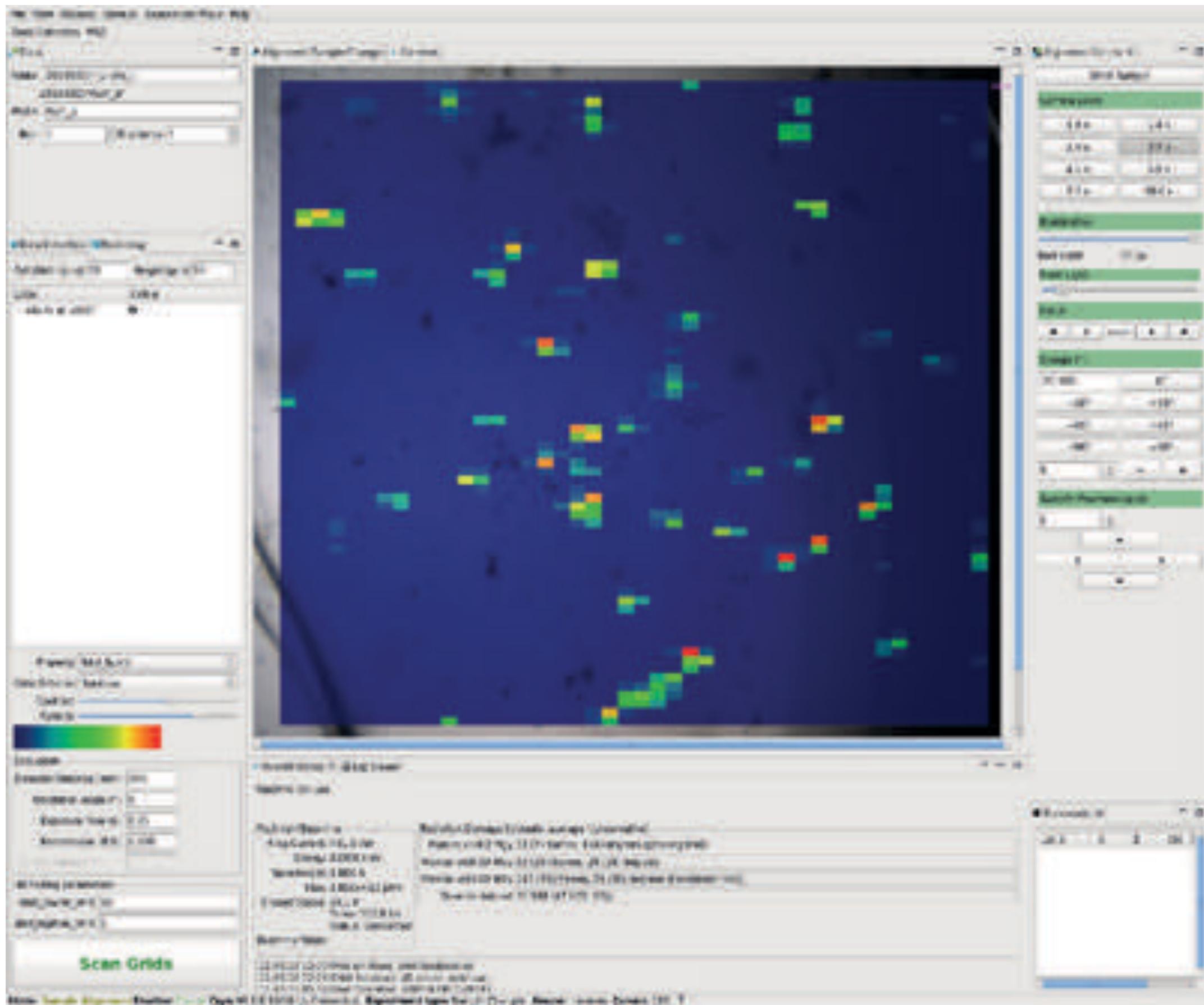


Grid scan & CY+ in sync

DA+ GUI

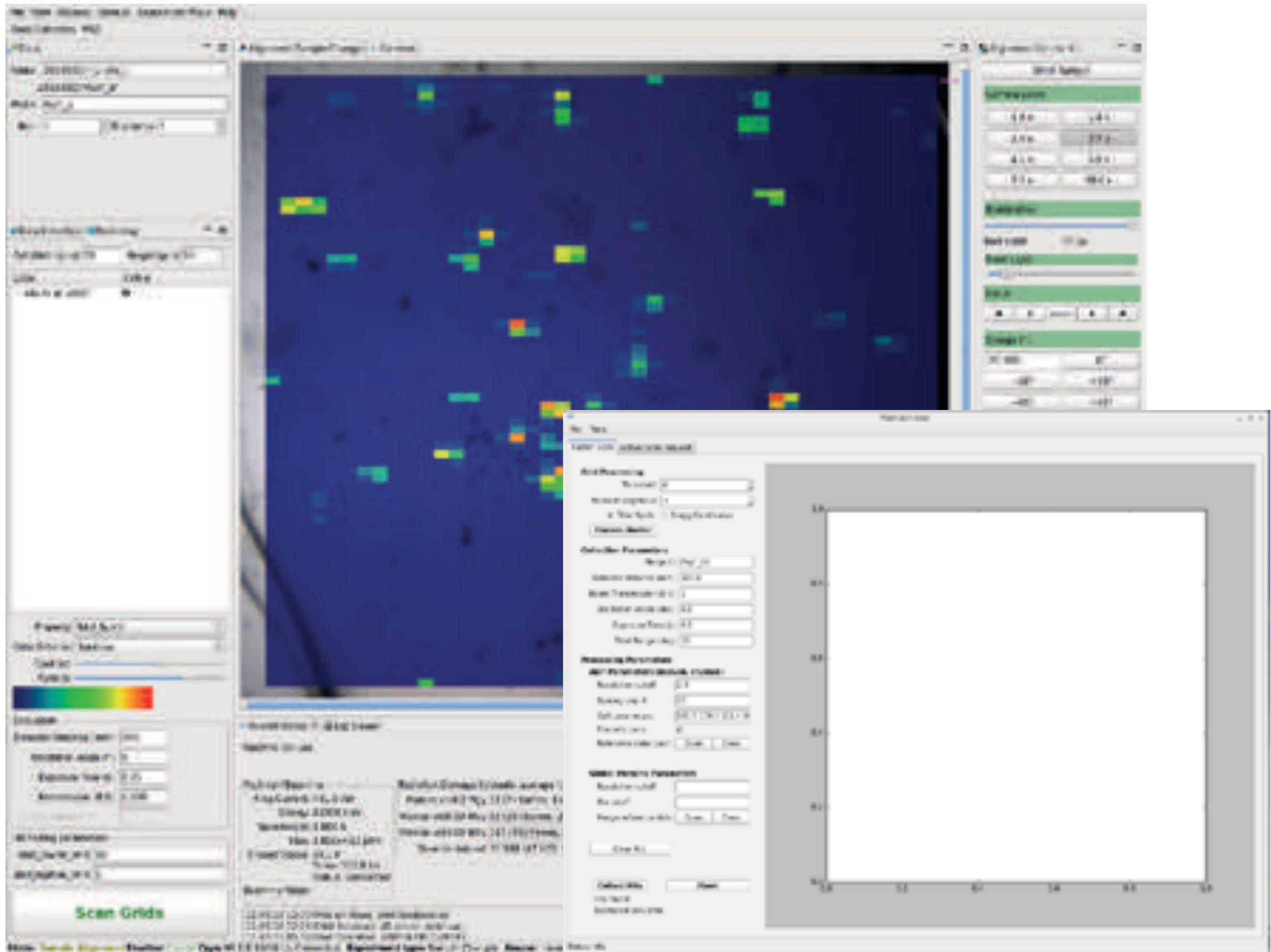


Grid scan & CY+ in sync



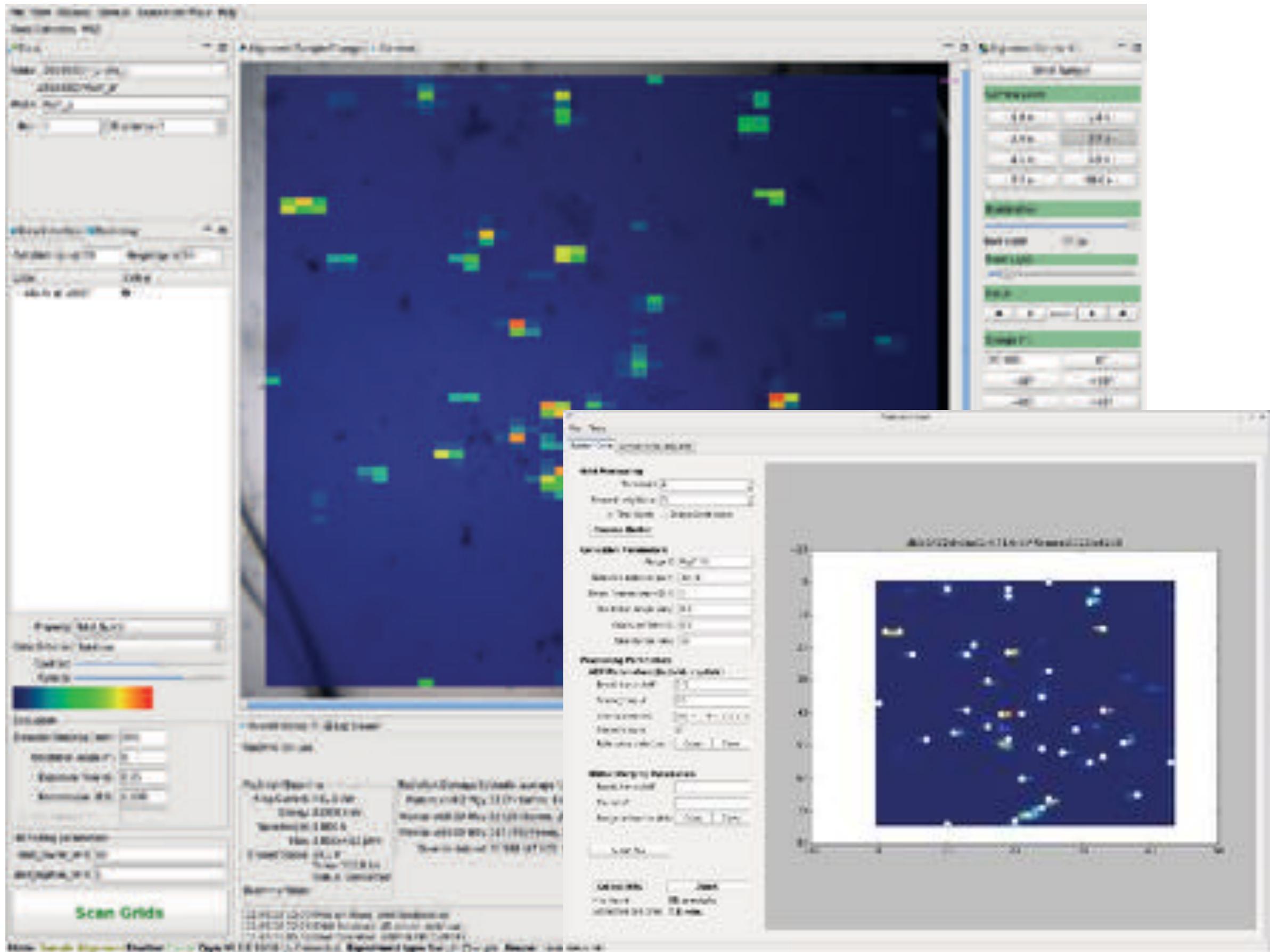
Grid scan & CY+ in sync

CY+ GUI

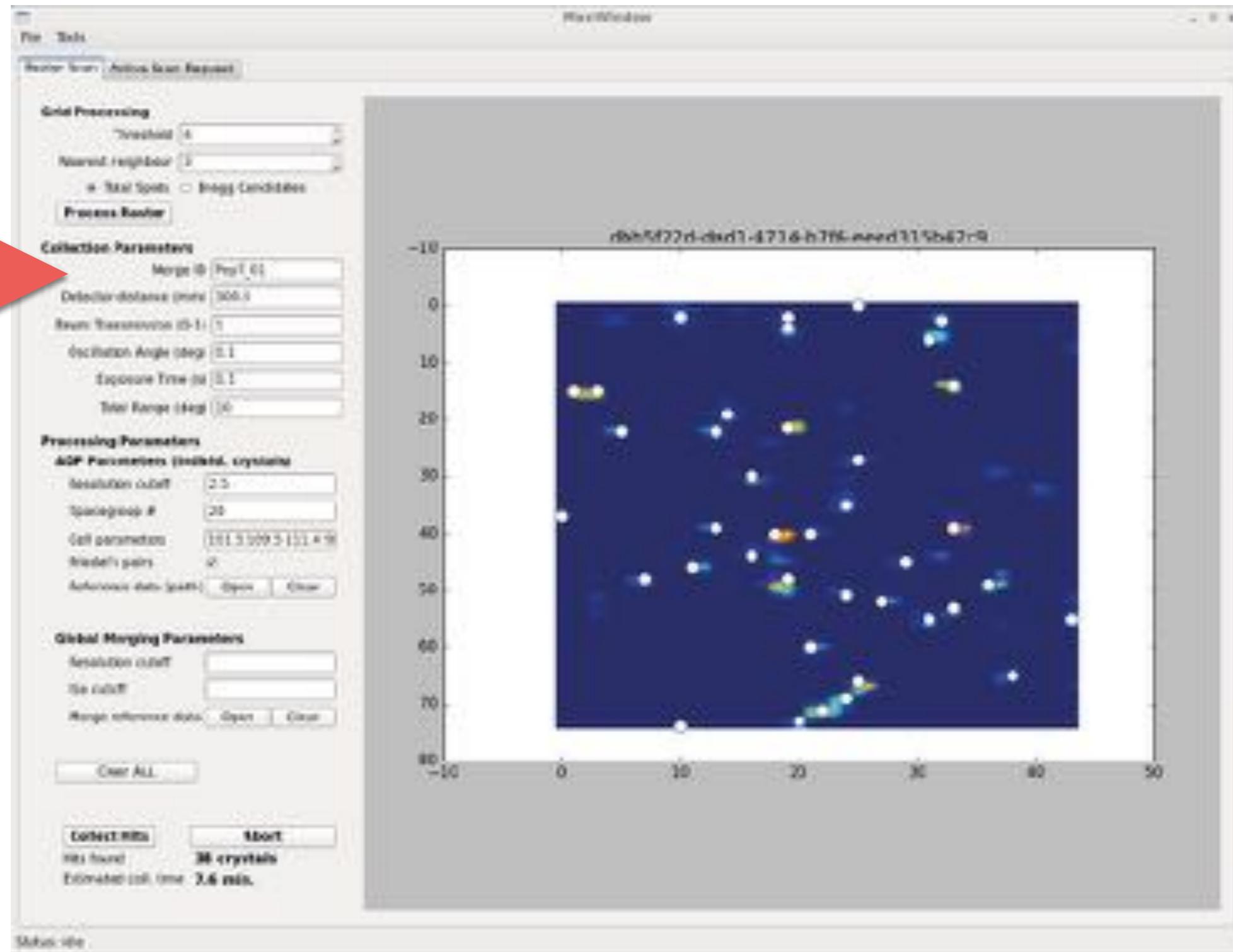


Grid scan & CY+ in sync

CY+ GUI

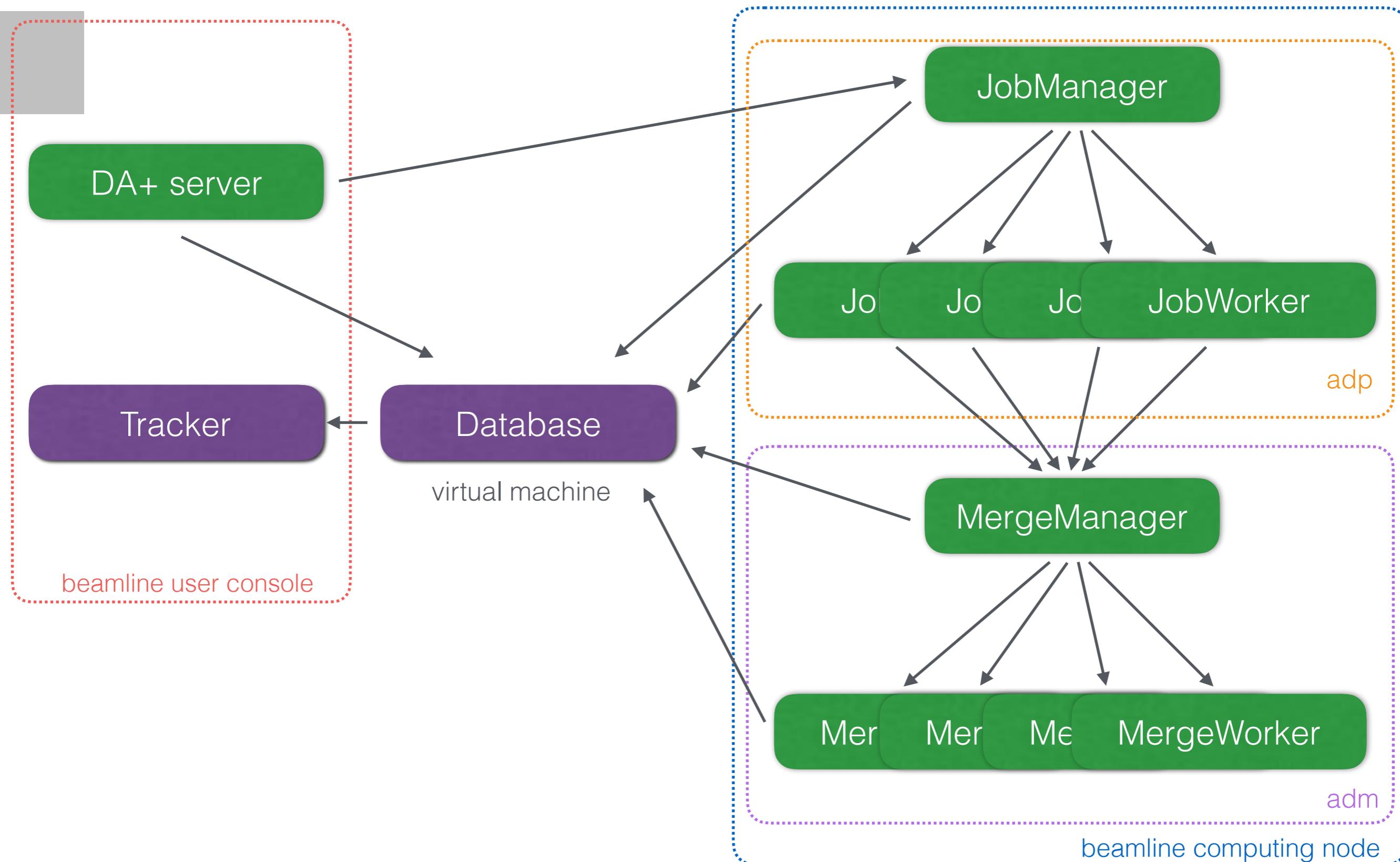


Merge_ID

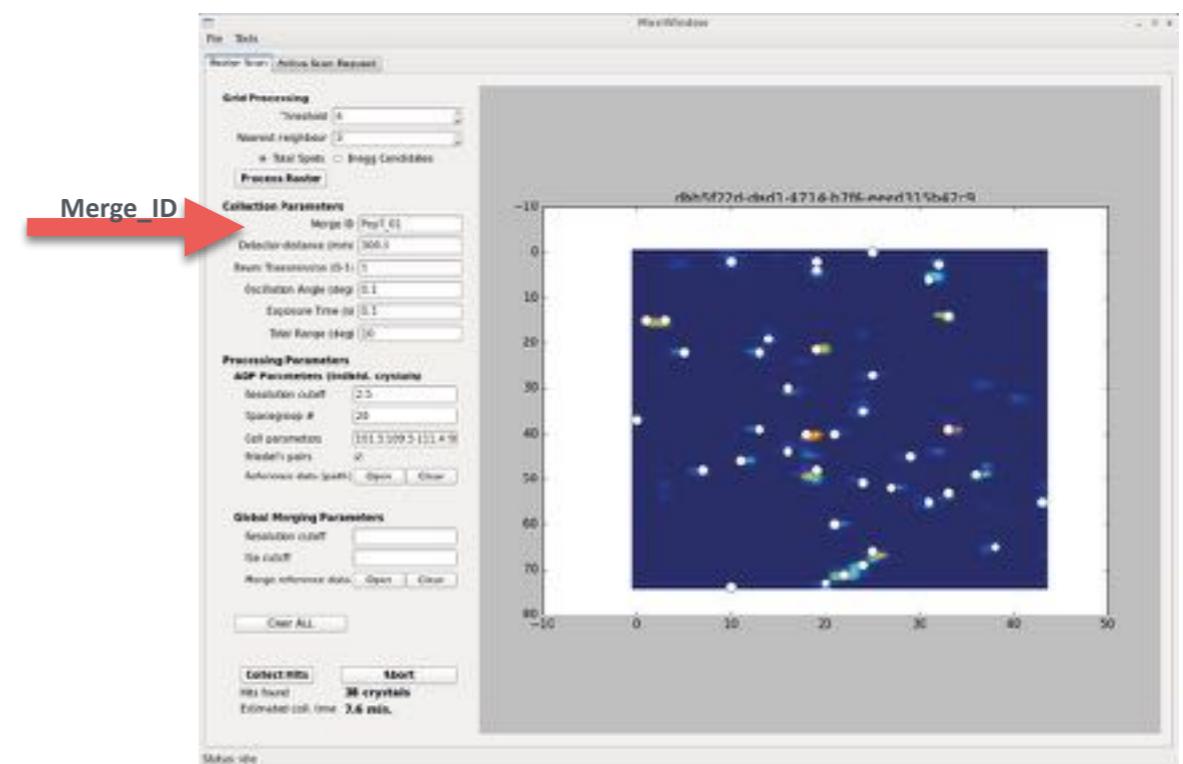


Automatic data merging

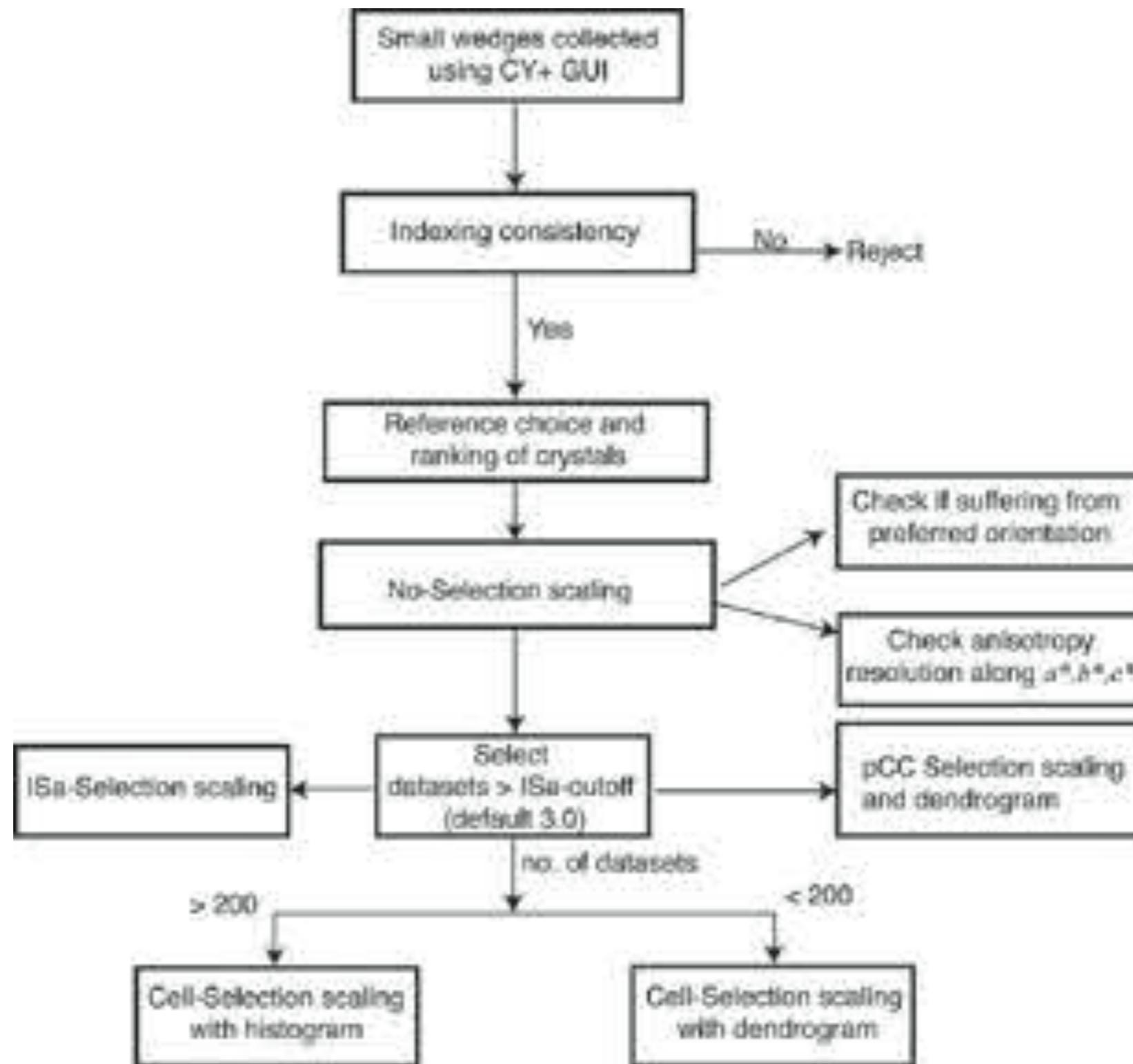
adm



- 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



The sxdm package

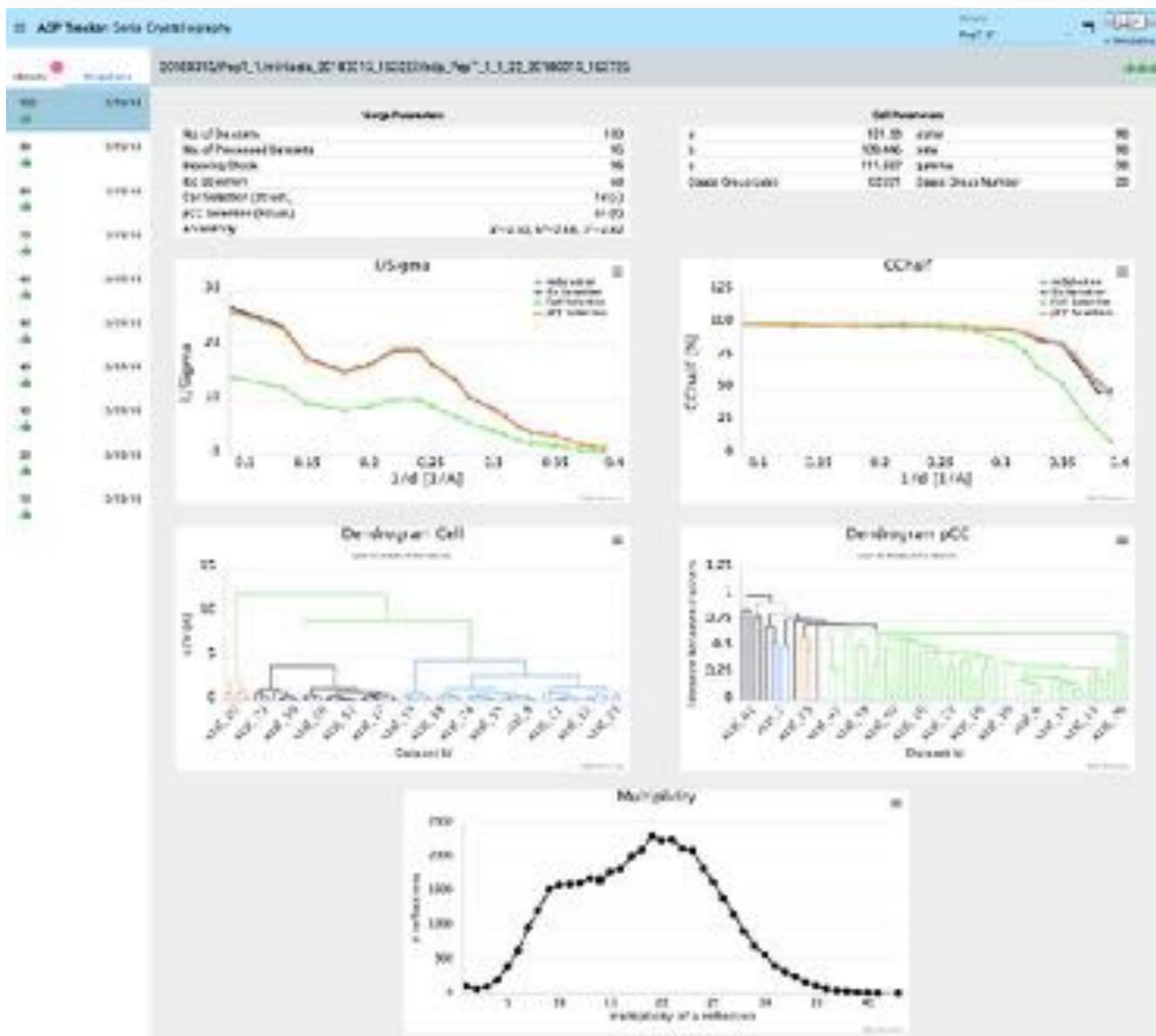


Database & tracker

Tracker

ADP Tracker: Serial Crystallography										PepT	Pept	PEI
Lastest	Minutes	Merged info	20171026/serial-xtal/PepT/minisets_20171026_165051/adp_PepT_1_20171026_165205								details	
PepT	10/26/17	ad ad ad	Experimental Parameters					Crystal Parameters: fast Processing				
PepT	10/26/17	ad ad ad	Collection Angle	0.1	#	182.02	alpha		90			
PepT	10/26/17	ad ad ad	Exposure Time	0.1	#	109.03	beta		90			
PepT	10/26/17	ad ad ad	Max Transverse	1	#	105.45	gamma		90			
PepT	10/26/17	ad ad ad	Number of Images	100	Space Group	C2221	Space Group Number		90			
PepT	10/26/17	ad ad ad	Orientation Estimate	0.000	Sensitivity	0.000	RFA		90			
PepT	10/26/17	ad ad ad	Wavelength	0.9999	Wilson B Factor	45.511						
PepT	10/26/17	ad ad ad	Detector	FR40105004								
Fast processing (angularRange: 20)												
PepT	10/26/17	ad ad ad	mean sin theta / c	0.09	mean sigma / c	0.79	Completeness	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.10	0.09	0.79	0.80	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.11	0.08	0.79	0.81	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.10	0.09	0.79	0.82	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.09	0.09	0.80	0.83	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.08	0.09	0.80	0.84	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.07	0.09	0.80	0.85	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.06	0.09	0.80	0.86	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.05	0.09	0.80	0.87	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.04	0.09	0.80	0.88	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.03	0.09	0.80	0.89	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.02	0.09	0.80	0.90	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.01	0.09	0.80	0.91	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	0.00	0.09	0.80	0.92	0.00	0.00	0.00	0.00	0.00	0.00
Fast indexing (angularRange: 10)												
PepT	10/26/17	ad ad ad	Previous Lattice	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
PepT	10/26/17	ad ad ad	ad	0	75.3	75.4	129.3	90.3	90.3	90.3	90.3	90.3
PepT	10/26/17	ad ad ad	ad	1.0	262.0	126.3	129.3	90.1	90.4	90.4	90.4	90.4
PepT	10/26/17	ad ad ad	ad	1.9	75.3	75.4	129.3	90.7	90.3	90.3	90.3	90.3
PepT	10/26/17	ad ad ad	ad	7.2	75.3	126.3	79.4	90.3	90.3	90.3	90.3	90.3
PepT	10/26/17	ad ad ad	ad	7.7	262.0	126.3	129.3	90.1	90.4	90.4	90.4	90.4
PepT	10/26/17	ad ad ad	ad	22.6	129.3	126.3	129.3	90.5	90.1	90.1	90.1	90.1
PepT	10/26/17	ad ad ad	ad	37.6	75.3	75.4	129.3	90.3	90.3	90.3	90.3	90.3
PepT	10/26/17	ad ad ad	ad	38.8	262.0	79.4	129.3	90.4	90.2	90.2	90.2	90.2
PepT	10/26/17	ad ad ad	ad	42.2	75.3	75.4	126.3	129.3	90.3	90.2	90.2	90.2

Database & tracker



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
- Jakub Kaminski
- Simon Ebner
- Jose Gabadinho
- Shibom Basu
- Chia-Ying Huang
- MX team
- Controls
- IT support

Local contact persons

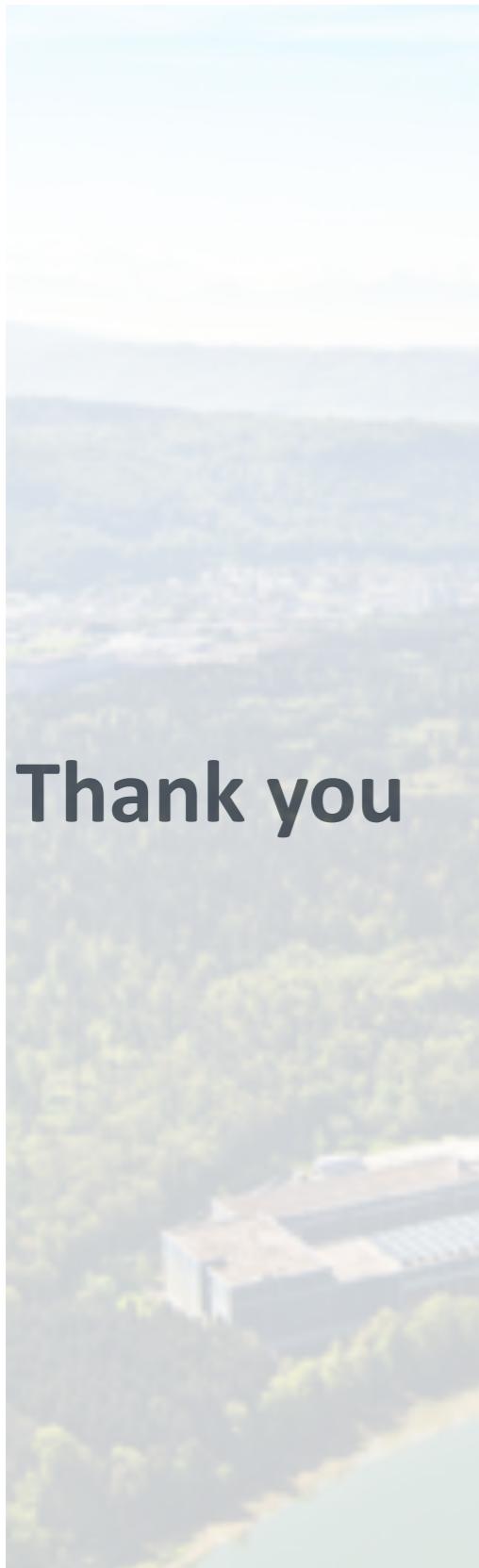
						
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<https://www.psi.ch/macromolecular-crystallography/>



Thank you

