Integrated Real-Time Auto-Processing at Diamond Light Source

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R. Gildea, T. Snow, S. Maheswaran

Introduction

Things used to be both harder and easier…

…Now they are both easier and harder.

Challenges

- Many Beamlines
- All the 4 V's of Big Data
- Driven by relatively uniform systems
  - EPICS + GDA
  - NeXus/HDF5
- Analysis less so...
  - XRD != SAXS != XPDF != XES != XRF != STXM != Ptychography != Tomography....
  - Sometimes best analysis code not developed in-house
  - Faster Experiments -> "Raw-er" data -> more post-processing required
  - Hard work for beamline staff and users
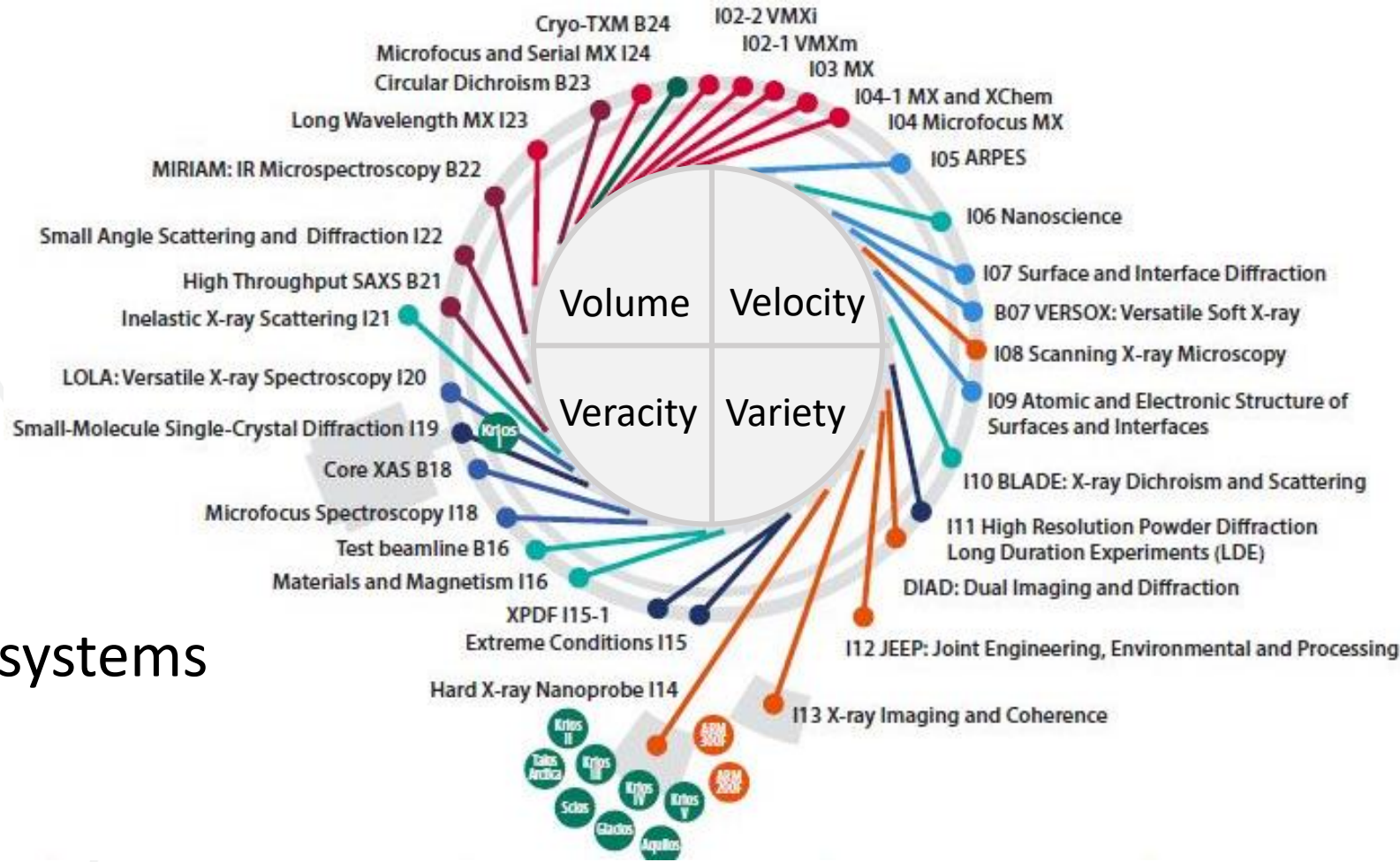
Target Beamline UX

- Experiment/Measurement/Scan triggered
- Start triggers real-time processing for live experiment feedback
    - Raw and Processed data visible during scan
    - (Feedback from real-time processing guides acquisition)
- At end of scan (or live processing), down-stream processing starts
    - Notification of additional processing sent
    - Results of down-stream processing available
- All Results + Provenance visible in LIMS system and (where appropriate) acquisition software
    - Because just generating more files is not good enough – need to see the results
- Ideally, triggering of reprocessing through the same system (SaaS)
- Basically, like an MX experiment…

Available Infrastructure

- Acquisition System

- Access to Metadata/Data

- Access to Compute

- Auto-processing Launcher
  - And applications to actually perform the processing…

- Laboratory Information Management System (LIMS)
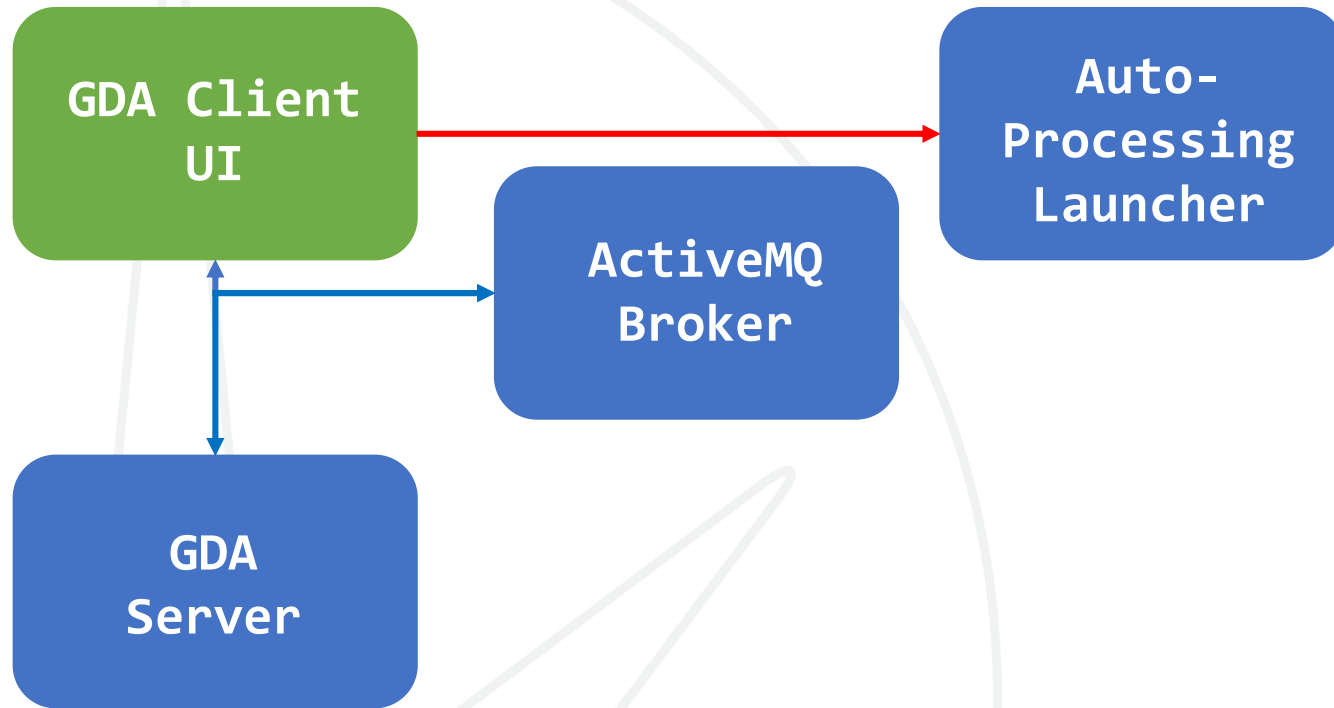
- Mechanisms for all the above to work together!

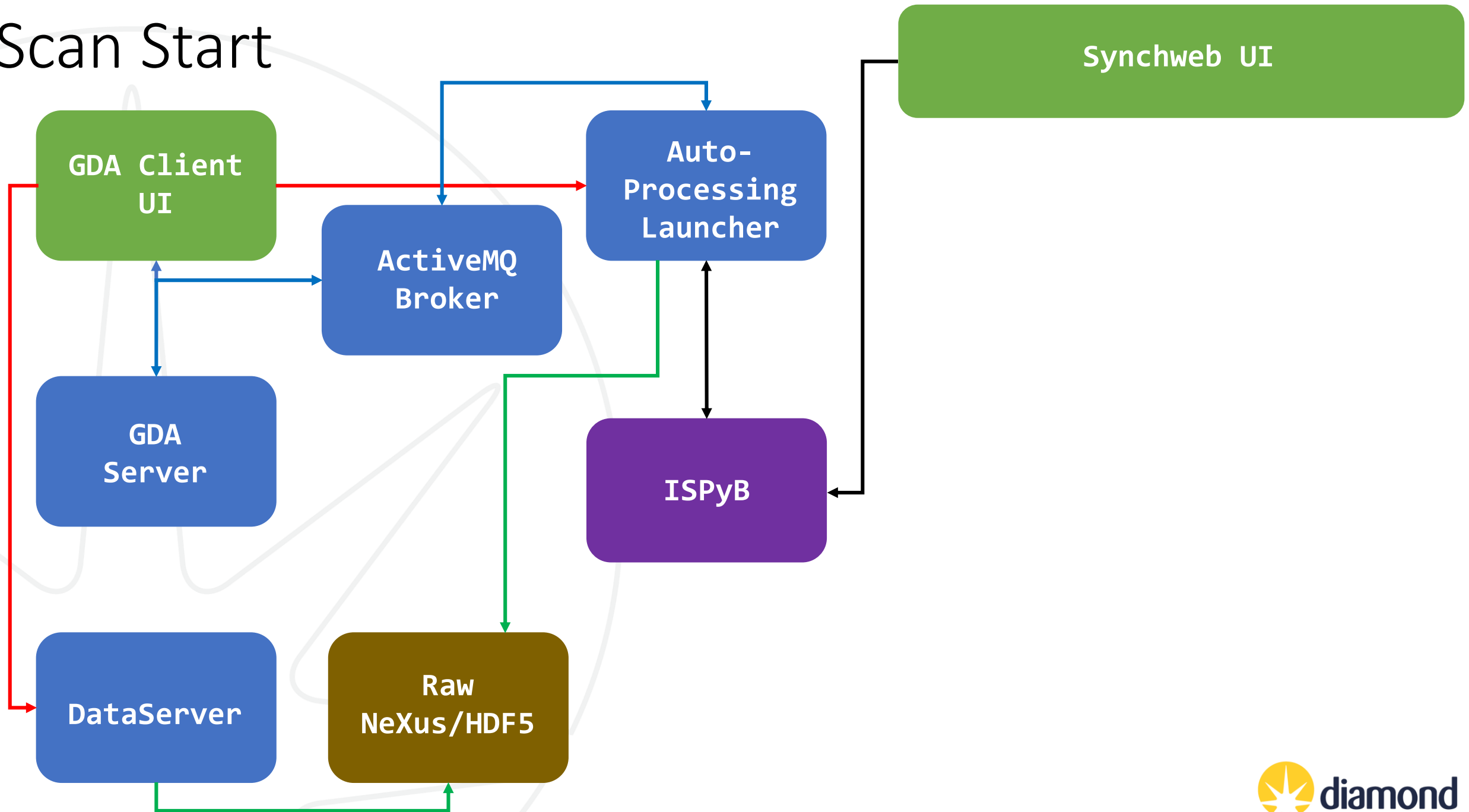# Behind the scenes…
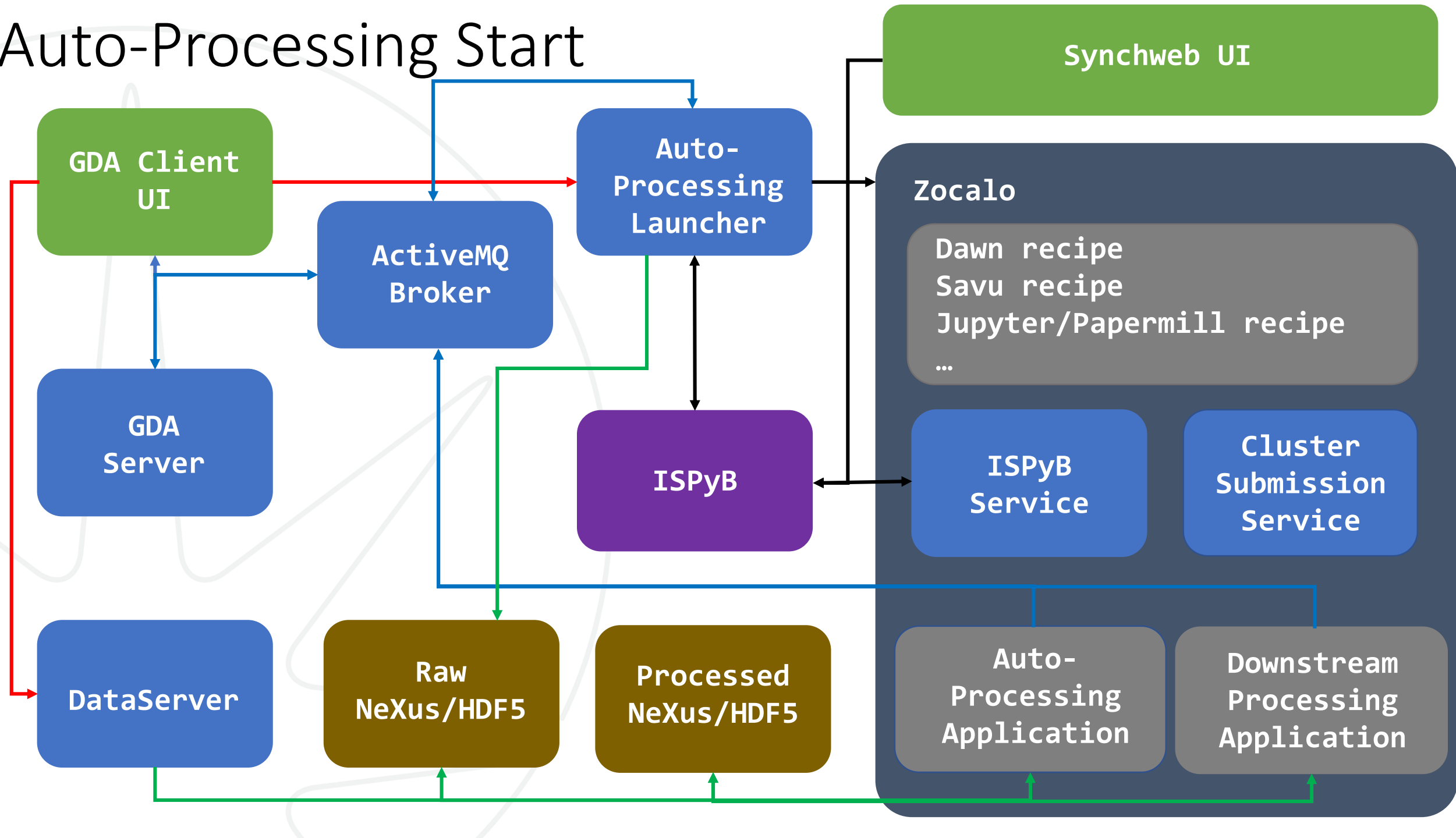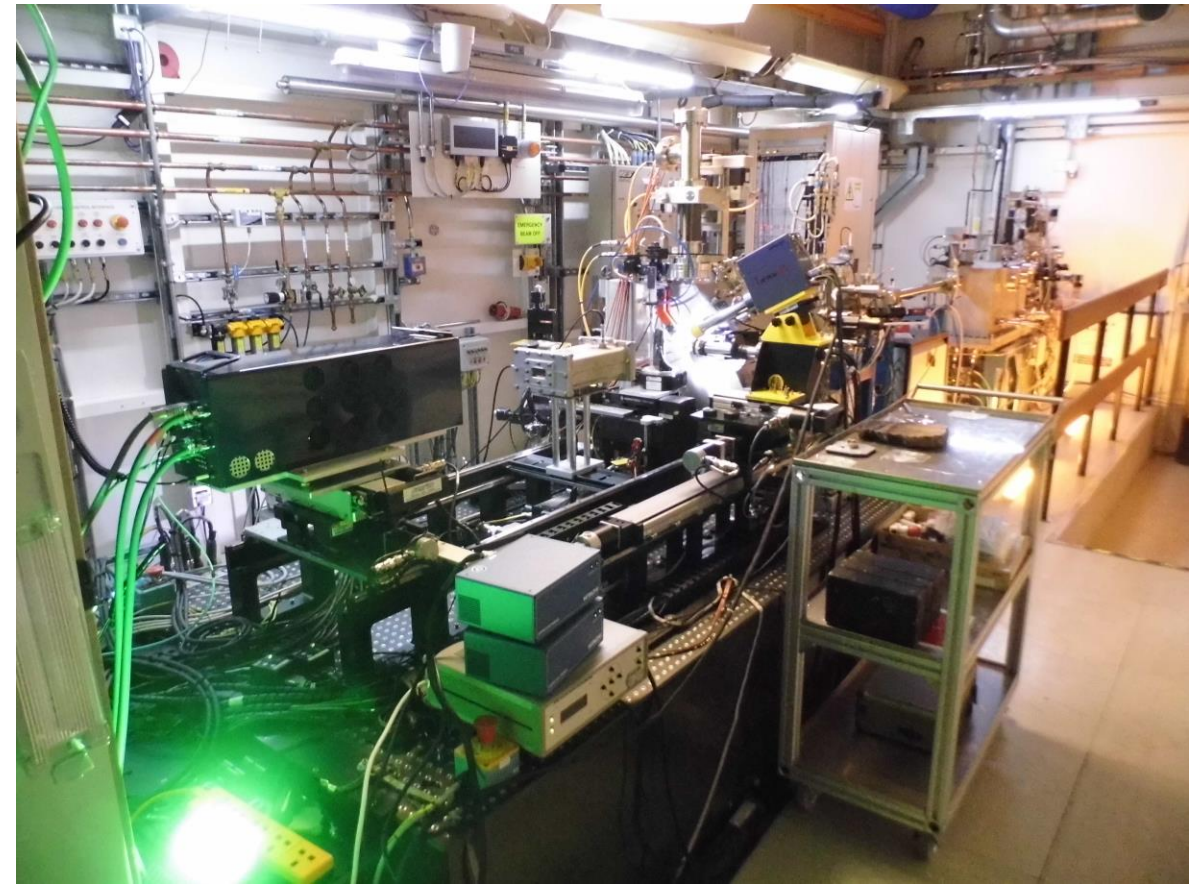
Scan Configuration…

Scan Start

Auto-Processing Start

On The Beamline…

I18 - The Micro-Focus Beamline

- …the analysis of heterogeneous materials in all fields of science in microscopic detail

- XRF and XRD mapping, XRF and XRD tomography, XAS and XANES mapping (+ optical microscope)

- XRF @ 1 kHz (8 x 4K channels – Xspress3)

- XRD @ 100 Hz (3.7 Mpixel – Excalibur)

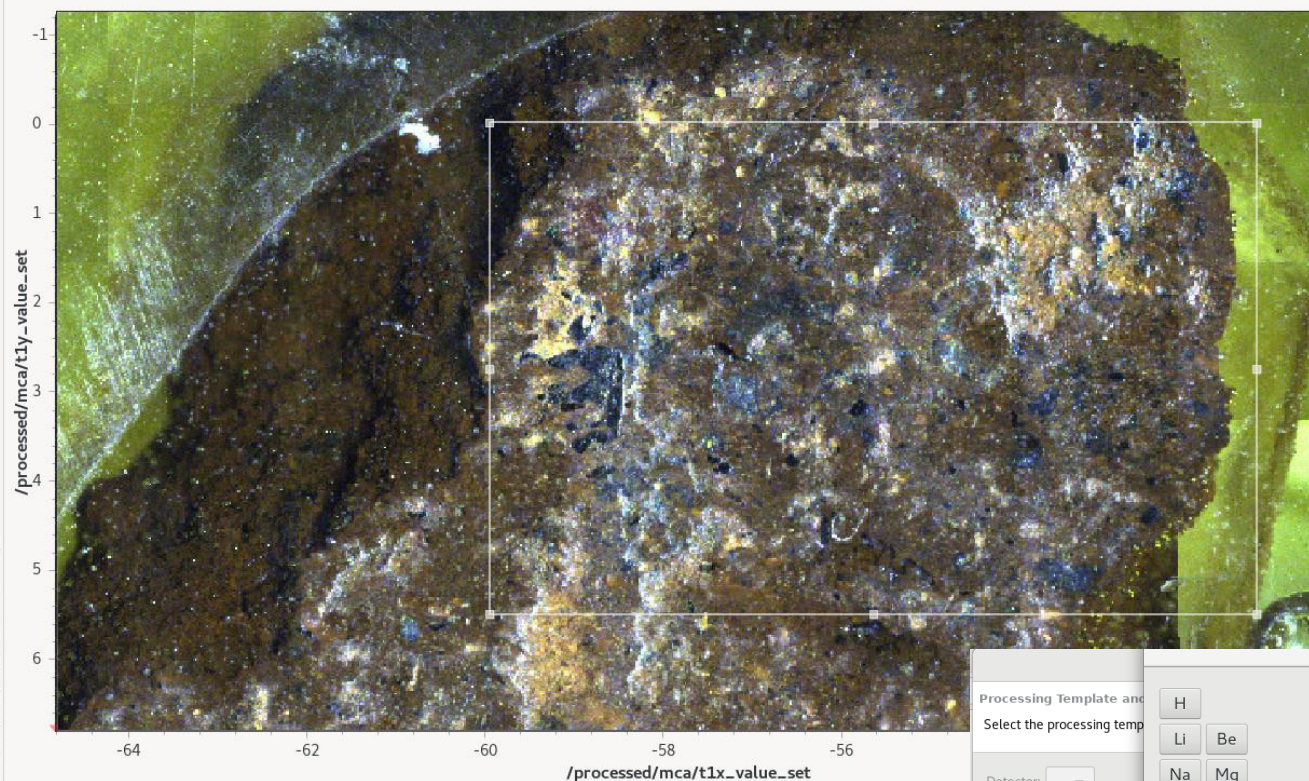Data Acquisition Client - Beamline I18 - 9.26.0

File   Edit   Search   Run   File   Tools   Detector   Window   Help

Reset perspective   Live Background   XY Scan Plot   Run   Experiment   Plot   Scripts   Mapping   DataVis

Mapped Data

Search:

- i18-180440_x_vmastitch.nxs
  - registered_image

Map

/processed/mca/t1y-value_set

/processed/mca/t1x_value_set

Jython Console   Queue

Name	Status	Complete	Date Submitte
Unnamed Sample - Raster Scan	COMPLETE	100%	12 Sep 2022, 21
Unnamed Sample - Raster Scan	TERMINATE	33%	12 Sep 2022, 15
Unnamed Sample - Raster Scan	TERMINATE	71%	12 Sep 2022, 15
Unnamed Sample - Raster Scan	TERMINATE	71%	12 Sep 2022, 14
Unnamed Sample - Raster Scan	TERMINATE	64%	12 Sep 2022, 11
Unnamed Sample - Raster Scan	TERMINATE	67%	10 Sep 2022, 21
Unnamed Sample - Raster Scan	TERMINATE	74%	10 Sep 2022, 10
Unnamed Sample - Raster Scan	TERMINATE	55%	9 Sep 2022, 13:
Unnamed Sample - Raster Scan	TERMINATE	66%	9 Sep 2022, 12:
Unnamed Sample - Raster Scan	TERMINATE	75%	8 Sep 2022, 18:
Unnamed Sample - Raster Scan	TERMINATE	34%	8 Sep 2022, 17:
Unnamed Sample - Raster Scan	TERMINATE	64%	8 Sep 2022, 16:
Experiment_1-MultipleScan_1-Scan_1	COMPLETE	100%	7 Sep 2022, 14:
Experiment_1-MultipleScan_1-Scan_1	COMPLETE	100%	7 Sep 2022, 14:
Experiment_1-MultipleScan_1-Scan_1	COMPLETE	100%	7 Sep 2022, 14:
Experiment_1-MultipleScan_1-Scan_1	COMPLETE	100%	7 Sep 2022, 14:
Unnamed Sample - Raster Scan	TERMINATE	77%	7 Sep 2022, 13:
Unnamed Sample - Raster Scan	COMPLETE	100%	7 Sep 2022, 12:
Unnamed Sample - Raster Scan	COMPLETE	100%	7 Sep 2022, 12:
Unnamed Sample - Raster Scan	TERMINATE	66%	6 Sep 2022, 21:

Mapping Experiment Setup   **Exafs Selection**

Configure Beamline

Script Files

Other Scan Axes

energy_nogap   7100 7150 10;7150 7200 5   6562.5

Detectors

- Xspress3A   1
- Excalibur   0.05
- Xspress3   0.05
- Xspress3 + Excalibur   0.01
- Xspress3 [*]   0.05

Region shape: Rectangle   Scan path: Raster

t1x Start -61.731 mm   t1x Step 0.1 mm
t1x Stop   -58.58   mm   t1y Step 0.1 mm
t1y Start 4.25   mm   Alternating
                         Continuous
t1y Stop   6.233   mm   Orientation Horizontal

Detector Data

800
600
400
200
0
        0   5   10   15   20   25
                  X-Axis

—data[654,425,:] —data[552,309,:] —data[689,1306,:]

Processing Template and

Select the processing temp

Detector:

- Create a new processing
  Processing Template Fi
- Use an existing process
  Processing File:
- Specify application and
  App Name:
  Config File:
- Specify application and s

xrf-i18

Name	
Element List	Fe-Ka, Cu-Ka XRF
Width	20 channels

Periodic table:
H   He
Li Be   B   C   N   O   F   Ne
Na Mg   Al Si P   S   Cl Ar
K   Ca Sc Ti V   Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr
Rb Sr Y   Zr Nb Mo Tc Ru   Ag Cd In Sn Sb Te I   Xe
Cs Ba Lu Hf Ta W   Re Os   Au Hg Tl Pb Bi Po At Rn
Fr Ra Lr Rf Db Sg

La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb
Ac Th Pa U   Np Pu Am Cm Bk Cf Es Fm Md No

- Ka
- Kb
- La
- Lb
- Ma

Cancel   OK

< Back   Next >   Cancel   Finish

i18user   Baton held   No S

File   Edit   Search   Run   File   Tools   Detector   Window   Help

Reset perspective   Live Background   XY Scan Plot   Run   Experiment   Plot   Scripts   Mapping   DataVis

Mapped Data

Search:

- i18-180440_x_vmastitch.nxs
  - registered_image
- i18-186156.nxs
  - Xspress3A
  - Xspress3A_sum [:1156,:1835,0]

Map

/processed/mca/t1y-value_set

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t1y Stop   6.233   mm   Continuous ☑
                           Orientation   Horizontal

Sample Name   Unnamed Sample   Edit metadata...

Processing   Add Processing...

Jython Console   **Queue**

Name   Status   Complete   Date Submitted
Unnamed Sample - Raster Scan   COMPLETE   100%   12 Sep 2022, 21
Unnamed Sample - Raster Scan   TERMINATE   33%   12 Sep 2022, 15
Unnamed Sample - Raster Scan   TERMINATE   71%   12 Sep 2022, 15
Unnamed Sample - Raster Scan   TERMINATE   71%   12 Sep 2022, 14
Unnamed Sample - Raster Scan   TERMINATE   64%
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Unnamed Sample - Raster Scan   TERMINATE   55%
Unnamed Sample - Raster Scan   TERMINATE   66%
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Experiment_1-MultipleScan_1-Scan_1   COMPLETE   100%
Experiment_1-MultipleScan_1-Scan_1   COMPLETE   100%
Experiment_1-MultipleScan_1-Scan_1   COMPLETE   100%
Experiment_1-MultipleScan_1-Scan_1   COMPLETE   100%
Unnamed Sample - Raster Scan   TERMINATE   77%
Unnamed Sample - Raster Scan   COMPLETE   100%
Unnamed Sample - Raster Scan   COMPLETE   100%
Unnamed Sample - Raster Scan   TERMINATE   66%

0   0   22-04-2022 01:37:02 -   /dls/i18/data/2022/cm31141-2/i18-186156.nxs

Group: 1 Data Collections   Beam Centre: NaN x NaN
Wavelength: 0.0000Å   Detector Distance: NaNmm
Exposure: 0.0029s   Beamsize: 0x0µm
No. Images: Detector: Quantum Detectors Xspress 3
Comment: Unnamed Sample - No description provided.
Scan Parameters:

Data Files   Download

Auto Processing

Jupyter Autoprocessing:

Data Acquisition Client - Beamline I18 - 9.26.0

File   Edit   Search   Run   File   Tools   Detector   Window   Help

Reset perspective   Live Background   XY Scan Plot   Run   Experiment   Plot   Scripts   Mapping   DataVis

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- i18-186156.nxs
  - Xspress3A
  - Xspress3A_sum
- i18-186156_xrf_window_jf.nxs
  - mca
  - Zn-Ka
  - Ni-Ka
  - Fe-Ka

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/processed/mca/t1y-value_set

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t1y Start   4.25   mm   Alternating ☑
t1y Stop   6.233   mm   Continuous ☑
                        Orientation   Horizontal

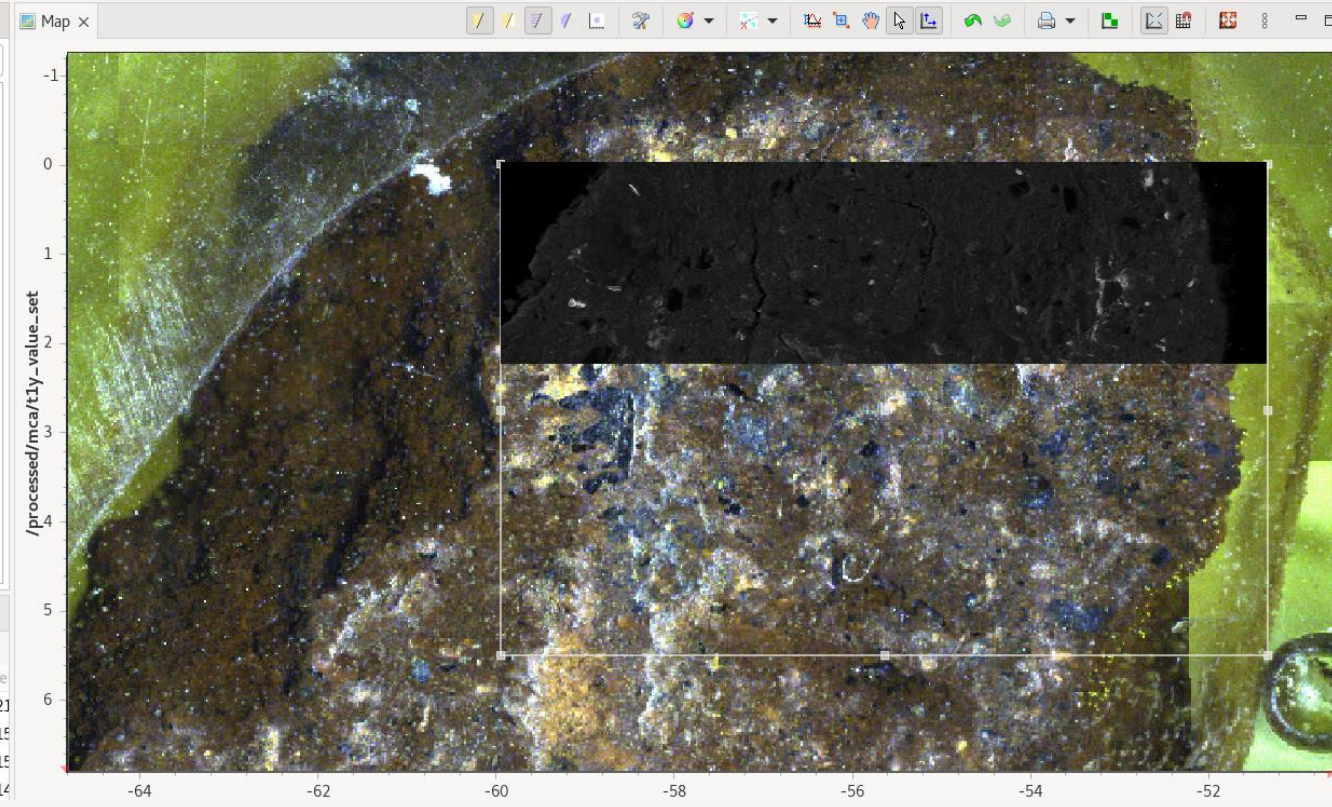Sample Name   Unnamed Sample   Edit metadata...

Processing   Add Processing...

Jython Console   Queue

Name   Status   Complete   Date Submitte
Unnamed Sample - Raster Scan   COMPLETE   100%   12 Sep 2022, 2
Unnamed Sample - Raster Scan   TERMINATE   33%   12 Sep 2022, 15
Unnamed Sample - Raster Scan   TERMINATE   71%   12 Sep 2022, 15
Unnamed Sample - Raster Scan   TERMINATE   71%   12 Sep 2022, 14
Unnamed Sample - Raster Scan   TERMINATE   64%
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Experiment_1-MultipleScan_1-Scan_1   COMPLETE   100%
Experiment_1-MultipleScan_1-Scan_1   COMPLETE   100%
Unnamed Sample - Raster Scan   TERMINATE   77%
Unnamed Sample - Raster Scan   COMPLETE   100%
Unnamed Sample - Raster Scan   COMPLETE   100%
Unnamed Sample - Raster Scan   TERMINATE   66%

22-04-2022 01:37:02 -   /dls/i18/data/2022/cm31141-2/i18-186156.nxs

Group: 1 Data Collections   Beam Centre: NaN x NaN

Wavelength: 0.0000Å   Detector Distance: NaNmm

Exposure: 0.0029s   Beamsize: 0x0µm

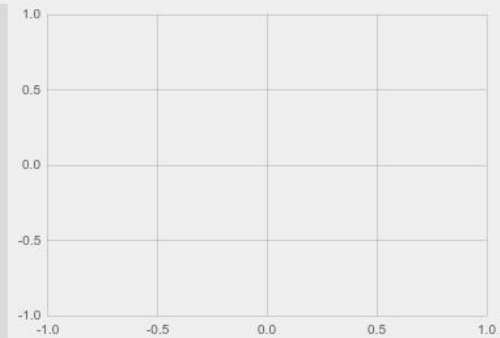No. Images: Detector: Quantum Detectors Xspress 3

Comment: Unnamed Sample - No description provided.

Scan Parameters:

Data Files   Download

Auto Processing

Jupyter Autoprocessing:

Data Acquisition Client - Beamline I18 - 9.26.0

File Edit Search Run File Tools Detector Window Help

Reset perspective Live Background XY Scan Plot Run Experiment Plot Scripts Mapping DataVis

Mapped Data

Search:

- i18-180440_x_vmastitch.nxs
  - registered_image
- i18-186156.nxs
  - Xspress3A
  - Xspress3A_sum
- i18-186156_xrf_window_jf.nxs
  - mca
  - Zn-Ka
  - Ni-Ka
  - Fe-Ka

Map

/processed/mca/t1y-value.set

-64   -62   -60   -58   -56   -54   -52

Jython Console   Queue

Name | Status | Complete | Date Submitte
Unnamed Sample - Raster Scan | COMPLETE | 100% | 12 Sep 2022, 21
Unnamed Sample - Raster Scan | TERMINATE | 33% | 12 Sep 2022, 15
Unnamed Sample - Raster Scan | TERMINATE | 71% | 12 Sep 2022, 15
Unnamed Sample - Raster Scan | TERMINATE | 71% | 12 Sep 2022, 14
Unnamed Sample - Raster Scan | TERMINATE | 64% |
Unnamed Sample - Raster Scan | TERMINATE | 67% |
Unnamed Sample - Raster Scan | TERMINATE | 74% |
Unnamed Sample - Raster Scan | TERMINATE | 55% |
Unnamed Sample - Raster Scan | TERMINATE | 66% |
Unnamed Sample - Raster Scan | TERMINATE | 75% |
Unnamed Sample - Raster Scan | TERMINATE | 34% |
Unnamed Sample - Raster Scan | TERMINATE | 64% |
Experiment_1-MultipleScan_1-Scan_1 | COMPLETE | 100% |
Experiment_1-MultipleScan_1-Scan_1 | COMPLETE | 100% |
Experiment_1-MultipleScan_1-Scan_1 | COMPLETE | 100% |
Experiment_1-MultipleScan_1-Scan_1 | COMPLETE | 100% |
Unnamed Sample - Raster Scan | TERMINATE | 77% |
Unnamed Sample - Raster Scan | COMPLETE | 100% |
Unnamed Sample - Raster Scan | COMPLETE | 100% |
Unnamed Sample - Raster Scan | TERMINATE | 66% |

Mapping Experiment Setup   Exafs Selection

Configure Beamline

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Other Scan Axes

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Xspress3 [*]   0.05

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t1x Start -61.731 mm   t1x Step 0.1   mm
t1x Stop -58.58   mm   t1y Step 0.1   mm
t1y Start 4.25   mm   Alternating
t1y Stop 6.233   mm   Continuous
                        Orientation Horizontal

Sample Name Unnamed Sample   Edit metadata...

Processing   Add Processing...

22-04-2022 01:37:02 - /dls/i18/data/2022/cm31141-2/i18-186156.nxs

Group: 1 Data Collections   Beam Centre: NaN x NaN
Wavelength: 0.0000Å   Detector Distance: NaNmm
Exposure: 0.0029s   Beamsize: 0x0µm
No. Images: Detector: Quantum Detectors Xspress 3
Comment: Unnamed Sample - No description provided.
Scan Parameters:

1500
1250
1000
750
500
250
0
   0   5   10   15   20   25   30   35   40

Data Files   Download

Auto Processing

Jupyter Autoprocessing:

https://ispyb.diamond.ac.uk/dc/visit/cm31141-2/s/615

Comment:

Scan Params:
  title:scan t1x -58.775 -58.754 0.001 counterTimer01 0.2

Data Files   ⬇ Download

Auto Processing   Jupyter Autoprocessing: ✔

22-04-2022 07:24:26 - ▶ i18-186159.nxs

Group: 1 Data Collections   Beam Centre: NaN x NaN

Wavelength: 0.0000Å   Detector Distance: NaNmm

Exposure: 0.0029s   Beamsize: 0x0µm

No. Images: Detector: Quantum Detectors Xspress 3

Comment: Unnamed Sample - No description provided.

Scan Parameters:

Attachments: jupyter autoprocessing

Attachments

File	Type	
i18-186159_xrf_window_jf.nxs	Result	⬇ Download
i18-186159_xrf_window_jf.ipynb	Result	⬇ Download
i18-186159_xrf_window_jf.html	Log	⬇ Download 🔍 View

15 ▾ Page « ‹ 1 › »

Close

Data Files   ⬇ Download

Auto Processing   Jupyter Autoprocessing: ✔

jupyter autoprocessing

🗎 Archive   🗎 Logs & Files

Processing Programs	Comments	Message	Start Time	End Time
Jupyter Autoprocessing	Running Jupyter on /dls/i18/data/2022/cm31141-2/i18-186159.nxs	Processing Successful	2022-04-22 07:24:29	2022-04-22 07:54:41

In [1]:
```python
# Parameters
element_list = "C-Ka Co-Ka Fe-Ka Ni-Ka Zn-Ka"
window_width = 40
inpath = "/dls/i18/data/2022/cm31141-4//i18-190813.nxs"
outpath = "/dls/i18/data/2022/cm31141-4/processed/i18-190813_xrf.nxs"
```

diamond

Key Components…

Live Processing using SWMR

- NeXus tagging used for metadata
- DAWN or SWMRtools (python)
- High performance SWMR not completely trivial…
- For write performance data is Blosc compressed, direct-chunk written
  - Either with or without Virtual Dataset (VDS)
- Best read performance using direct-chunk read
  - Need to then decompress
  - Fast small reads/writes can slow file writer (on GPFS @ 1kHz)
  - VDS not chunked – need to access the source datasets
- With this can read fast in a single process
  - currently benchmarking direct chunk read -> blosc -> pyFAI on GPU for real time XRD

GDA-Zocalo-Connector (Autoprocessing Launcher)

- Subscribes to GDA scan messages

- Unpacks metadata from NeXus
  - Record ISPyB DataCollectionGroup/DataCollection

- Determines default processing
  - Beamline name and NeXus structure
  - i.e. If B18 and XAFS -> run Larch
  - Adds to processing request

- Unpacks processing request from scan message
  - Inserts appropriate ProcessingJob/Parameters
  - Submits to Zocalo

- Exposes Processing Types and associated Parameters via REST api
  - For guided configuration in the GDA client

ISPyB/Synchweb/Zocalo

- ISPyB
  - Rich set of tables for structural biology LIMS
  - Some tables contain generic information
  - Allows recording of metadata from scans and auto-processing
  - (and the relationships between them)

- Synchweb
  - Auth/Auth access to ISPyB
  - Visit event view shows generic information

- Zocalo
  - "Runs processing"
  - Integrates with compute and ISPyB

`qsub …`

Sample: ins7	Group: 14 Data Collections
Flux: 9.20e-1	Ω Start: -32.5°
Ω Osc: 0.10°	Ω Overlap: 0°
No. Images: 50	Resolution: 1.82Å
Wavelength: 0.6702Å	Exposure: 0.0100s
Transmission: 100.00%	Beamsize: 7x7µm
Type: SAD	
Comment: (-6,-3879,1115)	

15-07-2022 13:53:09 - ▶ Test_Insulin/ins7/ins7_b104_1_master.h5

Auto Processing — fast_dp: ✓ xia2 dials: ✗ xia2 3dii: ✓ autoPROC: ✓ autoPROC+STARANISO: ✓

Downstream Processing — fast_ep: ✗

Inside Zocalo…

- Richards Talk…
- For Physical Sciences:
    - Largely applications ran in wrappers
    - Data goes from HDF5 to HDF5
    - **DAWN/Savu/Ptypy** but also Python using Papermill and Jupyter (which give **PyMCA**, **PyFAI**, **TomoPy**, **Larch**, **Scikit-learn**, **Scikit-image**….)
    - Main benefit of Zocalo is the abstraction around LIMS and HPC

diamond

Papermill wrapper

- Template notebook written by Analysis/Beamline/User

- Takes parameters from ISPyB database

- Papermill – Injects params into a template Jupyter notebook

- Executes notebook in the specified python environment (currently using Module and Conda)

- Broadcasts the result files back to zocalo for further processing

- Basic visualisation and provenance

i18-190813_xrf.html Log File

```
In [1]:    # Parameters
           element_list = "C-Ka Co-Ka Fe-Ka Ni-Ka Zn-Ka"
           window_width = 40
           inpath = "/dls/i18/data/2022/cm31141-4//i18-190813.nxs"
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```

XRD-Tomography

- 2D Scan of stage_x, stage_theta

- Live reduction of data with PyFAI

- Post-reduction reconstruction with TomoPy

- Post-reconstruction investigation with Scikit-Learn
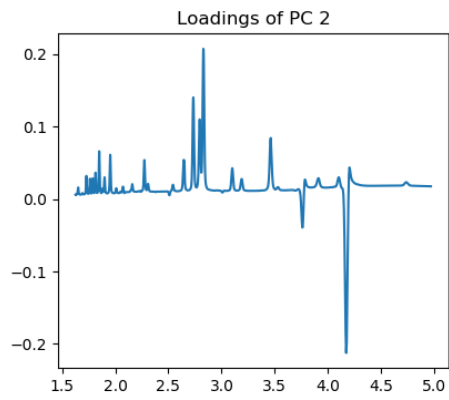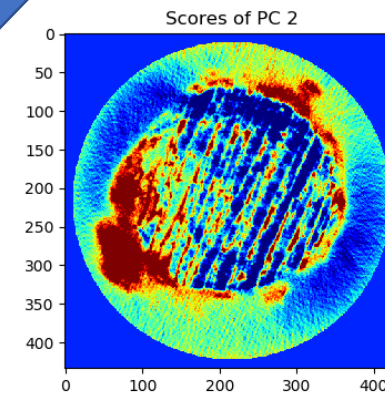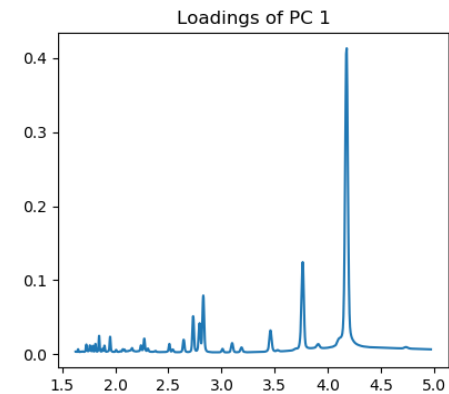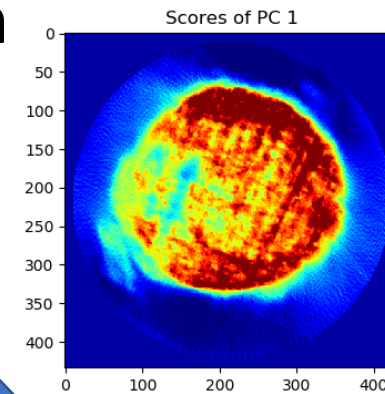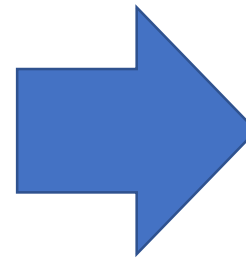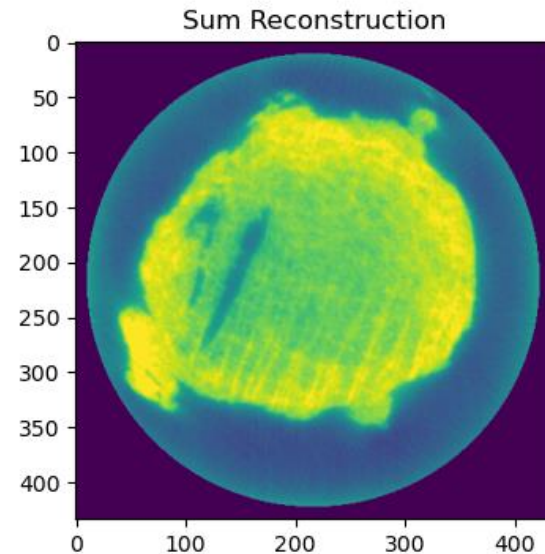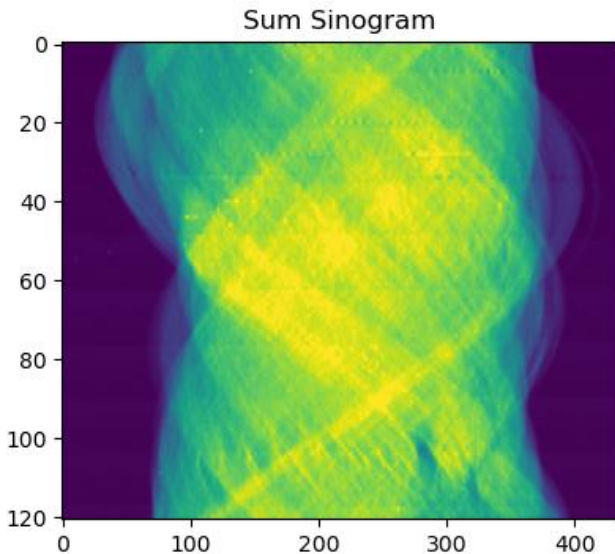
Conclusions

- Generic deployment of real-time auto-processing is complicated
- Lots of infrastructure needed
- Making results easily findable is critical
- As is provenance
- Information management systems are key
- Lots of good open-source tools
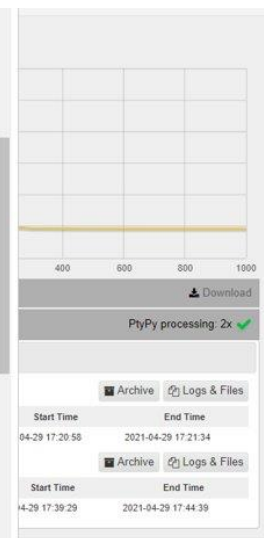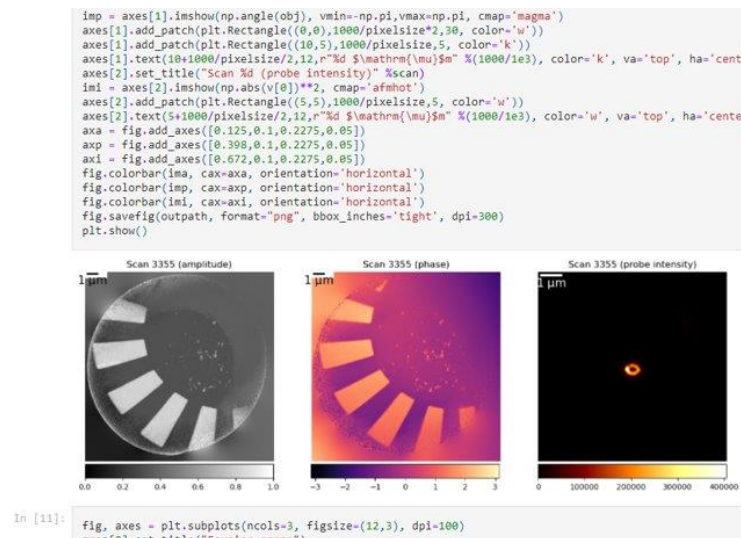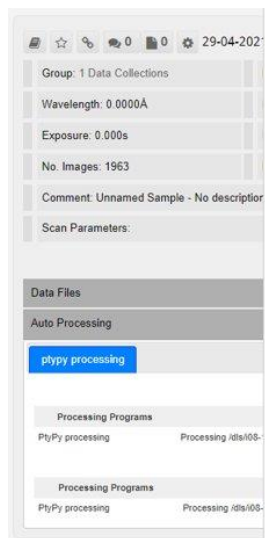
If you are interested in ptychography there is a PtyPy workshop at DLS 12/13th Jan 2023