Detectors and Calibration (Processing)

Data Analysis & Karabo Workshop, 23.01.2018

Steffen Hauf

Overview

- Detectors @ European XFEL
- Detector Calibration
  - Tools we use
  - Online Calibration
  - Offline Calibration
  - Characterization Processing
  - Documentation
  - Simulations

- With contributions from AGIPD, DSSC and LPD consortia, first users and instruments, DET, CAS, ITDM, ….

- 5 user beam times, 2 commissioning beam times + commissioning time → ~300 hours of data taking for both detectors.
  Detector up-time currently ~ 90%

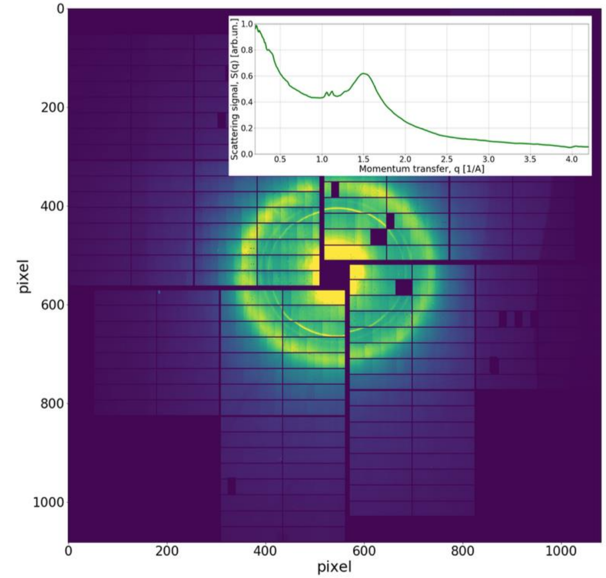
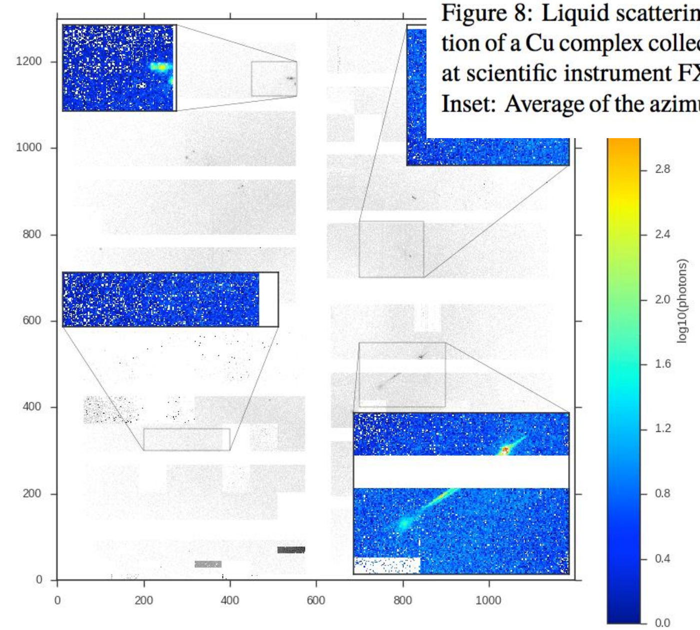


Figure 8: Liquid scattering pattern of tetrahydrofuran solution of a Cu complex collected with the LPD detector [23,24] at scientific instrument FXE [25](corrected for dark offset). Inset: Average of the azimuthally integrated set of 150 image.

LPD 1M

AGIPD 1M



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LPD @ FXE

Experiment/proposal	Number of hours	Raw data size [TB]
p2016	60	4.1
p2073	60	2.3
p2052	60	3.9
p2072	48	20
p2050	60	27
Total	**288 h**	**57 TB**

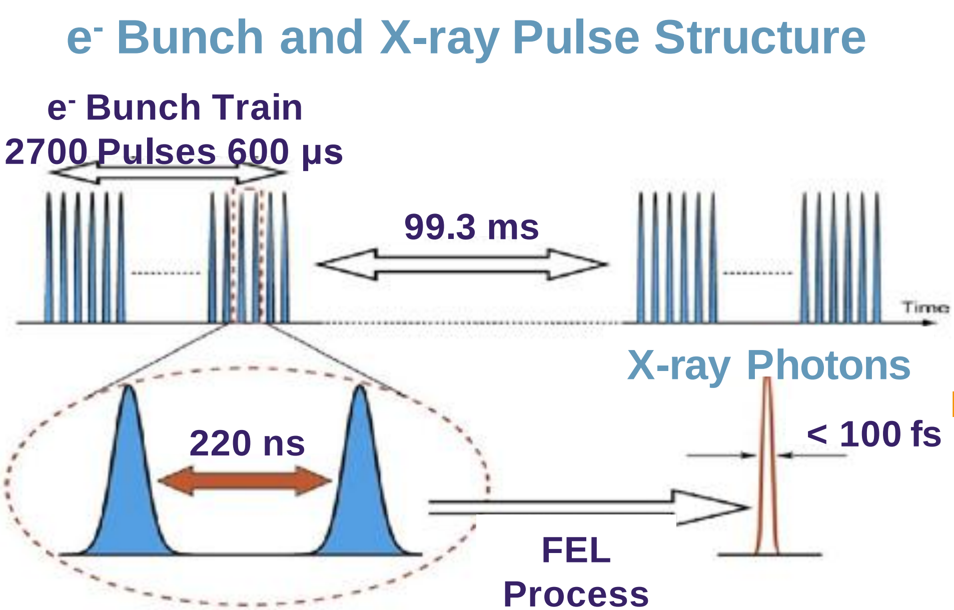
AGIPD @ SPB

Experiment/proposal	Number of hours	Raw data size [TB]
p2012	60	57
p2042	60	87
p2017	60	49
p2066	48	80
p2013	60	116
Total	**288 h**	**389 TB***

*** Double size images, X-rays in every 2nd image**

Detectors: from First Ideas to User Operation – 2006 til 2017

- The European XFEL pulse structure poses strict constraints on detectors (e.g. intensity and time structure)
- No commercial imaging detectors available
- Call for expression of interest launched in 2006
- 3 project proposals were selected with the goal to finally have at least one fast 2D imaging detector




European XFEL Project Team
c/o Deutsches Elektronen-Synchrotron DESY
in der Helmholtz-Gemeinschaft,
Notkestraße 85,
D-22607 Hamburg, Germany

XFEL
X-Ray Free-Electron Laser

Call by the:

European Project Team for the X-ray Free-Electron Laser

for:

Expressions of Interest

to:

Develop and Deliver
Large Area Pixellated X-ray Detectors.

Deadline: 30 September 2006
http://xfel.desy.de/xfelhomepage

- Selected proposals

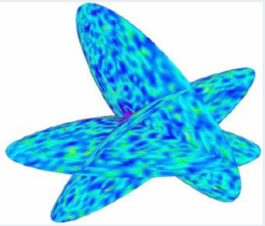
Adaptive Gain Integrating Pixel Detector
Large Pixel Detector
DEPFET Sensor with Signal Compression

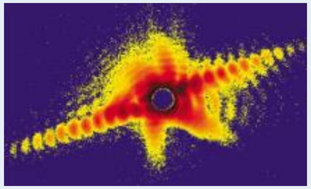
XFEL Scientific Instruments

Hard X-Rays

SPB **Single Particles, Clusters and Biomolecules and Serial Femtosecond Crystallography**

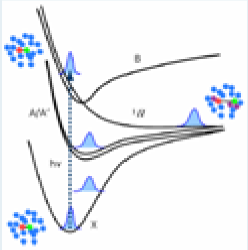
Will determine the structure of single particles, such as atomic clusters, viruses and biomolecules





MID **Materials Imaging & Dynamics**

Will be able to image and analyse nano-sized devices and materials used in engineering

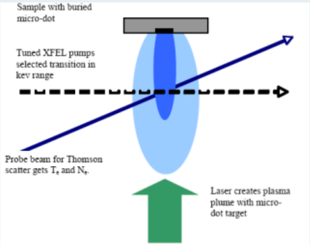


FXE **Femtosecond X-Ray Experiments**

Will investigate chemical reactions at the atomic scale in short time scales molecular movies

HED **High Energy Density Matter**

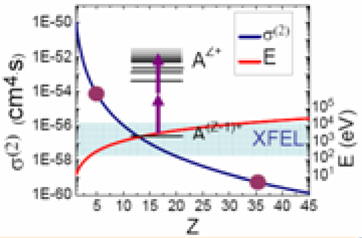
Will look into some of the most extreme states of matter in the universe, such as the conditions at the center of planets



Soft X-Rays

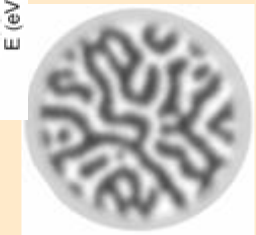
SQS **Small Quantum Systems**

Will examine the quantum mechanical properties of atoms and molecules.



SCS **Soft X-Ray Coherent Scattering/Spectroscopy**

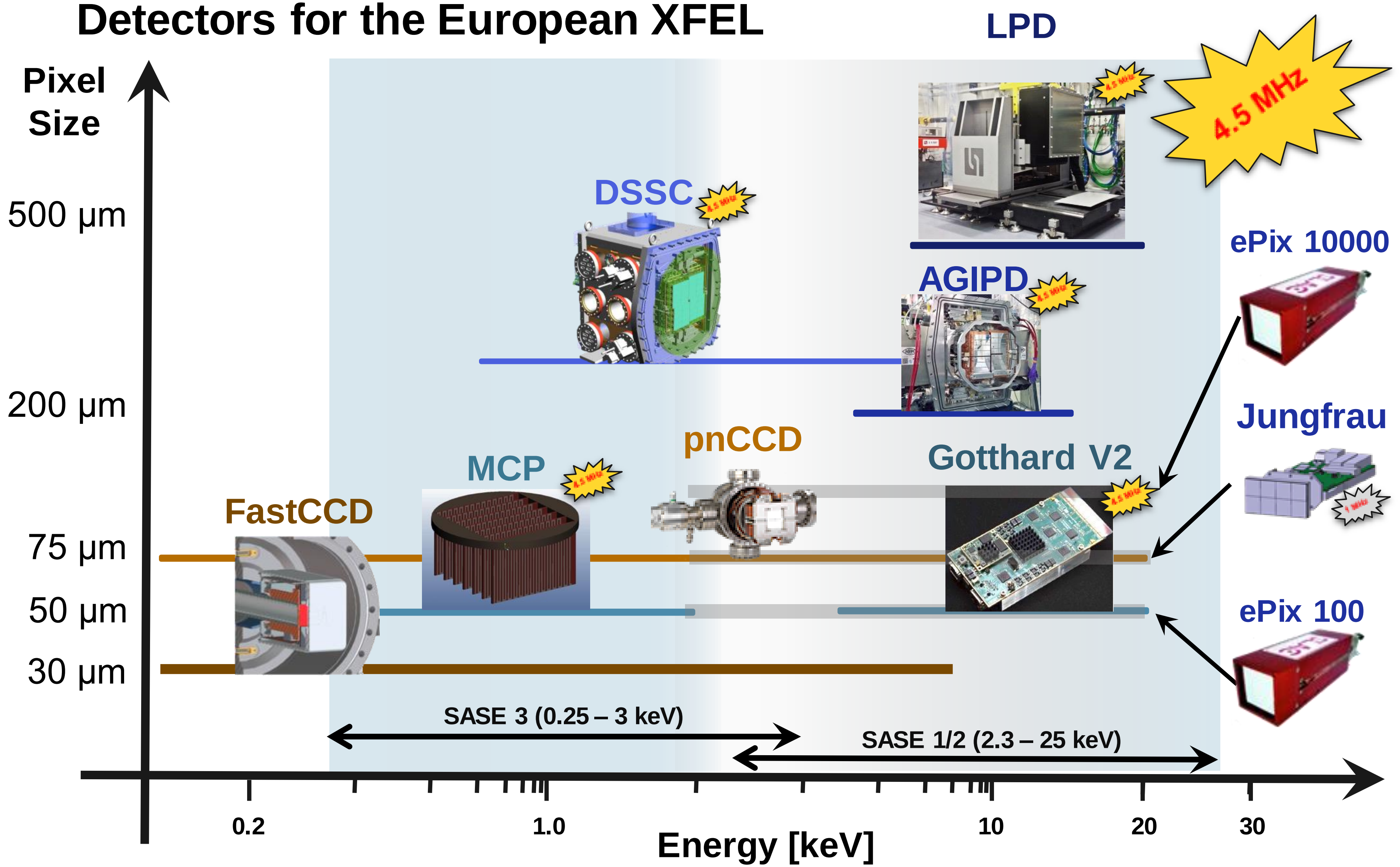
Will determine the structure and properties of large, complex molecules and nano-sized structures.



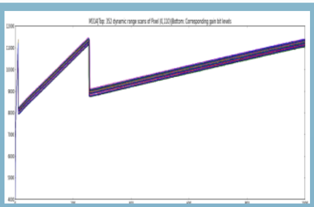
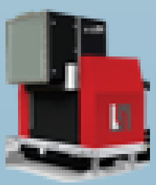
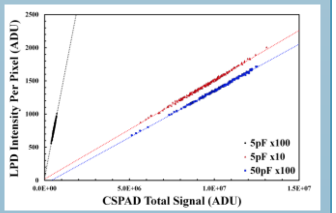
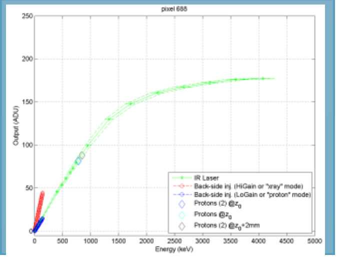
Detectors for the Scientific Instruments

Beamline	Energy	Instrument	Detectors			
SASE I	High E	Single Particles, Clusters and Biomolecules (SPB)	AGIPD	Gotthard V1/2		Jungfrau
SASE I	High E	Materials Imaging & Dynamics (MID)	AGIPD	Gotthard V1/2	ePix	Jungfrau
SASE II	High E	Femtosecond X-ray Experiments (FXE)	LPD	Gotthard V1/2		Jungfrau
SASE II	High E	High Energy Density Matter (HED)	Jungfrau	Gotthard V1/2	ePix	Jungfrau
SASE III	Low E	Small Quantum Systems (SQS)	DSSC	Fast CCD	pnCCD	MCP
SASE III	Low E	Spectroscopy and Coherent Scattering (SCS)	DSSC	Fast CCD	pnCCD	MCP

Detectors for the European XFEL



MHz Rate, High Dynamic Range Detectors – Challenges for Calibration

Detector	Specs	Modularity	Gain Switching	Gain Curve
AGIPD 	1 Mpixel, 4.5 MHz 352 memory cells 200µm sq. pixels 1-10^4 ph@ 12 keV 3 – 13 keV	16 modules in 2 cols x 8 rows on 4 quadrants	3 gain stages with automatic switching	
LPD 	1 Mpixel, 4.5 MHz 508 memory cells 500µm sq. pixels 1-10^5 ph@ 12 keV 5 – 25 keV	16 modules per supermodule (2x8) 16 SM on 4 quadrants	3 gain stages with on front-end selection	
DSSC 	1 Mpixel, 4.5 MHz 800memory cells 204µm hex. pixels 1-10^4 ph@ >1keV 0.5 – 6 keV	16 modules in 2 cols x 8 rows on 4 quadrants	Non-linear gain in ASIC (miniSDD), in sensor (DePFET)	

MHz Rate, High Dynamic Range Detectors – Challenges for Calibration

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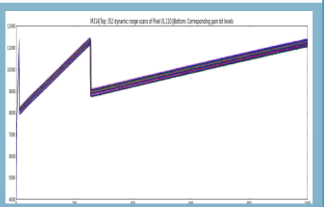
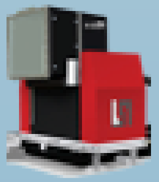
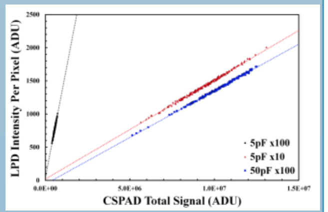
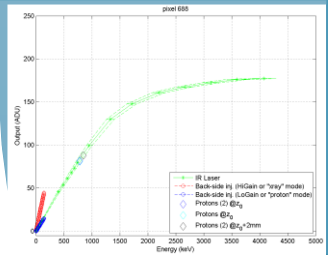
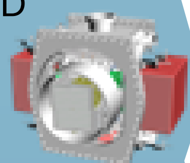
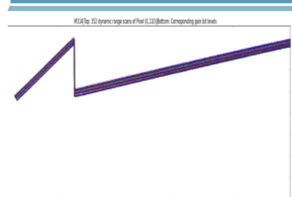
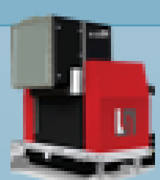
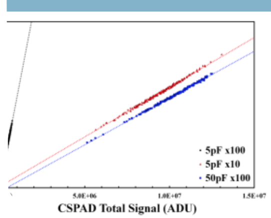
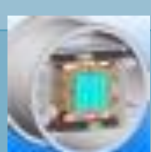
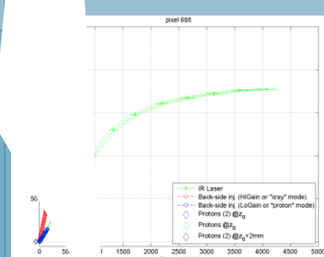
AGIPD 	1 Mpixel, 4.5 M 352 memory c 200µm sq. pixel 1-10^4 ph@ 12 k 3 – 13 keV	
LPD 	1 Mpixel, 4.5 M 508 memory ce 500µm sq. pixe 1-10^5 ph@ 12 k 5 – 25 keV	
DSSC 	1 Mpixel, 4.5 MH 800memory cells 204µm hex. pixe 1-10^4 ph@ >1ke 0.5 – 6 keV	

- Three gains per pixels
- Offsets depend on signal
- Analogue gain evaluation
- ….

- Six gains per pixels
- Offset errors multiply
- Air scattering in FF
- ….

- Non-linear gain
- One ADU per photon
- ….

MHz Rate, High Dynamic Range Detectors – Challenges for Calibration

Detector	Gain Curve
AGIPD 	
LPD 	
DSSC 	

AGIPD:
- Three gains per pixels
- Offsets depend on signal
- Analogue gain evaluation
- ….

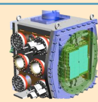
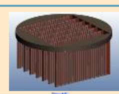
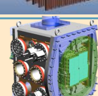
LPD:
- Six gains per pixels
- Offset errors multiply
- Air scattering in FF
- ….

DSSC:
- Non-linear gain
- One ADU per photon
- ….

Calibration is non-trivial!

Facility-side calibration recommended

Detectors – Timeline and Status

Detector System	Beam Line	Scientific Instrument	Project Status	Arrival at XFEL	Installation at Experiment
AGIPD 	SASE I	SPB	Calibration/User Operation	December 2016	August 2017
LPD 	SASE I	FXE	Calibration/User Operation	February 2017	July 2017
FastCCD 	SASE III	SCS	Commissioning/ Calibration	May 2016	May 2018
AGIPD 	SASE II	MID	Integration	March/April 2018	August 2018
Gotthard V2 	SASE I-III	FXE/HED/MID/ SPB/Diagnostic s	Development	July 2018	August 2018
DSSC MiniSDD 	SASE III	SCS	Integration	September 2018	November 2018
pnCCD 	SASE III	SCS/SQS	Integration	July 2018	November 2018
MCP DLD 	SASE III	SQS	Development	≈ First half of 2018	Approx. 1 year after delivery
DSSC DEPFET 	SASE III	SCS/SQS	Development	January 2020	November 2020

External

Development → Integration → Testing → Commissioning Calibration DAQ/Control Integration → End-2-End Test

at XFEL

→ Beam Line Integration Commissioning → User Operation

Detectors – Timeline and Status

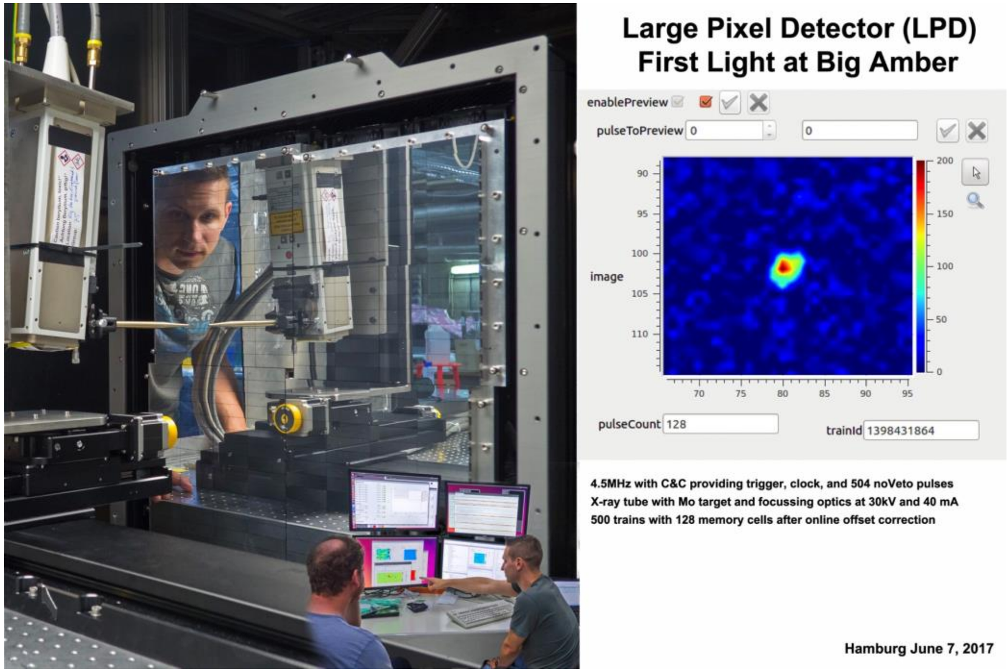
Detector System	Beam Line	Scientific Instrument	Project Status	Arrival at XFEL	Installation at Experiment
ePix100 	SASE II	MID	Integration	February 2018	September 2018
ePix100 	SASE II	HED	Integration	February 2018	December 2018
Jungfrau 	SASE I	SPB	Development / Integration (1 mem cell)	April 2018	August 2018
Jungfrau 	SASE I	FXE	Development/ Integration (1 mem cell)	April 2018	August 2018
Jungfrau 	SASE II	MID	Development/ Integration (1 mem cell)	September 2018	October 2018
Jungfrau 	SASE II	HED	Development/ Integration (1 mem cell)	December 2018	January 2019

External: Development → Integration → Testing → Commissioning Calibration DAQ/Control Integration

at XFEL: → End-2-End Test → Beam Line Integration Commissioning → User Operation

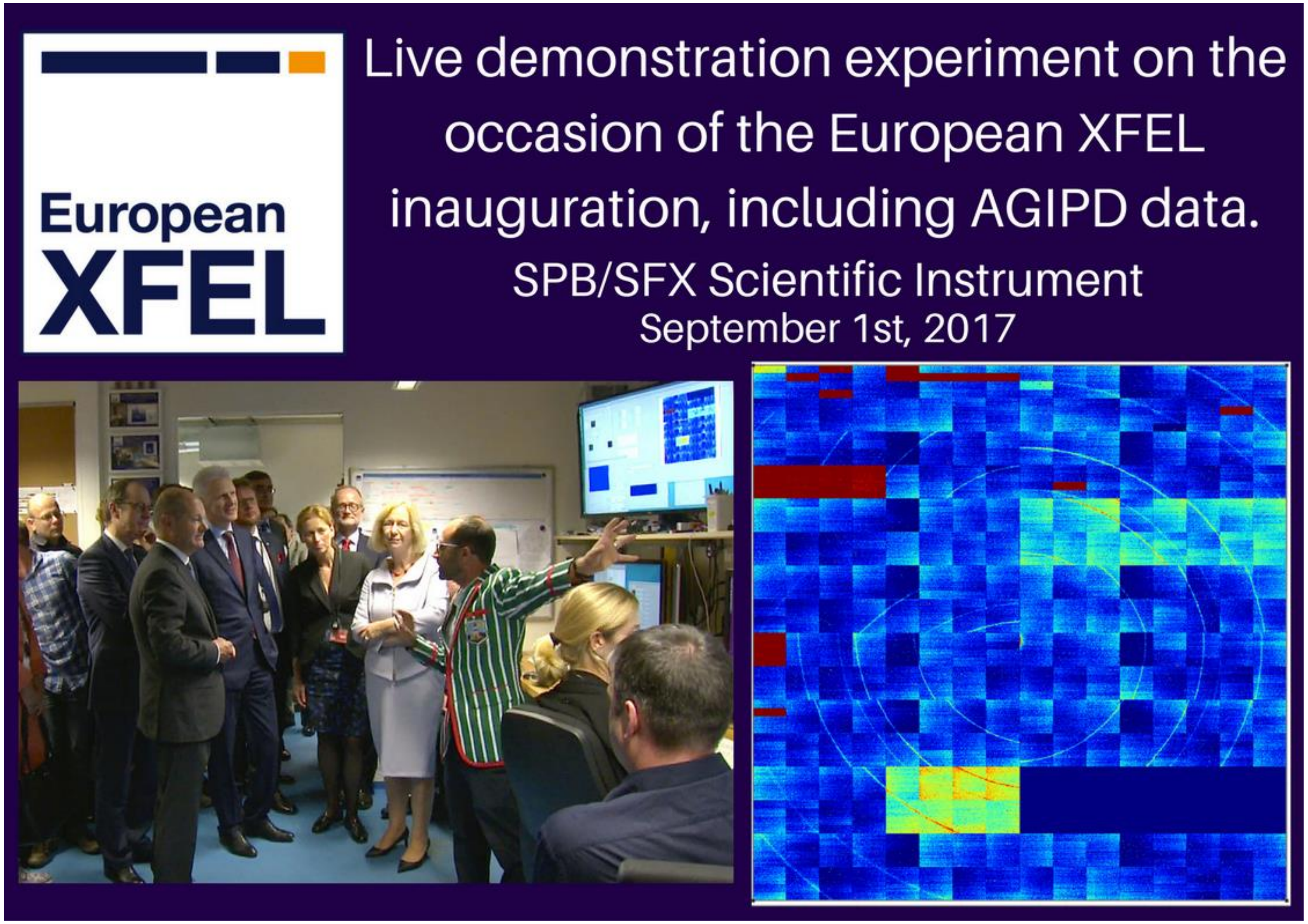
On the way to user operation – Detector End-to-End tests

- Status @ last XDAC: LPD and AGIPD in the HERA South lab, prepared for user operation.
- LPD and AGIPD transported from HERA South to Schenefeld in July 2017 (LPD) and middle of August (AGIPD)



- Much less time for E2E tests than originally planned. Some tests had to be postponed after the beam line installation.
  - Inauguration event on September 1st: first images on AGIPD. **User operation started on September 14th!**

The AGIPD detector at SPB/SFX



LPD at FXE

- System worked stably
- Small problems with hardware were solved quickly (coolant leak, broken transceiver, etc.)
- Detector illuminated with X-rays at FXE for commissioning purposes
- Uses veto system to reject ‘empty’ images

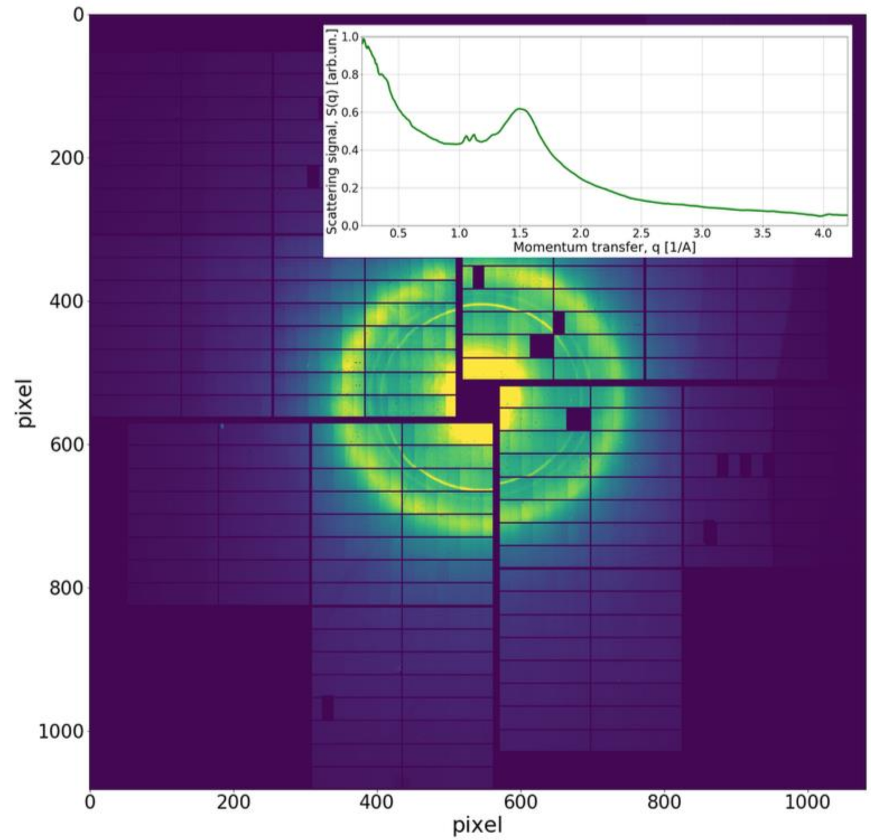


Figure 8: Liquid scattering pattern of tetrahydrofuran solution of a Cu complex collected with the LPD detector [23,24] at scientific instrument FXE [25](corrected for dark offset). Inset: Average of the azimuthally integrated set of 150 image.

LPD at FXE

- System worked stably
- Small problems with hardware were solved quickly (coolant leak, broken transceiver, etc.)
- Detect
  for cor
- Uses v

Successful first user operation due to the contribution of many different people and groups:
the AGIPD and LPD Collaborations
the XFEL groups Detectors, CAS, ITDM, AE, PSPO,
and the instruments SPB/SFX, FXE

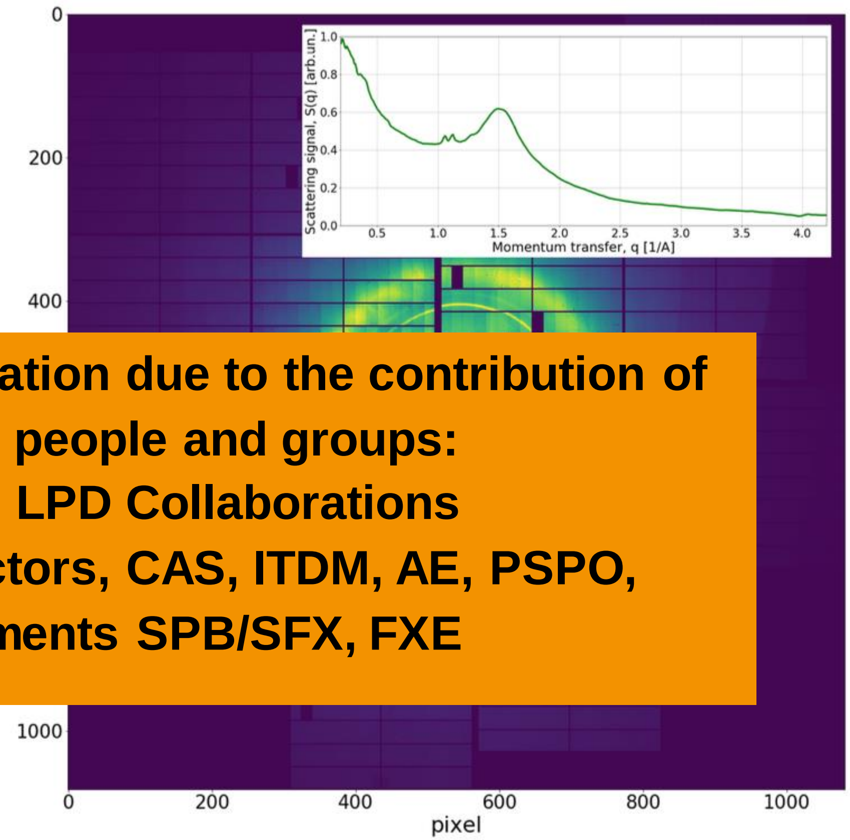
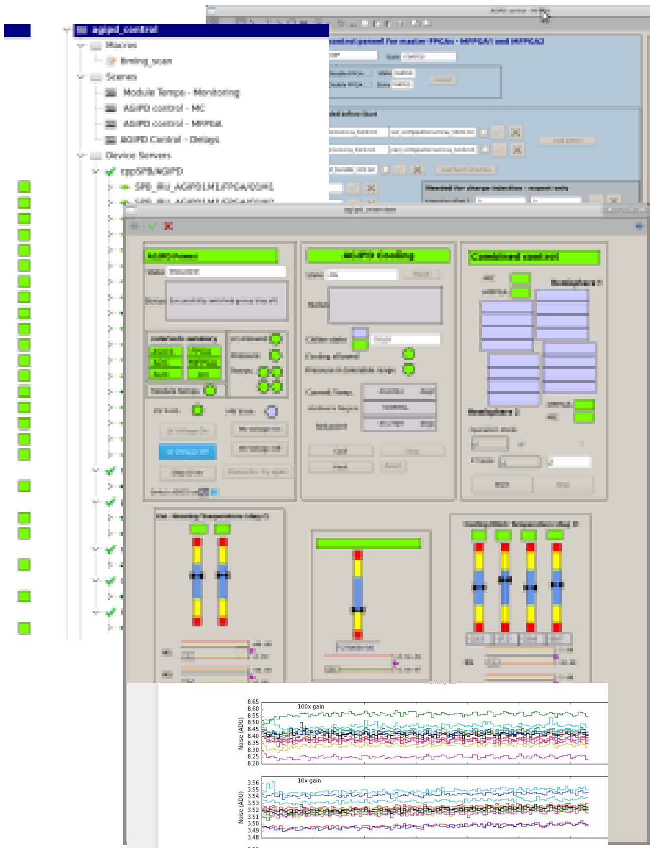


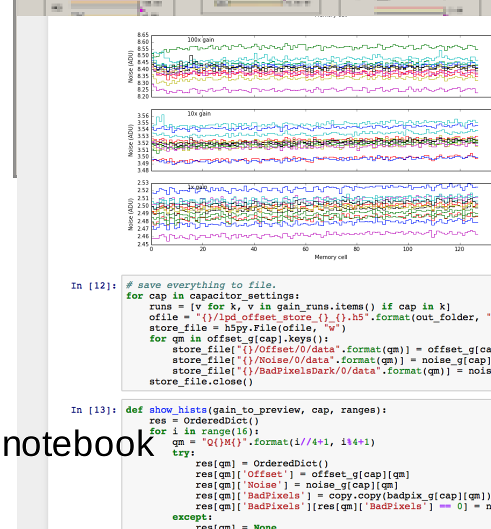
Figure 8: Liquid scattering pattern of tetrahydrofuran solution of a Cu complex collected with the LPD detector [23,24] at scientific instrument FXE [25](corrected for dark offset). Inset: Average of the azimuthally integrated set of 150 image.

Tools we use

- Karabo – the European XFEL Control and Analysis Framework
  - DAQ, online corrections, multi-module combination, and user exposure are all implemented in this framework. See e.g. *Kuster et al.: Detectors and Calibration Concept for the European XFEL; Fangohr et al.: Data Analysis Support at European XFEL*
  - Detector Control is implemented in Karabo, working on top of consortia-provided libraries
  - Karabo now follows a 2-4 week release schedule, with bug fixes made quickly available
    - ► Many improvements in responsiveness during last 6 months as mandated with ever growing installations
    - ► DAQ and calibration and detector control follow relevant updates in these release cycles, leading to stability and performance improvements
    - ► Beam-time like conditions are a must for proper evaluation
- IPython and project Jupyter
  - For offline analysis and characterization
  - For transparency of what we do
- ZMQ
  - For exposing data to users via a well-established path

Karabo GUIs



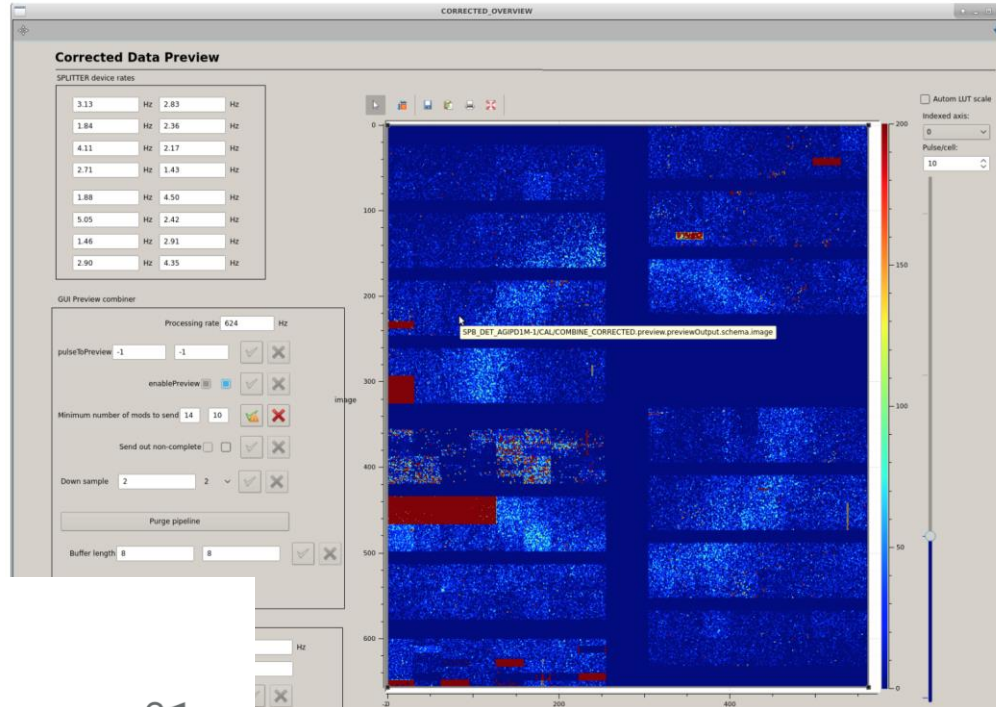


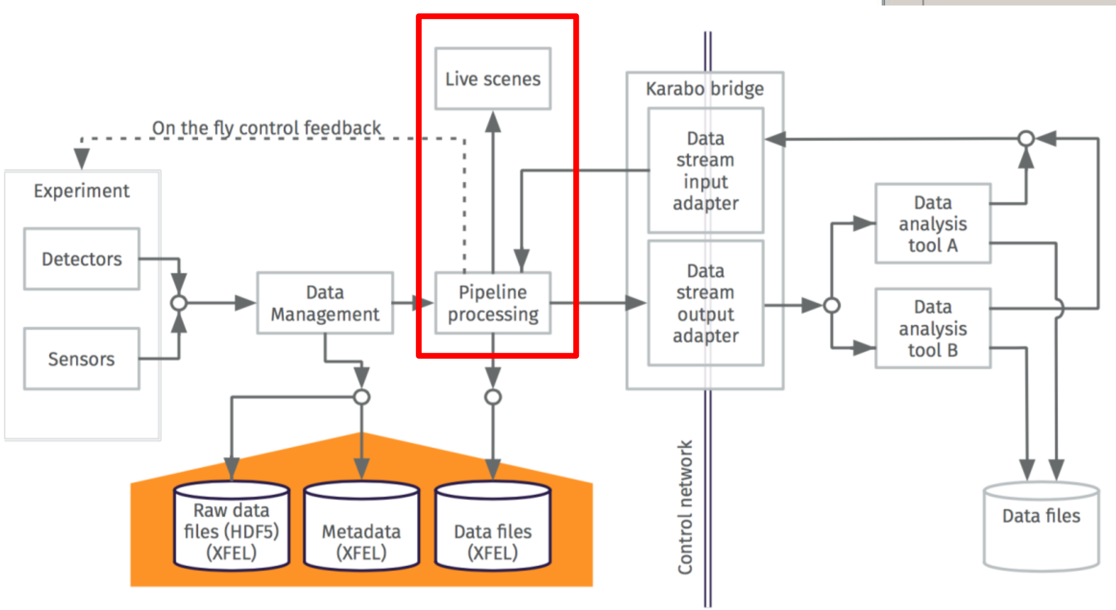
Jupyter notebook

Online Calibration

- Has seen extensive use at both instruments for rapid feedback
- Feeds user-provided online tools via a Karabo-ZMQ adapter device
- GPU algorithms available if data rates require

Corrected online preview for AGIPD



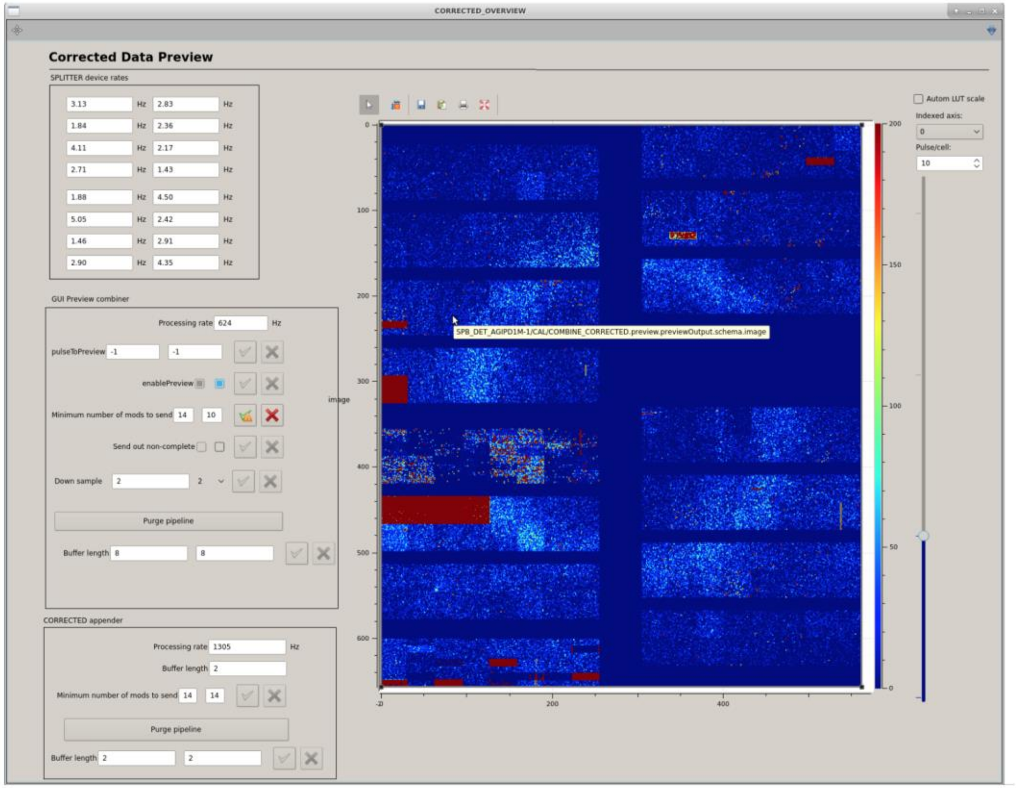


	AGIPD	LPD
Gain evaluation	X	X
Offset correction	X	X
Relative gain correction	X	X
Bad pixels	G/O/N	G/O/N
KRB devices for MPIX	103	69

Online Calibration

- Has seen extensive use at both instruments for rapid feedback
- Feeds user-provided online tools via a Karabo-ZMQ adapter device
- GPU algorithms available if data rates require
- Online processing is module parallel, chunks size always one train
  - “Splitter” devices as entry points to pipelines from → pass every nth train, safe guard DAQ by dropping on slowness
  - “Combiner” device as exit points:
    - ► Combine modules into stack: [pulse, module, x y]
    - ► Combine modules into image: [pulse, x’, y’]

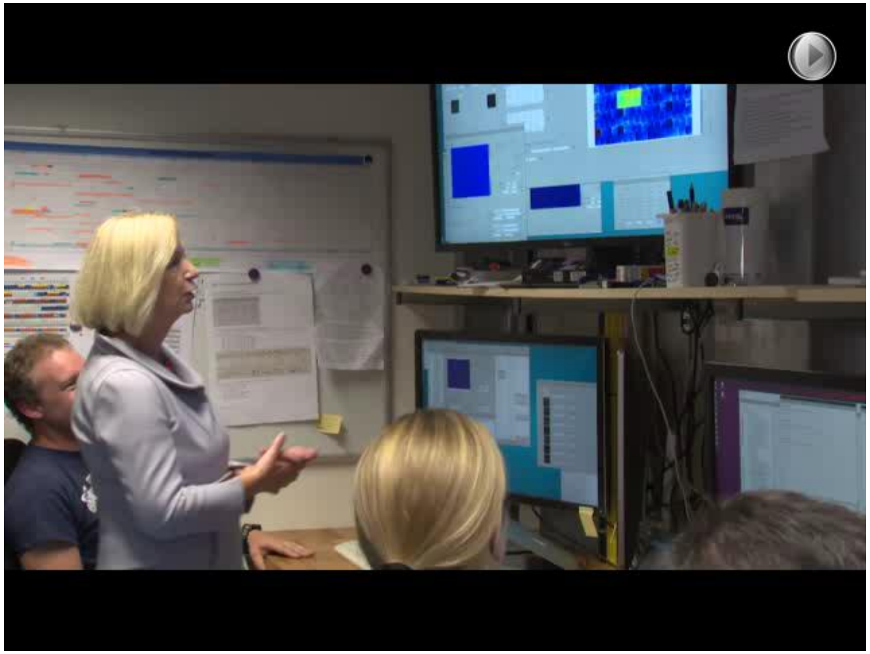
Corrected online preview for AGIPD



- Needs to combine 16 data streams @1.6 Gb/s tot.
- Can optionally mask BP
- Configurable number of modules to “wait” for

Online Calibration

Corrected online preview for AGIPD



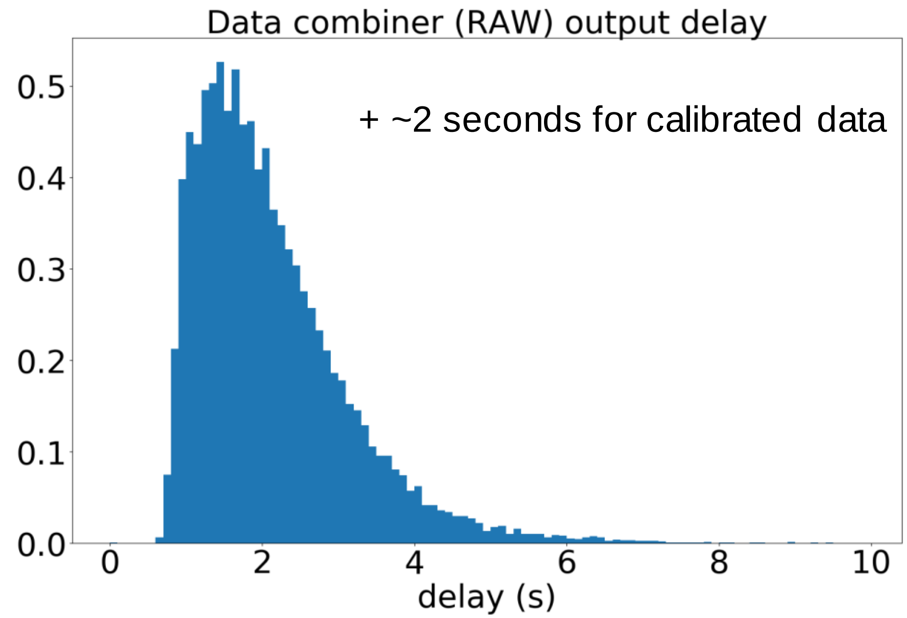
- Has seen extensive use at both instruments for rapid feedback
- Feeds user-provided online tools via a Karabo-Bridge device
- GPU algorithms available if data rates require
- Online processing is module parallel, chunks size always one train
  - "Splitter" devices as entry points to pipelines from → pass every nth train, safe guard DAQ by dropping on slowness
  - "Combiner" device as exit points:
    - ► Combine modules into stack: [pulse, module, x y]
    - ► Combine modules into image: [pulse, x', y']

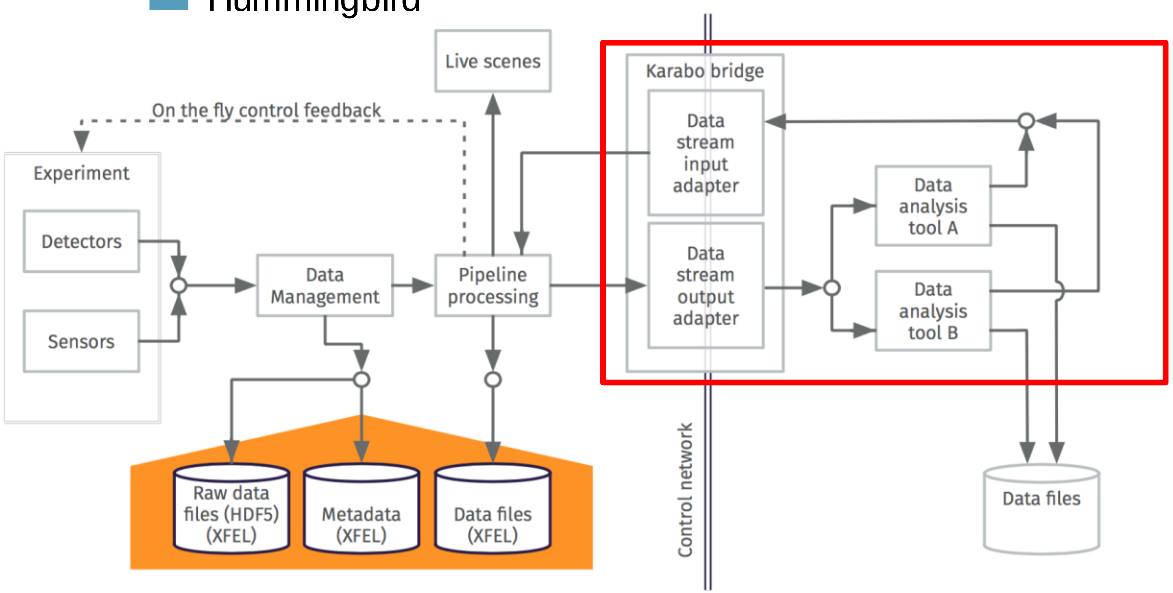
- Needs to combine 16 data streams @1.6 Gb/s tot.
- Can optionally mask BP
- Configurable number of modules to "wait" for

Online Calibration

- Feeds user-provided online tools via a Karabo-Bridge device (T. Michelat)
  - Usually combiner in appender mode
  - Connects to CAS-provided ZMQ bridge
  - 3-5 Hz rate at 64 cells measured
  - 2-4s latency with 64 memory cells

- Applications so far:
  - ONDA
  - CASS
  - Hummingbird





- Latency includes:
  - Data acquisition
  - Data formatting on DAQ
  - Data forwarding to pipelines
  - Data selection at pipeline entry points:
    - ► Every nth train
    - ► Cells containing FEL pules
  - Combining of 16 streams from modules
  - Data advertising on ZMQ

Offline Calibration

- Two approaches under investigation:
  - Docker containing Karabo pipeline
    - ▶ Same codebase as online processing
    - ▶ Access to ITDM reader/writers
    - ▶ Unit tests of pyDetLib
  - Python scripts containing correction code
    - ▶ Less overhead
    - ▶ Less opaque
- Common front-end script
- Both run module concurrent on server node and run concurrent on many nodes
- Both feature automated processing whenever data is migrated from online to offline processing via MDC

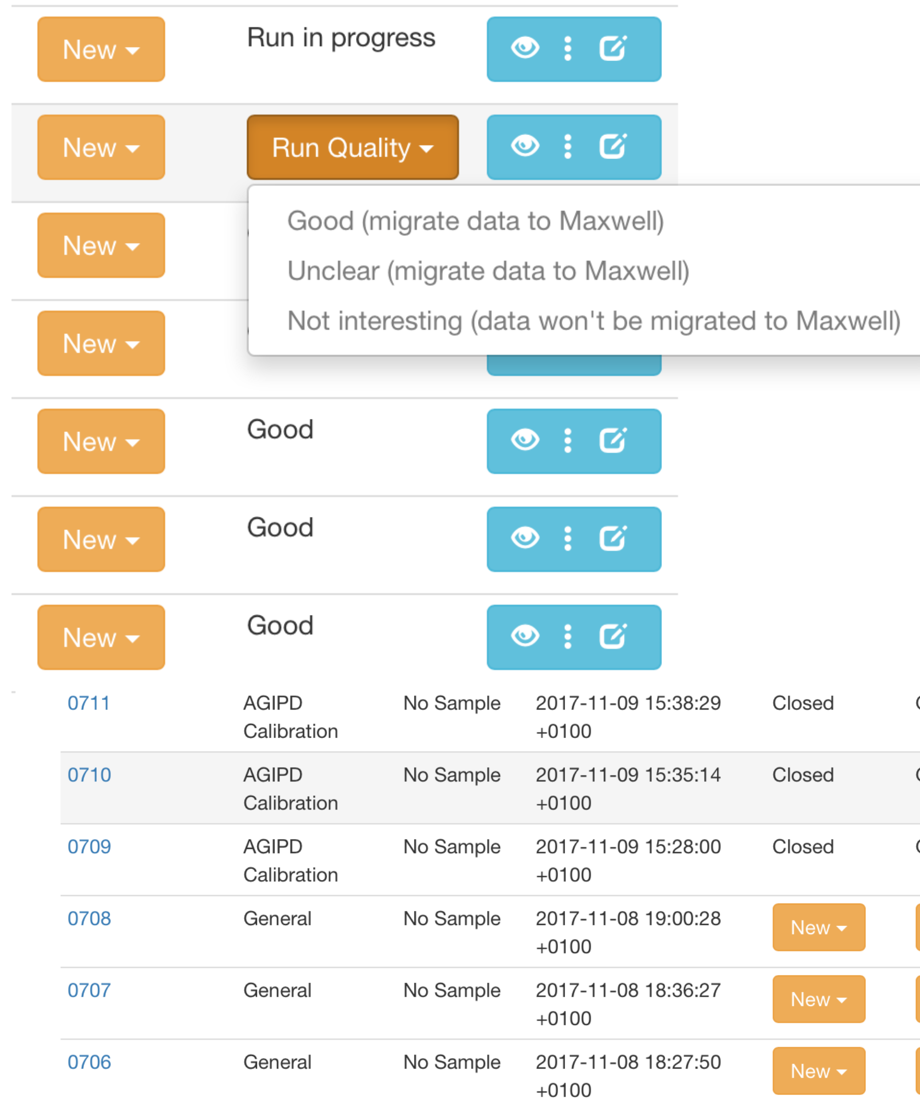
```
% python calibrate.py --help
usage: calibrate.py [-h] [--input INPUT]
                    [--output OUTPUT]
                    [--base-cal-store BASE_CAL_STORE]
                    [--offset-cal-store OFFSET_CAL_STORE
                    [--mem-cells MEM_CELLS]
                    [--detector DETECTOR]
                    [--sequences SEQUENCES]
                    [--overwrite] [--no-relgain]
                    [--uuid UUID]
                    [--ff-cal-store FF_CAL_STORE]
                    [--no-ff]

Main entry point for offline calibration

optional arguments:
 -h, --help            show this help message and exit
 --input INPUT
 --output OUTPUT
 --base-cal-store BASE_CAL_STORE
 --offset-cal-store OFFSET_CAL_STORE
 --mem-cells MEM_CELLS
 --detector DETECTOR
 --sequences SEQUENCES
 --overwrite
 --no-relgain
 --uuid UUID
 --ff-cal-store FF_CAL_STORE
 --no-ff
```

Offline Calibration

- Two approaches under investigation:
  - Docker containing Karabo pipeline
    - ▶ Same codebase as online processing
    - ▶ Access to ITDM reader/writers
    - ▶ Unit tests of pyDetLib
  - Python scripts containing correction code
    - ▶ Less overhead
    - ▶ Less opaque
- Common front-end script
- Both run module concurrent on server node and run concurrent on many nodes
- Both feature automated processing whenever data is migrated from online to offline processing via MDC



Offline Calibration

- File and directory structure from RAW files is preserved:
  - ./raw/r0012 → ./proc/r0012
  - All data not touched by corrections is simply copied
- During correction data format may be sanitized and RAW format changes hidden:
  - AGIPD interlaced and AGIPD non-IL have different raw data layouts but same layout in corrected data

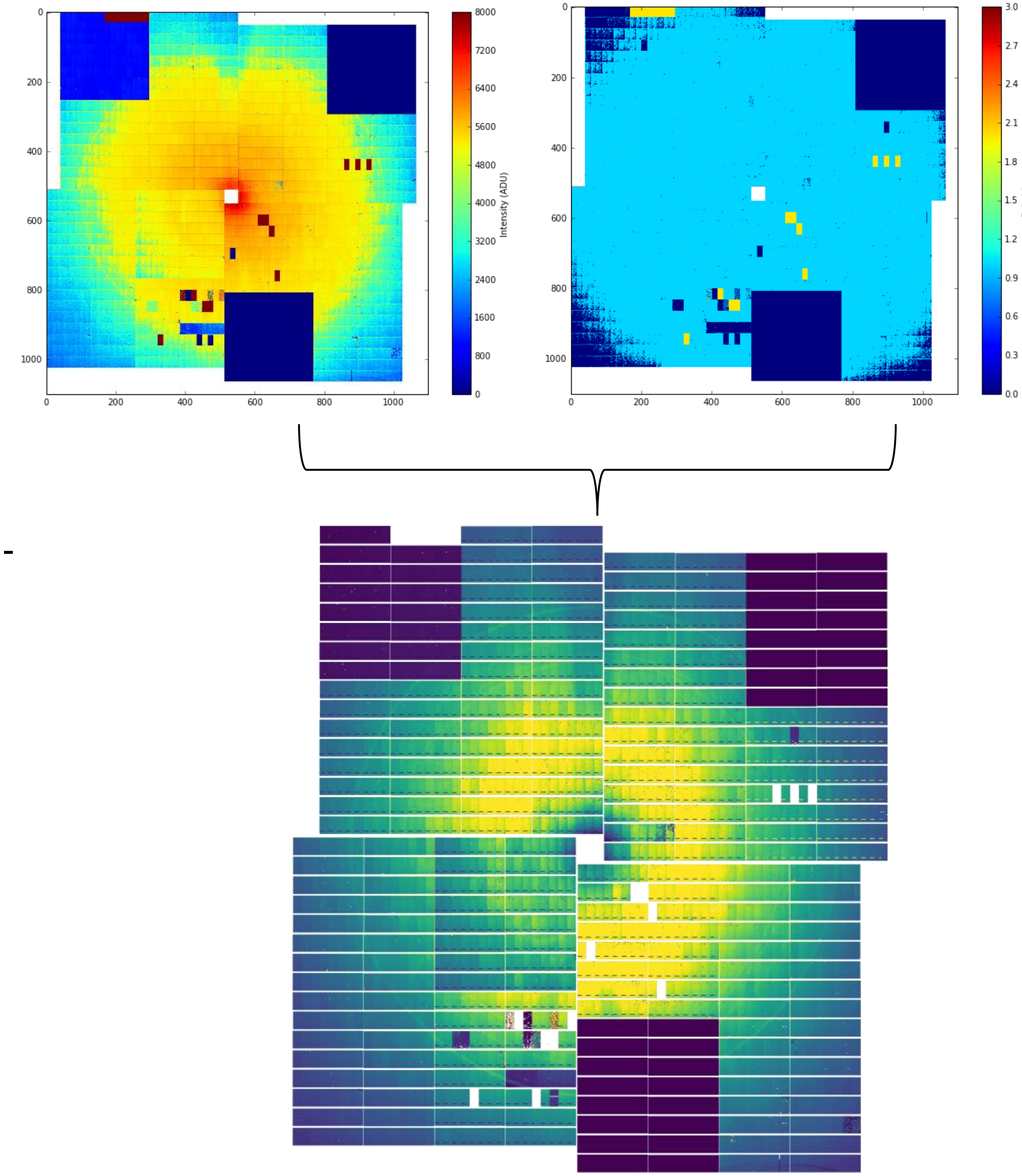
	AGIPD	LPD
Gain evaluation	X	X
Offset correction	X	X
Relative gain correction	X	X
Bad pixels	G/O/N	G/O/N
Run time (1000 trains)	~3m	~3m

Offline Calibration

- Pending algorithmic improvements:
  - AGIPD gain correction and evaluation
    - ► Nonlinear region
    - ► Artifacts through offset correction
    - ► Bad pixels / outliers
  - LPD
    - ► Artifacts at low gain → pin cushion effect
    - ► Flat fields needed for CI data with X-ray correlation

- Upcoming technical improvements:
  - Enable usage of remote calibration database
  - Integrate into metadata catalogue

LPD Offline Corrections



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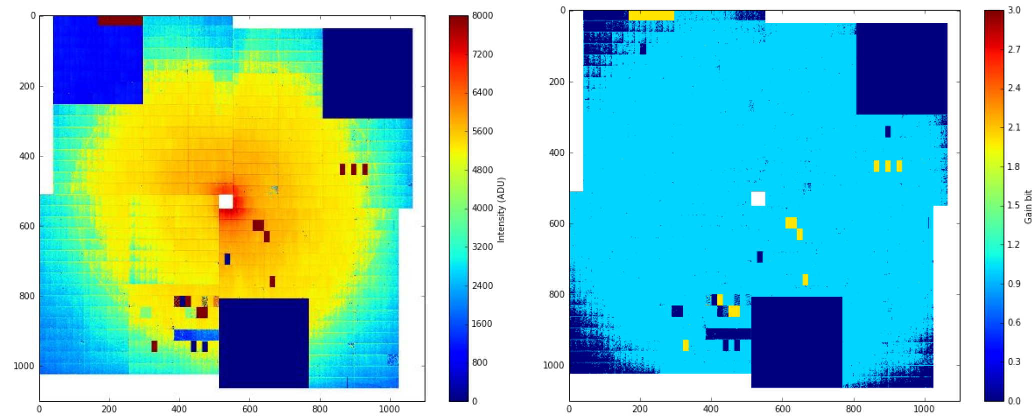
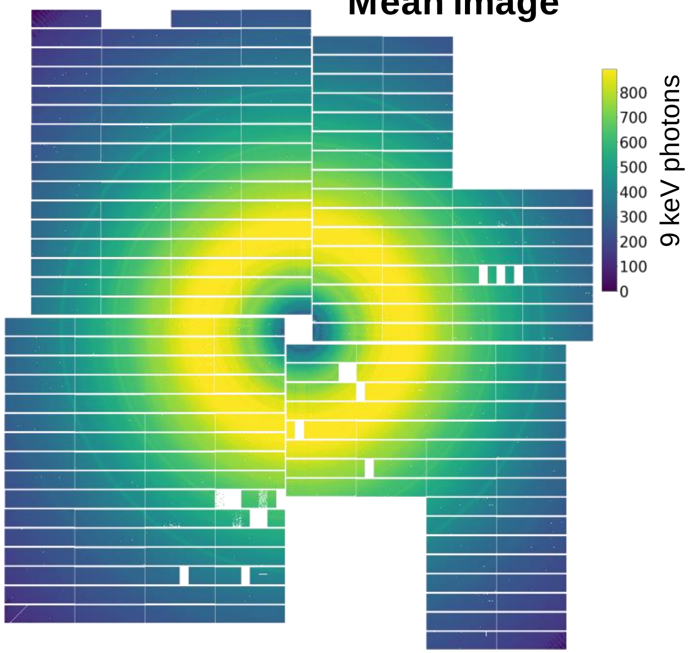


Mean image



Offline Calibration

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    - ▶ Nonlinear region
    - ▶ Artifacts through offset correction
    - ▶
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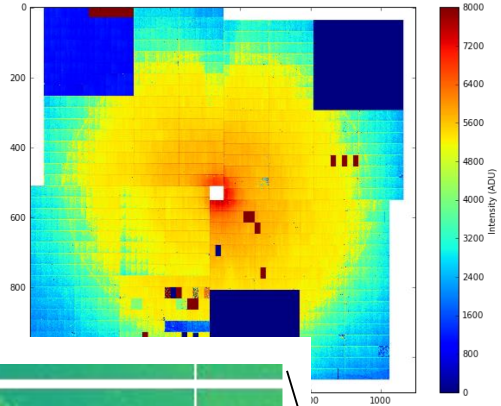
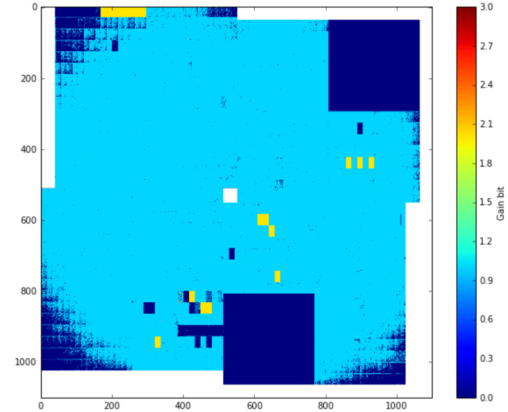
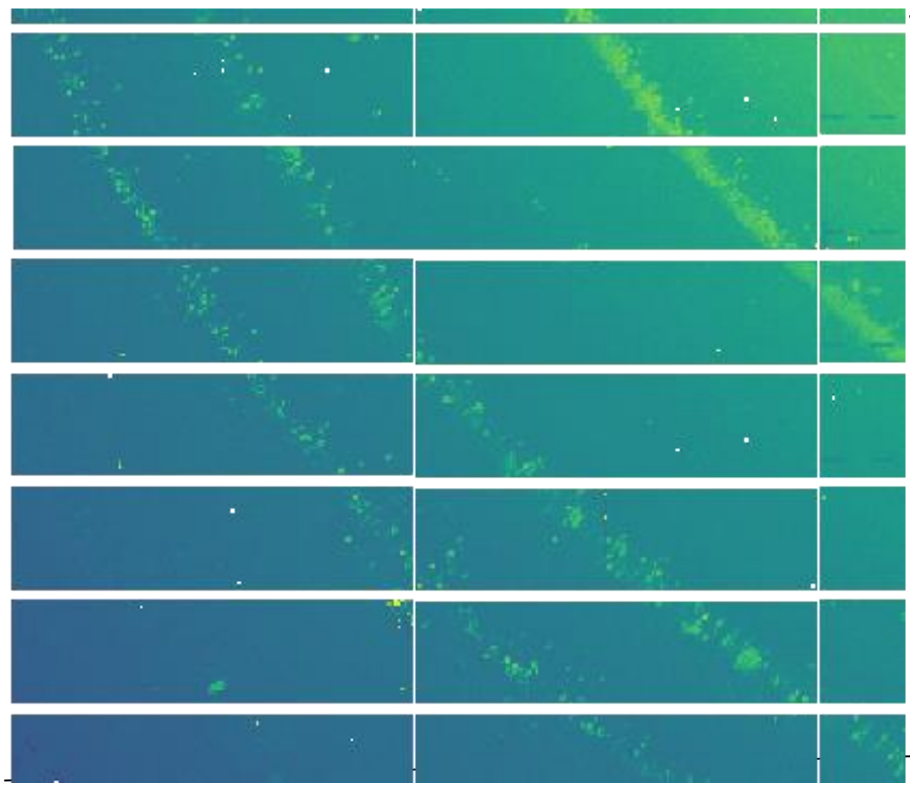
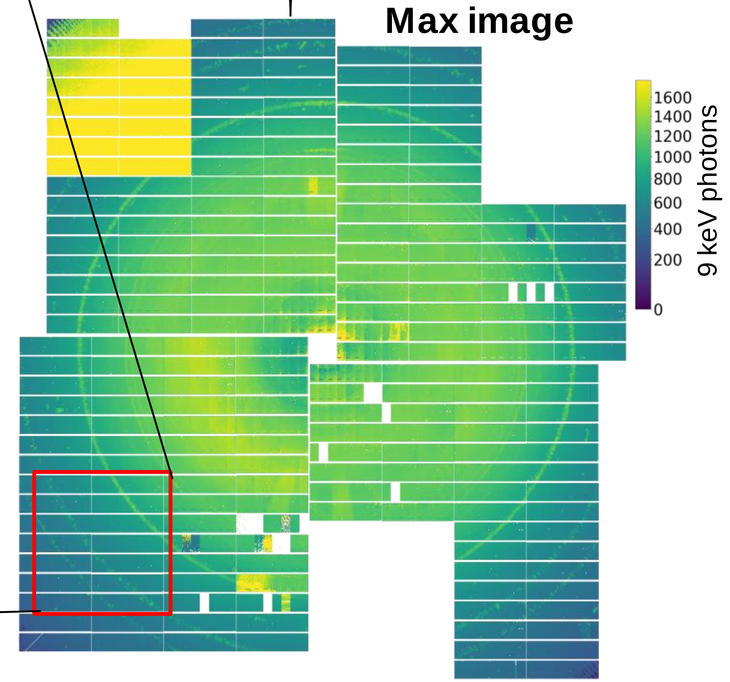
LPD Offline Corrections









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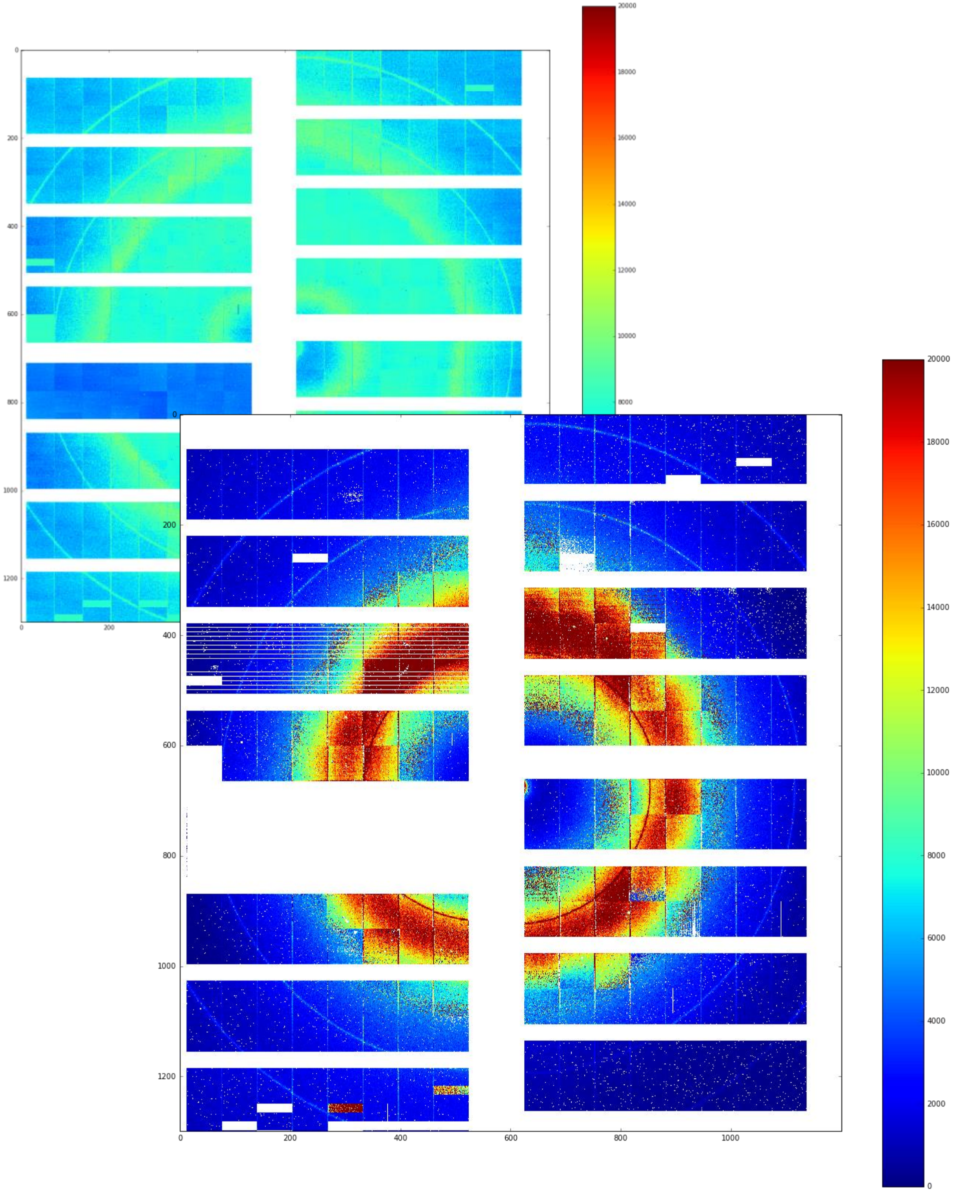

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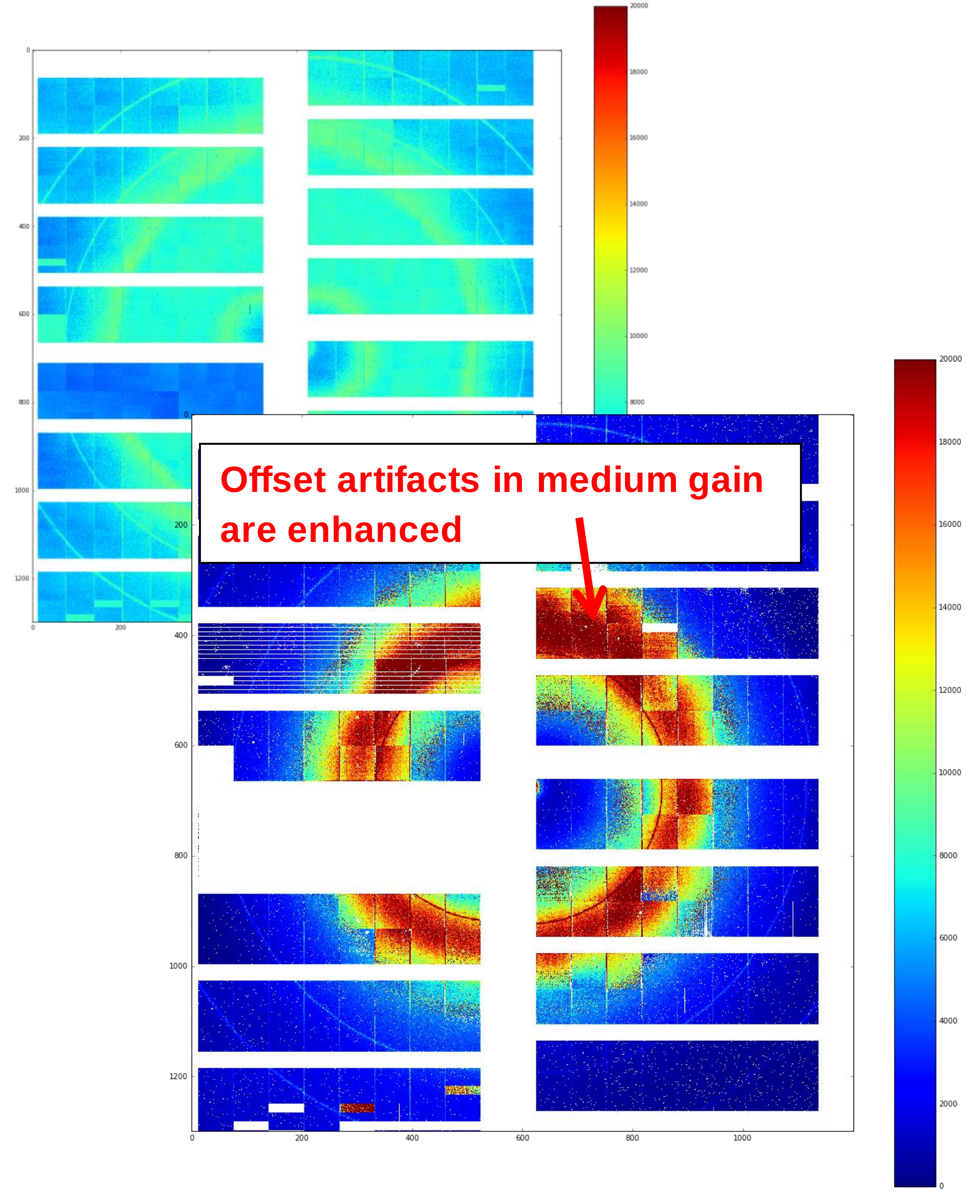

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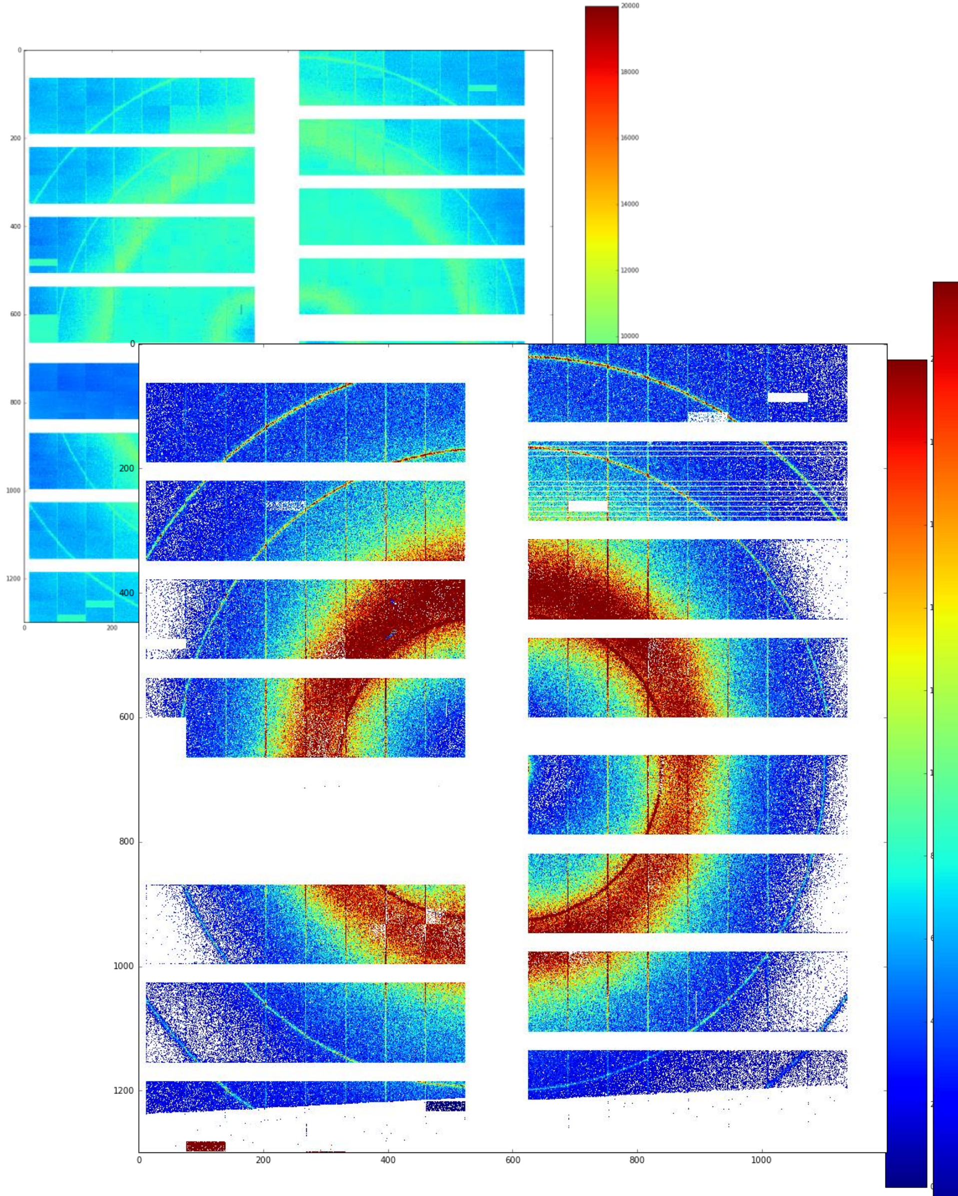
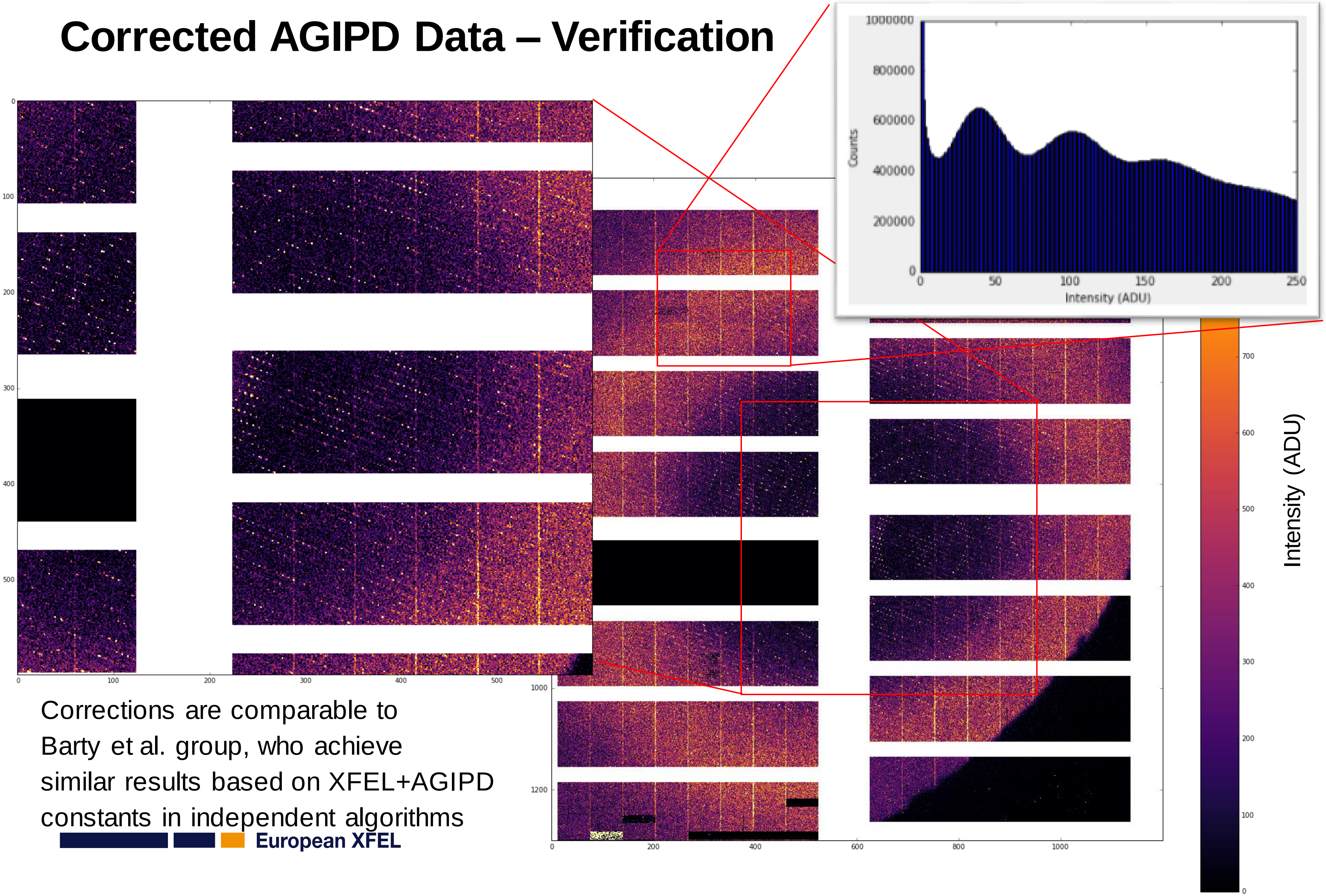


Corrected AGIPD Data – Verification



Corrections are comparable to Barty et al. group, who achieve similar results based on XFEL+AGIPD constants in independent algorithms

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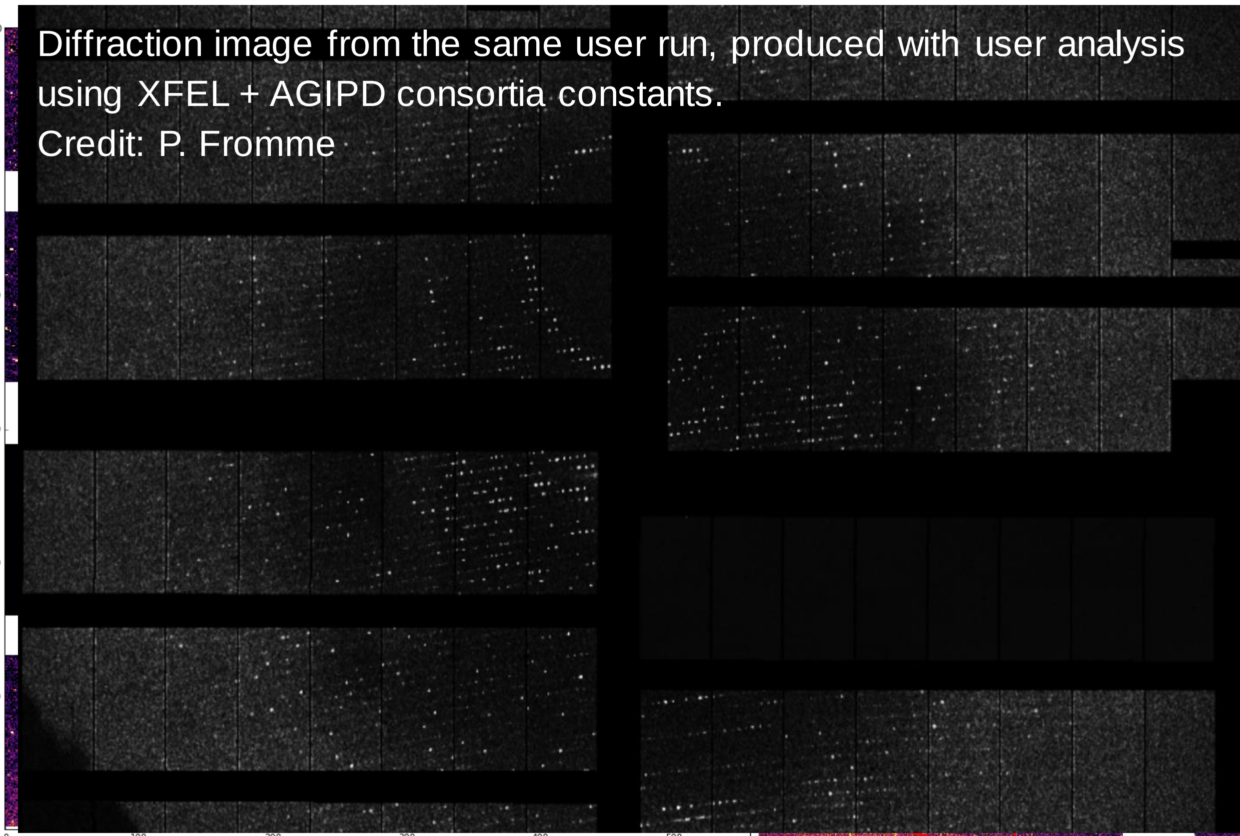

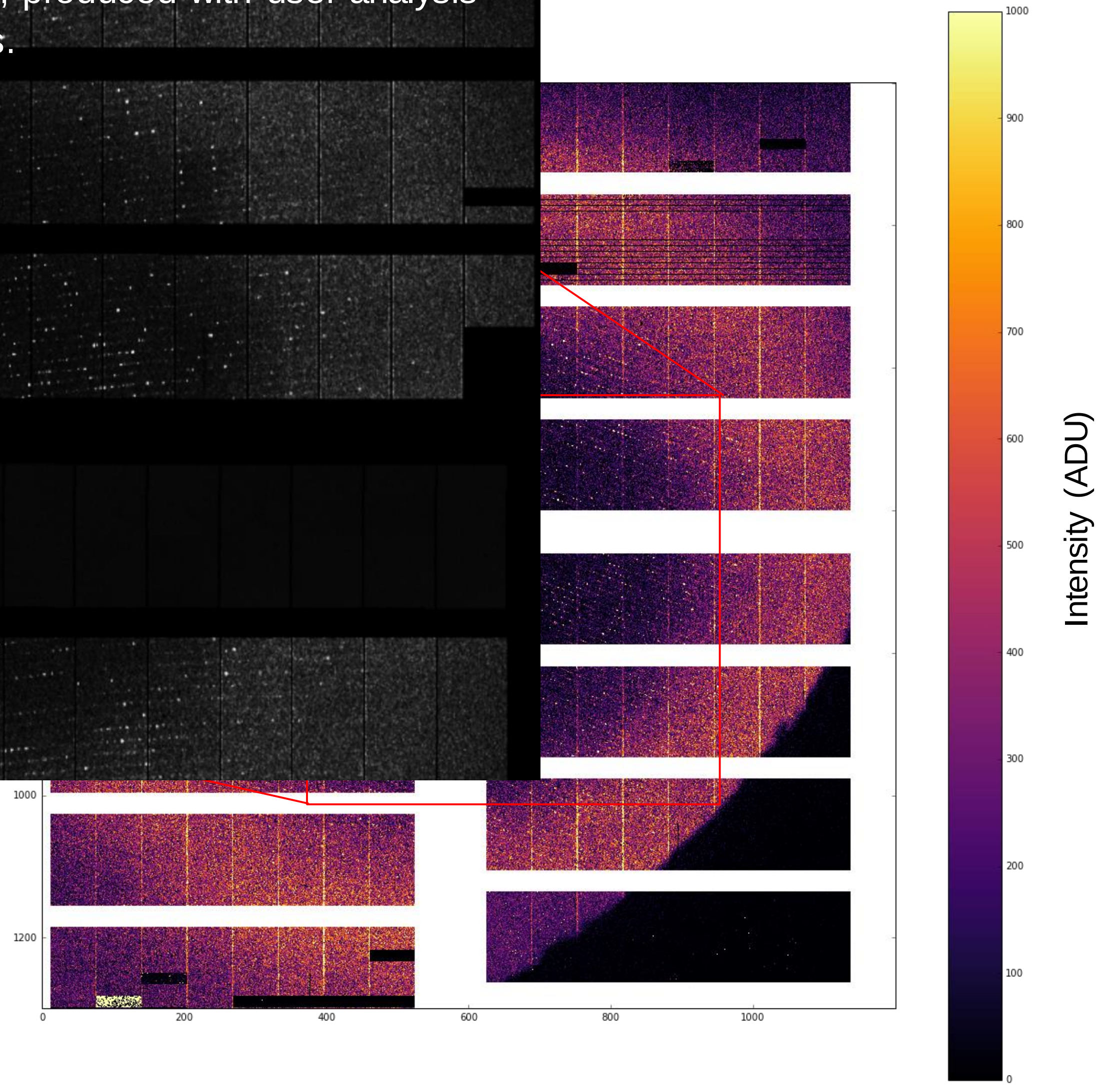

Corrections are comparable to Barty et al. group, who achieve similar results based on XFEL+AGIPD constants in independent algorithms

Characterization Processing

- Frequently use Jupyter notebooks
- For AGIPD:
  - Dark image analysis → offset, noise, bad pixels, gain thresholds
  - Pulse capacitor data → medium/high gain relation, bad pixels, gain thresholds
  - Current source data → medium/low gain relation, bad pixels, gain thresholds
  - Flat fields: → X-ray/charge injection relation, bad pixels

Frequent updates, 5min processing

More static, Each about 2-4 hours processing each

- For LPD
  - Dark image analysis → offset, noise, bad pixels
  - Charge injection data →gain stage relations, bad pixels
  - Flat fields: → X-ray/charge injection relation, bad pixels

Frequent updates, 5min processing

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Frequent updates,
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Data is produced via Karabo processing pipelines storing only pixels with charge injected: 1.75 TB/d, 10GB/s peak

Characterization Processing

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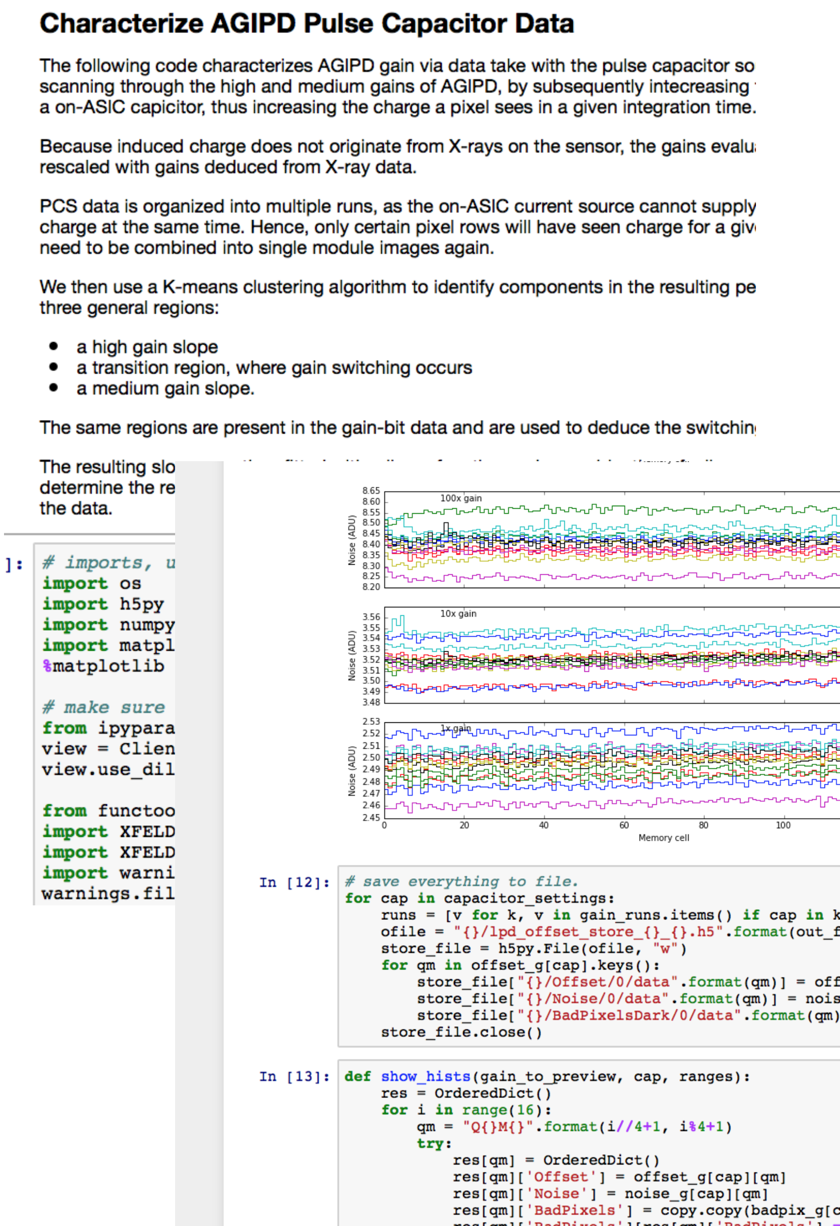
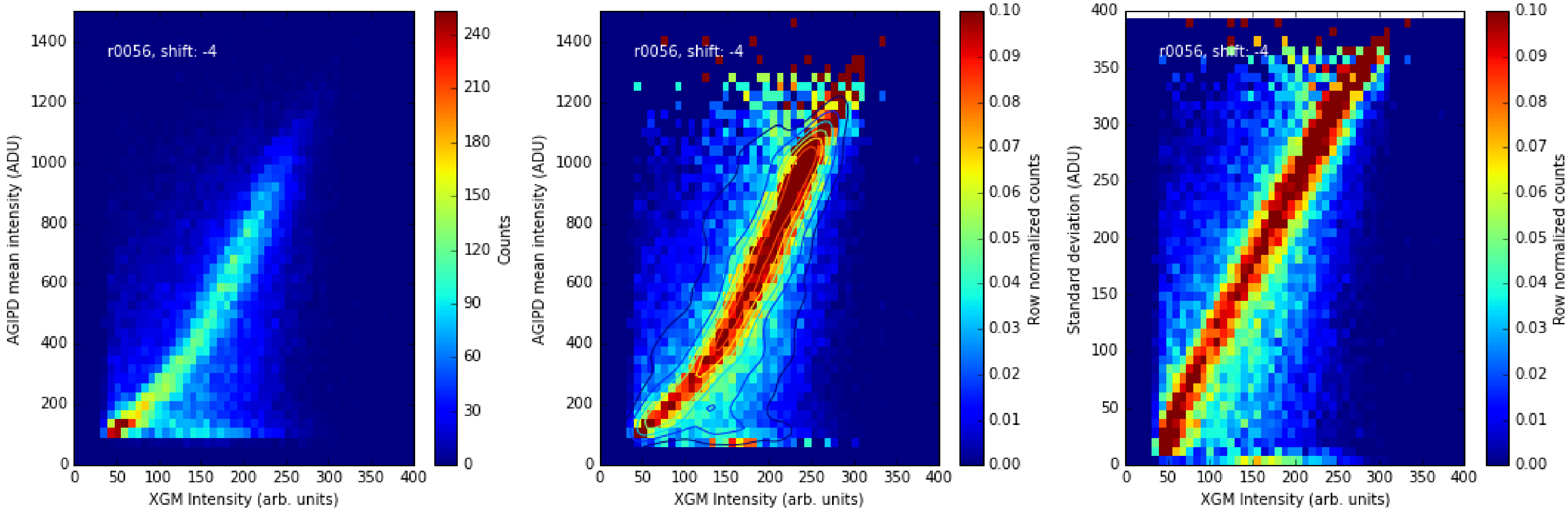


Characterization Processing – Data Correlation with XGM

AGIPD: module mean and std dev. vs XGM signal

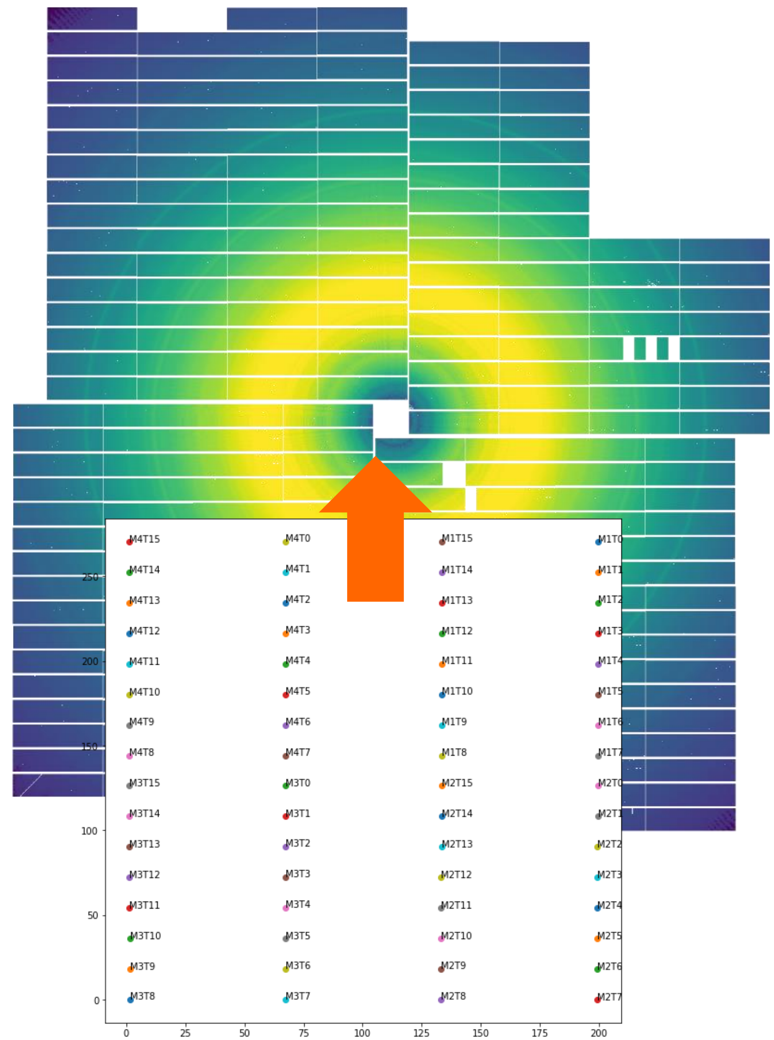


- Requires correlation between different data sources on a per-pulse level → relatively straight forward using indexing meta-data

Alignment Data

- Goal: Facility-side provide initial module positions on segmented detectors → possible refine in situ if needed
- In verification with FXE for LPD for positions up to quadrant level determined using photographic metrology data (procedure and analysis by T. Rüter)
- AGIPD to be produced
- Data store in HDF5 file matching the hierarchical layout of the detector, will be made available through calibration database in the future.
- Python code provided to get position of a given module in terms of top left corner pixel.
- Within module lithography assumed as “perfect”

Corrected LPD (5 train mean, modules positioned)



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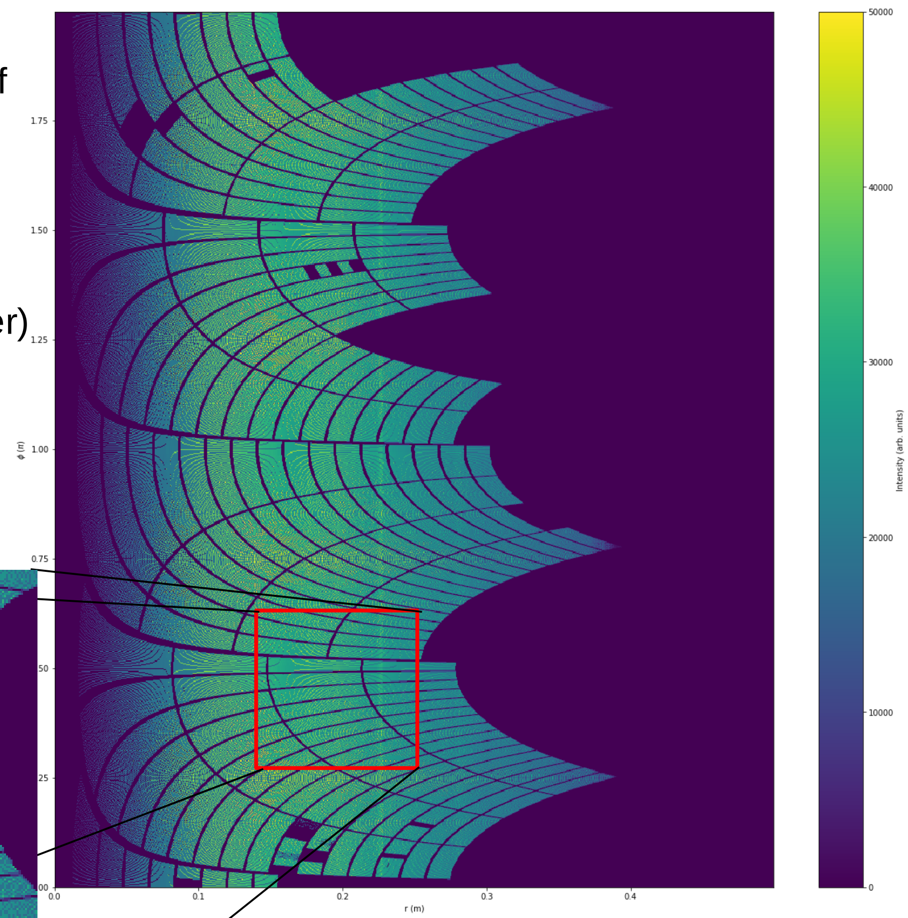

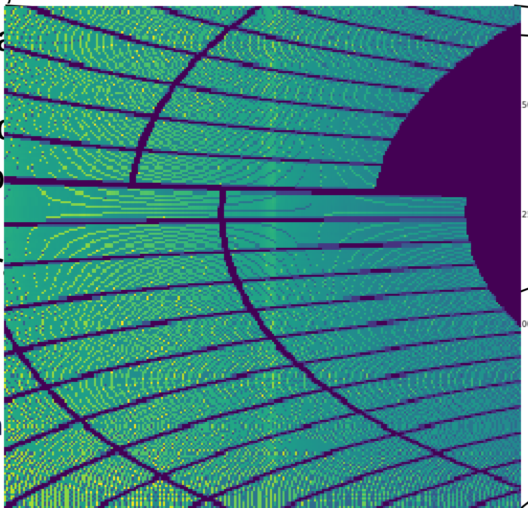

- Plotted in polar coordinates, diffraction rings show as straight lines

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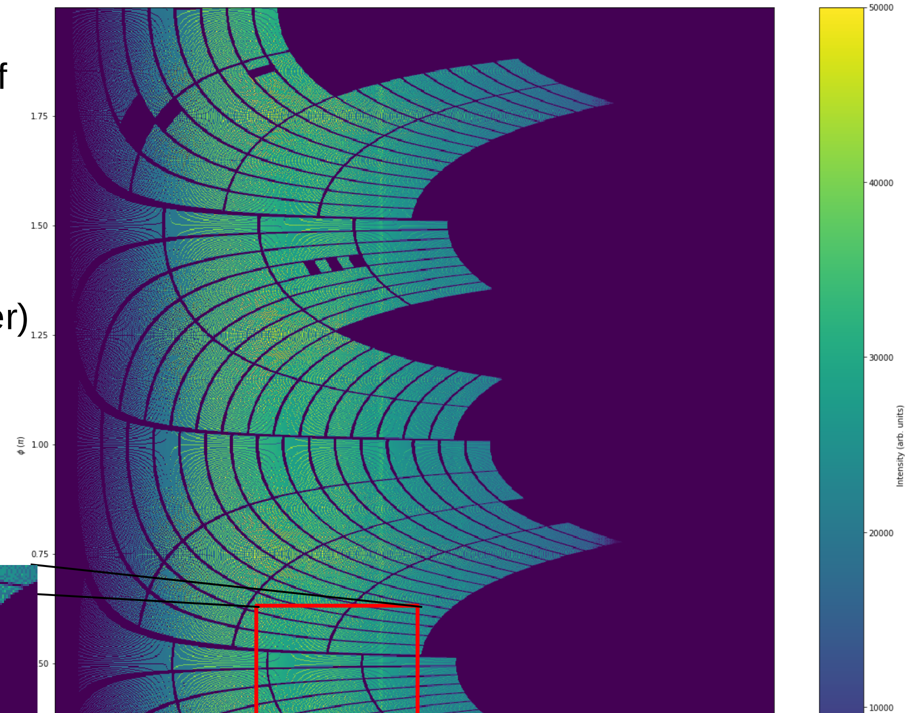

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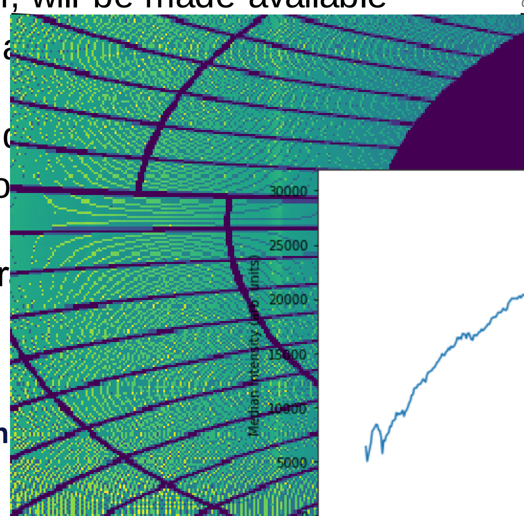
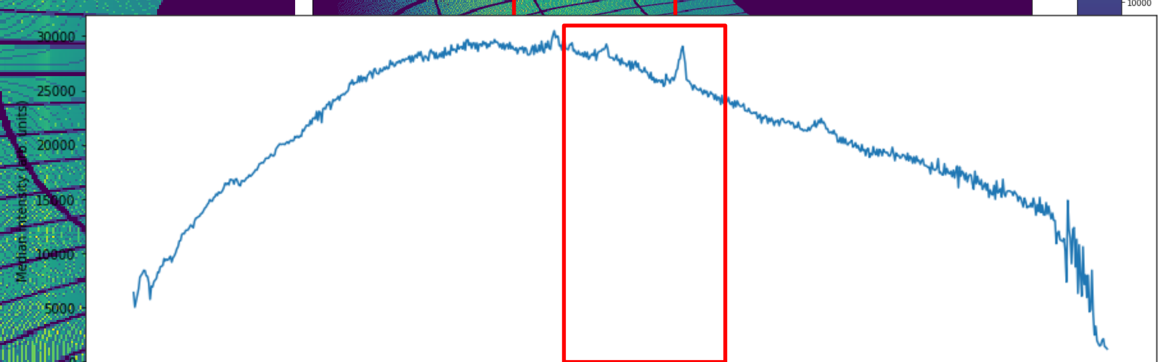
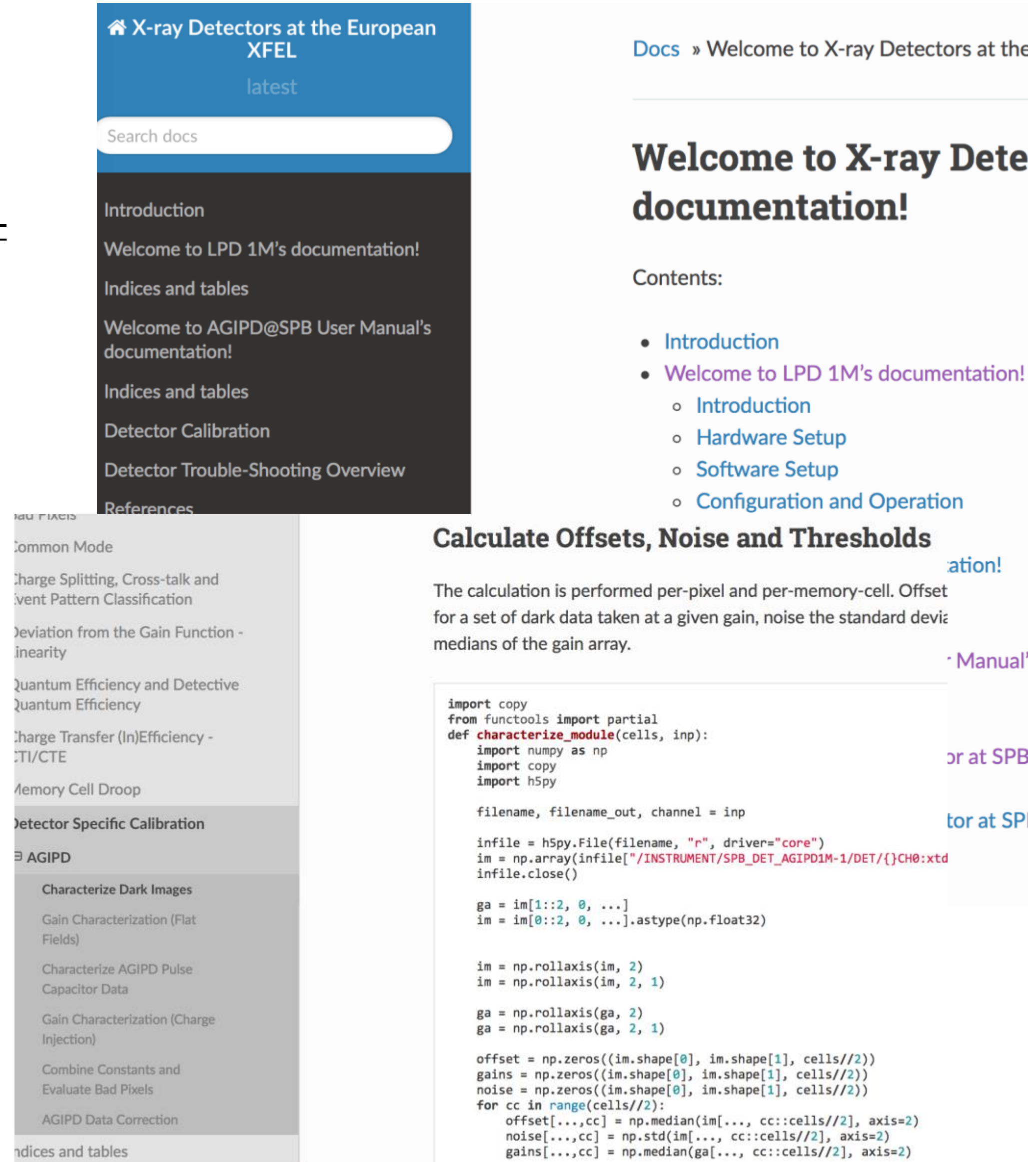




Documentation

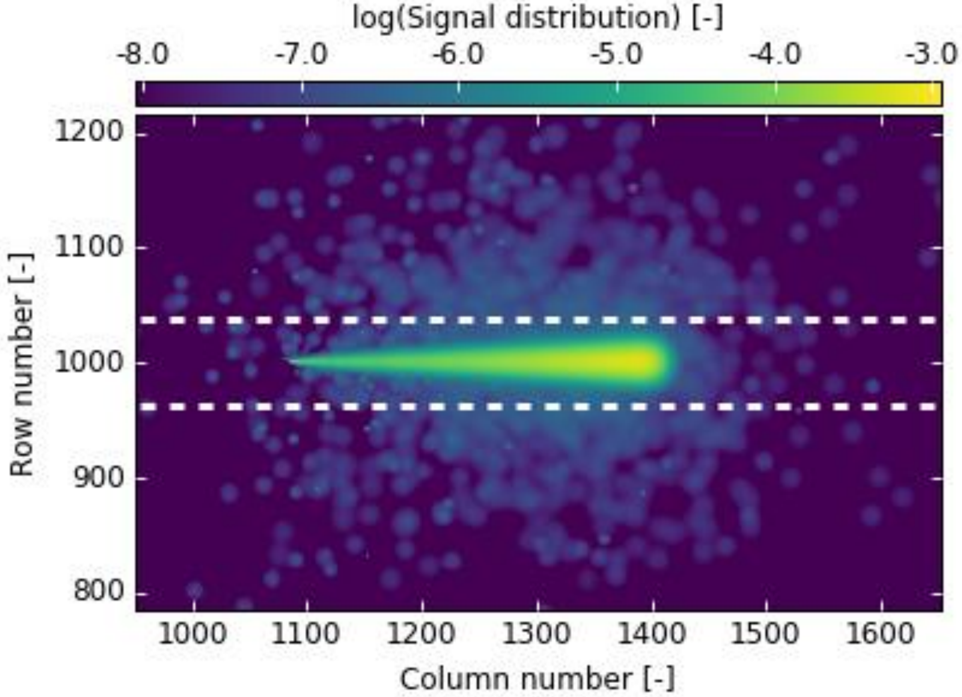
- Documentation is on readthedocs: https://in.xfel.eu/readthedocs/docs/detector-documentation/en/latest/index.html
- General detector documentation
- General calibration documentation
- Detector specific calibration documentation
  - Also documents how constants are derived

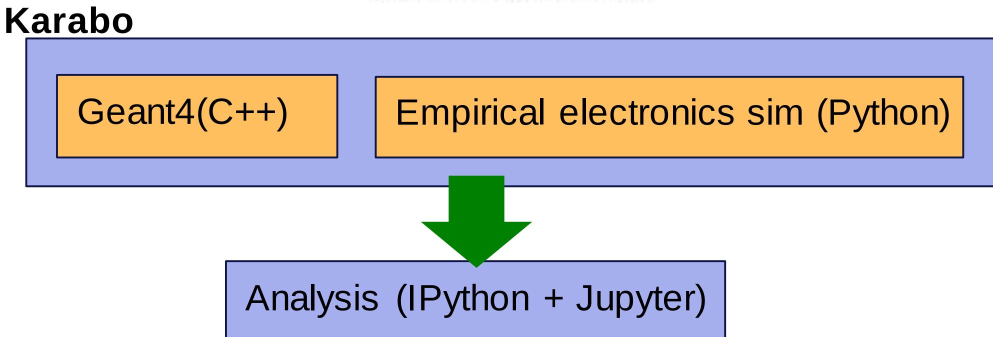


Simulation Activities: Angular Resolution Studies

- Work by T. Rüter
- Simulation framework now allows to study event mis-location for large parameter space:
  - Energy (6 keV – 25 keV, 1 keV steps)
  - Pixel size (> 1um, min. bin size)
  - Angle of incidence (0° - 50°, 2.5° steps)
- Validation experiment planned jointly with Uni Siegen for 2018
- Work has been presented at IEEE NSS&MIC 2017, publication of results as peer-reviewed paper planned
- Mid-term goals: study implication on representative XFEL experiments and evaluate in combination with accuracy of metrology measurements (p.o.c for LPD exists)

Simulated signal distribution of mono-energetic 10keV X-rays at 30° AOI





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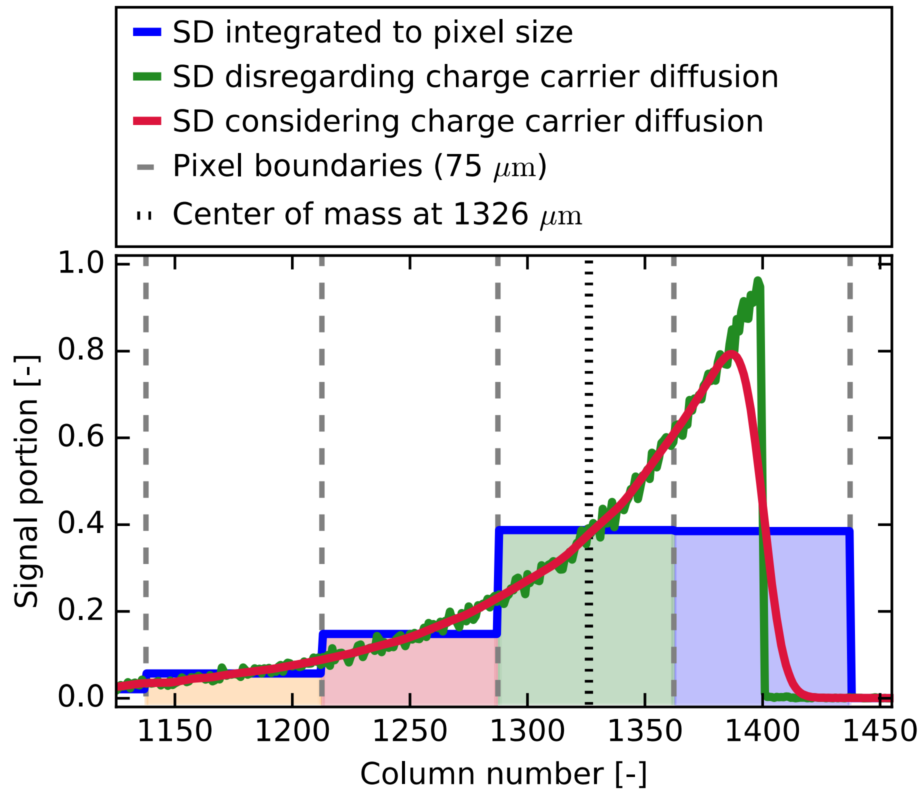
1-D charge distribution in sensor and effect on 75um detector



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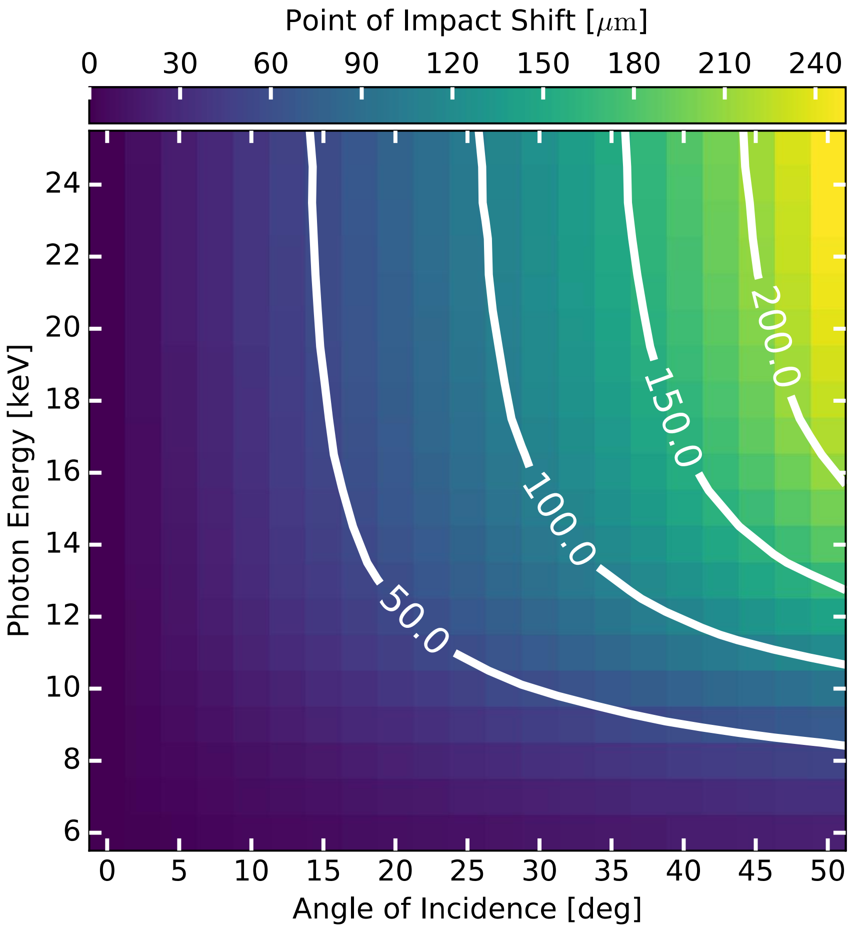
Point of impact shift w.r.t. photon energy and angle of incidence



Summary

- Online feedback (raw & calibrated) and offline corrections are available to instruments and users during beam times
  - Continuous improvements since first FEL light on AGIPD and LPD in August
  - Good and frequent feedback from instruments and users
  - By now: low latency with max. few seconds delay
- Online data can be passed to user tools via CAS-provided Karabo bridge
- Offline corrections still being optimized for both detectors
  - More characterization data is needed → dedicated commissioning time
  - Algorithms also still being optimized as result of further characterization

Outlook

- December/January shutdown
  - Remote calibration database for online and offline
  - Triggering and configuring offline calibration from metadata catalogue
  - Optimization of characterization for both detectors
  - (GPUs on online calibration)
  - Initial DSSC integration
- Longer term
  - Enable full GPU support on offline
  - Automated performance tracking of selected parameters and signals of interest
  - DSSC integration
  - User pluggable components in offline calibration allowing for pre-selection
  - Calibration data release policy & quality assurance
- **Technical and performance papers to cite are under preparation**