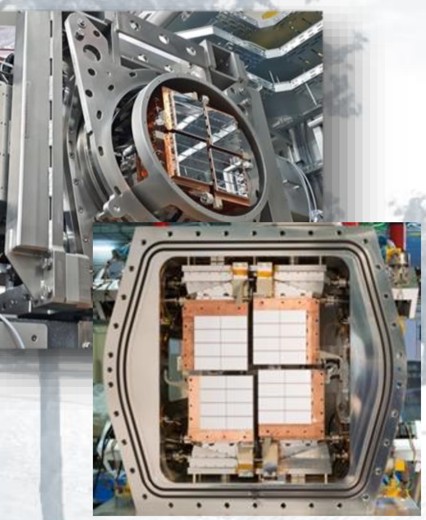
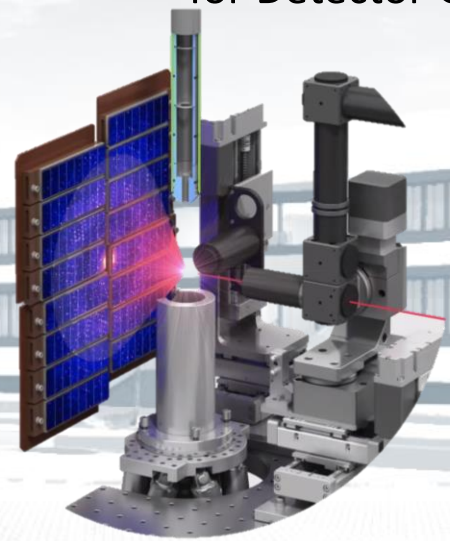
European XFEL

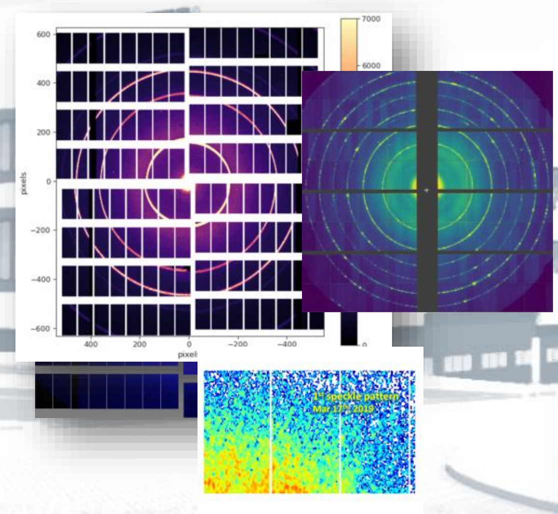
Operational Experience and Lessons Learned with Existing Detectors

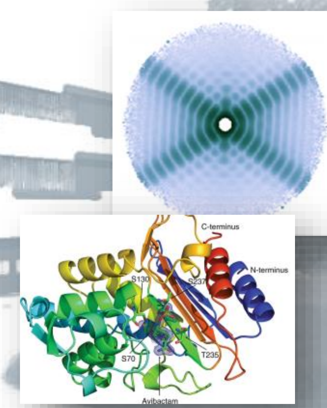
(Hardware, Interlocks and Calibration)

Jola Sztuk-Dambietz
for Detector Group







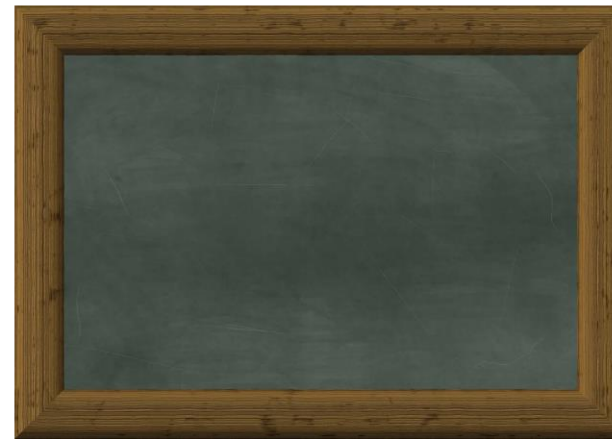


Future Detectors for the European XFEL Workshop

Schenefeld, 18th September 2023

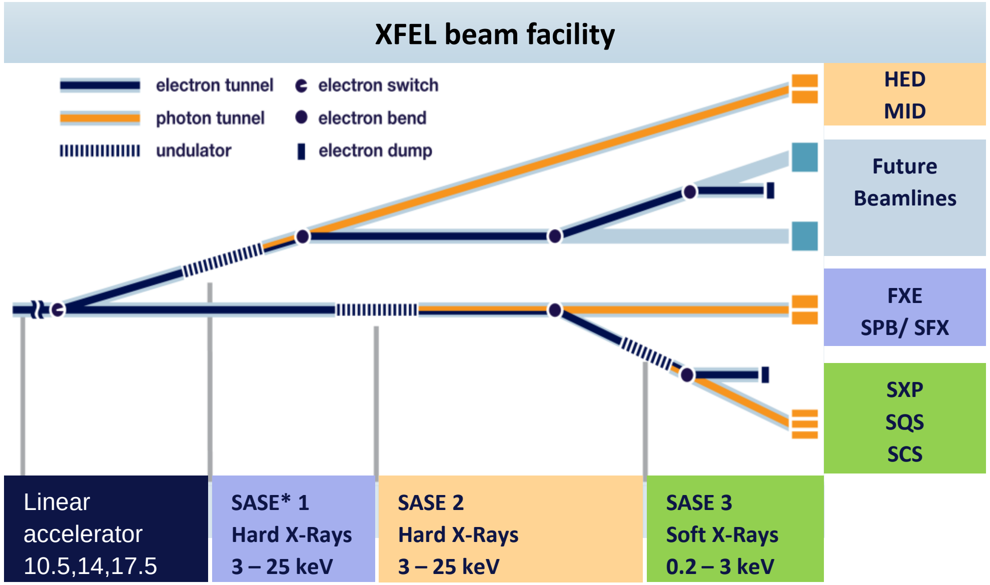
Outline

- First-Generation Detectors for EuXFEL: Navigating the Unique Time Structure
  - Our path to the current stage
- Operation and Lessons Learned
  - Insights gained from integration, commissioning and operations

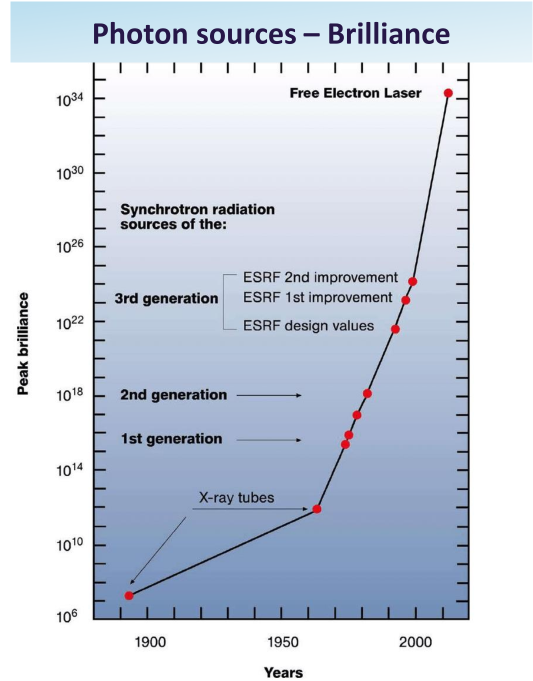


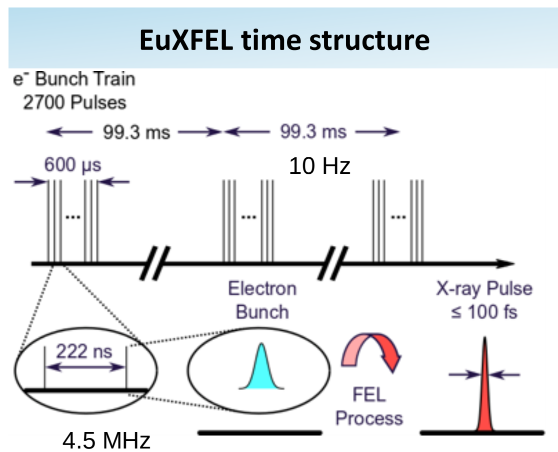
EuXFEL facility : 3 beamlines, 7 Instruments

Start of operation – July 2017



*Self-Amplified Spontaneous Emission





Challenges for Detectors → Demanding Intensity and Timing Constraints

- High dynamic range (10^4 ph/pixel/pulse) with single photon sensitivity for soft and hard X-ray instruments
- Radiation hardness
- MHz operation (in the burst mode)
- **No commercial imaging detectors available**

First Generation of EuXFEL detectors: A journey from concept to user operation

- **For the first-generation detectors, EuXFEL initiated a dedicated call for proposals from external development groups**
  - **2006:** Launched a Call for Expression of Interest
  - **Selected Proposals** → Three different projects adopting different solutions to solve the EuXFEL challenges
    - ▶ Adaptive Gain Integrating Pixel Detector
    - ▶ Large Pixel Detector
    - ▶ DEPFET Sensor with Signal Compression
  - **Goal:** Developing at least one MHz 2D Imaging Detector
  - Development started ca. 2009


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

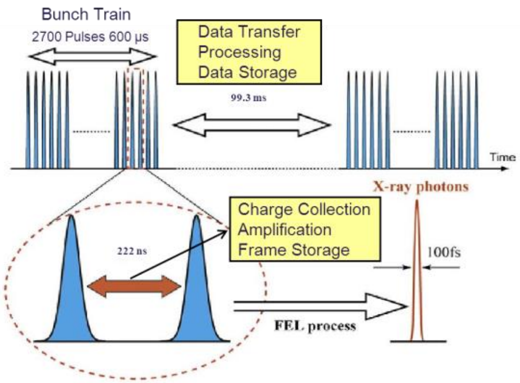
for:

Expressions of Interest

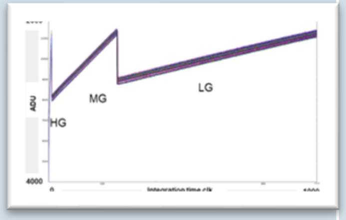
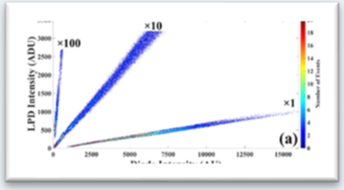
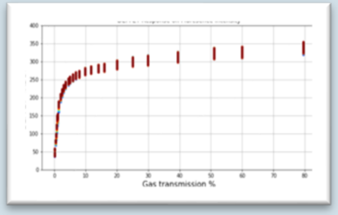
to:

Develop and Deliver Large Area Pixellated X-ray Detectors.

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



The first MHz detector generation at the EuXFEL

Detector	Specs	Gain Mechanism	Gain	Start of Operation
AGIPD 	352 memory cells (analog) 200µm x 200µm sq. pixels 1-10^4 12 keV ph 3-20 keV Modular: 16 (1MPix) or 8 (0.5MPix) modules	3 gains with automatic switching		AGIPD1M (SPB/SFX): 2017 AGIPD1M (MID): 2019 AGIPD500K: 2020 (new gen.) AGIPD4M (SPB/SFX): 2024 (new. gen) AGIPD1M (HED): 2024 (new gen)
LPD 	(3x)512 memory cells (analog) 500µm x 500µm sq. pixels 1-10^5 12 keV ph 7- 20 keV Modular: 16 module (1MPix)	3 parallel gain stages with on front-end selection		LPD (FXE): 2017
DSSC 	800 memory cells (digital) 204µm x 236µm hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ f≤2.2 MHz N ≤ 1 for single ph sensitivity 0.5 – 6 keV Modular: 16 modules (1MPix)	Linear response (miniSDD), non-linear signal compression in sensor (DEPFET)		DSSC1M (SCS): 2019 DSSC DEPFET: 2024

A Journey from Concept to User Operation <u>> 10 years</u>

Detectors at EuXFEL

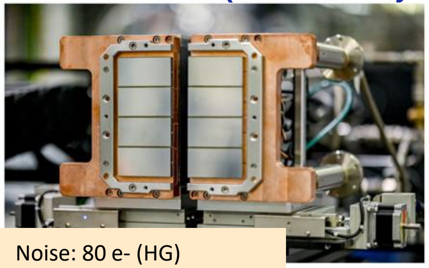
X-ray energy

Hard X-rays 6-25 keV

ePix100 (MID, HED)

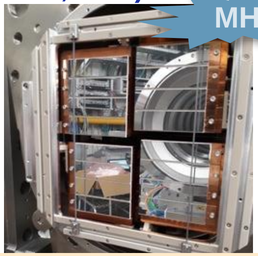
Noise: 50 e- (HG)
Dyn range: 100 8 keV ph

JUNGFRAU x 18 (all hard X-ray inst.)



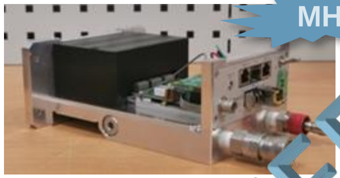
Noise: 80 e- (HG)
Dyn range: 10^4 12 keV ph

AGIPD (SPB/SFX, MID, HED) MHz

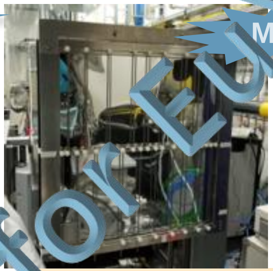


Noise: 350 e- (HG)
Dyn range: 10^4 12 keV ph

GOTTHARD-II MHz



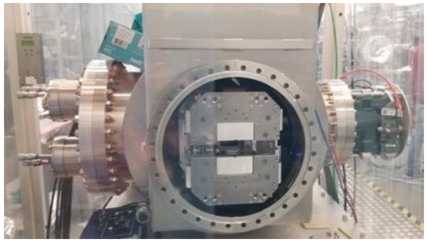
LPD (FXE) MHz



Noise: 2010 e- (HG)
Dyn range: 10^5 12 keV ph

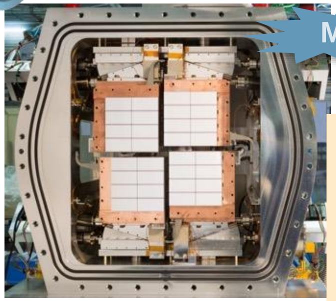
Soft X-rays 0.5-3 keV

pnCCD (SQS)



Noise: 3 e-
Dyn range: 1500-3000 1 keV ph

DSSC (SCS, SQS) MHz



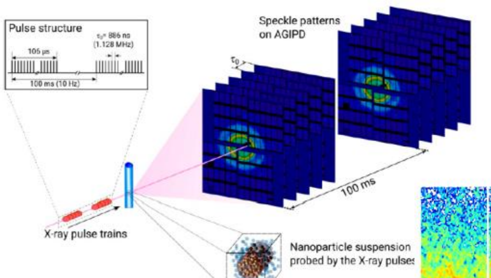
Noise: 60 e-
Dyn range:
N x 256 ph @ 4.5 Mhz
–
N x 512 @ f≤2.2 MHz
N ≤ 1 for single ph sens.

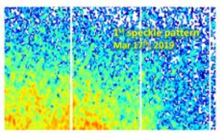
Developed for EuXFEL

10 Hz
4.5 MHz
Rate

European XFEL Detectors: enabling scientific excellence

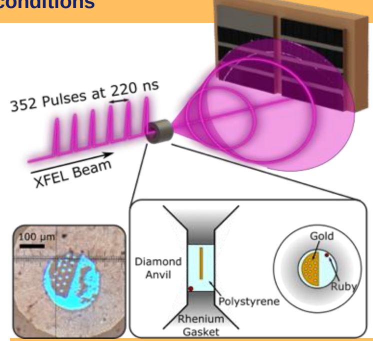
MHz XPCS to look at system dynamics



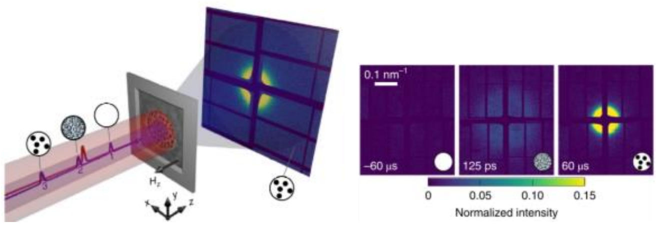


Lehmkühler et al. PNAS 117:24110-24116(2020)

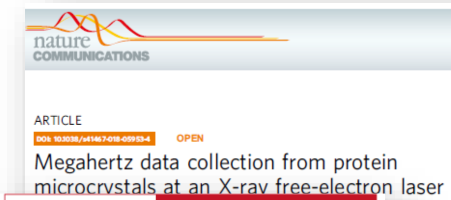
Study of materials in extreme conditions



M. Frost et al., accepted by Nature Astronomy (2023)



F. Büttner et al., Nat. Mater., 20, 30-37 (2021)


nature COMMUNICATIONS

ARTICLE

OPEN

Megahertz data collection from protein microcrystals at an X-ray free-electron laser

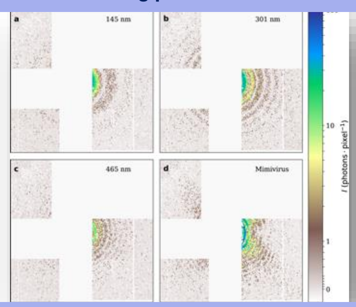

nature methods ARTICLES

Time-resolved serial femtosecond crystallography at the European XFEL


ARTICLES nature materials

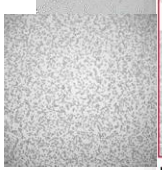
Observation of fluctuation-mediated picosecond nucleation of a topological phase

Examples of scattering patterns from IrCl3 and Mimivirus.

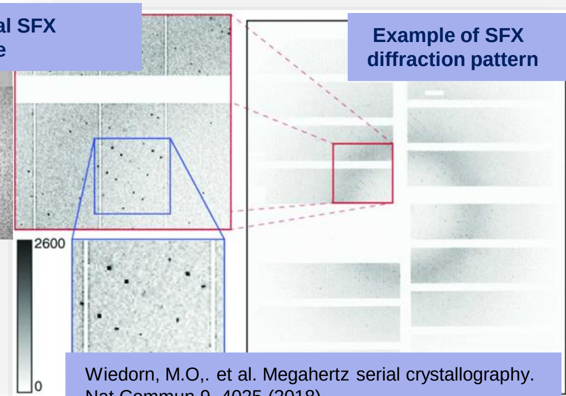


Sobolev, E. et al. Megahertz single-particle imaging at the European XFEL Commun Phys 3, 97 (2020)

Typical SFX sample



Example of SFX diffraction pattern

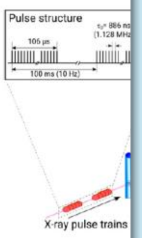


Wiedorn, M.O,. et al. Megahertz serial crystallography. Nat Commun 9, 4025 (2018)

European XFEL Detectors: enabling scientific excellence

Study of materials in extreme conditions

MHz XPCS to look at system dynamics



- Significant role of EuXFEL detectors in facilitating high-quality scientific outcomes → the data provided by the detectors allows production of high-quality scientific results
- Integration, commissioning, operation, data collection and dedicated studies have also led to the identification and quantification of challenges related to detector performance and operation

Lehmkühl

Examples of s


ARTICLES

graphy

Austin Echelmeier, Diandra Doppler, Moritz Emons, Matthias Frank, Raimund Fromme, Yaroslav Gevorkov, Gabriele Giovanetti, Man Jiang, Daihyun Kim, Yoonhee Kim, Henry Kirkwood, Anna Klimovskaia, Juraj Knoska, Faisal H. M. Koua, Romain Letrun, Stella Lisova, Luis Maia, Victoria Mazalova, Domingo Meza, Thomas Michelat, Abbas Ourmazd, Guido Palmer, Marco Ramilli, Robin Schubert, Peter Schwander, Alessandro Silenzi, Jolanta Sztuk-Dambietz, Alexandra Tolstikova, Henry N. Chapman, Alexandra Ros, Anton Barty, Petra Fromme, Adrian P. Mancuso and Marius Schmidt

Sobolev, E. et al. Megahertz single-particle imaging at the European XFEL.
Commun Phys 3, 97 (2020)

Wiedorn, M.O,. et al. Megahertz serial crystallography.
Nat Commun 9, 4025 (2018)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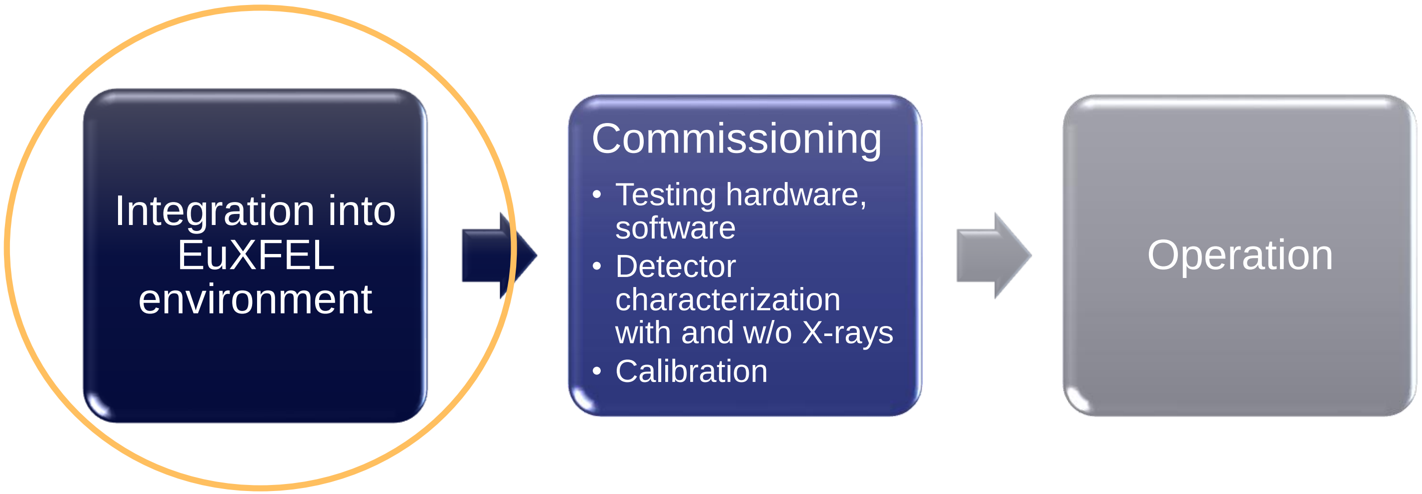
nature materials

Observation of fluctuation-mediated picosecond nucleation of a topological phase

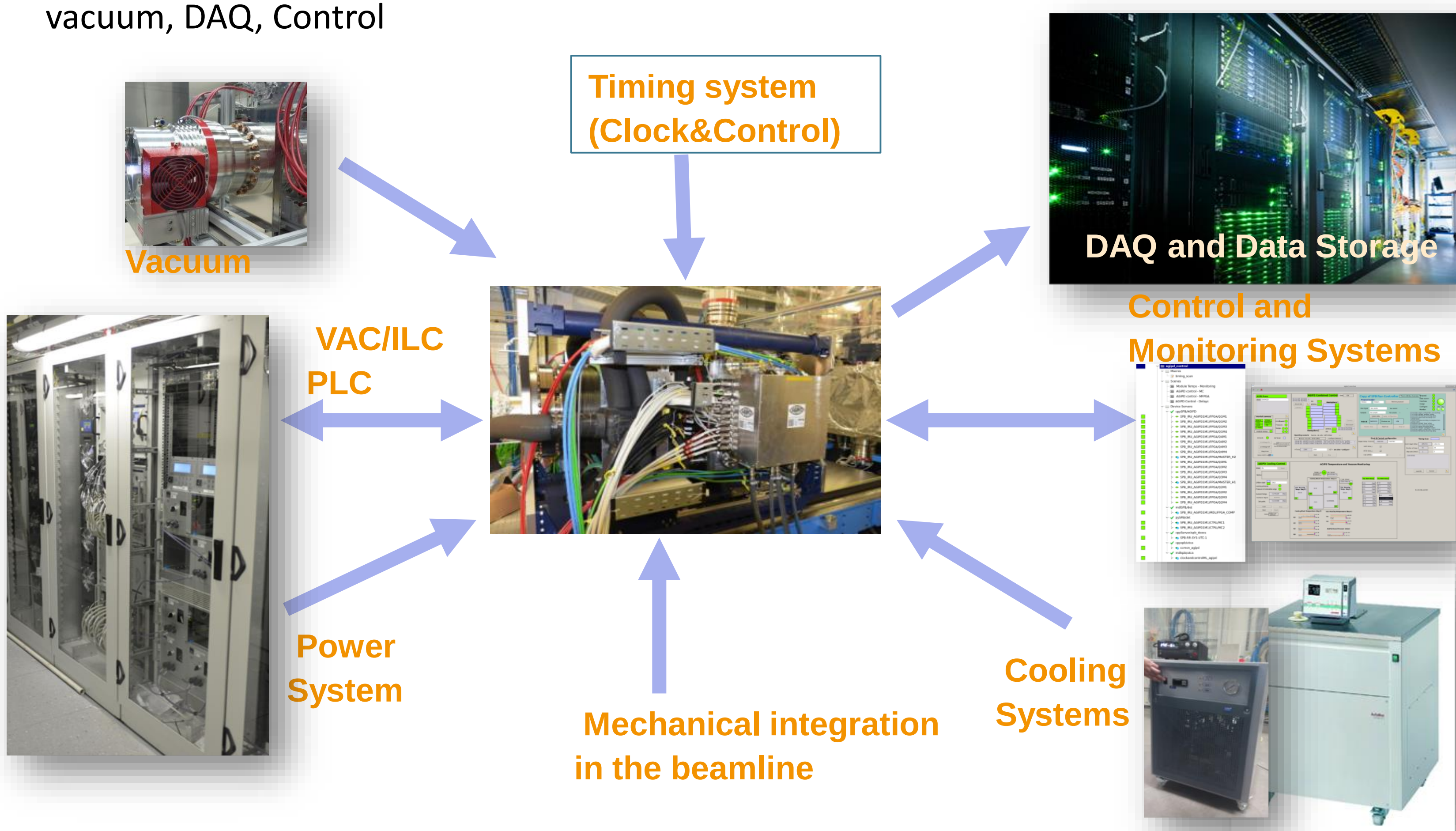
Felix Büttner, Bastian Pfau, Marie Böttcher, Michael Schneider, Giuseppe Mercurio, Christian M. Günther, Piet Hessing, Christopher Klose, Angela Wittmann, Kathinka Gerlinger,

What have we learned from the first-generation detectors?



Integration: A complex task

- EuXFEL detectors were fully integrated into our infrastructure: mechanics, cooling, power, vacuum, DAQ, Control



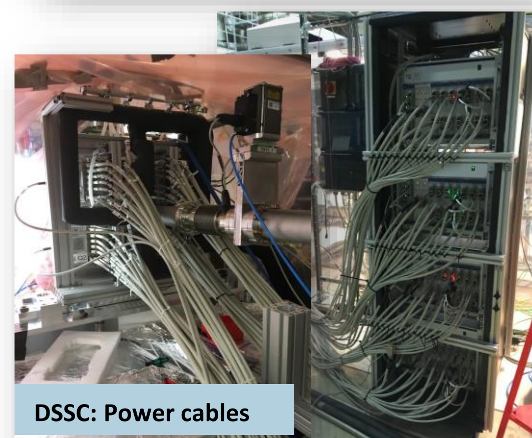
Integration is a highly complex task → Start early to define interfaces

It is all about the cables…

- The challenge of cables and cooling is often underestimated
- The "HEP approach" for powering the detector is not well-suited for XFEL applications, especially considering the number of cables that need to be managed when detectors must be moved
  - this approach significantly increases the risk of damaging the detector or other beamline instrumentation.
  - it limits access to the detector electronics in case of failure or routine maintenance

More compact design and optimization of the power/cooling system are needed

AGIPD at MID



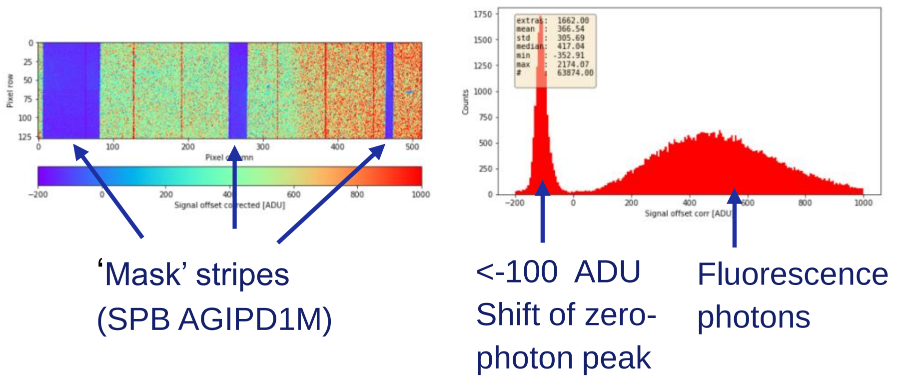
DSSC: Power cables

What have we learned from the first-generation detectors?

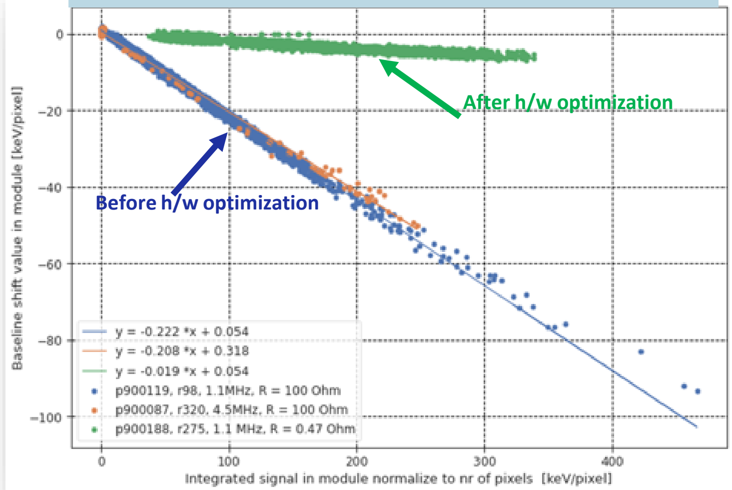
Testing in real experimental conditions

- We can test at the same time all detector properties only with the EuXFEL beam
  - Identifying features related to high intensity at high speed can be challenging
  - Dedicated beam time for detector characterization is essential to optimize detector performance
  - Characterizing the detectors requires a joint effort between EuXFEL and DET developers

Baseline shift - effect in offset corrected image (Cu fluorescence)

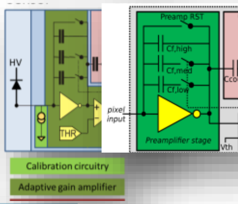


AGIPD: Baseline shift as a function of X-ray intensity



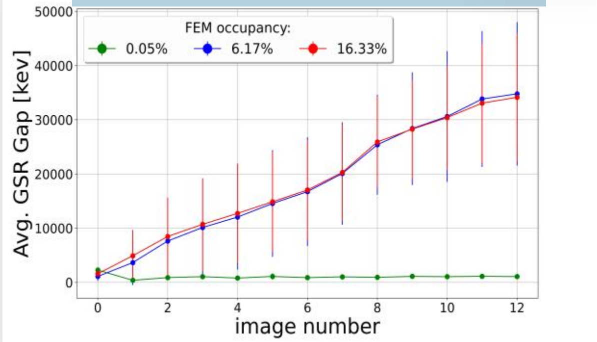
Effective detector optimization requires the XFEL beam and is a continuous processes that necessitates collaboration and feedback from DET developers, instrument scientists and users

Data Quality: Adaptive gain and its transition region

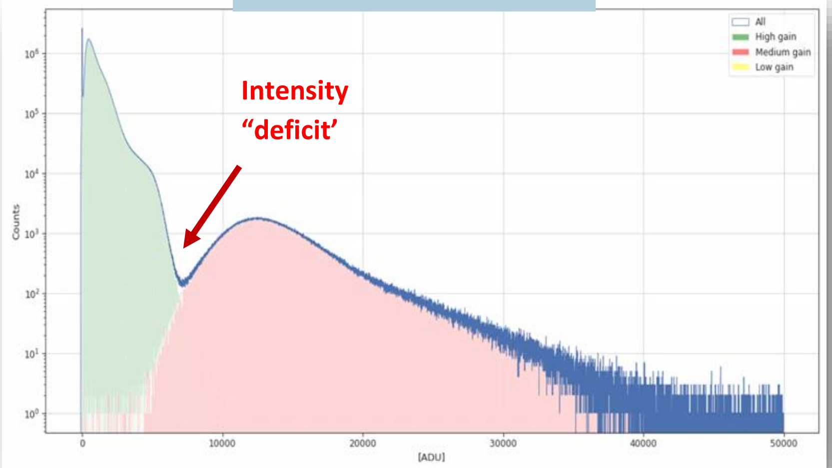


- Adaptive gain, an elegant method to achieve a high dynamic range, faces challenges in the transition region
  - Issue with proper determination of “baseline’ for lower gain stages
  - Both AGIPD and JUNGFRAU affected
  - Preliminary findings indicate an issue in that region with GOTTHARD-II as well

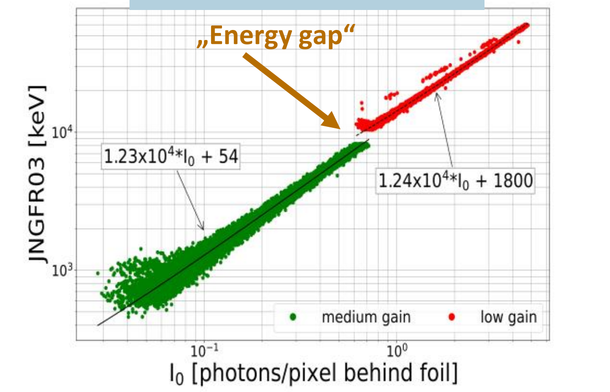
JUNGFRAU: Energy gap vs. mem. cell



AGIPD: Intensity spectrum

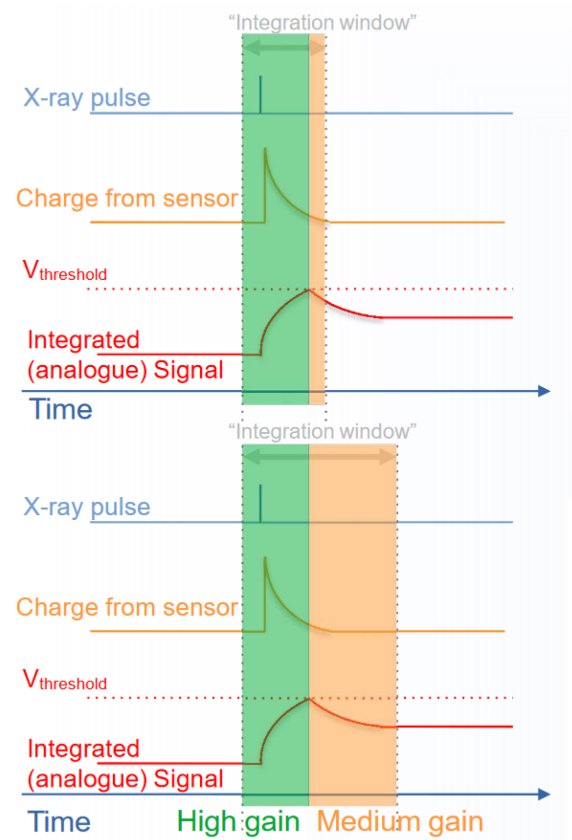


JUNGFRAU: Intensity scan



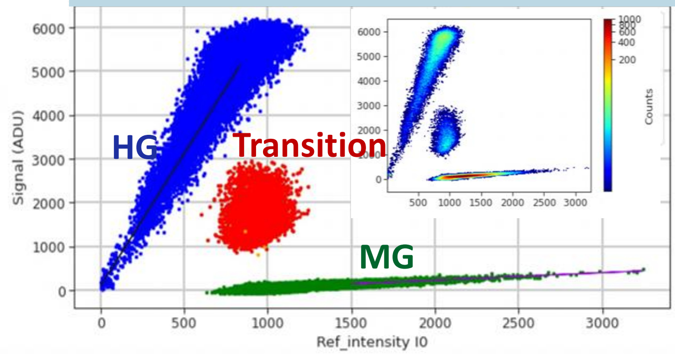
Data Quality: Adaptive gain and its transition region

- Fast (4.5MHz) operation → 'late gain switching' ("snowy pixels")

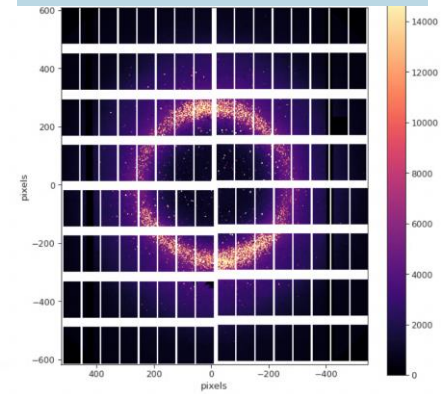


Courtesy of Ulrich Trunk (DESY FS-DS)

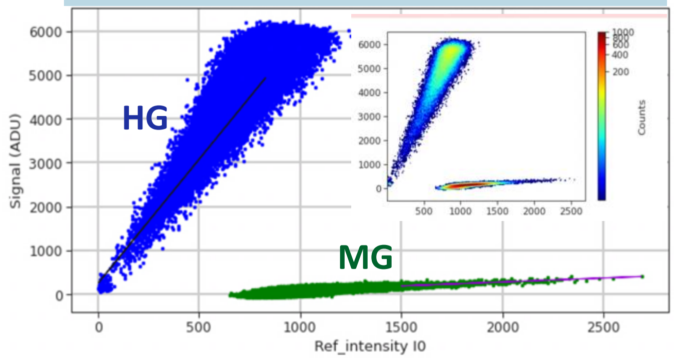
Intensity scan (single pixel, all mem. cells) – 120 ns



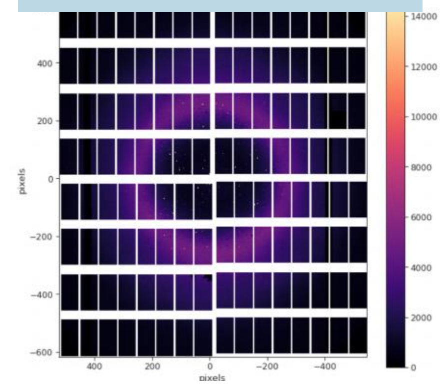
Lysozyme data – 120 ns int. time



Intensity scan (single pixel, all mem. cells) – 200 ns



Lysozyme data – 200 ns int. time

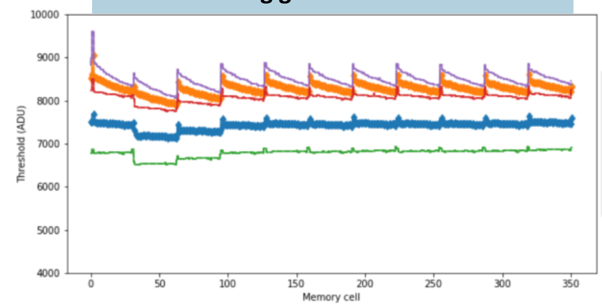


For the next generation of detectors, addressing the observed issue with the adaptive gain mechanism is crucial, and alternatives should be explored

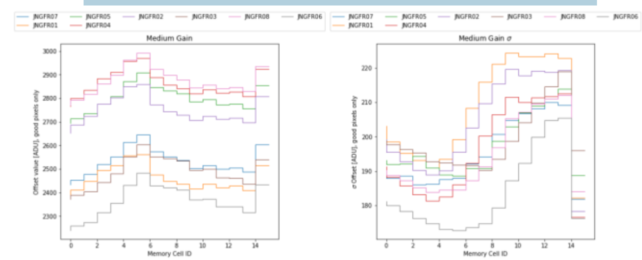
Data Quality: Analog memory cells

- Analog memory cells are used to temporarily store signals before they can be read out → this storage technique is employed in several detectors, including AGIPD, LPD, and JUNGFRAU
  - Analog memory cells impact data quality with offset and gain variations
  - Cross-talk observed between adjacent memory cells
  - Extensive calibration required to mitigate the issues

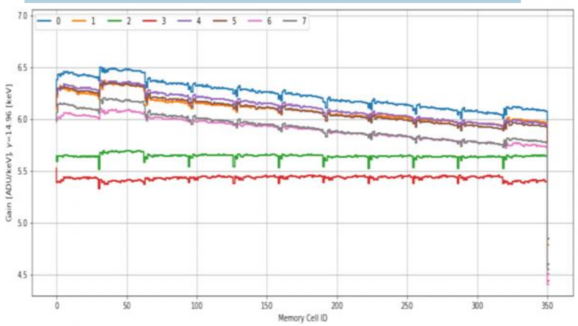
AGIPD: Analog gain value vs. mem. cell



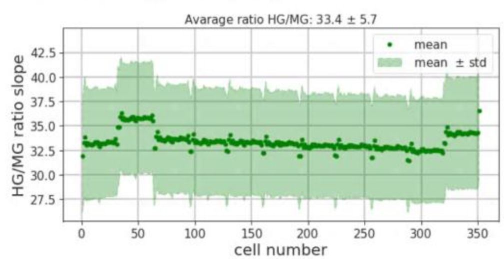
JNGF4M: Average Offset MG vs. mem. cell



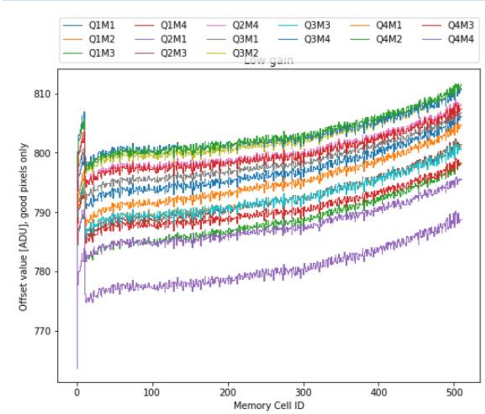
AGIPD: Average Gain (HG) vs. mem. cell



AGIPD: Average HG/MG ratio vs. mem. cell



LPD1M: Average Offset LG vs. mem. cell



Move away from analog memory cells for the next generation of the detectors

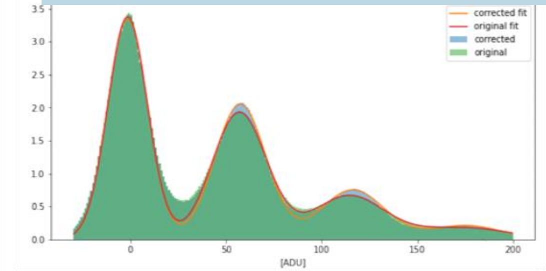
Data Quality: Addressing issues with dedicated operation modes

- The detector 'artefacts' impact scientific analyses

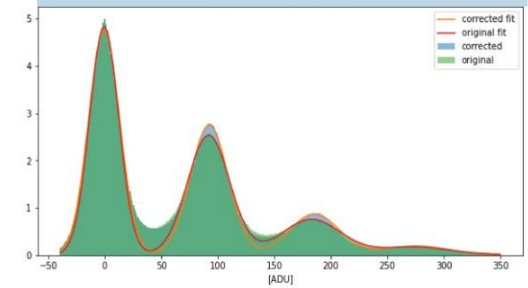
- Enable "experiment-specific" operation modes (detector configurations)
  - "**Very High Gain mode**" with improved noise performance
    - low intensity data (i.e. no dynamic range required)
  - **Fixed (medium) Gain mode**
    - solution for experiments which does not required single ph. sensitivity
  - **Operation with longer int. time** (for acq < 4.5MHz) to avoid snowy pixels

- Implement **image-topology dependent corrections**
    - Low intensity data: Common mode corrections (across ASIC and memory cell rows) for very low intensity data

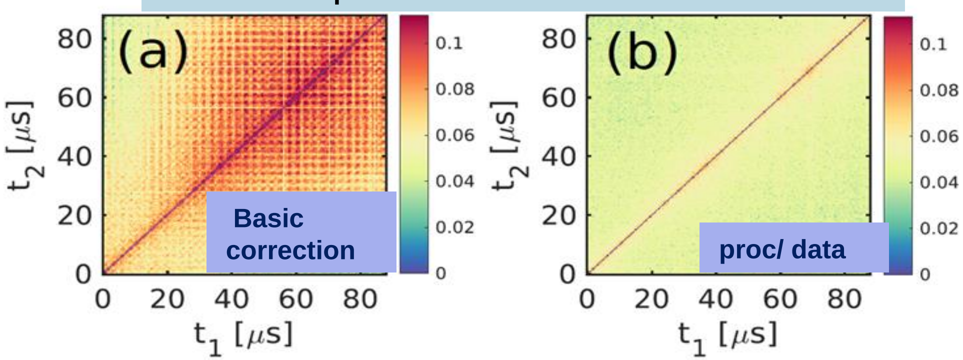
Cu fluorescence in 'default' High Gain



Cu fluorescence in Very High Gain

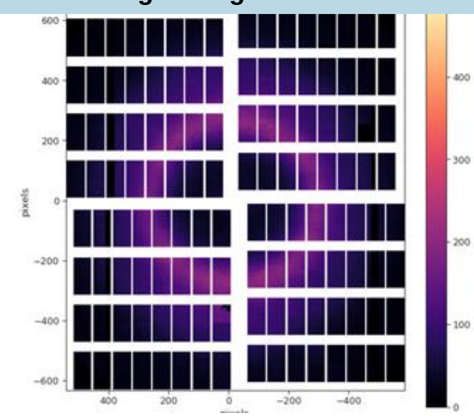


XPCS – Example of Double correlation function – MID



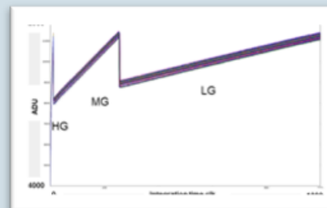
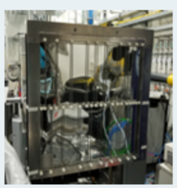
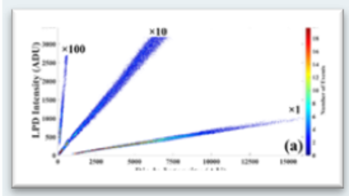
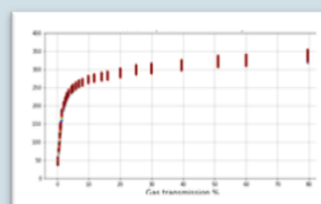
Francesco Dallari et. al., Applied Sciences, vol. 11, no. 17, p. 8037, 2021.

SFX – single image in fixed MG mode



MHz, MPix & high dynamic range detectors – challenges for calibration

- Calibration needs to be performed whenever there are significant changes in detector hardware or performance
  - Routinely done after each maintenance period for the hard X-ray detectors
  - Calibrating the full dynamic range is a major challenge

Detector	Specs	Gain Mechanism	Gain
AGIPD 	352 memory cells (analog) 200µm x 200µm sq. pixels 1-10^4 12 keV ph 3-20 keV Modular: 16 (1MPix) or 8 (0.5MPix) modules	3 gains with automatic switching	
LPD 	(3x)512 memory cells (analog) 500µm x 500µm sq. pixels 1-10^5 12 keV ph 7- 20 keV Modular: 16 module (1MPix)	3 parallel gain stages with on front-end selection	
DSSC 	800 memory cells (digital) 204µm x 236µm hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ f≤2.2 MHz N ≤ 1 for single ph sensitivity 0.5 – 6 keV Modular: 16 modules (1MPix)	Linear response (miniSDD), non-linear signal compression in sensor (DEPFET)	

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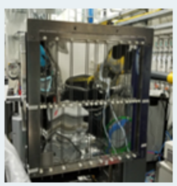
LPD 	(3x)512 memory cells (analog) 500µm x 500µm sq. pixels 1-10^5 12 keV ph 7- 20 keV Modular: 16 module (1MPix)	- Three gain stages per pixel - Analog memory cells - Detector artefacts	
DSSC 	800 memory cells (digital) 204µm x 236µm hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ f≤2.2 MHz N ≤ 1 for single ph sensitivity 0.5 – 6 keV Modular: 16 modules (1MPix)	- Non-linear gain to be evaluated	

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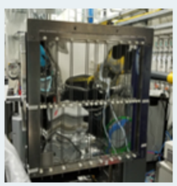
LPD 	(3x)512 memory cells (analog) 500µm x 500µm sq. pixels 1-10^5 12 keV ph 7- 20 keV Modular: 16 module (1MPix)		
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Challenges

AGIPD:
- Three gain stages per pixel
- Analog memory cells
- Analog gain evaluation
- Many operation modes to mitigate detector artefact

LPD:
- Three gain stages per pixel
- Analog memory cells
- Detector artefacts

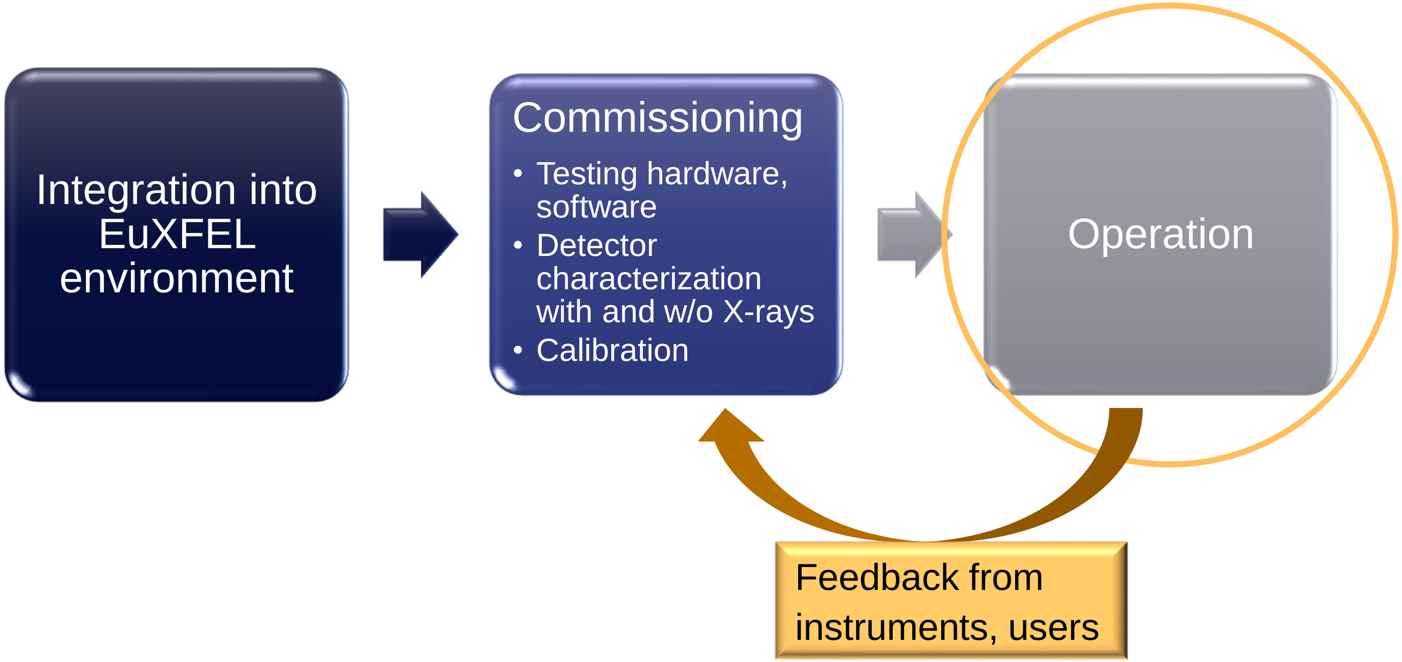
DSSC:
- Non-linear gain to be evaluated

Example AGIPD (one operation scenario)
x 1 million pixels
x 352 memory cells
x 3 gain stages
x number of needed calibration constants
→ > 10^9 parameters

The constants have to be generated for different operation modes:
→ rep. rate
→ Number of mem. cells
→ Integration time

For the next detector generation, prioritize a design that is calibration-friendly and supports reliable in-situ calibration sources

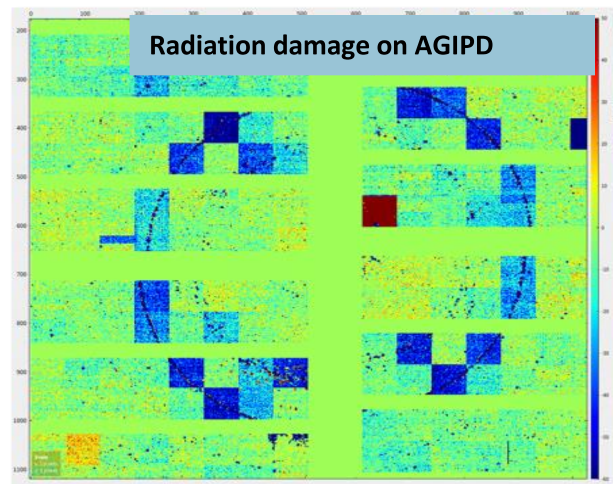
What have we learned from the first-generation detectors?

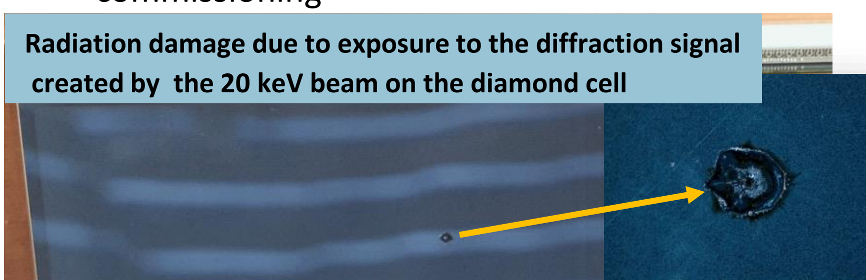


The significance of ease of operation and interlocks

- Incidents happen → Interlock system has saved detectors from severe damage on several occasions:
  - Chillers, cooling water failures
  - Vacuum quality during liquid jet injection, pump failure
  - Power cuts
  - Human error
- Radiation damage and hardware failure happens
  - An online monitoring and alarm system is a necessity
  - Easy access and the ability to quickly exchange modules
  - Fast access to electronics is crucial
  - Protection against e.g. ice formation would help, under commissioning


Deformed DSSC cooling pipes

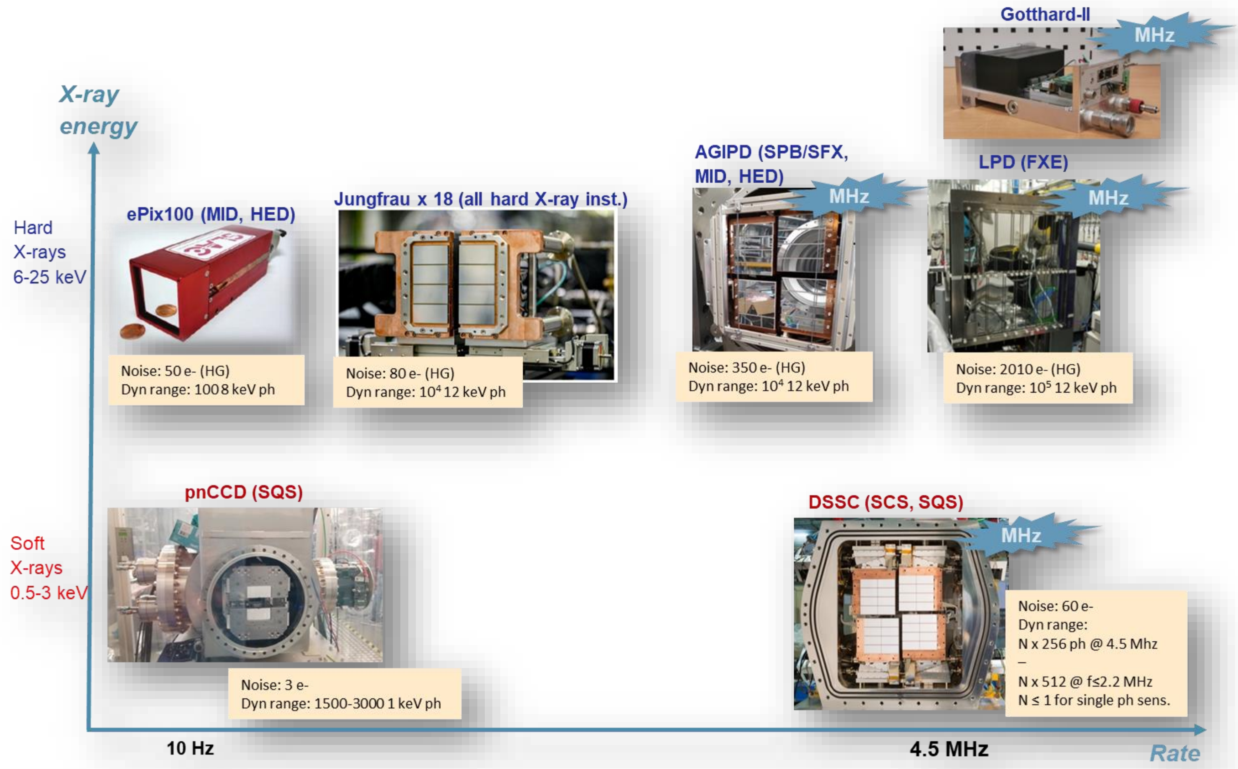

Radiation damage on AGIPD


Radiation damage due to exposure to the diffraction signal created by the 20 keV beam on the diamond cell

Courtesy of DESY FS-DS

A self-protecting, robust system with easy access to electronics components in the detector vessel and the availability of spare parts is essential

The impact of having a detector ‘zoo’

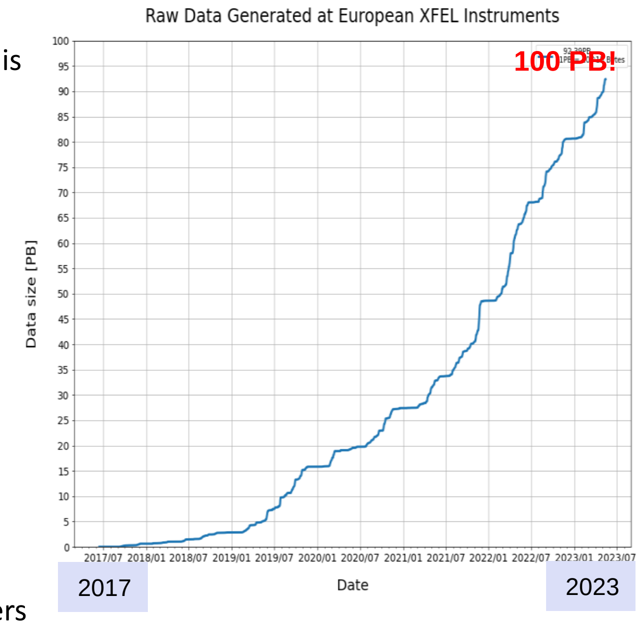


- Different technologies require different experts
- Standardization in controls, interlocks, and calibration is challenging, if not impossible
- We heavily rely on developers for tasks like firmware updates.

To address these challenges for the next generation of detectors, standardization efforts and investments in "In-House Expertise" are necessary

Data volume challenge (more in K. Wrona's talk)

- The amount of collected data is huge (> 100 PB of raw data)
- The initial strategy of indefinitely storing all data beyond the embargo period is no longer sustainable
- Data reduction addressed starting from policy down to specific online and offline data reduction implementations:
  - **Data management plan (DMP)** to include data reduction early and throughout the proposal process
  - **Operation-specific**, e.g.: automatic detection of non-illuminated frames
  - **Technique-specific,** e.g. event reconstruction, hit finding (*SFX*, *SPI*), $g^{(2)}$ correlation functions (*XPCS*, *XCCA*)
- First attempts with real-time reduction before saving to disk
- Currently preparing to apply techniques to past data in collaboration with users



In the next detector generation, consider implementing data reduction as near to the detector head as possible

Key Takeaways

- Integrating the first detector generation into EuXFEL was a complex task
  - The required infrastructure poses challenges for integration and operation
  - More compact, efficient power and cooling design with standardized interfaces are needed

- EuXFEL provided around 8000 hours of user beamtime last year:
  - Ease operation and reliability are essential
  - Accessible detector components for maintenance and replacement
  - Hardware interlocks are crucial (consider self-protecting detectors)

- Data quality is the primary measure of detector performance
  - Testing detectors under real XFEL conditions already on prototype level is essential
  - Methods for achieving high dynamic range need evaluation
  - A design that is calibration-friendly and supports reliable in-situ calibration sources is necessary
  - Collaborative efforts involving experts with diverse backgrounds and investment in “In-House Expertise” are vital for optimizing detector performance and addressing observed issues

- Standardizing technologies is essential to reduce the operational burden

- Managing the enormous volume of generated data requires early design-level reduction strategies

Lessons learned today shape the detectors of tomorrow

European XFEL

Thank you

Acknowledgment

UKRI Science and Technology Facilities Council

DSSC

DESY

POLITECNICO MILANO

HALBLEITERLABOR DER MAX-PLANCK-GESELLSCHAFT MPG HLL

PNSensor

UNIVERSITATIS STUDIORUM BERGOMENSIS

INFN Istituto Nazi… di Fisica Nuc…

AGIPD

UHH Universität Hamburg

universitätbonn

PAUL SCHERRER INSTITUT PSI

DESY.

Backup slides

XFEL Science: 7 Instruments

SASE 1 (Hard X-Rays)

SPB/SFX (start Sep 2017)
Single Particles, Clusters and Biomolecules /
Serial Femtosecond Crystallography

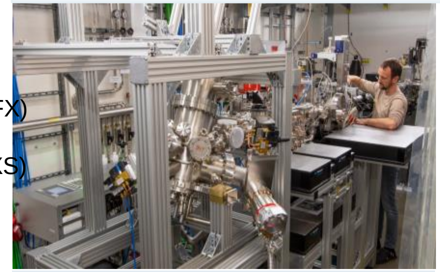
FXE (start Sep 2017)
Femtosecond X-Ray Experiment

SASE 2 (Hard X-Rays)

MID (start Apr 2019)
Materials Imaging & Dynamics

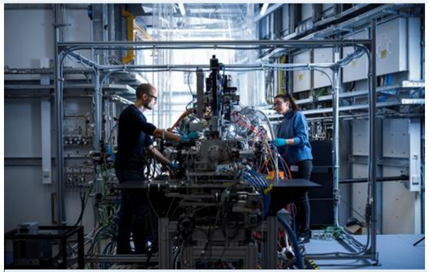
HED (start May 2019)
High Energy Density Matter

SASE 3 (Soft X-Rays)



SXP (start summer 2023)
Soft Xray Port

SCS (start Nov 2018)
Soft X-Ray Coherent Scattering / Spectroscopy



SQS (start Nov 2018)
Small Quantum Systems

Main Technics:

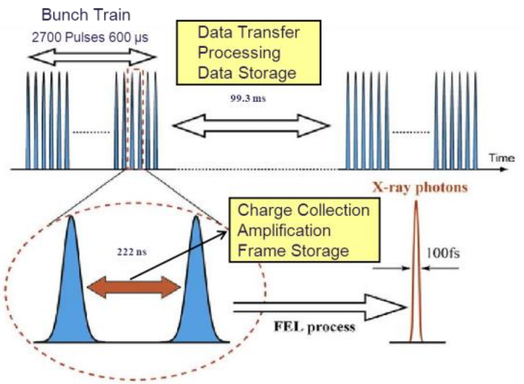
- Single Particle Imaging (SPI)
- X-ray scattering (WAXS/ SAXS)
- Serial Femtosecond Crystallography (SFX)
- X-ray Spectroscopies (XES/ XAS)
- Resonant Inelastic X-ray Scattering (RIXS)
- ….

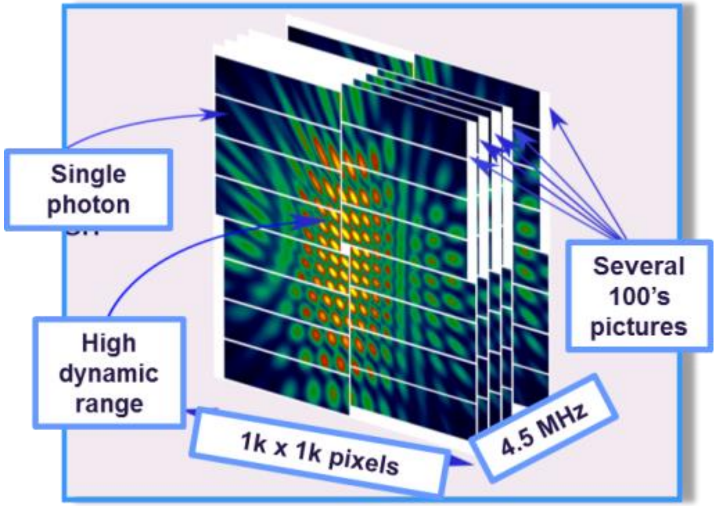
→ **More constraints on detectors**

First Generation Detectors for EuXFEL

Detector requirements from < 2010

- Energy range 0.2 – ~25 keV
- Single photon sensitivity
  - High quantum efficiency (>0.8)
  - Low noise
- High dynamic range 10^4 ph/pixel/pulse
- Vacuum compatible (< 10-6 bar)
- Flexible central hole
- Sufficiently rad. hard for operation at XFEL
- EuXFEL timing compliant

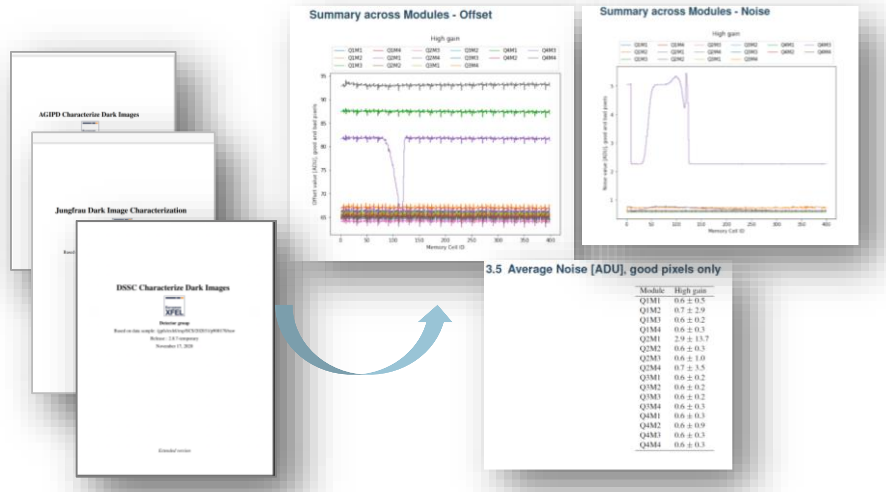


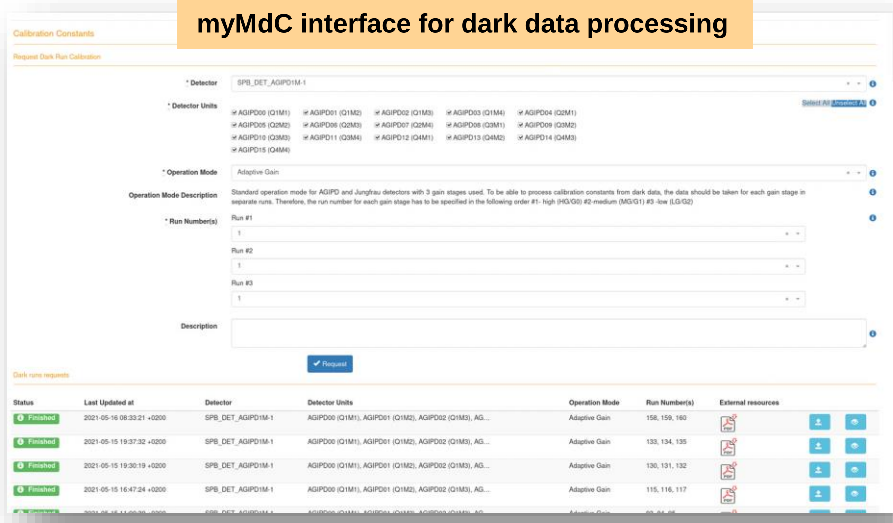


Characterization of the detectors – Calibration constants

Overview – current status

- Characterization with dark data → Offset, Noise and Bad Pixels
  - Generation of the constants for **all detectors** in use is a **part of the experiment routine** → performed **at least twice during the shift**
  - Automatic procedure for data taking and interface via myMdC to start dark data processing → do not requires expert level to create constants
  - Calibration constants are produced and injected to calibration data base
  - Automatically generated reports available to monitor the performance of the detector:
    - ► Configuration information, status of the processing
    - ► Control plots including comparison to the previous version of the calib. constants
  - Time: below 30 mins
    - ► Data collection < 5 mins
    - ► Migration to offline < 5 min
    - ► Processing and generation of reports < 15 min

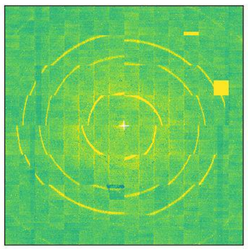




myMdC interface for dark data processing

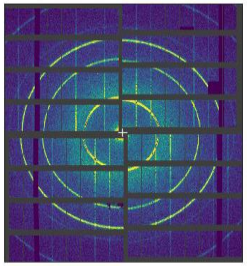
Detectors setups: data correction

- Corrected data proposed for each detector

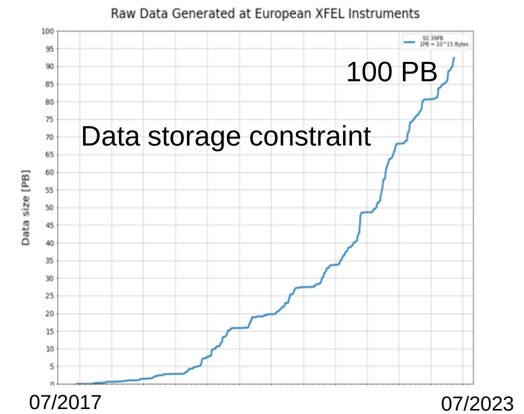


Raw data

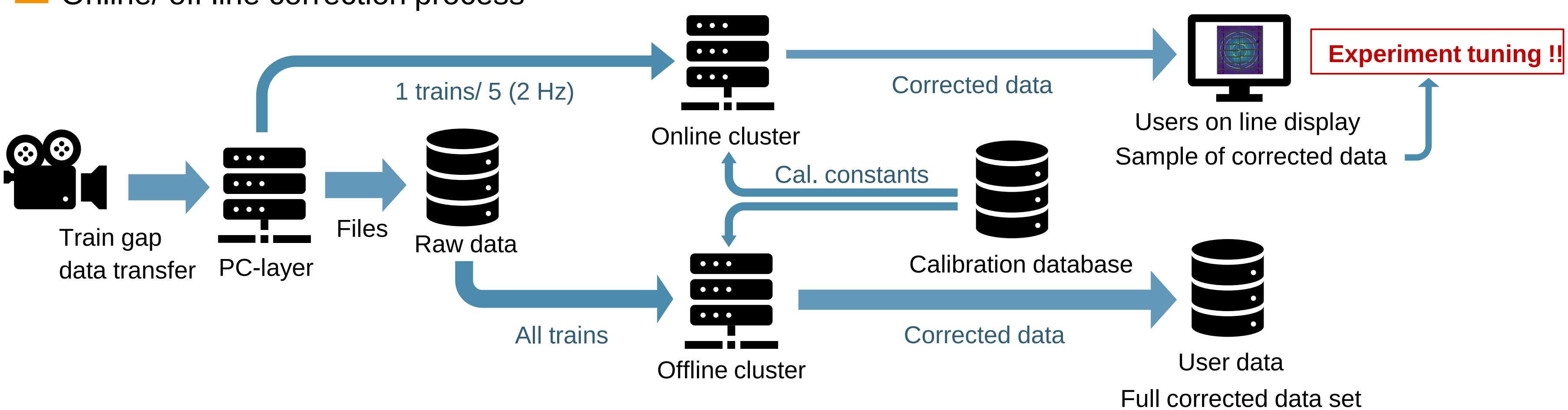
- Offset Correction
- Gain corrections
- Bad Pixel Maps
- ….



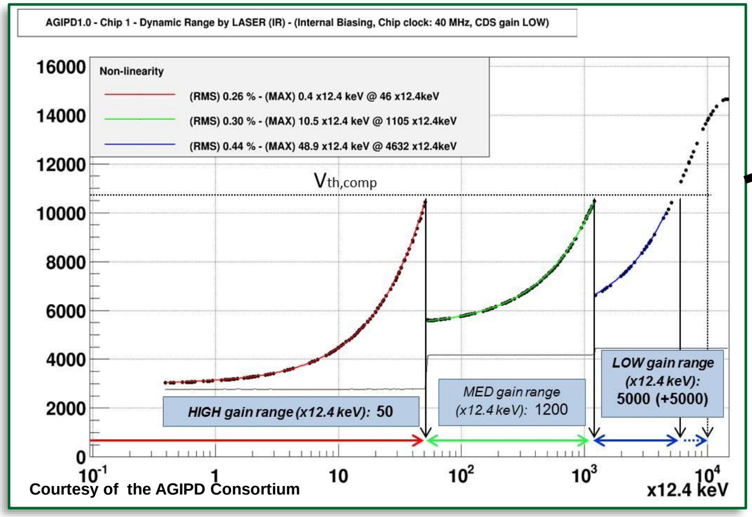
Corrected data

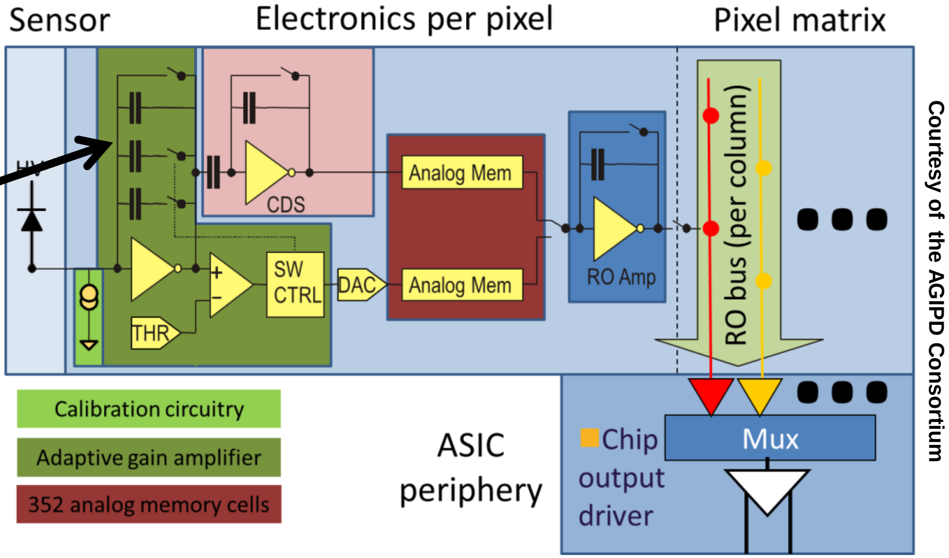


- Online/ off line correction process



AGIPD Pixel Design for Fast Imaging and High Dynamic Range

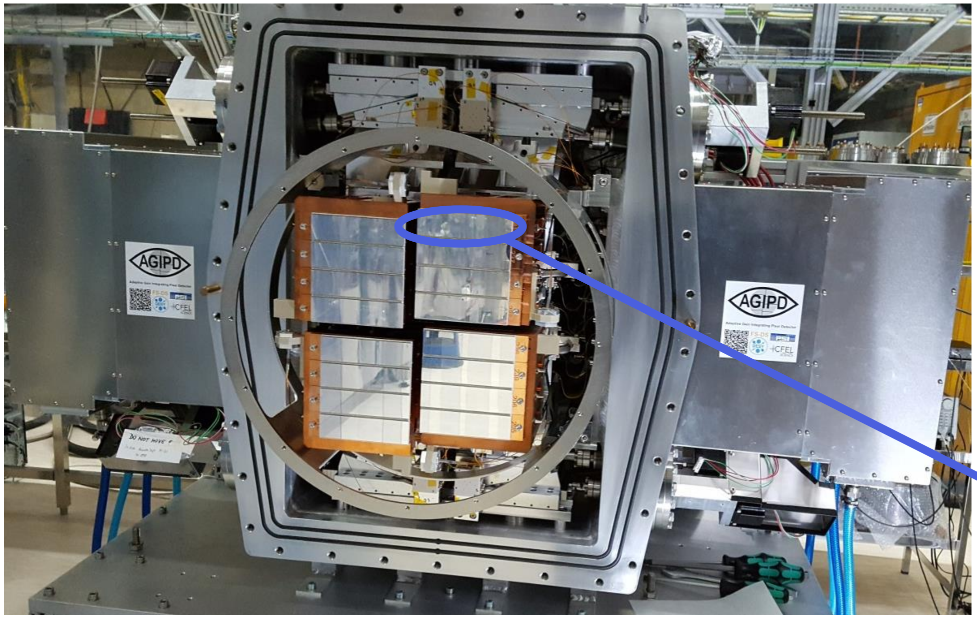




- **200 µm x 200 µm** pixels
- **352 storage cells** for **4.5 MHz** frame rate
- Veto & trigger capabilities by overwriting unfit/obsolete images
- Dynamic range:
  from single photon to 10^4 @ 12 keV

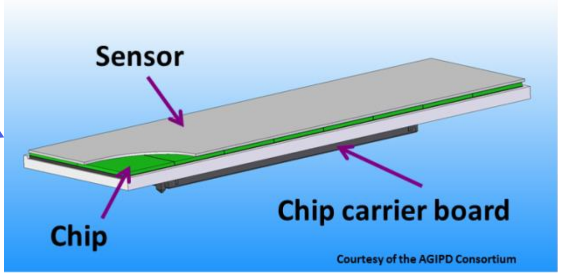
- Preamplifier with **adaptive gain** by insertion of additional feedback capacitors to lower sensitivity and increase dynamic range once a defined threshold is crossed
- Correlated Double Sampling (CDS) stage to remove reset noise and reduce low frequency noise
- Analogue memory, which can store 352 images
- Read out of stored signals are through the pixel buffer, column buffer and off-chip driver in between the bunch

AGIPD detector system for SPB/SFX and MID instruments



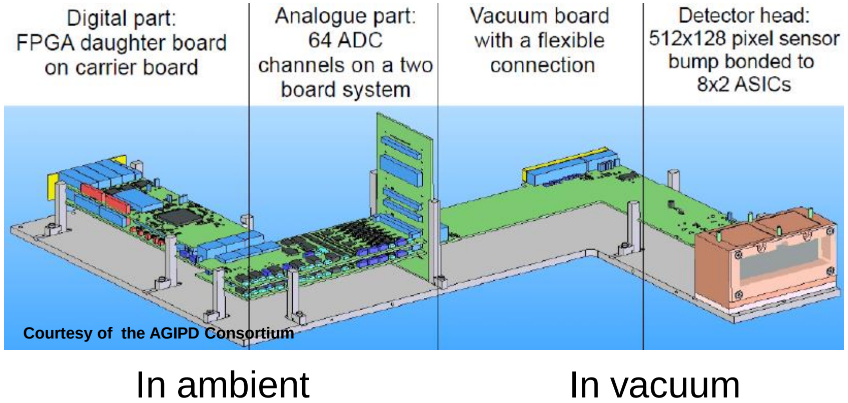
Hybrid detector module

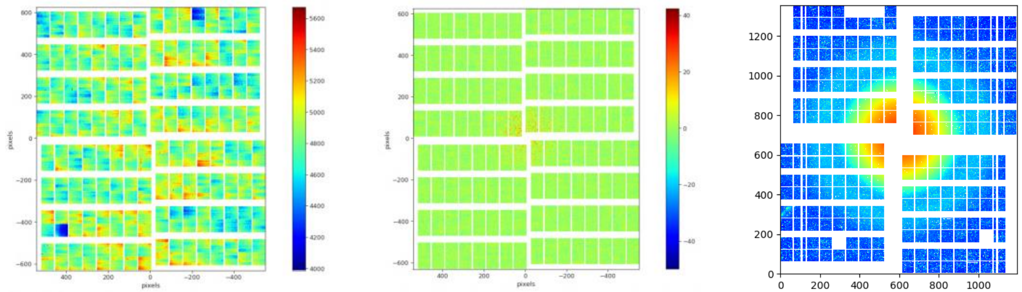
- Sensor:
  - 128 x 512 pixels
  - 500 um thick silicon
- 2 x 8 read-out chips connected to sensor via bump-bonding
- Size: ~26 x 105 mm^2



1M AGIPD system

- 16 modules are mounted on four independently movable quadrants
- Vacuum operation (P< 10^{-5} mbar)
- Electronics/Control: two independent detectors: 'half 1' and 'half 2'
- Readout: 16 independent detectors



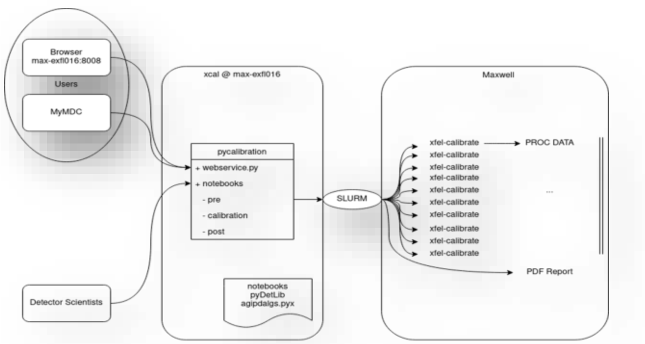


raw proc averaged

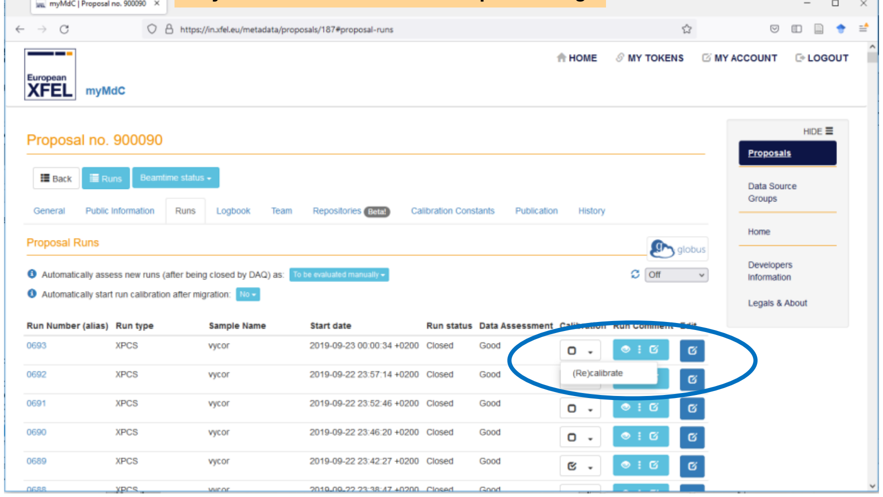
single shot

Offline Calibration Pipeline

- Many 2D detectors require corrections to process “raw” detector data into analysis-ready “proc”
- Raw data processing (calibration request through myMdC (metadata catalogue, in.xfel.eu/metadata)
- XFEL offline calibration (xfel-calibrate) runs on DESY HPC cluster (Maxwell), jobs are distributed across nodes using SLURM



myMdC interface for raw data processing



Online Calibration Pipeline

- Online calibration:
  - Correction of data “on-the-fly” with limited number of corrections
  - Possibility to interface external analysis tool via Karabo bridge
  - Next generation pipeline with improved performance in development
  - For analysis during the experiment only
    - ▶ No files saved
    - ▶ Offline calibration