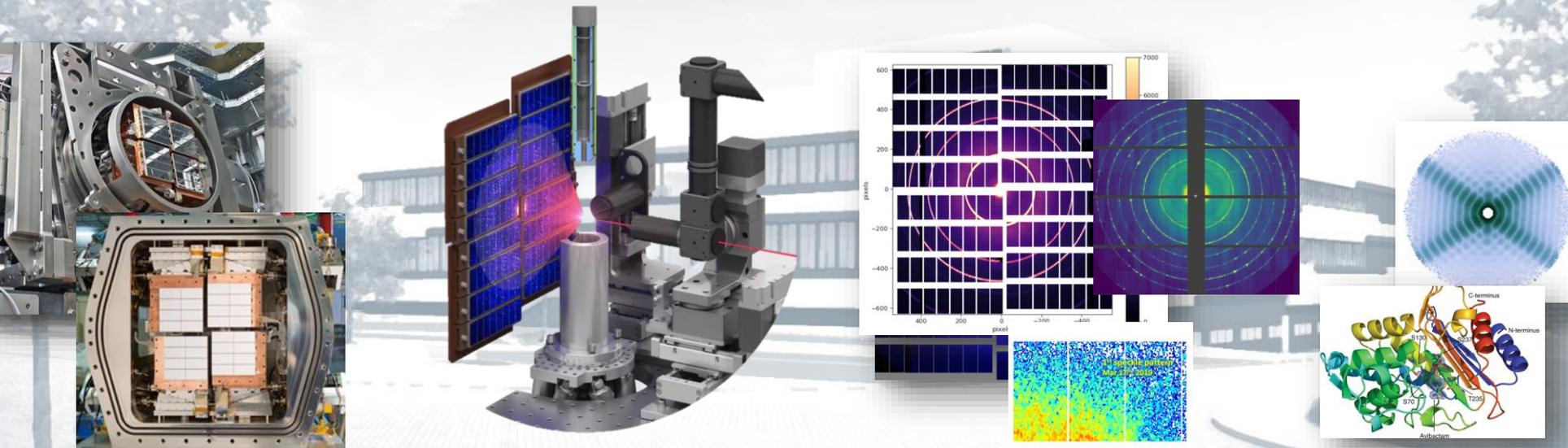


# Operational Experience and Lessons Learned with Detectors at European XFEL (mostly based on AGIPD)

Jola Sztuk-Dambietz  
European XFEL



DESY Joint Instrumentation Seminar  
Hamburg, 1<sup>st</sup> December 2023

# Outline & Acknowledgment

## Outline

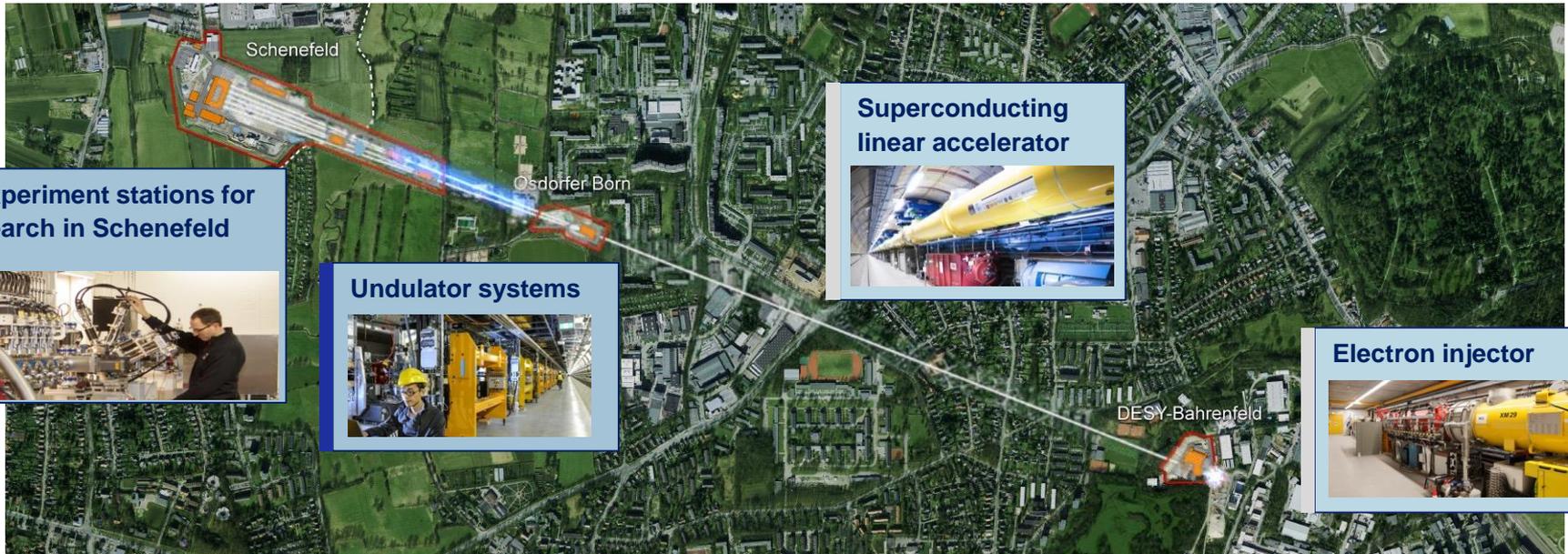
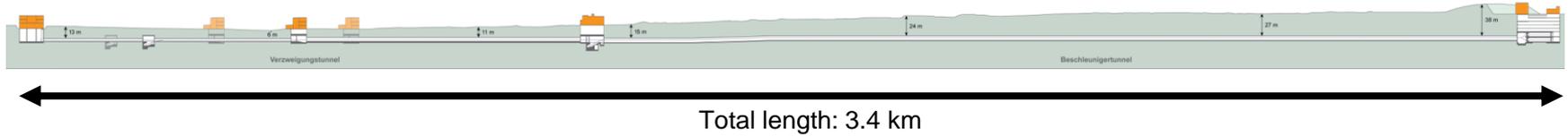
- Introduction
- First-Generation Detectors for EuXFEL: Navigating the Unique Time Structure
  - Our path to the current stage
- Operation and Lessons Learned
  - Insights gained from integration, commissioning and operations

## People



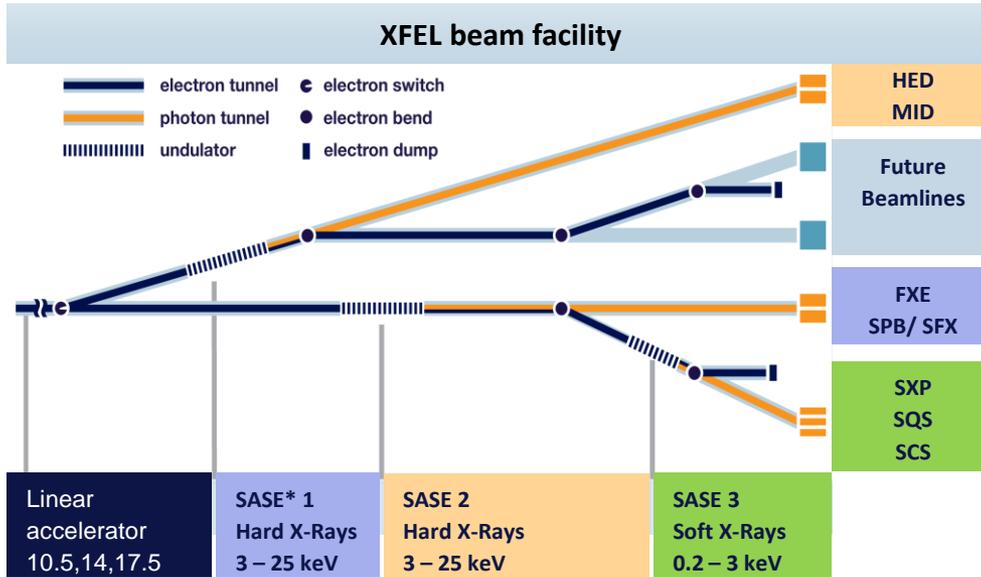
- **AGIPD Consortium (H. Graafsma)**
  - DESY, PSI, Uni Bonn, Uni Hamburg
- **STFC UKRI (M. Hart)**
- **DSSC consortium (M. Porro)**
  - EuXFEL, DESY, PoliMi, Uni BG, Uni Heidelberg, pnSensor, MPG-HLL
- **European XFEL**
  - Data Department (S. Aplin)
    - ▶ **DET Group**, Controls, ITDM, EEE, DA
  - SPB/SFX instrument (A. Mancuso/R. Bean)
  - MID instrument (A. Madsen)
  - FXE (Ch. Milne)
  - HED (U. Zastra)
  - SCS (A. Scherz)
  - SQS (M. Meyer)

# The European XFEL in Schenefeld, Germany



# EuXFEL facility : 3 beamlines, 7 Instruments

Start of operation – July 2017



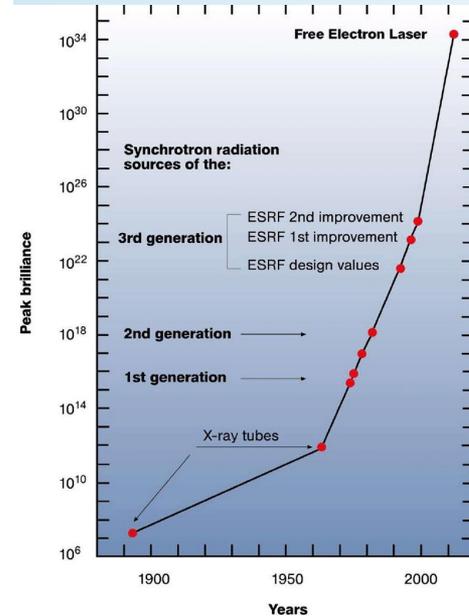
\*Self-Amplified Spontaneous Emission

## Challenges for Detectors → Demanding Intensity and Timing Constraints

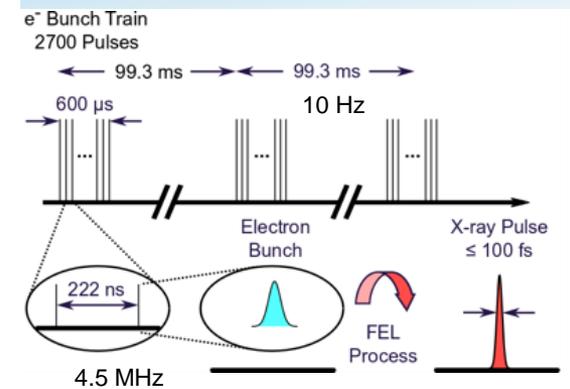
- High dynamic range (  $10^4$  ph/pixel/pulse) with single photon sensitivity for soft and hard X-ray instruments
- Radiation hardness
- MHz operation (in the burst mode)
- No commercial imaging detectors available

European XFEL

## Photon sources – Brilliance



## EuXFEL time structure



# 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

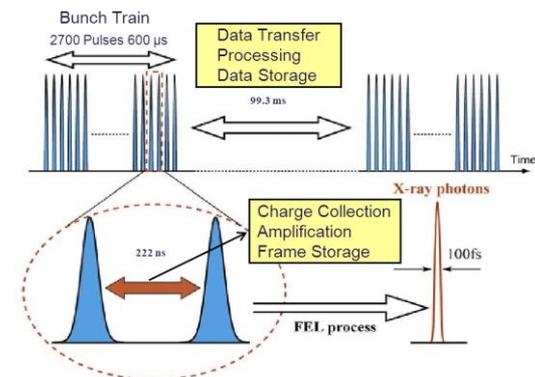
■ **2006:** Launched a Call for Expression of Interest

■ **Selected Proposals** → Three different projects adopting different solutions to solve the EuXFEL challenges

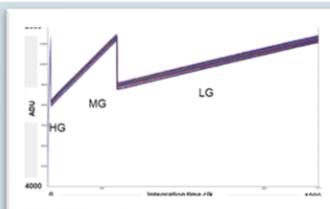
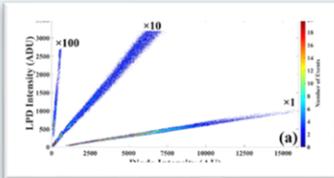
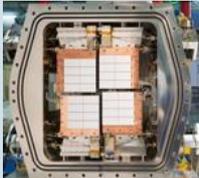
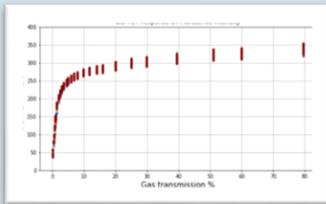
- ▶ Adaptive Gain Integrating Pixel Detector
- ▶ Large Pixel Detector
- ▶ DEPFET Sensor with Signal Compression

■ **Goal:** Developing at least one MHz 2D Imaging Detector

■ Development started ca. 2009



## The first MHz detector generation at the EuXFEL

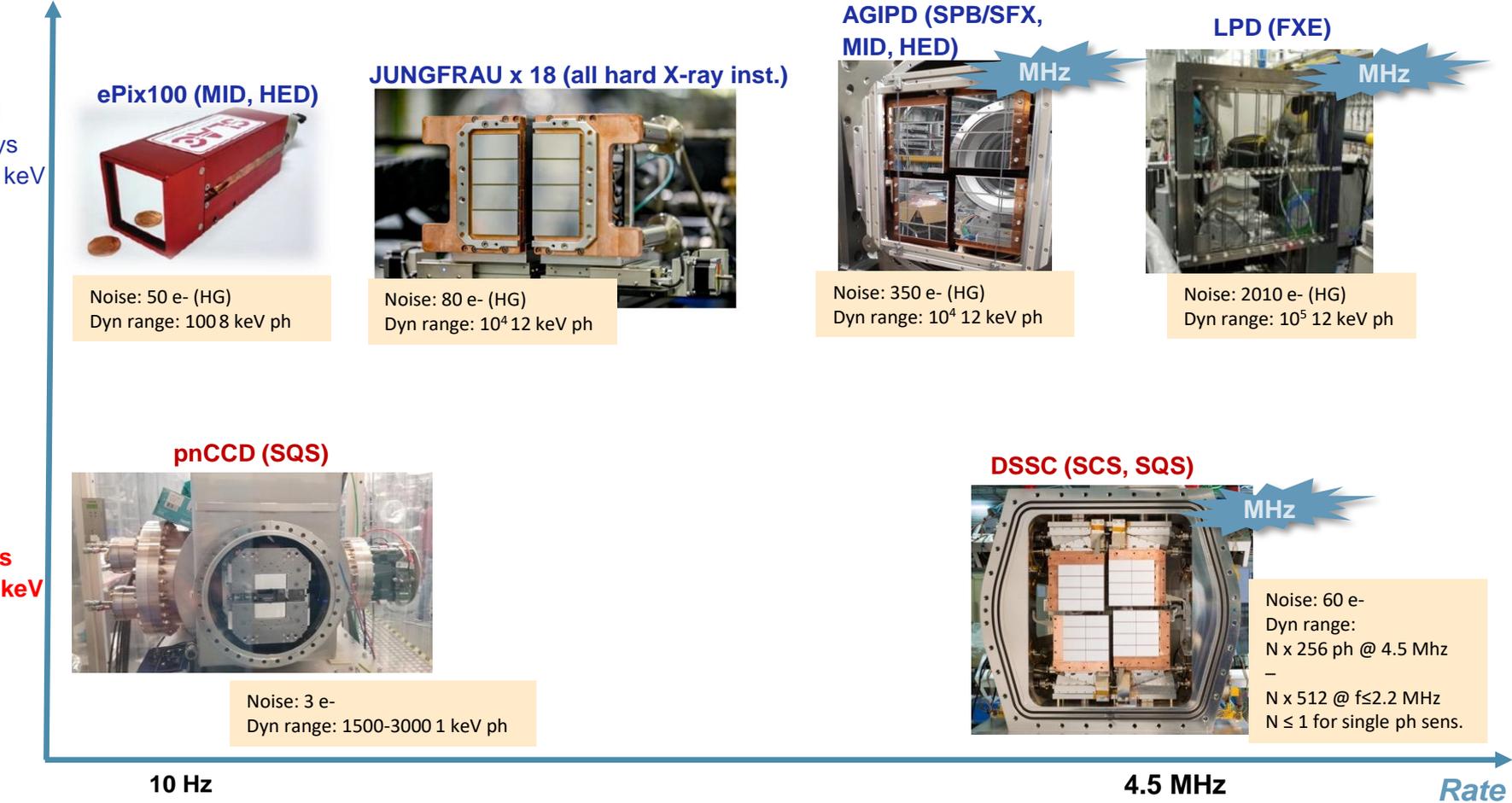
Detector	Specs	Gain Mechanism	Gain	Start of Operation
<b>AGIPD</b> 	352 memory cells (analog) 200 $\mu$ m x 200 $\mu$ m sq. pixels 1-10 <sup>4</sup> 12 keV ph 3-20 keV Modular: 16 (1MPix) or 8 (0.5MPix) modules	3 gains with automatic switching		AGIPD1M (SPB/SFX): 2017 AGIPD1M (MID): 2019 AGIPD500K: 2020 (new gen.) AGIPD4M (SPB/SFX): 2024 (new. gen.) AGIPD1M (HED): 2024 (new gen)
<b>LPD</b> 	(3x)512 memory cells (analog) 500 $\mu$ m x 500 $\mu$ m sq. pixels 1-10 <sup>5</sup> 12 keV ph 7- 20 keV Modular: 16 module (1MPix)	3 parallel gain stages with on front-end selection		LPD (FXE): 2017
<b>DSSC</b> 	800 memory cells (digital) 204 $\mu$ m x 236 $\mu$ m hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ f $\leq$ 2.2 MHz N $\leq$ 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 DEP FET: 2024



**A Journey from Concept to User Operation > 10 years**

# Detectors at EuXFEL

X-ray energy



GOTTHARD-II



MHz

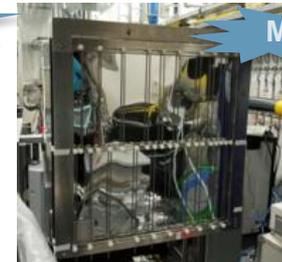
AGIPD (SPB/SFX, MID, HED)



MHz

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

LPD (FXE)



MHz

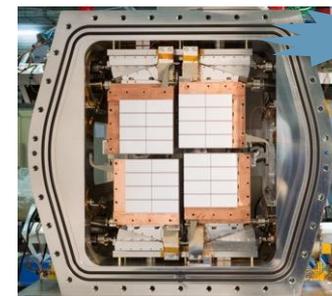
Noise: 2010 e- (HG)  
Dyn range:  $10^5$ :12 keV ph

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 @  $f \leq 2.2$  MHz  
 $N \leq 1$  for single ph sens.

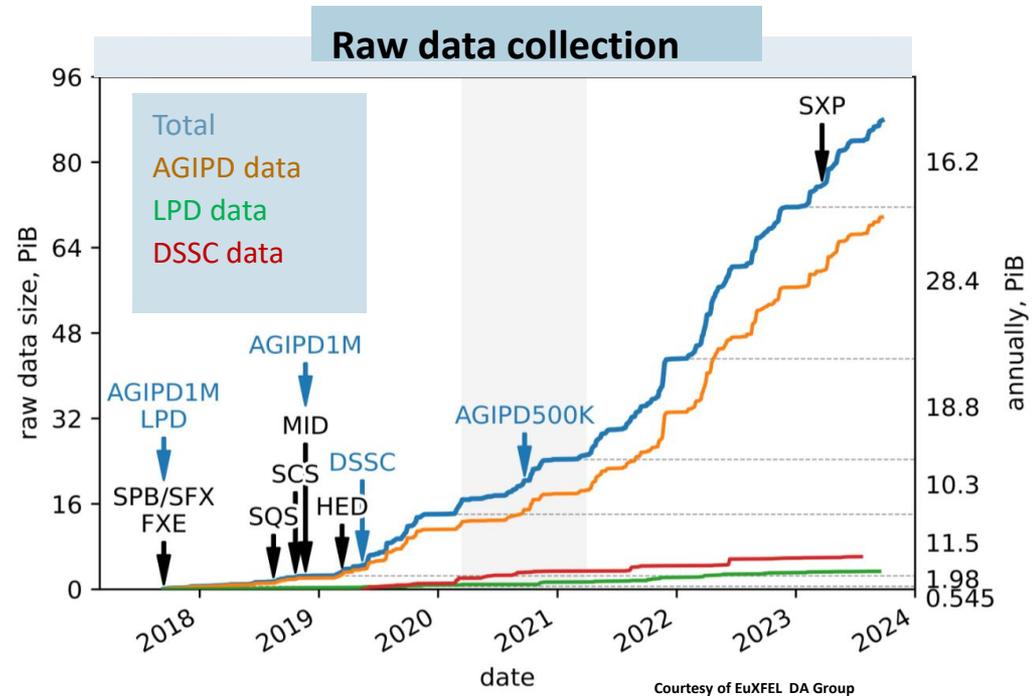
## Why “mostly based on AGIPD” detectors?

### Most Frequent Usage:

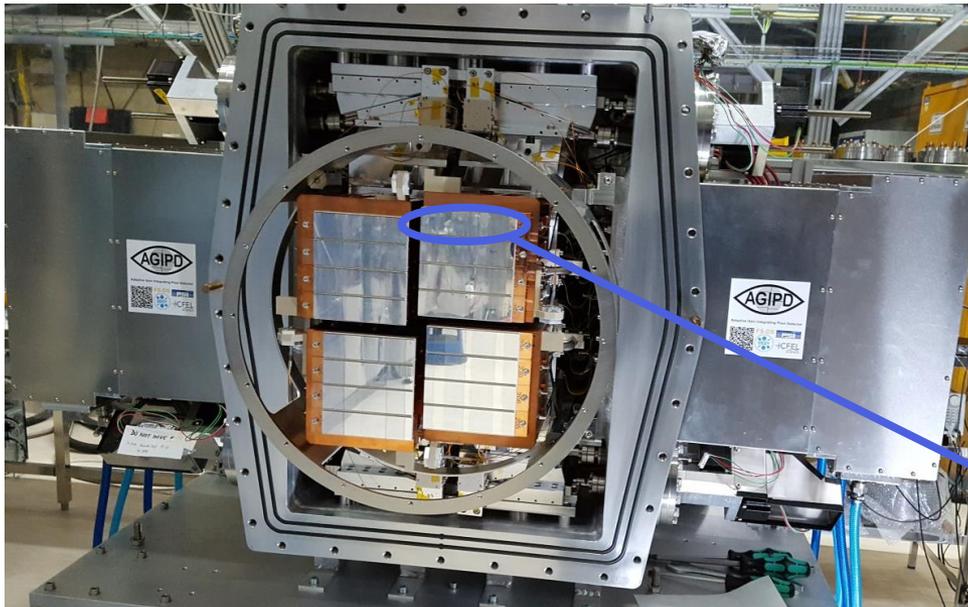
- AGIPD detectors are the most frequently used 2D MHz detectors at EuXFEL
- Primary detectors at SPB/SFX and MID

### Operational Demands:

- One of the most demanding detectors at EuXFEL in terms of infrastructure and operational requirements

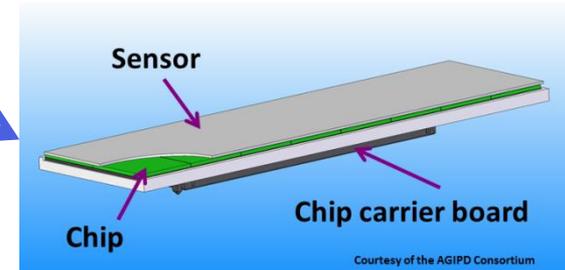


# AGIPD1M detector system for SPB/SFX and MID instruments



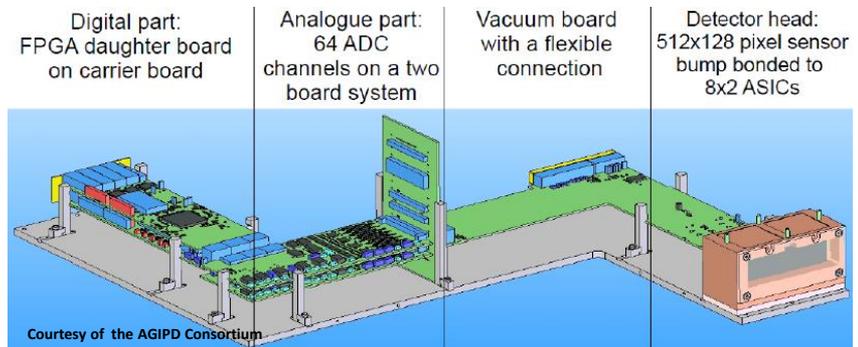
## Hybrid detector module

- Sensor:
  - 128 x 512 pixels
  - 500 μm thick silicon
- 2 x 8 read-out chips connected to sensor via bump-bonding
- Size: ~26 x 105 mm<sup>2</sup>



## 1M AGIPD system

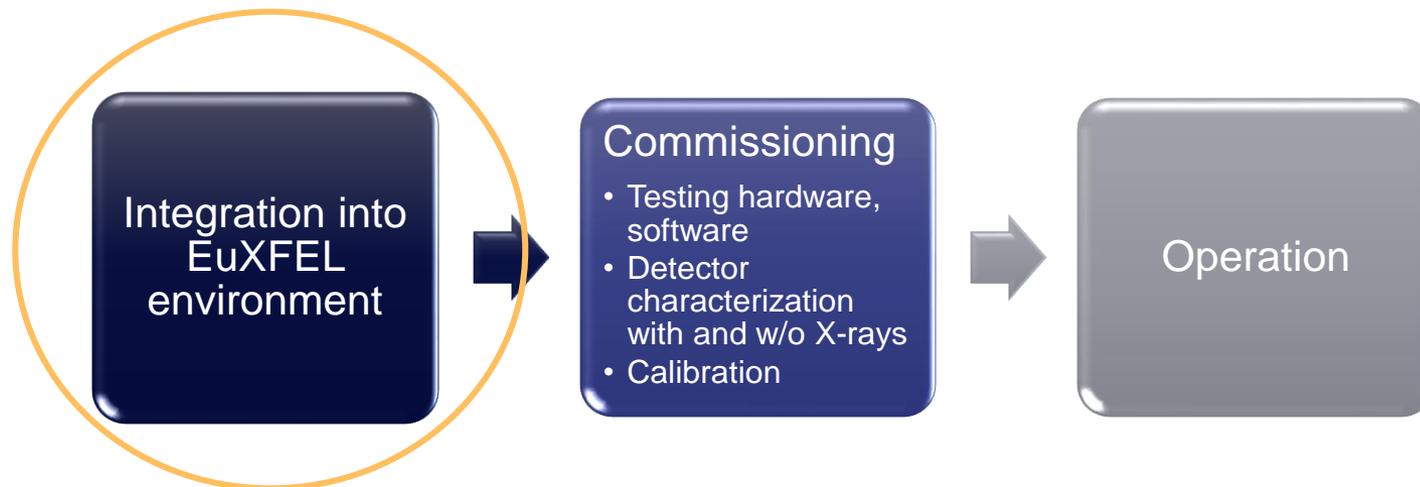
- 16 modules are mounted on four independently movable quadrants
- Vacuum operation ( $P < 10^{-5}$  mbar)
- Electronics/Control: two independent detectors: 'half 1' and 'half 2'
- Readout: 16 independent detectors



In ambient

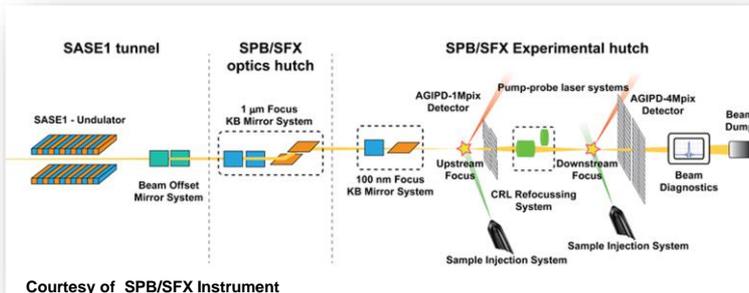
In vacuum

# What have we learned from the first-generation detectors?

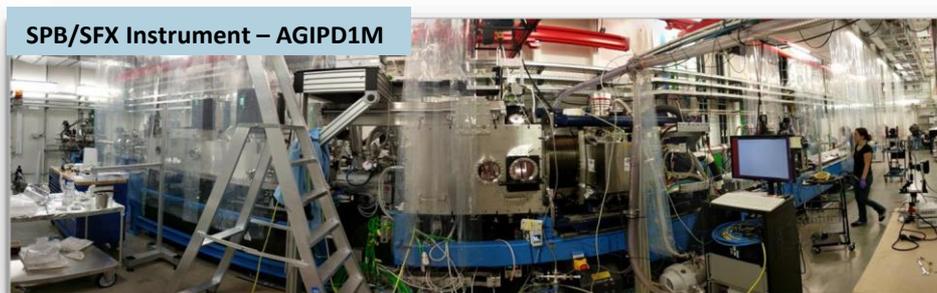


# AGIPD1M detectors are integral part of the instruments

General layout of the SPB/SFX instrument.



Courtesy of SPB/SFX Instrument

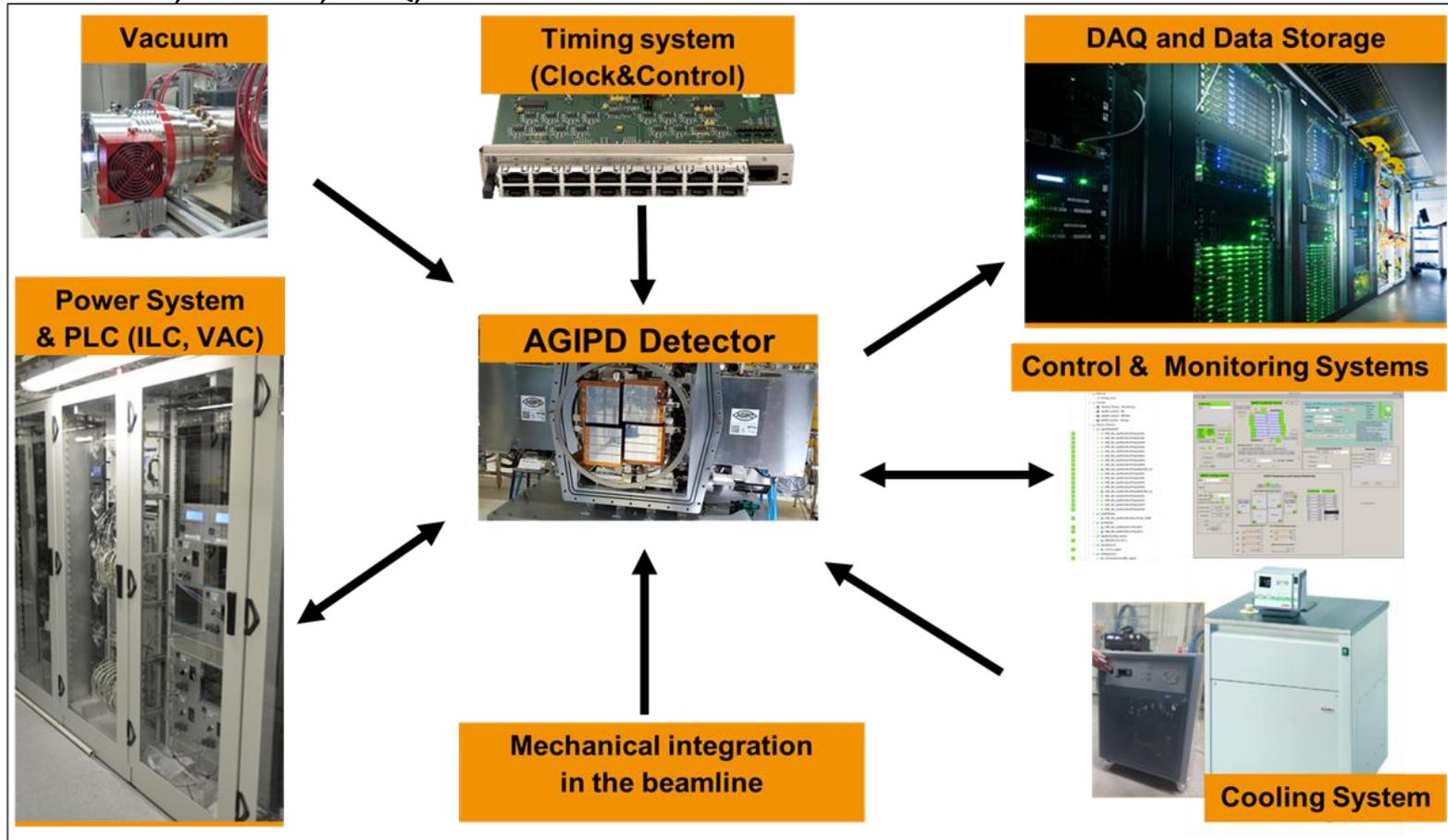


MID Instrument - AGIPD1M in WAXS configuration



# Integration: A complex task

- EuXFEL detectors were fully integrated into our infrastructure: mechanics, cooling, power, interlock, 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 (more than 100 cables for one AGIPD1M detector)
  - 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 would make integration and operation easier**



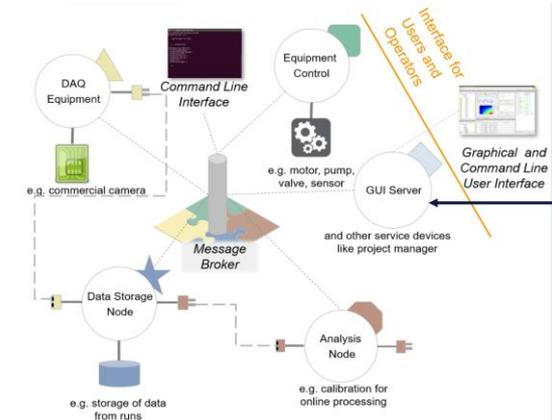
# Interlock system for detector protection

- Relies on Programmable Logic Controllers (PLCs)
- Monitors:
  - Vacuum quality and cooling efficiency
  - Detector cooling block temperatures
  - Pressure values in detector vessel and sample chamber
  - Chiller conditions
  - Internal detector conditions (hardware and FEM temperatures)
- PLCs initiate appropriate actions when needed
  - Switching off power
  - Warming up detector
  - Close valves to protect vacuum

Input	ILC Trigger	ILC Action
Vacuum status	Pressure $P > 10^{-3}$ mbar or pump failure	Warm up detector to RM, Switch off HV, Close relevant valves
Cooling blocks Temperature (in vacuum)	Temp. $> 0^{\circ}\text{C}$	Switch off power for components in vacuum (HV, ASICs, vacuum boards)
Electronics temperature (outside vacuum)	Temp. $> 35^{\circ}\text{C}$	Switch off power for all components (except MicroController)
$\mu$ Controller signals (internal detector conditions)	FEM temp. not OK Electronics boards status not OK	Switch off power for all components (except MicroController)

# Detector integration in Karabo

- Karabo - European XFEL's Control System framework for control, DAQ and monitoring
  - Distributed system of devices (physical and 'logical') that communicate with each other through a message broker
  - Devices are aggregated in topics (one topic per instrument)
  - GUI Client facilitates interaction and control of devices
- Tight coupling of controls and DAQ
  - DAQ is generic for all data source (e.g. detector, motors, sensors, etc)
  - Data is stored centrally, ensuring easy accessibility
- Integration of detectors in Karabo
  - Enables control of the detector and its infrastructure
  - Supports complex procedures, including detector startup and calibration data collection
  - Provides monitoring capabilities (e.g., temperatures, power, detector status) and 2nd level detector protection
  - Data online viewers offer near real-time experiment feedback



### DAQ Run Controller

Group	Type	Behavior	Alarm	Data source	Alias	Data aggregator	Status (Alert)	Unit	Level
1	AGP001A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT01	MONITORING	12020	
2	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT02	MONITORING	12020	
3	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT03	MONITORING	12020	
4	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT04	MONITORING	12020	
5	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT05	MONITORING	12020	
6	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT06	MONITORING	12020	
7	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT07	MONITORING	12020	
8	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT08	MONITORING	12020	
9	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT09	MONITORING	12020	
10	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT10	MONITORING	12020	
11	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT11	MONITORING	12020	
12	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT12	MONITORING	12020	
13	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT13	MONITORING	12020	
14	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT14	MONITORING	12020	
15	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT15	MONITORING	12020	
16	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT16	MONITORING	12020	
17	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT17	MONITORING	12020	
18	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT18	MONITORING	12020	
19	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT19	MONITORING	12020	
20	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT20	MONITORING	12020	
21	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT21	MONITORING	12020	
22	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT22	MONITORING	12020	
23	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT23	MONITORING	12020	
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26	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT26	MONITORING	12020	
27	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT27	MONITORING	12020	
28	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT28	MONITORING	12020	
29	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT29	MONITORING	12020	
30	MID_ASP01A_CTRL			MID_DET_AGI...	AGP011	MID_DET_ASP01A_LDETECT30	MONITORING	12020	

# Primary AGIPD1M control panel

The screenshot displays the 'agipd\_overview' control panel, which is divided into several functional sections:

- In-Vacuum Cooling Control:** Shows system state (STOPPED), pressure, and temperature controls. Includes buttons for 'Cool' and 'Heat'.
- AGIPD Power Control:** Features an interlock summary for ASICS, FPGA, ADC, MFPGA, AUX, and HV. Includes 'Get Detector Ready' and 'Detector Shutdown' buttons.
- AGIPD Combined Control:** Displays the status of various components like MC2, MFPGA2, Hemisphere 1, Hemisphere 2, and MFPGA1. Includes a 'Pattern Type' dropdown and gain settings.
- AGIPD Dark Runs:** Contains 'Operation scenarios for dark data' and 'Run and Sample types for dark data' sections. Includes a table for dark run parameters (HG, MG, LG) and sample types.
- AGIPD Pulse Capacitor Runs:** Similar to dark runs but for pulse capacitor data.
- AGIPD Monitoring:** A central monitoring area showing 'AGIPD Position (Z) and Gate Valve State', 'Cooling Block Temperature (deg C)', and 'Information from uControllers (MC)'. It includes a diagram of the cooling system and a table of temperatures.
- AGIPD C&C and VETO control:** Manages DAQ controller state and veto data.
- Timing scan:** A section for configuring and executing timing scans.
- SPB Run Controller:** A separate window showing 'Copy of SPB Run Controller' with proposal number 4417, run type 'agnostics', and a progress indicator at 100%.
- AGIPD CALNG - Overview:** A section with links to manager scenes (Main Overview, Constants Overview) and online preview scenes (Raw Preview, Corrected Preview).

# Primary AGIPD1M control panel

More than 200 Karabo devices for AGIPD1M

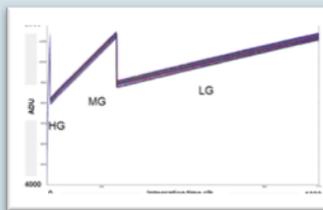
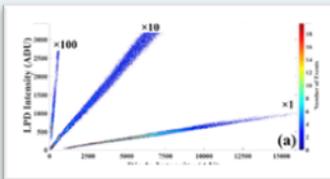
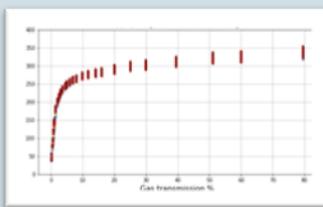
- Detector
- Motors
- Interlocks
- Infrastructure (power supplies, chillers, pumps)
- Timing system
- DAQ
- Procedures (“get detector ready”, “take calibration data”)
- Online Data Corrections and Visualization

# What have we learned from the first-generation detectors?



# 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
<b>AGIPD</b> 	352 memory cells (analog) 200 $\mu$ m x 200 $\mu$ m sq. pixels 1-10 <sup>4</sup> 12 keV ph 3-20 keV Modular: 16 (1MPix) or 8 (0.5MPix) modules	3 gains with automatic switching	
<b>LPD</b> 	(3x)512 memory cells (analog) 500 $\mu$ m x 500 $\mu$ m sq. pixels 1-10 <sup>5</sup> 12 keV ph 7- 20 keV Modular: 16 module (1MPix)	3 parallel gain stages with on front-end selection	
<b>DSSC</b> 	800 memory cells (digital) 204 $\mu$ m x 236 $\mu$ m hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ fs $\leq$ 2.2 MHz N $\leq$ 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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<b>LPD</b> 	(3x)512 memory cells (analog) 500 $\mu$ m x 500 $\mu$ m sq. pixels 1-10 <sup>5</sup> 12 keV ph 7- 20 keV Modular: 16 module (1MPix)			<ul style="list-style-type: none"> <li>■ Three gain stages per pixel</li> <li>■ Analog memory cells</li> <li>■ Detector artefacts</li> </ul>	
<b>DSSC</b> 	800 memory cells (digital) 204 $\mu$ m x 236 $\mu$ m hex. pixels N x 256 ph @ 4.5 MHz N x 512 @ fs2.2 MHz N $\leq$ 1 for single ph sensitivity 0.5 – 6 keV Modular: 16 modules (1MPix)				

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  - Calibrating the full dynamic range is a major challenge

Detector	Specs	Gain	Gain	
<b>AGIPD</b> 	352 memory cells (analog) 200µm x 200µm sq. pixels 1-10 <sup>4</sup> 12 keV ph 3-20 keV Modular: 16 (1MPix) or 8 (0.5MPix) modules	<b>Challenges</b> <ul style="list-style-type: none"> <li>■ Three gain stages per pixel</li> <li>■ Analog memory cells</li> <li>■ Analog gain evaluation</li> <li>■ Many operation modes</li> </ul>	<ul style="list-style-type: none"> <li>■ Three gain stages per pixel</li> <li>■ Analog memory cells</li> <li>■ Detector artefacts</li> </ul>	
<b>LPD</b> 	(3x)512 memory cells (analog) 500µm x 500µm sq. pixels 1-10 <sup>5</sup> 12 keV ph 7- 20 keV Modular: 16 module (1MPix)			<ul style="list-style-type: none"> <li>■ miniSDD – linear gain evaluated</li> <li>■ DEPFET - non-linear gain to be evaluated on full DSSC1M camera</li> </ul>
<b>DSSC</b> 	800 memory cells (digital) 204µm x 236µm hex. pixels N x 256 ph @ 4.5 Mhz N x 512 @ fs2.2 MHz N ≤ 1 for single ph sensitivity 0.5 – 6 keV Modular: 16 modules (1MPix)			

**Example AGIPD (one operation scenario)**

- x 1 million pixels
- x 352 memory cells
- x 3 gain stages
- x number of needed calibration constants
- > 10<sup>9</sup> parameters

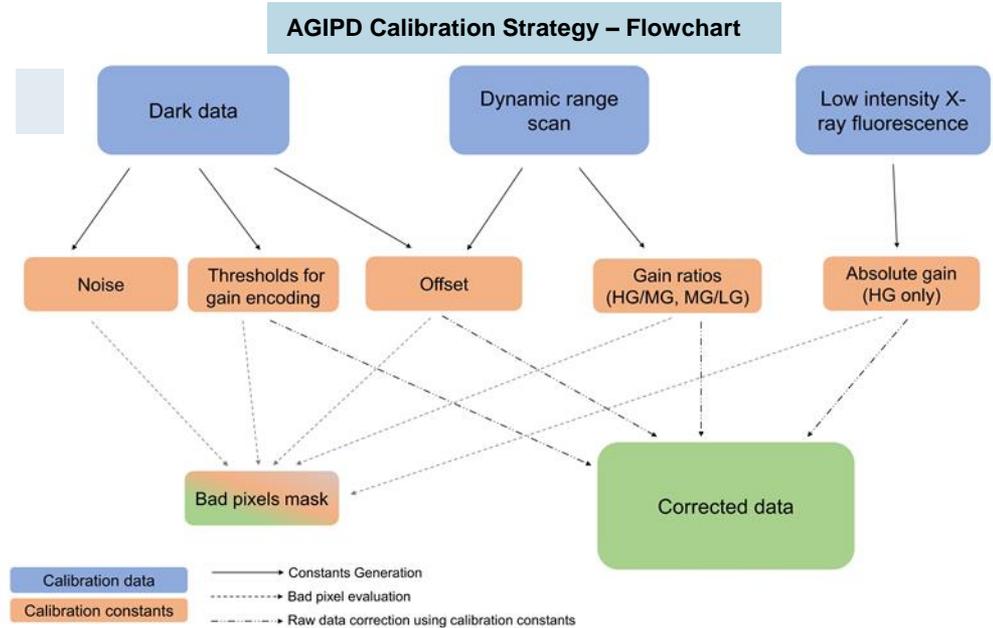
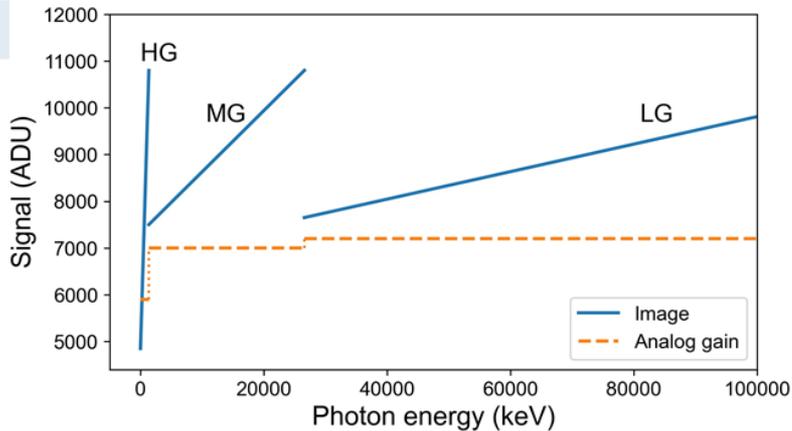
**The constants have to be generated for different operation modes:**

- 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**

# AGIPD Calibration Process - Overview



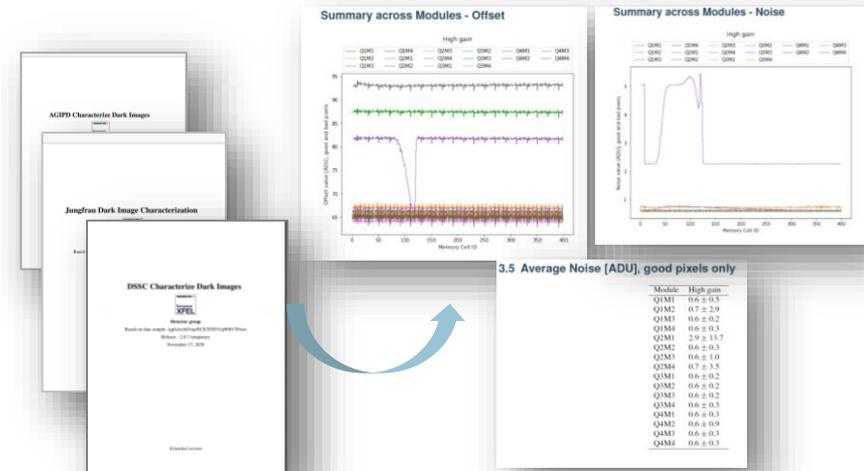
## AGIPD Calibration for one operation mode

Data Type	Data Size	Measurement Time	Data Processing Time	Frequency
Dark Data	2.2 TB	5 mins	~ 10 mins	at least once per shift
Dynamic Range Scan - Pulsed Capacitor	8.2 TB	20 mins	~ 100 mins	6 months
Dynamic Range Scan - Current Source	21 TB	65 mins	~ 180 mins	6 months
Fluorescence Data	15-20 TB	25-30 mins	up to 720 mins	6-12 months

- Generated calibration constants is centrally stored and indexed in the Calibration Catalogue (CalCat)
- CalCat allows easy retrieval based on detector identifier, creation time, and specific conditions (e.g. bias voltage, integration time, etc.)

# Characterization of the detectors – Calibration constants

- 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 once per shift**
  - Automatic procedure for data taking and interface via myMdC web interface to start dark data processing → do not requires expert level to generate new set of calibration constants
  - 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 < 10 min



### myMdC interface for dark data processing

Request Dark Run Calibration

\* Detector: SPB\_DET\_AGPDM-1

\* Detector Units:
 

- ⊞ AGPD00 (Q1M1) ⊞ AGPD01 (Q1M2) ⊞ AGPD02 (Q1M3) ⊞ AGPD03 (Q1M4) ⊞ AGPD04 (Q2M1)
- ⊞ AGPD05 (Q2M2) ⊞ AGPD06 (Q2M3) ⊞ AGPD07 (Q2M4) ⊞ AGPD08 (Q3M1) ⊞ AGPD09 (Q3M2)
- ⊞ AGPD10 (Q3M3) ⊞ AGPD11 (Q3M4) ⊞ AGPD12 (Q4M1) ⊞ AGPD13 (Q4M2) ⊞ AGPD14 (Q4M3)
- ⊞ AGPD15 (Q4M4)

\* Operation Mode: Adaptive Gain

Operation Mode Description: Standard operation mode for AGPD and Jungfrau detectors with 3 gain stages used. To be able to process calibration constants from dark data, the data should be taken for each gain stage in separate runs. Therefore, the run number for each gain stage has to be specified in the following order #1- high (HS/G0) #2-medium (MS/G1) #3-low (LS/G2)

\* Run Number(s):

Run #1: 1

Run #2: 1

Run #3: 1

Description:

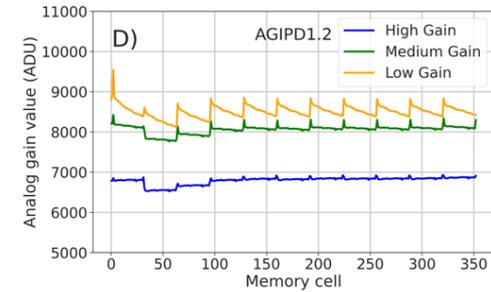
Request

Status	Last Updated at	Detector	Detector Units	Operation Mode	Run Number(s)	External resources
Finished	2021-05-16 08:33:21 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	156, 159, 160	
Finished	2021-05-15 19:37:32 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	133, 134, 135	
Finished	2021-05-15 19:30:19 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	130, 131, 132	
Finished	2021-05-15 16:47:24 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	115, 116, 117	

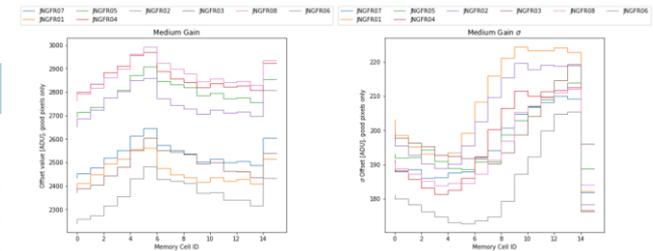
# Data Quality: Analog memory cells

- 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 JUNGFRU
- 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

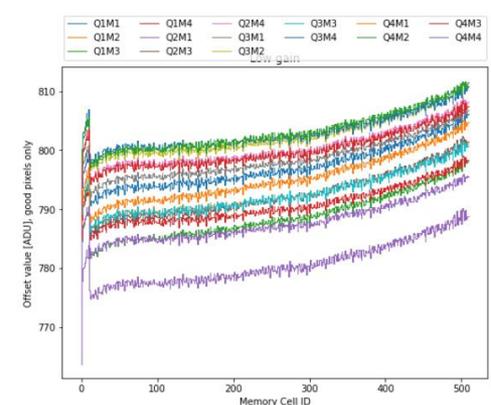
**AGIPD: Analog gain value vs. mem. cell**



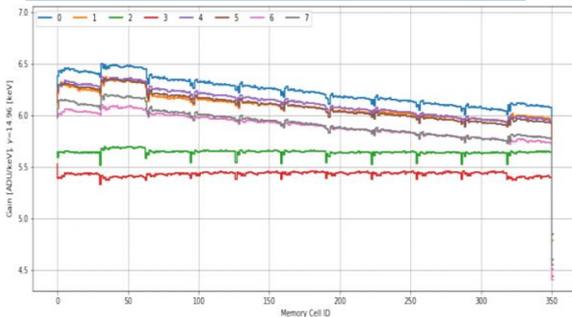
**JNGF4M: Average Offset MG vs. mem. cell**



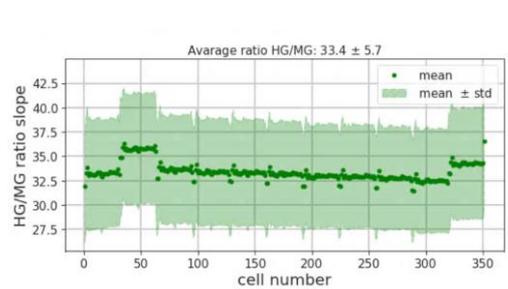
**LPD1M: Average Offset LG vs. mem. cell**



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



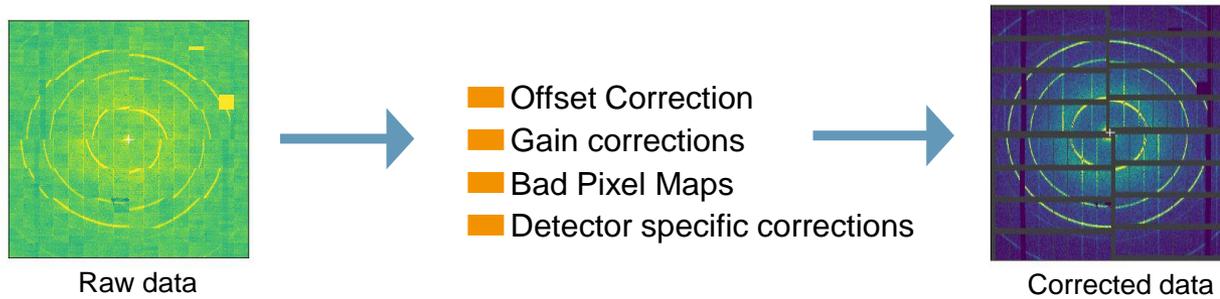
**AGIPD: Average HG/MG ratio vs. mem. cell**



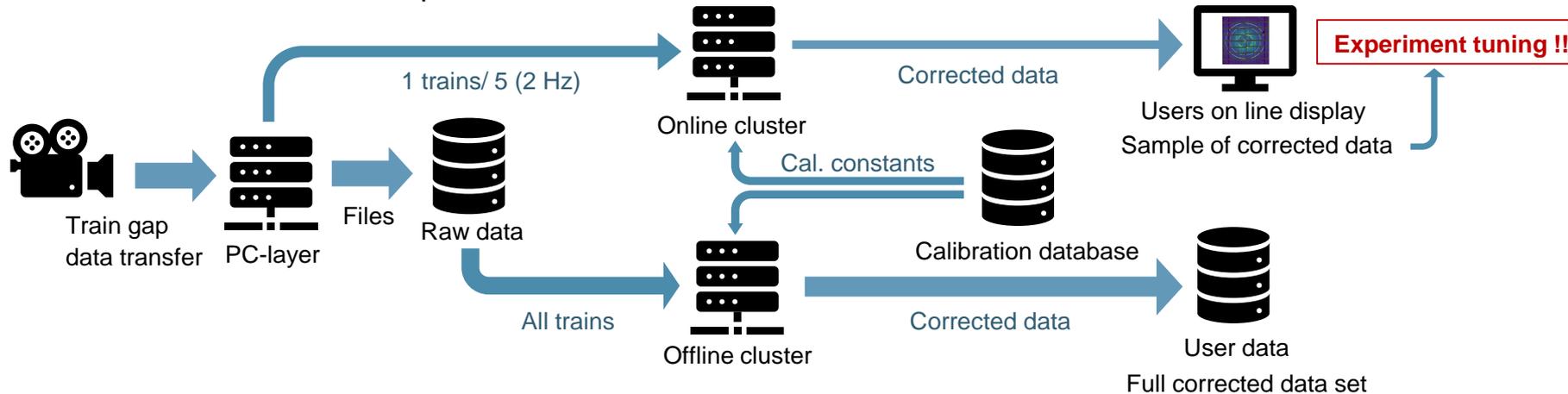
**Move away from analog memory cells for the next generation of the detectors**

# Detectors data correction

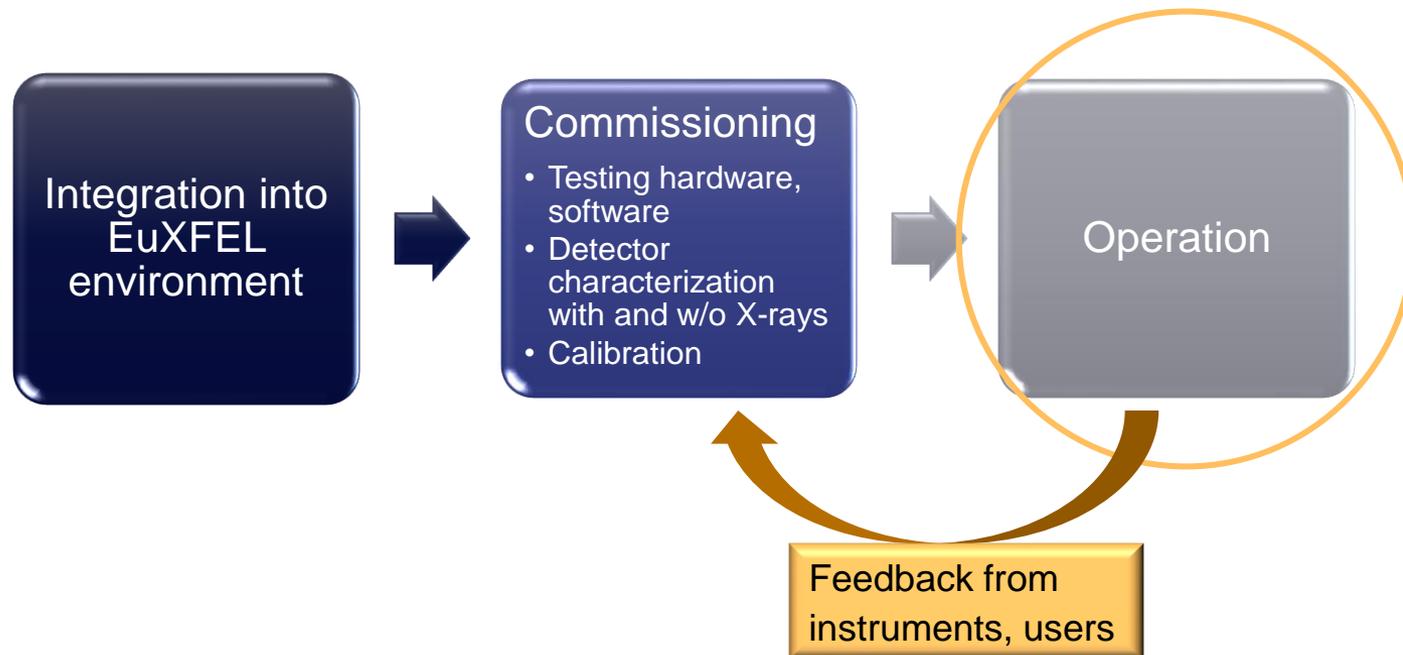
Corrected data proposed for each detector



Online/ off line correction process

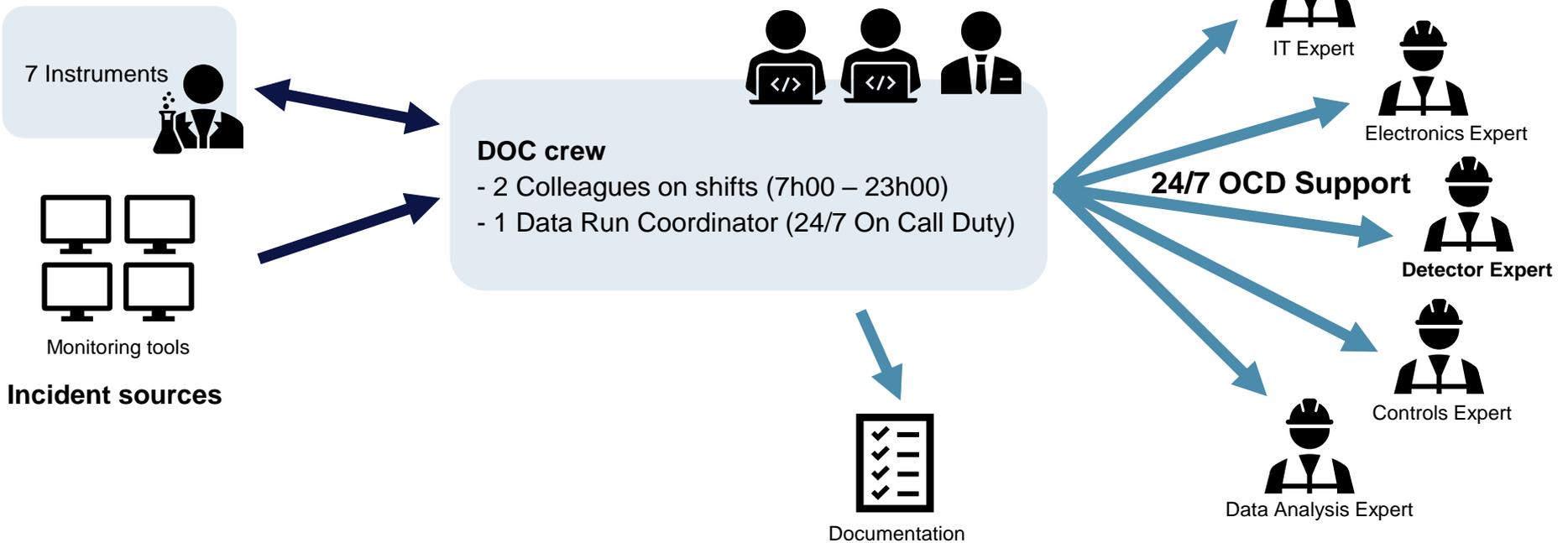


# What have we learned from the first-generation detectors?



# Support for User Operation

- Each week: 3 instruments run Tuesday-Sunday 24h/day
- Data Operation Center (DOC): single contact point for support



# User Operation

- User experiments at EuXFEL:
  - Mostly performed with a beam at repetition rate 2.25 MHz, 1.125 MHz and lower
  - Experiments performed at 4.5MHz  $\ll$ 10% (~ 1-2 weeks per year)
- Detectors run stable and provide high quality data for scientific publications
- An example: Functionality of SPB/SFX Instrument with liquid jet and AGIPD1M detector

# User Operation



# European XFEL Detectors: enabling scientific excellence

**MHz XPCS to look at system dynamics**

Pulse structure:  $\nu_p = 880 \text{ ns}$  (1.125 MHz), 100  $\mu\text{s}$ , 100 ms (10 Hz)

Speckle patterns on AGIPD

X-ray pulse trains

Nanoparticle suspension probed by the X-ray pulse

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

**Study of materials in extreme conditions**

352 Pulses at 220 ns

XFEL Beam

Diamond Anvil

Polystyrene

Rhenium Gasket

Gold

Ruby

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

Normalized intensity

0 0.05 0.10 0.15

0.1 nm<sup>-1</sup>

-60  $\mu\text{s}$  125 ps 60  $\mu\text{s}$

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

**Examples of scattering patterns from IrCl<sub>3</sub> and Mimivirus.**

a 145 nm

b 303 nm

c 465 nm

d Mimivirus

I (photons  $\mu\text{m}^{-2}$ )

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**

2600

0

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

nature COMMUNICATIONS

ARTICLE

DOI: 10.1038/s41467-018-0593-4 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

Suraj Pandey<sup>1\*</sup>, Richard Bean<sup>1,2\*</sup>, Takashi Sato<sup>1,3\*</sup>, Ishwor Poudyal<sup>1</sup>, Johan Bielecki<sup>1</sup>, Jorvani Cruz Villarreal<sup>1</sup>, Olexandr Yefanov<sup>1</sup>, Valerio Mariani<sup>1</sup>, Thomas A. White<sup>1</sup>, Christopher Kupitz<sup>1</sup>, Mark Hunter<sup>1</sup>, Mohamed H. Abdellatif<sup>1</sup>, Saba Bajaj<sup>1</sup>, Valerii Bondar<sup>1</sup>, Austin Echeimer<sup>1</sup>, Diandra Doppler<sup>1</sup>, Moritz Emons<sup>1</sup>, Matthias Frank<sup>1</sup>, Raimund Fromme<sup>1</sup>, Yaroslav Gevorgyan<sup>1,4</sup>, Gabriele Giovannetti<sup>1</sup>, Man Jiang<sup>1</sup>, Dahun Kim<sup>1</sup>, Younsuk Kim<sup>1</sup>, Henry Kirkwood<sup>1</sup>, Anna Klimovskaja<sup>1</sup>, Juraj Koska<sup>1,5</sup>, Faical H. M. Kous<sup>1</sup>, Romain Letrun<sup>1</sup>, Stella Lisova<sup>1</sup>, Luis Maia<sup>1</sup>, Victoria Mazalova<sup>1</sup>, Domingo Meza<sup>1</sup>, Thomas Michelat<sup>1</sup>, Abbas Ourmazd<sup>1</sup>, Guido Palmeri<sup>1</sup>, Marco Ramilli<sup>1</sup>, Robin Schubert<sup>1</sup>, Peter Schwander<sup>1</sup>, Alessandro Silenzi<sup>1</sup>, Jolanta Sztuk-Dambietz<sup>1</sup>, Alexandra Tobitkova<sup>1</sup>, Henry N. Chapman<sup>1,6,7,8,9</sup>, Alexandra Ross<sup>1</sup>, Anton Barfy<sup>1</sup>, Petra Fromme<sup>1</sup>, Adrian P. Mancuso<sup>1,10</sup> and Marius Schmidt<sup>1,11</sup>

ARTICLES

https://doi.org/10.1038/s41563-020-00828-1

nature materials

Check for updates

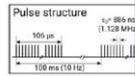
Observation of fluctuation-mediated picosecond nucleation of a topological phase

Felix Büttner<sup>1,12,13</sup>, Bastian Pfau<sup>1,14,15</sup>, Marie Böttcher<sup>1</sup>, Michael Schneider<sup>1</sup>, Giuseppe Mercurio<sup>1</sup>, Christian M. Günther<sup>1,16</sup>, Piet Hessing<sup>1</sup>, Christopher Klose<sup>1</sup>, Angela Wittmann<sup>1</sup>, Kathinka Gerlinger<sup>1</sup>, Lisa-Marie Kern<sup>1,17</sup>, Christian Strübar<sup>1</sup>, Clemens von Knorff-Schönhausen<sup>1,18</sup>, Ineffia Fuchs<sup>1</sup>, Dieter Engel<sup>1,19</sup>

# European XFEL Detectors: enabling scientific excellence

MHz XPCS to look at system dynamics

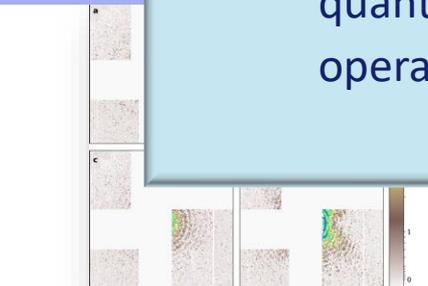
Study of materials in extreme conditions



X-ray pulse trains

Lehmkühn

Examples of s



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)

- 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

Austin Echelmeier<sup>1</sup>, Diandra Doppler<sup>2</sup>, Moritz Emons<sup>1</sup>, Matthias Frank<sup>3</sup>, Raimund Fromme<sup>4</sup>, Yaroslav Gevorgyan<sup>5</sup>, Gabriele Giovannetti<sup>6</sup>, Man Jiang<sup>7</sup>, Dahun Kim<sup>8</sup>, Younhee Kim<sup>9</sup>, Henry Kirkwood<sup>10</sup>, Anna Klimovskaya<sup>11</sup>, Juraj Kroska<sup>12</sup>, Faisal H. M. Kous<sup>13</sup>, Romain Letrun<sup>14</sup>, Stella Lisova<sup>15</sup>, Luis Maia<sup>16</sup>, Victoria Mazalova<sup>17</sup>, Domingo Meza<sup>18</sup>, Thomas Michelat<sup>19</sup>, Abbas Ourmazd<sup>20</sup>, Guido Palmeri<sup>21</sup>, Marco Ramilli<sup>22</sup>, Robin Schubert<sup>23</sup>, Peter Schwander<sup>24</sup>, Alessandro Silenzi<sup>25</sup>, Jolanta Sztuk-Dambietz<sup>26</sup>, Alexandra Tobilkova<sup>27</sup>, Henry N. Chapman<sup>28</sup>, Alexandra Rox<sup>29</sup>, Anton Barry<sup>30</sup>, Petra Fromme<sup>31</sup>, Adrian P. Mancuso<sup>32</sup> and Marius Schmidt<sup>33</sup>\*

ARTICLES

<https://doi.org/10.1038/s41563-020-00825-1>

nature materials

Check for updates

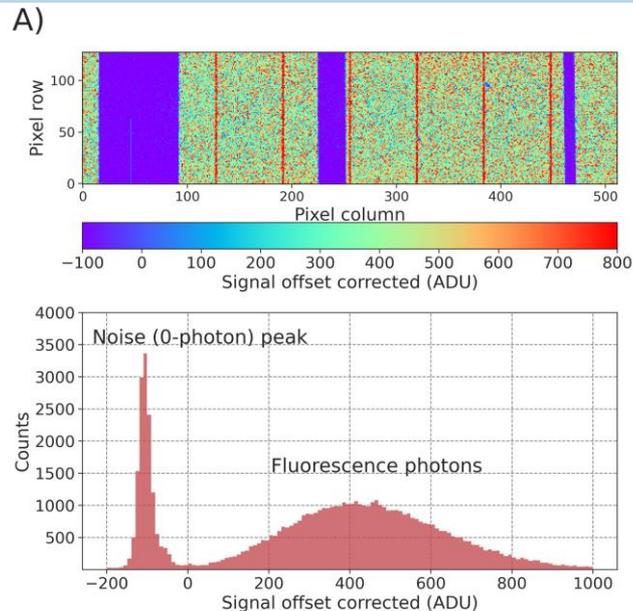
Observation of fluctuation-mediated picosecond nucleation of a topological phase

Felix Büttner<sup>1,2,3,4</sup>, Bastian Pfau<sup>5,6,7</sup>, Marie Böttcher<sup>8</sup>, Michael Schneider<sup>9</sup>, Giuseppe Mercurio<sup>10</sup>, Christian M. Günther<sup>11</sup>, Piet Hessing<sup>12</sup>, Christopher Klose<sup>13</sup>, Angela Wittmann<sup>14</sup>, Kathinka Gerlinger<sup>15</sup>, Lisa-Marie Kern<sup>16</sup>, Christian Strübel<sup>17</sup>, Clemens von Knorff-Schwinning<sup>18</sup>, Inesam Fuchs<sup>19</sup>, Dieter Enkel<sup>20</sup>

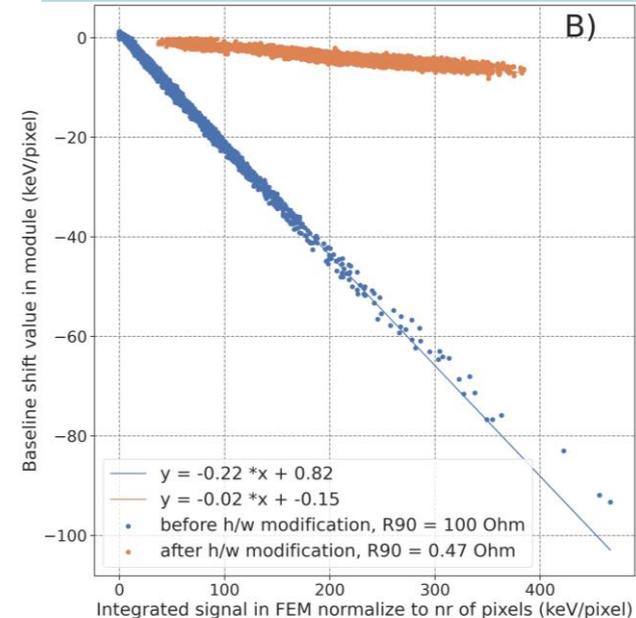
## Testing under real experimental conditions

- 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)

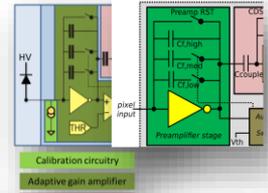


AGIPD: Baseline shift as a function of X-ray intensity

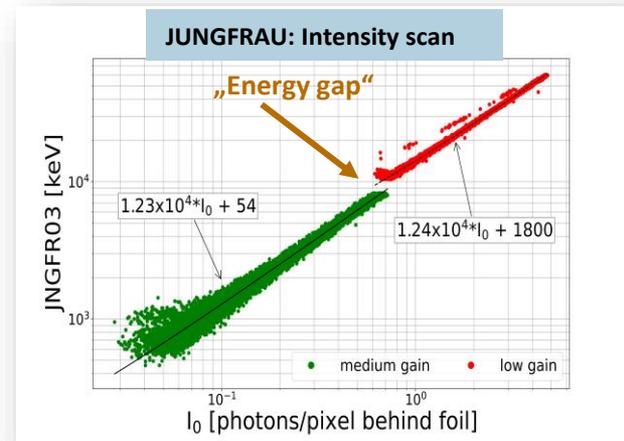
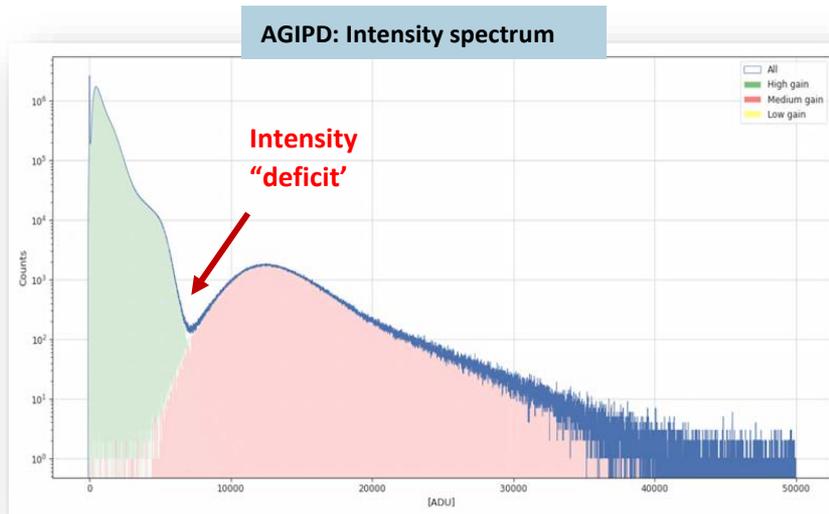
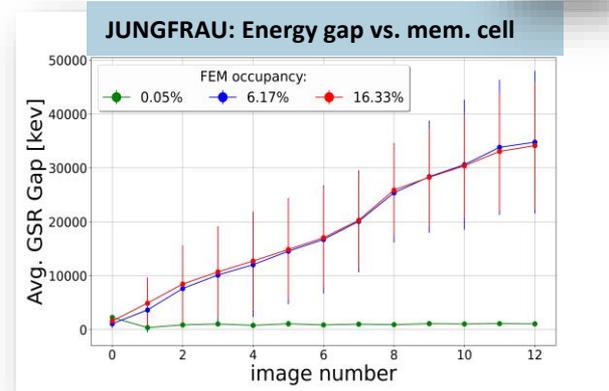


**Effective detector optimization requires the XFEL beam and is a continuous processes that necessitates collaboration and feedback from DET developers, instrument scientists and users**

# Data Quality: Adaptive gain and its transition region

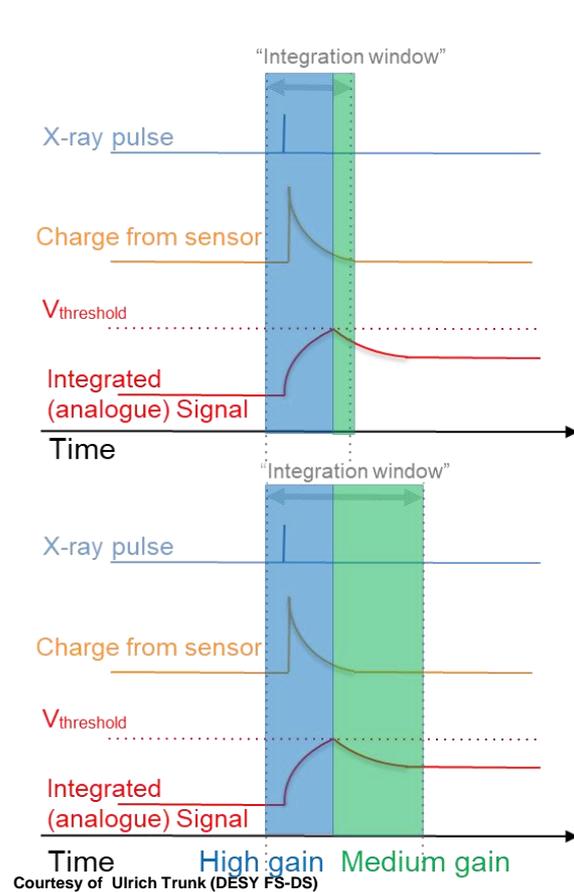


- Adaptive gain, an elegant method to achieve a high dynamic range, faces challenges in the transition region
- Issue with proper determination of “baseline’ for lower gain stages
- Both AGIPD and JUNGFRAU affected
- Preliminary findings indicate an issue in that region with GOTTHARD-II as well

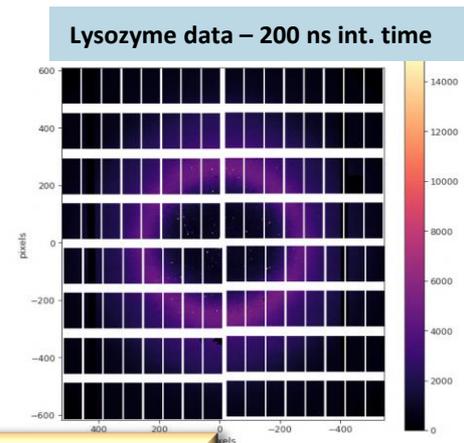
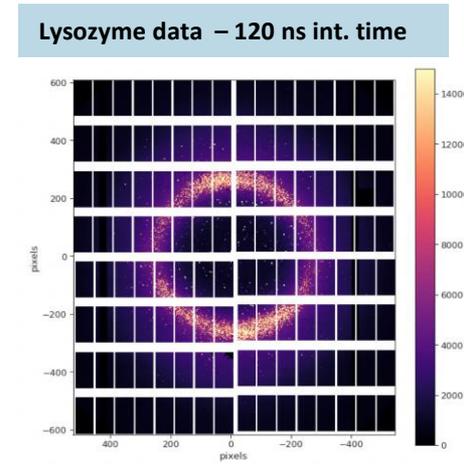
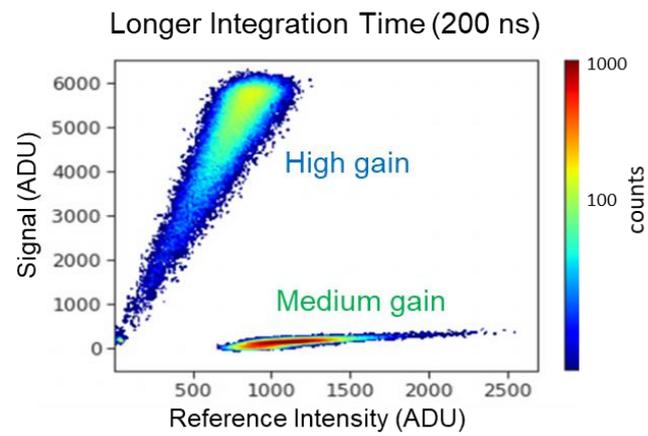
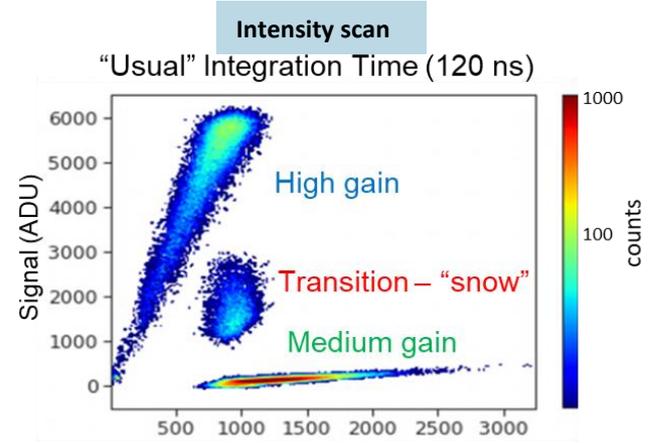


# Data Quality: Adaptive gain and its transition region

Fast (4.5MHz) operation → ‘late gain switching’ (“snowy pixels”)



Courtesy of Ulrich Trunk (DESY FS-DS)

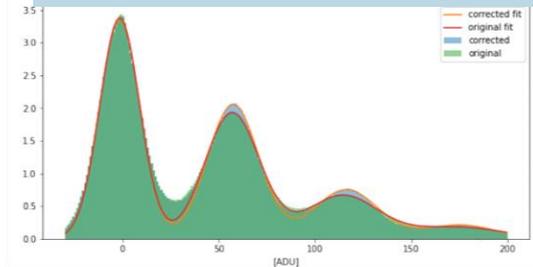


**For the next generation of detectors, addressing the observed issue with the adaptive gain mechanism is crucial, and alternatives should be explored**

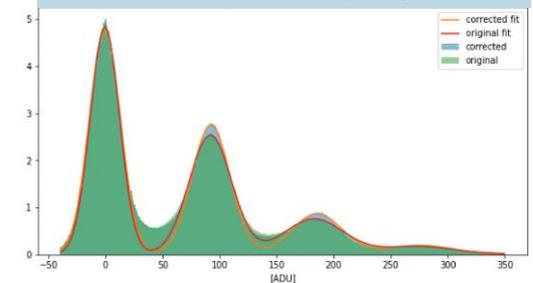
# Data Quality: Addressing issues with dedicated operation modes

- 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

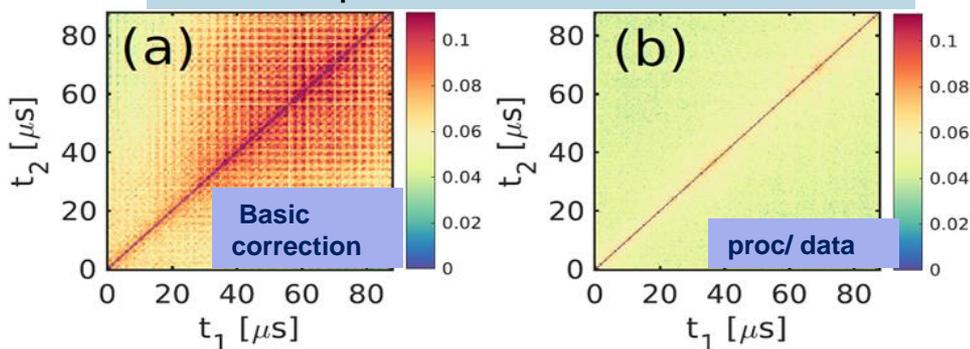
Cu fluorescence in ‘default’ High Gain



Cu fluorescence in Very High Gain

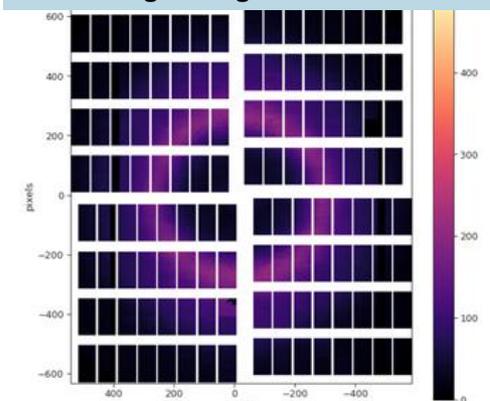


XPCS – Example of Double correlation function – MID



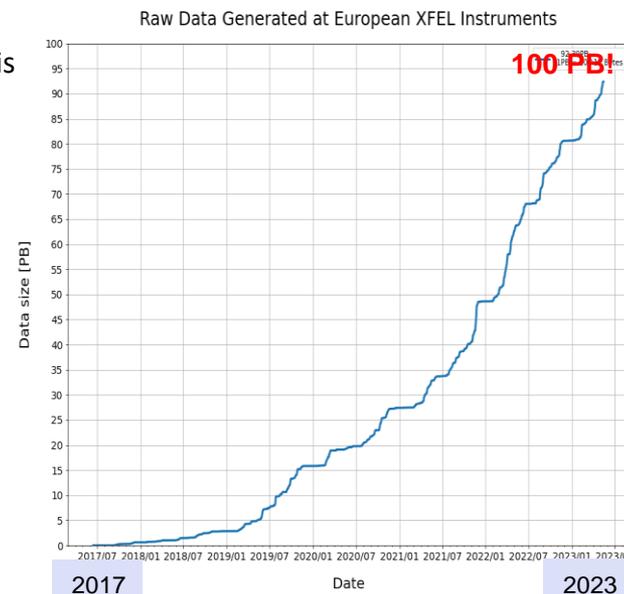
Francesco Dallari et. al., Applied Sciences, vol. 11, no. 17, p. 8037, 2021.

SFX – single image in fixed MG mode



## Data volume challenge

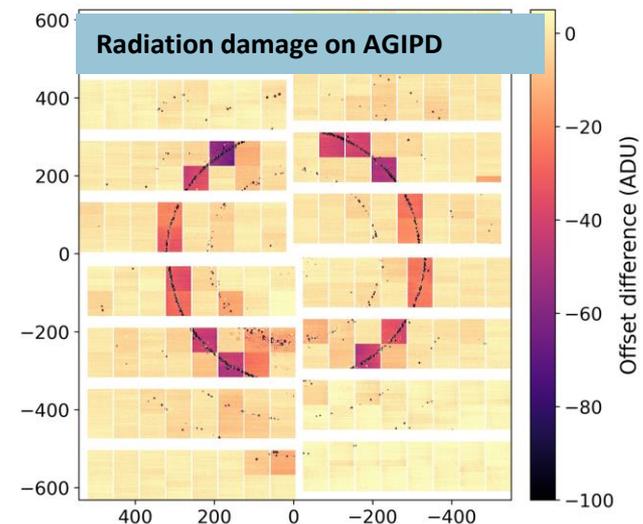
- The amount of collected data is huge (> 100 PB of raw data)
- The initial strategy of indefinitely storing all data beyond the embargo period is no longer sustainable
- Data reduction addressed starting from policy down to specific online and offline data reduction implementations:
  - **Data management 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



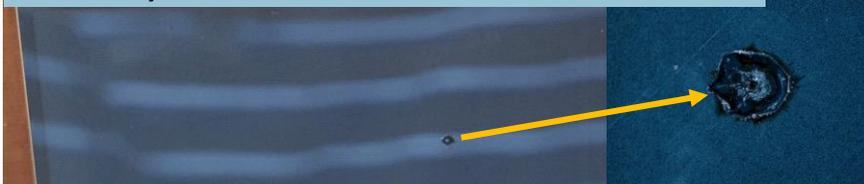
**In the next detector generation, consider implementing data reduction as near to the detector head as possible**

## 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



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

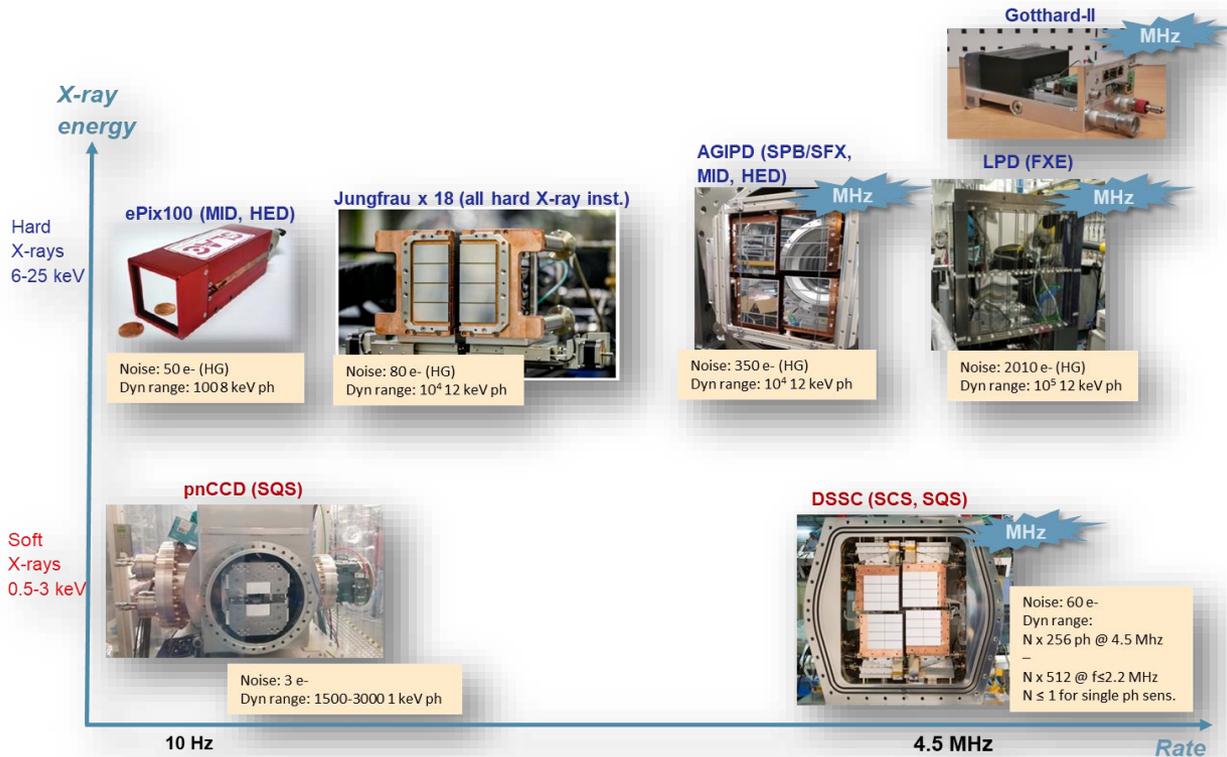


Courtesy of DESY FS-DS



**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 is required**

## Key Takeaways

- EuXFEL producing excellent scientific results based on data collected by the present detector generation
- Integration, commissioning, operation and dedicated studies have also led to the identification and quantification of challenges related to detectors performance and operation
- 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 this 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
  - Optimization is a continues process → Collaborative efforts involving experts with diverse backgrounds and investment in “In-House Expertise” are vital for optimizing detector performance and addressing observed issues
- Managing the enormous volume of generated data requires early design-level reduction strategies



**Lessons learned today shape the detectors of tomorrow**

# Thank you



Universität Hamburg



LPD



Science and  
Technology  
Facilities Council



HALBLEITERLABOR  
DER MAX-PLANCK-GESellschaft

PNSensor



# 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



**MID** (start Apr 2019)  
Materials Imaging & Dynamics



**HED** (start May 2019)  
High Energy Density Matter

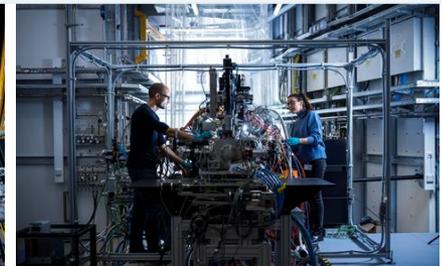
## SASE 3 (Soft X-Rays)



**SXP** (start summer 2023)  
Soft X-ray 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

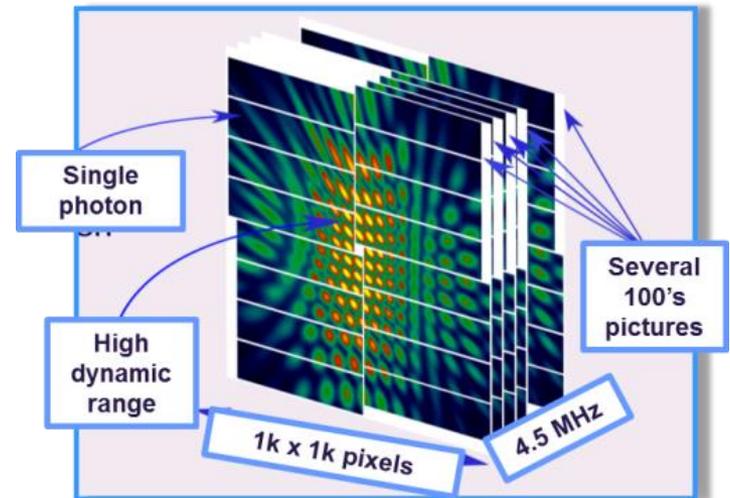
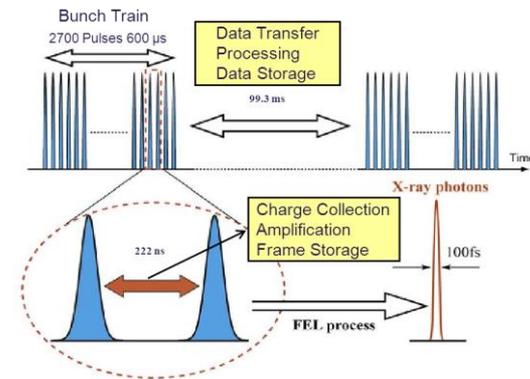
# First Generation Detectors for EuXFEL

## 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

Calibration Constants

Request Dark Run Calibration

\* Detector: SPB\_DET\_AGPDM-1

\* Detector Units:
 

- AGPD00 (Q1M1) AGPD01 (Q1M2) AGPD02 (Q1M3) AGPD03 (Q1M4) AGPD04 (Q2M1)
- AGPD05 (Q2M2) AGPD06 (Q2M3) AGPD07 (Q2M4) AGPD08 (Q3M1) AGPD09 (Q3M2)
- AGPD10 (Q3M3) AGPD11 (Q3M4) AGPD12 (Q4M1) AGPD13 (Q4M2) AGPD14 (Q4M3)
- AGPD15 (Q4M4)

\* Operation Mode: Adaptive Gain

Operation Mode Description: Standard operation mode for AGPD and Jungfrau detectors with 3 gain stages used. To be able to process calibration constants from dark data, the data should be taken for each gain stage in separate runs. Therefore, the run number for each gain stage has to be specified in the following order #1- high (HS/G0) #2-medium (MS/G1) #3-low (LS/G2)

\* Run Number(s):

Run #1: 1

Run #2: 1

Run #3: 1

Description:

Request

Status	Last Updated at	Detector	Detector Units	Operation Mode	Run Number(s)	External resources
Finished	2021-05-16 08:33:21 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	156, 159, 160	
Finished	2021-05-15 19:37:32 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	133, 134, 135	
Finished	2021-05-15 19:30:19 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	130, 131, 132	
Finished	2021-05-15 16:47:24 +0200	SPB_DET_AGPDM-1	AGPD00 (Q1M1), AGPD01 (Q1M2), AGPD02 (Q1M3), AG...	Adaptive Gain	115, 116, 117	

# Background information - AGIPD detectors @ EuXFEL

Detectors developed for EuXFEL by AGIPD Consortium ( DESY, PSI, Uni Bonn, Uni Hamburg)

Design for fast imaging and high dynamic range

Hybrid detector – module:

128 x 512 pixels, Pixel size: **200x200 um**, **500 um** thick Si, 2x8 chips

Module size: **~26 x 105 mm<sup>2</sup>**

Noise (HG)	350 e r.m.s.
Dynamic range	Upto 10 <sup>4</sup> 10 keV ph/pix/pulse
# images/train	Upto 352

Available detectors:

Instrument	#Pixels/ modules	In-vacuum operation	AGIPD (ASIC) version	Electronics	First User experiment
SPB/SFX	1MPix / 16	yes	AGIPD1.1	1 <sup>st</sup> generation	2017
MID	1MPix / 16	yes	AGIPD1.1	1 <sup>st</sup> generation	2019
HED/HiBEF	0.5MPix / 8	no	AGIPD1.2/1.1	2 <sup>nd</sup> generation	2021

1M AGIPD

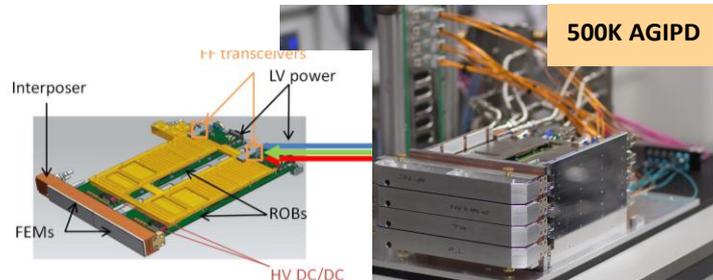


1M AGIPD

- 1<sup>st</sup> generation of electronics and AGIPD1.1 ASIC
- 16 modules are mounted on **four independently movable quadrants**
- Vacuum operation ( $P < 10^{-5}$  mbar)



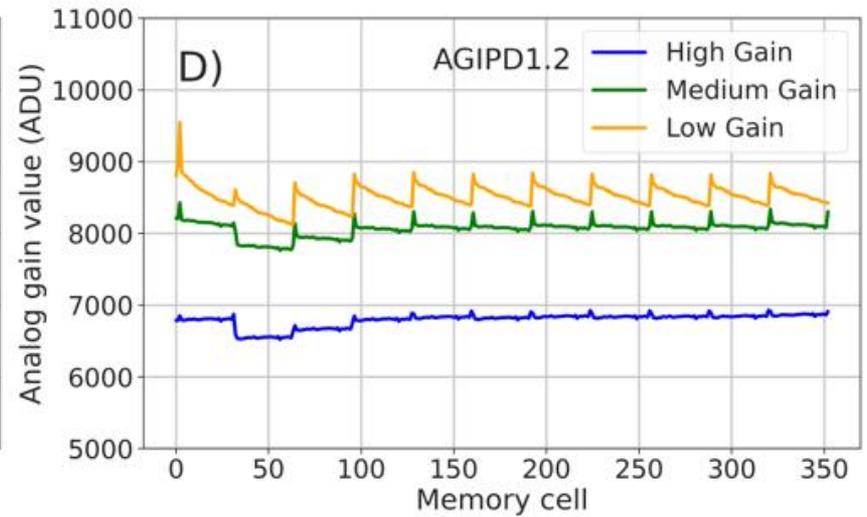
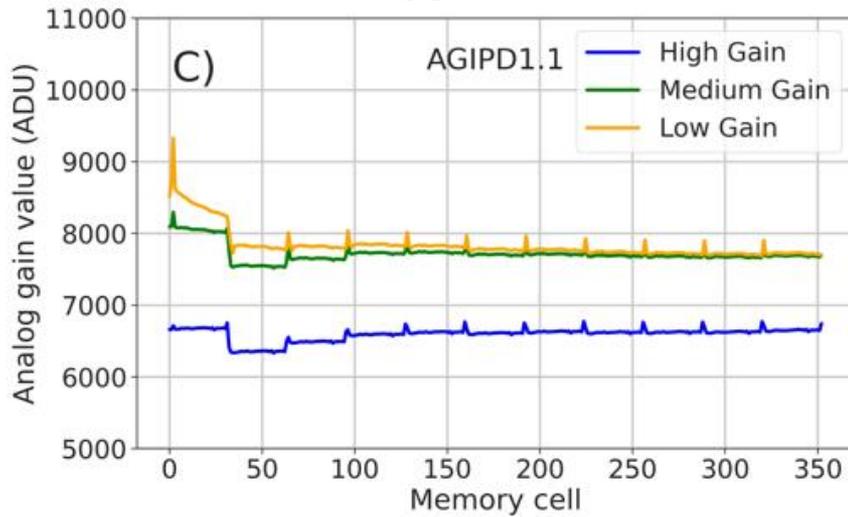
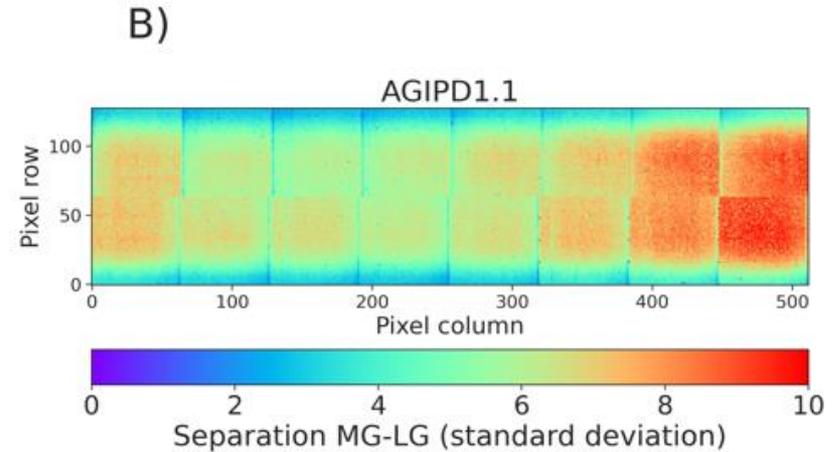
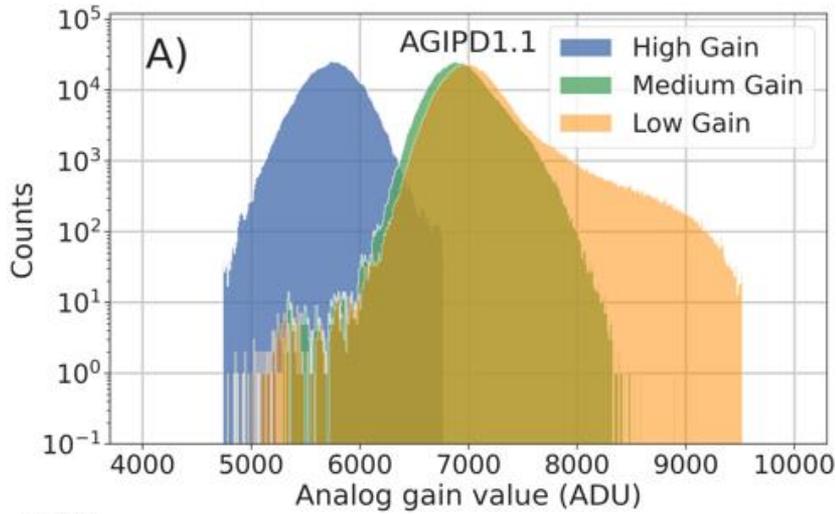
500K AGIPD



500K AGIPD system

- 8 modules
- New version of electronics (compact system)
- Operation in ambient

New generation AGIPD detectors to come next year :  
 1M AGIPD @ HED/HiBEF  
 4M AGIPD @ SPB/SFX



the bunch

## Radiation hardness sensor design

- **No bulk damage expected for  $E < 300$  keV**  
BUT

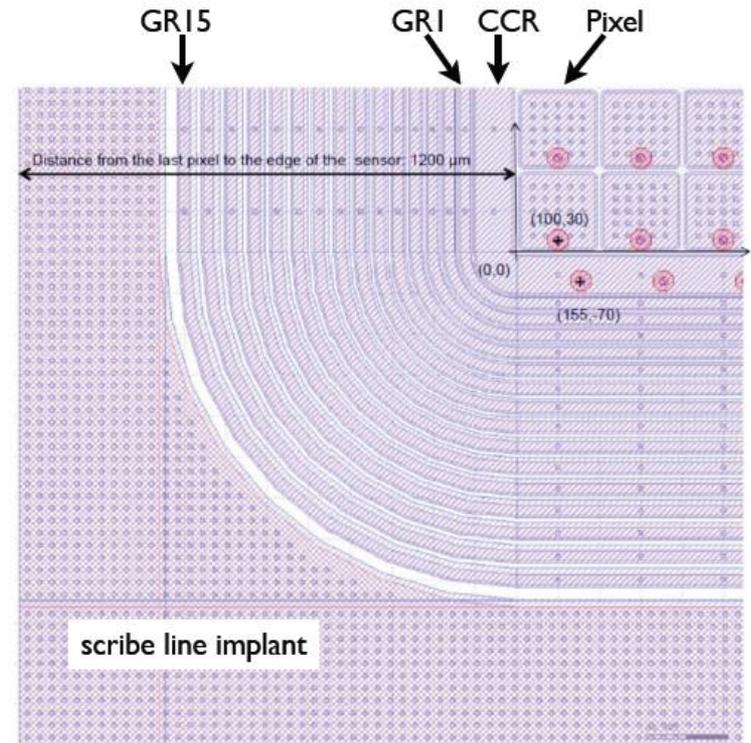
- **Surface and interface damage:**

- Higher leakage current
- Higher depletion voltage
- Lower breakdown voltage
- Charge losses at interface
- Increased inter-pixel capacitance

- ➔ **Special high voltage design with 15 guard rings:**

- radiation tolerant up to 1GGy 😊

- introduced additional non-sensitive area between detector modules ☹️



Distance from the last pixel to the edge of the sensor 1200 μm

JINST (2013) 8 C12015,  
DOI: 10.1088/1748-0221/8/01/C01015,  
e-Print: arXiv:1210.0430 [physics.ins-det]

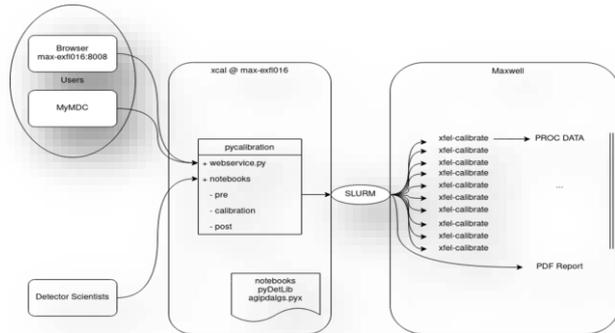
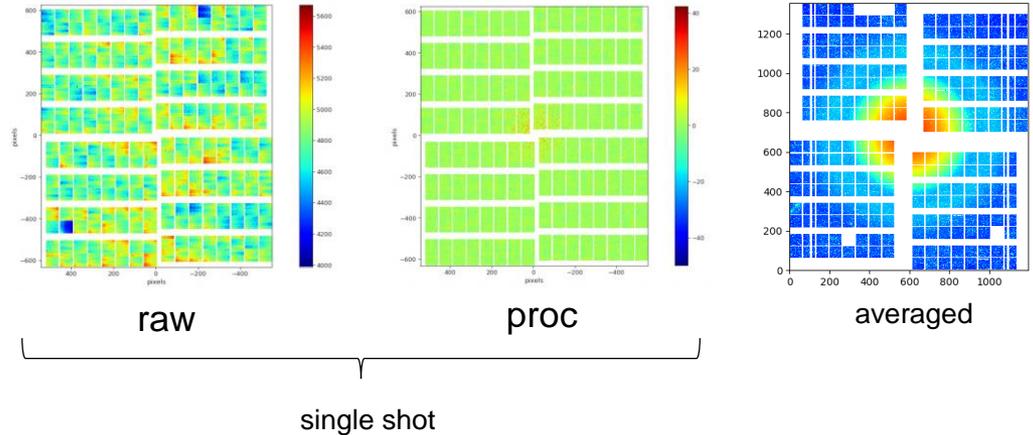
## Calibration constants – Gain

- Characterization with X-rays and internal calibration sources → det. response (gain, linearity)
  - Characterization is done by detector experts
  - Frequency: every 4-6 months, dedicated calibration beamtime or calibration campaign
  - Source requirements and techniques depends on the detector type: X-rays or combination of X-ray data and dedicated charge injection calibration sources
  - Charge injection calibration sources validated and cross-calibrated with X-rays are very useful (if not mandatory)
  
- All detectors - final validation of calibration should always be done under real conditions with the real scientific data!

Source	AGIPD	LPD	DSSC	pnCCD	Jungfrau	Epix100
XFEL beamlines (where the detectors belongs)	<ul style="list-style-type: none"> <li>- Cu flat-fields – single photon intensity</li> <li>Other:               <ul style="list-style-type: none"> <li>- Cu flat-fields Intensity scan</li> <li>- Water ring</li> <li>- Powder diffraction</li> <li>- SFX data</li> </ul> </li> </ul>	<ul style="list-style-type: none"> <li>- Cu flat-fields intensity scan</li> <li>- Single ph. with E&gt; 16keV (scattering)</li> <li>Other:               <ul style="list-style-type: none"> <li>- PP water scattering</li> </ul> </li> </ul>	(DSSC DEPFET will need FEL beam)	Al flat-fields	Cu flat-fields – intensity scan including single photons	Cu, Fe flat-fields – single ph. intensity
Laboratory X-ray sources			PulXar with different targets and filter (Cu and higher energies)	PulXar with different targets and filters at higher energies		
Charge injection calibration circuits	Yes, dynamic range scan for HG and MG with Pulse Capacitor (MG and LG with Current Source)		Yes, DAC injection sweep		Yes, dynamic range scan G0 and G1 (backplane pulsing), G1 and G2 – current source	

# 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

Run Number (alias)	Run type	Sample Name	Start date	Run status	Data Assessment	Calibration	Run Comment	PDF
0693	XPCS	vycor	2019-09-23 00:00:34 +0200	Closed	Good	[Dropdown]		
0692	XPCS	vycor	2019-09-22 23:57:14 +0200	Closed	Good	(Re)calibrate		
0691	XPCS	vycor	2019-09-22 23:52:46 +0200	Closed	Good	[Dropdown]		
0690	XPCS	vycor	2019-09-22 23:46:20 +0200	Closed	Good	[Dropdown]		
0689	XPCS	vycor	2019-09-22 23:42:27 +0200	Closed	Good	[Dropdown]		
0688	XPCS	vycor	2019-09-22 23:38:47 +0200	Closed	Good	[Dropdown]		

# European XFEL Storage Overview (

## Schenefeld

Online GPFS

Cache



- Extremely high performance
- Data available immediately
- Optimised for concurrency
- High redundancy
- Dedicated storage for each SASE
- Very high cost per PB
- Capacity for a few days

Offline GPFS

Performance



- High performance
- Large scale data analysis
- High redundancy
- High cost per PB
- Shared within XFEL
- Large capacity

## DESY Data Center

dCache

Capacity



- Lower performance
- Lower cost
- Scalability
- Shared within XFEL
- High capacity

Tape Archive

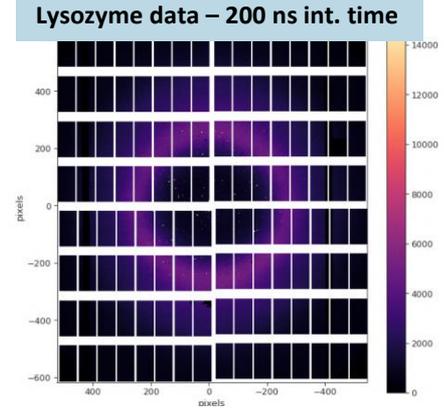
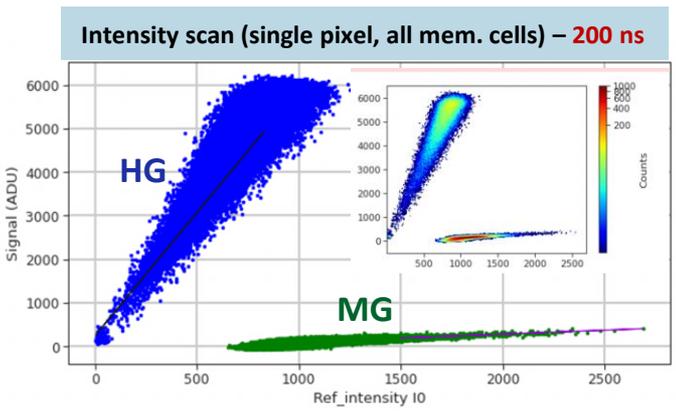
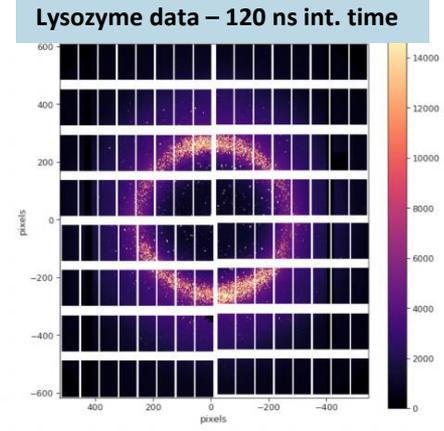
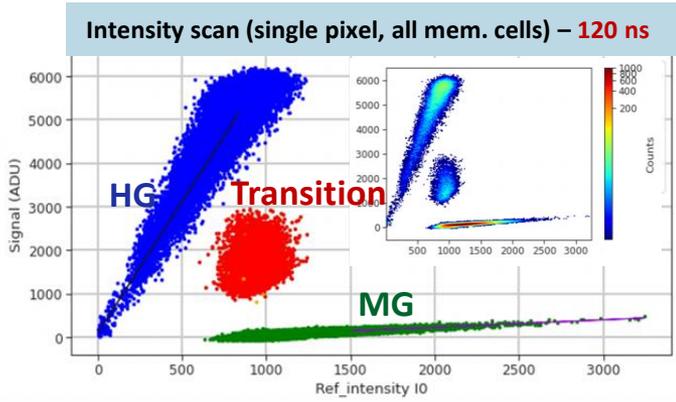
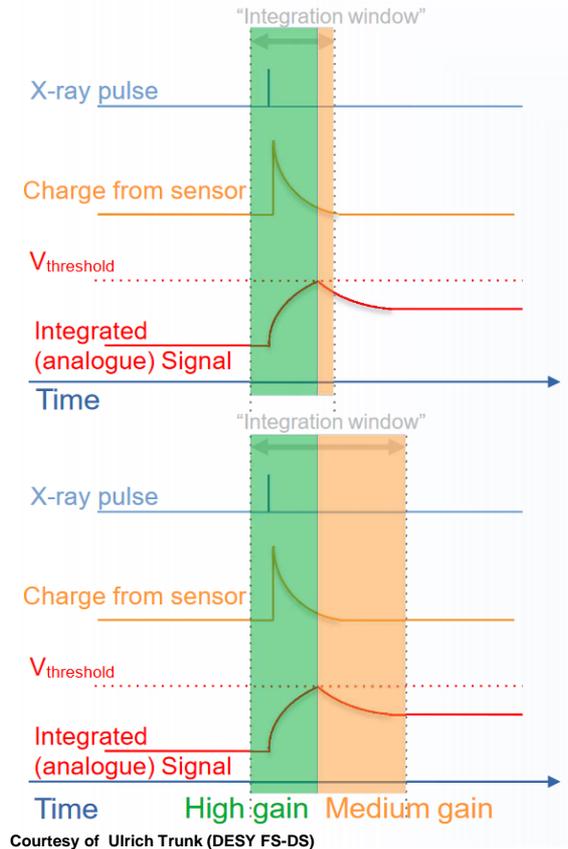
Safety



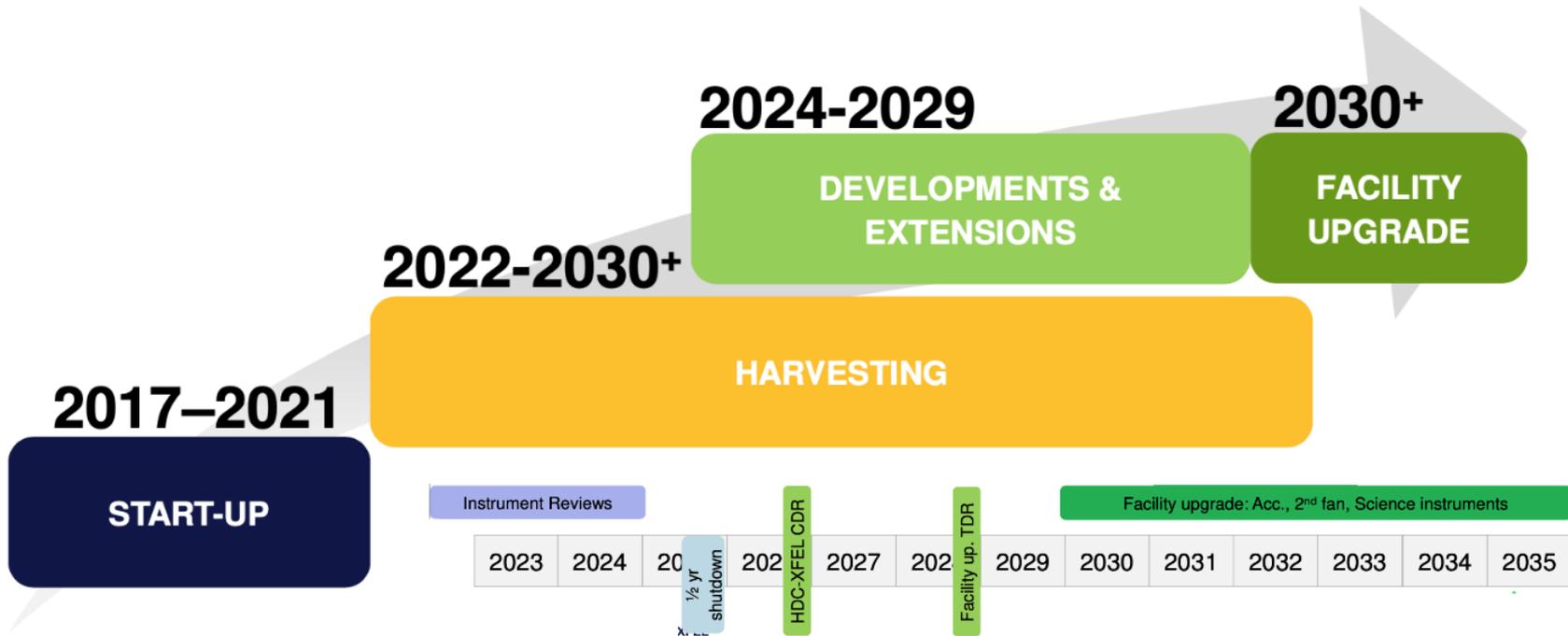
- Very slow
- Even lower cost
- Very high capacity
- Safety (second copy)
- Shared within DESY campus
- Long term

# Data Quality: Adaptive gain and its transition region

Fast (4.5MHz) operation → ‘late gain switching’ (“snowy pixels”)



# Where are we now?



*European XFEL plan for the next decade+*