Detector Calibration and Data Acquisition Environment at the European XFEL

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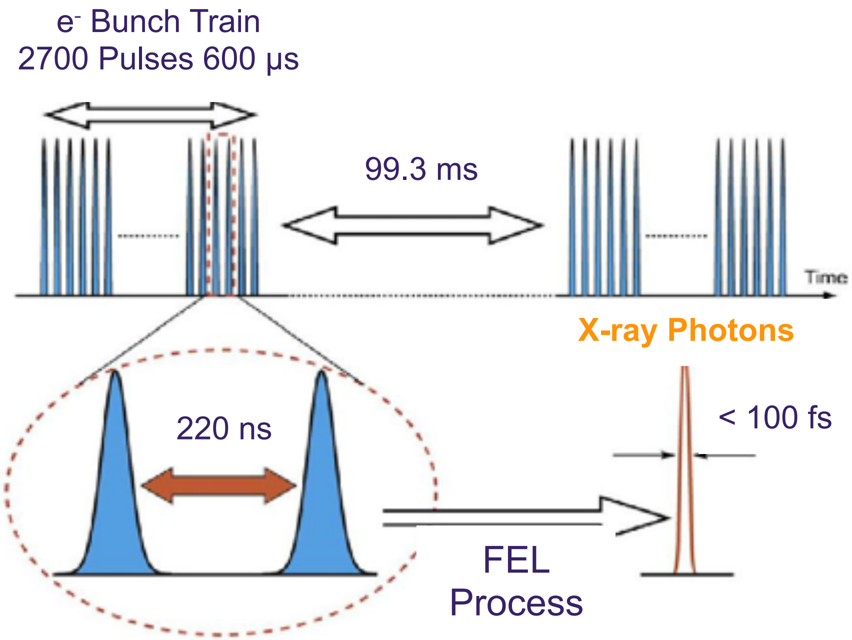
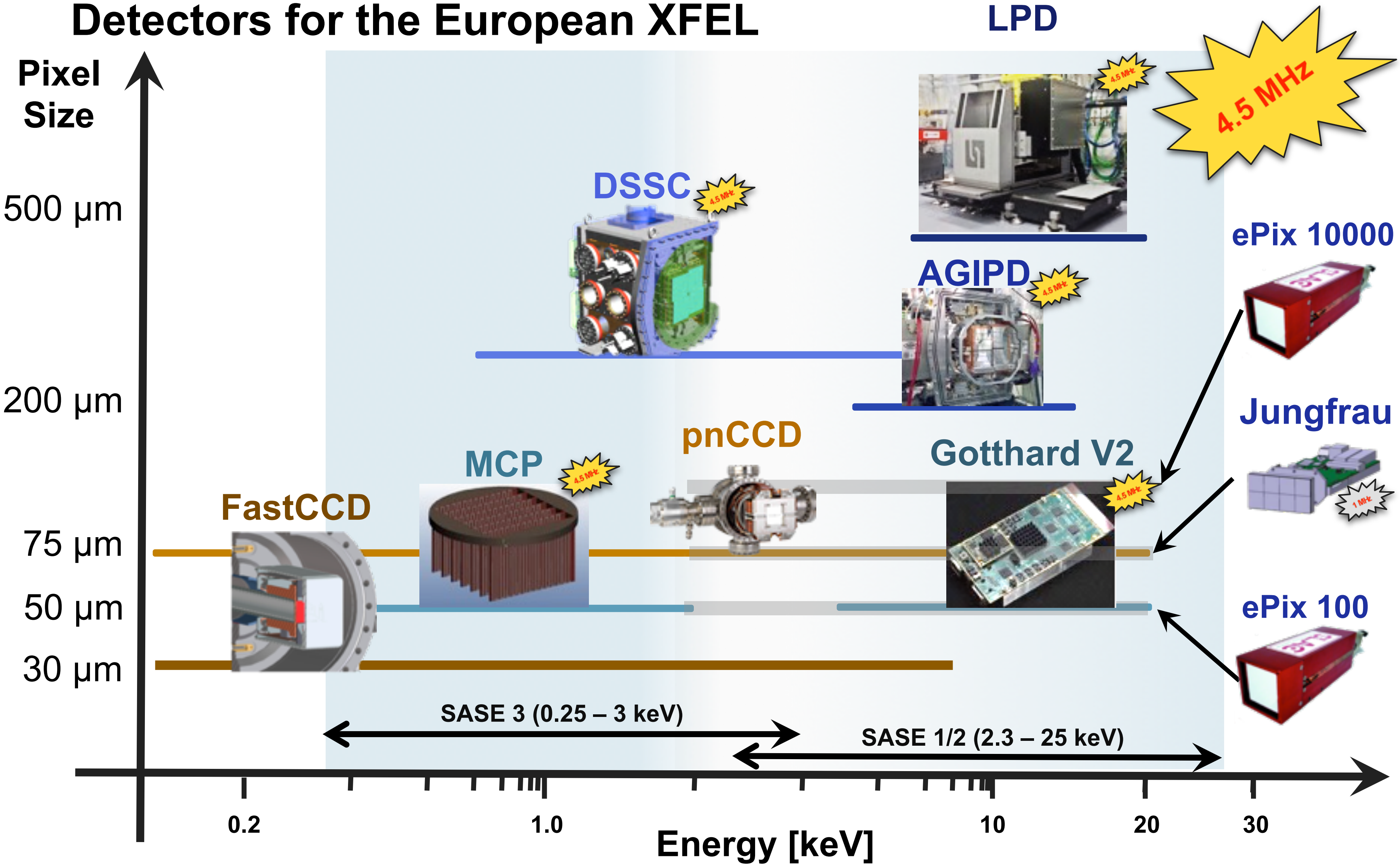
Overview

- Challenges related to data acquisition, calibration and data processing of MHz 2D imaging detectors
- DAQ infrastructure concept at the European XFEL and its implementation
- Calibration concept and its implementation
- Conclusions and summary

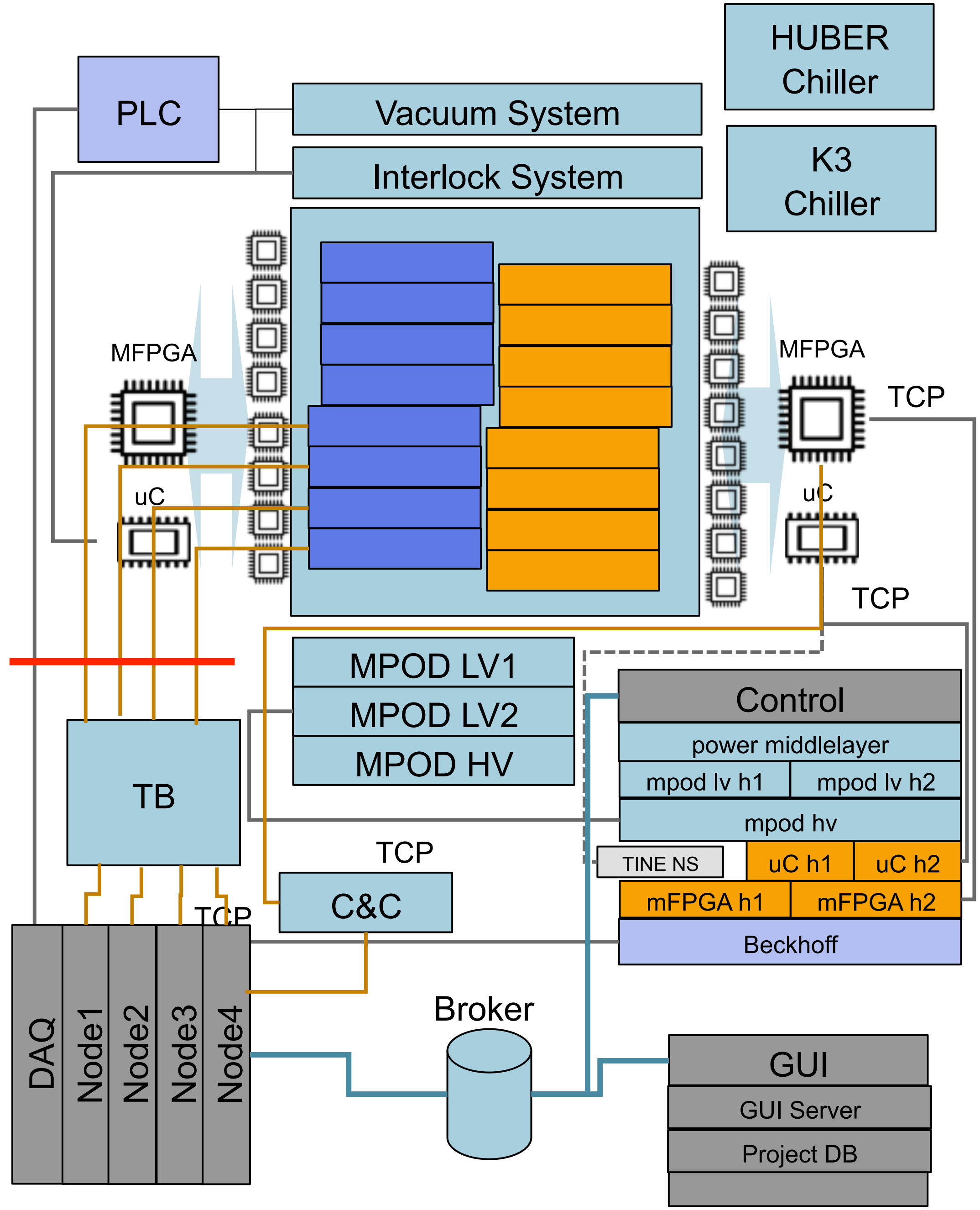


Detectors for the European XFEL



AGIPD System Overview

- Control is performed mostly on a hemisphere level:
  - Master FPGA
  - Microcontroller (via TINE interface)
- Vacuum and interlock system are controlled by Beckhoff PLC → Karabo acts on top of this
- Chillers are currently manually controlled
- Power system runs via MPOD crates, one for each hemisphere's LV, one HV
- Currently TINE name server in system but essentially not needed



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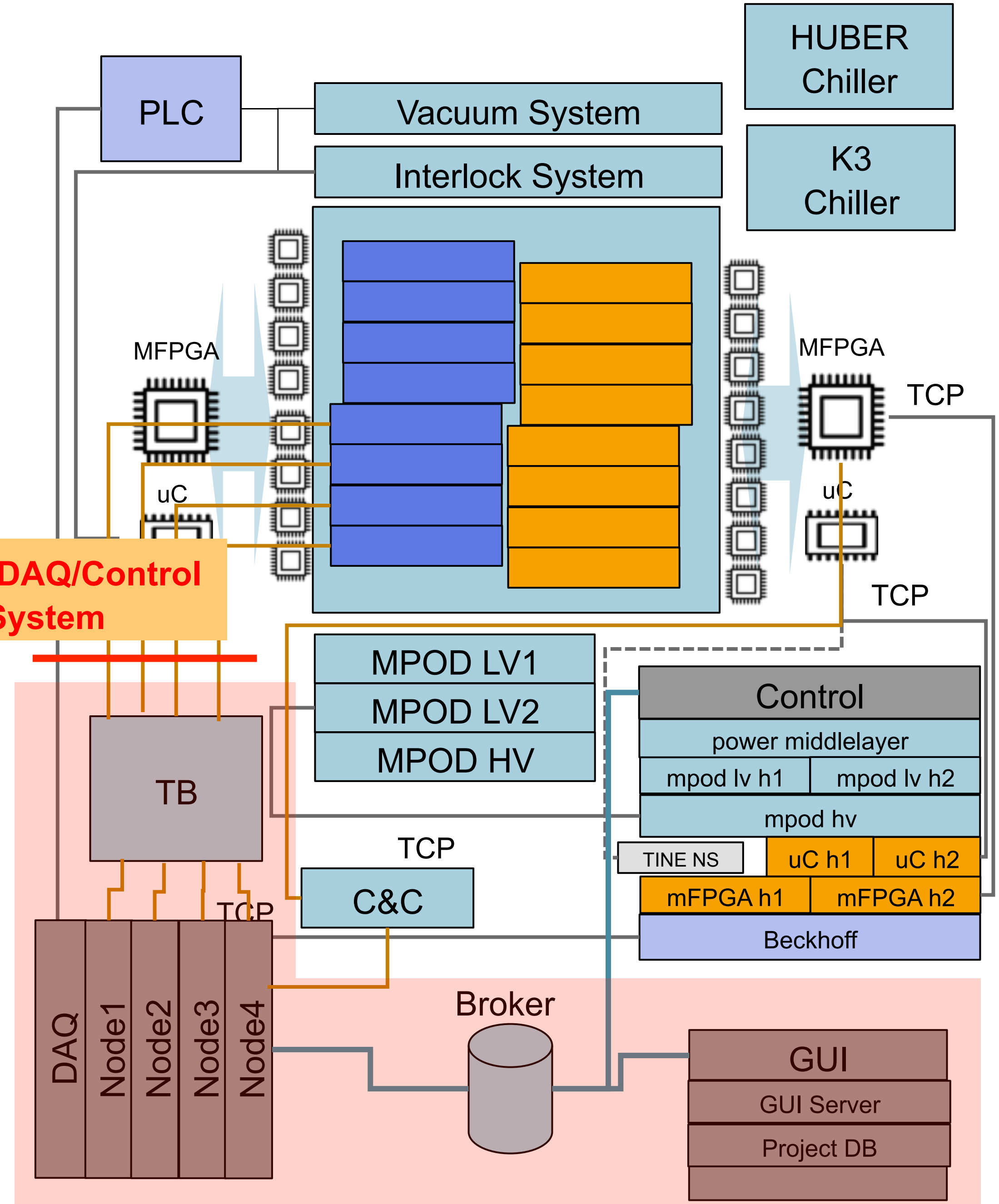
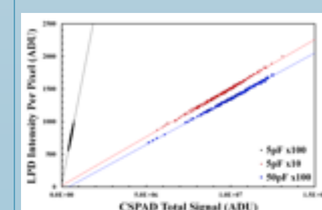
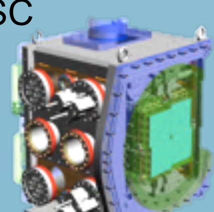
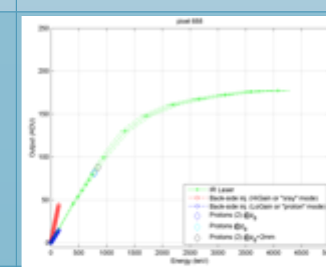
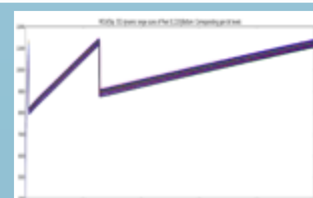
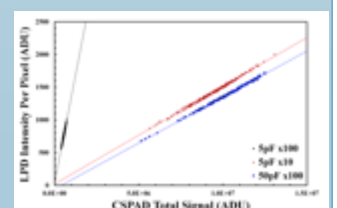
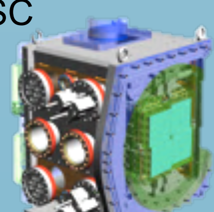
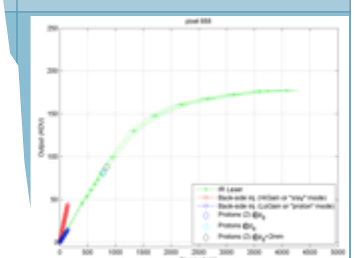


MHz Rate, High Dynamic Range Detectors – Challenges for Calibration and Data Acquisition

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

MHz Rate, High Dynamic Range Detectors – Challenges for Calibration and Data Acquisition

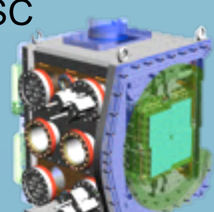
Detector	Specs	Gain Curve
AGIPD 	1 Mpixel, 4.5 M 352 memory ce 200µm sq. pixel 1-10⁴ ph@ 12 k 3 – 13 keV	
LPD 	1 Mpixel, 4.5 M 508 memory ce 500µm sq. pixe 1-10⁵ ph@ 12 k 5 – 25 keV	
DSSC 	1 Mpixel, 4.5 MH 800 memory cell 204µm hex. pixe 1-10⁴ ph@ >1ke 0.5 – 6 keV	

- Three gains per pixels
- Analogue gain evaluation
- Analogue memory
- ….

- Six gains per pixels
- Air scattering in FF
- Analogue memory
- ….

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

MHz Rate, High Dynamic Range Detectors – Challenges for Calibration and Data Acquisition

Detector	Specs
AGIPD 	1 Mpixe 352 me 200µm 1-10^4 p 3 – 13 k
LPD 	1 Mpixe 508 mem 500µm sq. pixe 1-10^5 5 – 2
DSSC 	1 Mp 800 204µ 1-10 0.5 -

Example LPD

x 512 memory cells
x 1 million pixel
= 5 x 10^8 parameters
and
3 Gain Stages
2 Gain Settings
~ 10^9 parameters

Parameter Dependence

Temperature,
integration time,
irradiated dose,
bias voltage and …

- Three gains per pixels
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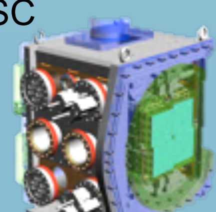
- Analogue memory
- ….

- Six gains per pixels
- Air scattering in FF
- Analogue memory
- ….

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

MHz Rate, High Dynamic Range Detectors – Challenges for Calibration and Data Acquisition

Detector	Spe
AGIPD 	1 M 352 200 1-10 3 –
LPD 	1 M 508 500 1-10 5 –
DSSC 	1 M 800 204 1-10 0.5 – 6 keV

Data rates: ~10-13 GB/s

What user community ideally would like to have:

1. **On the fly data correction**
2. **On the fly calibration**
3. **Near real time visualization and analysis (indexing, radial integration, …)**

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nalogue memory
..

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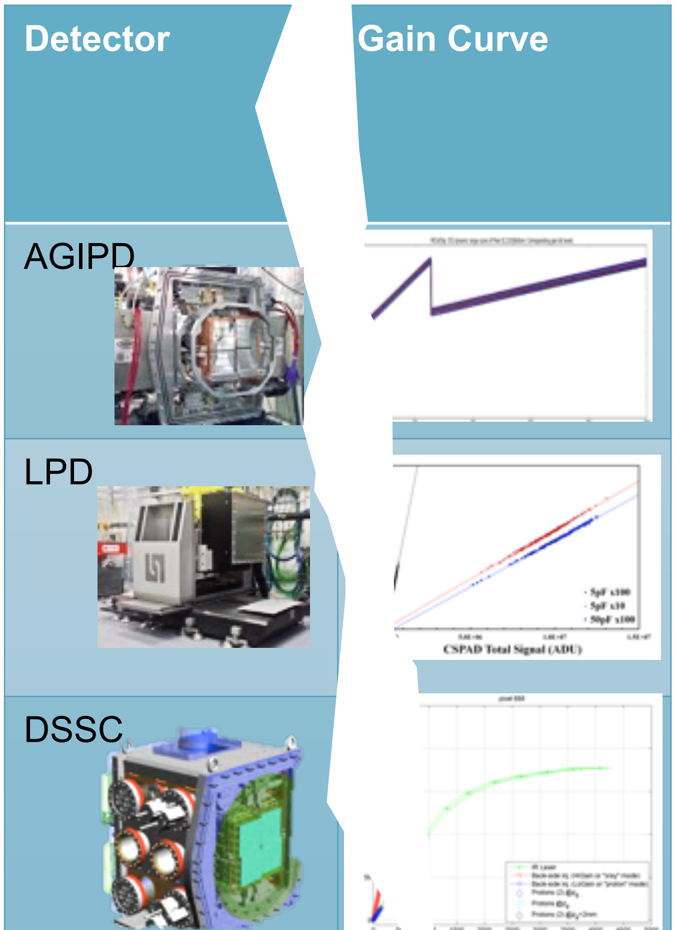
MHz Rate, High Dynamic Range Detectors – Challenges for Calibration and Data Acquisition



- Three gains per pixels
- Analogue gain evaluation
- Analogue memory
- …

- Six gains per pixels
- Air scattering in FF
- Analogue memory
- ….

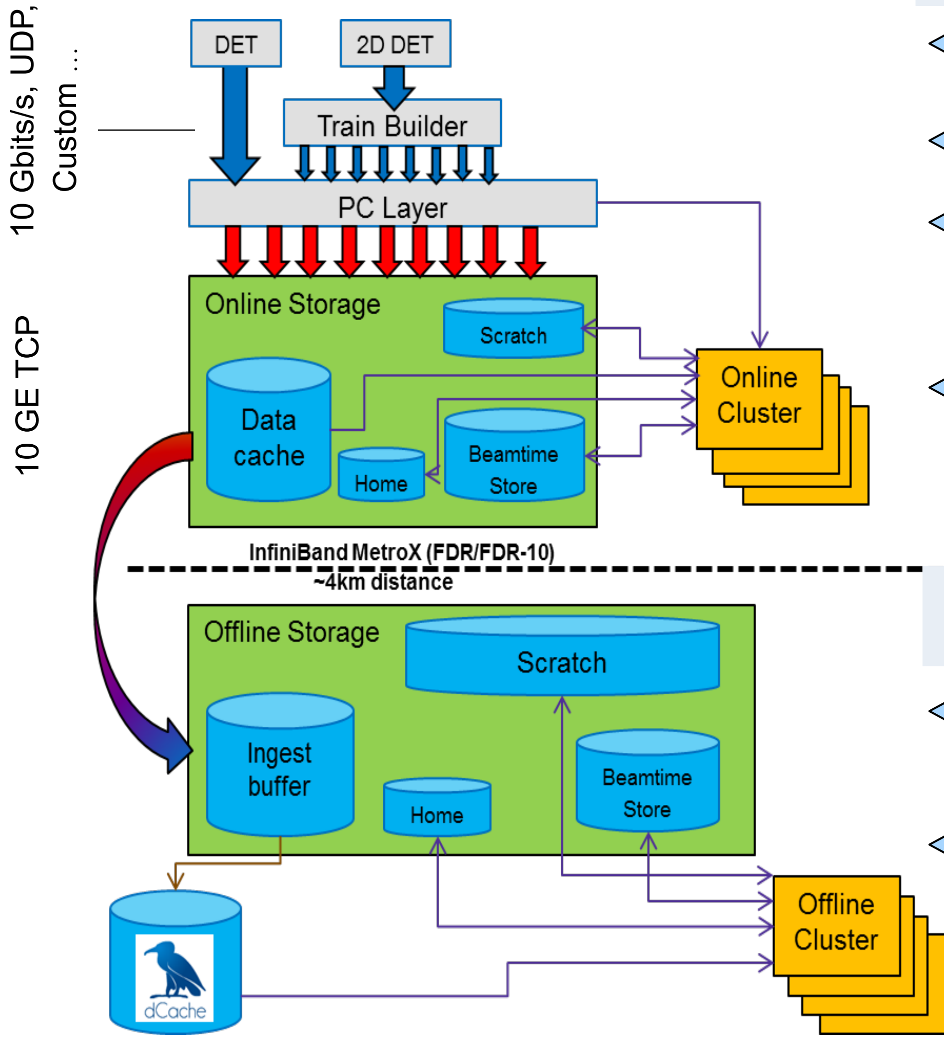
- Non-linear gain
- One ADU per photon
- ….

DAQ and calibration is non-trivial!

Flexible and scalable DAQ and data management environment.

Facility-side calibration recommended

XFEL DAQ Architecture



On Site per SASE

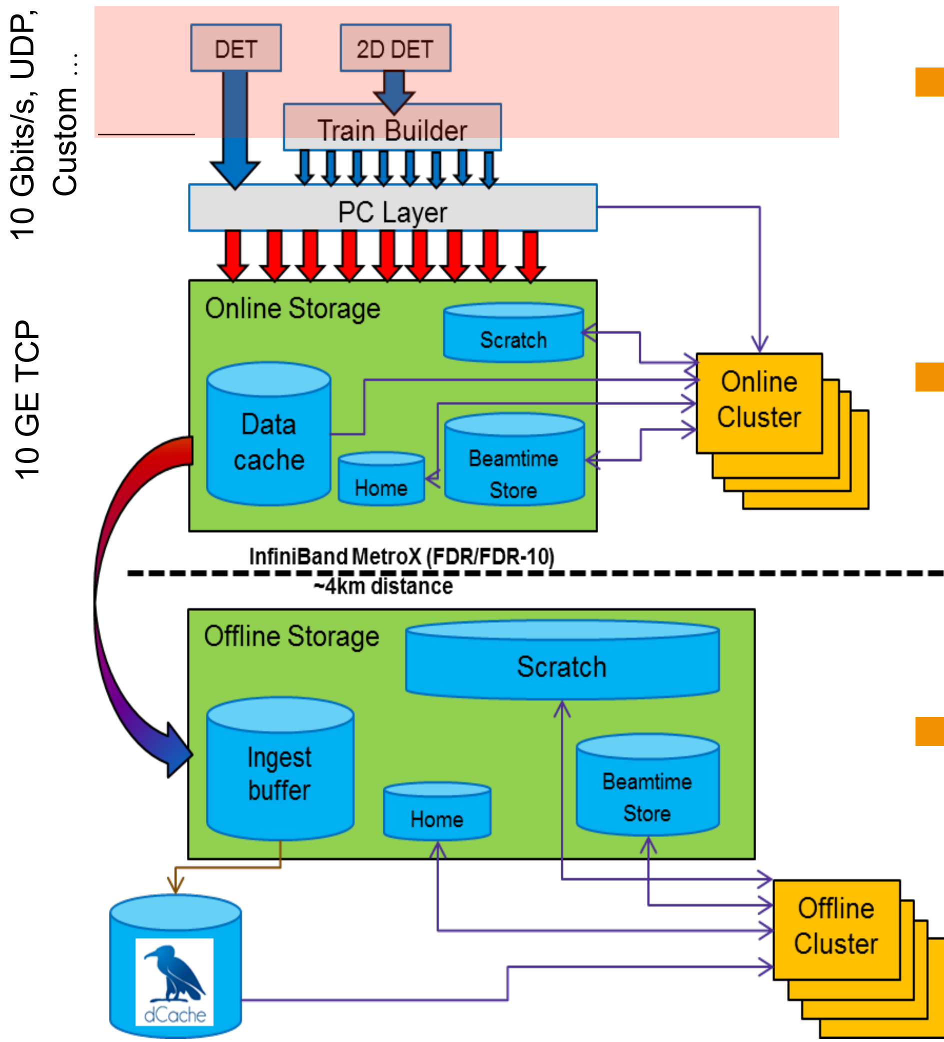
- Detector with Front End Electronics
- Front End Interface
- PC Layer
- Online storage and online analysis cluster

DESY Data Center – Shared for all SASE

- Offline storage and offline analysis cluster
- Archive

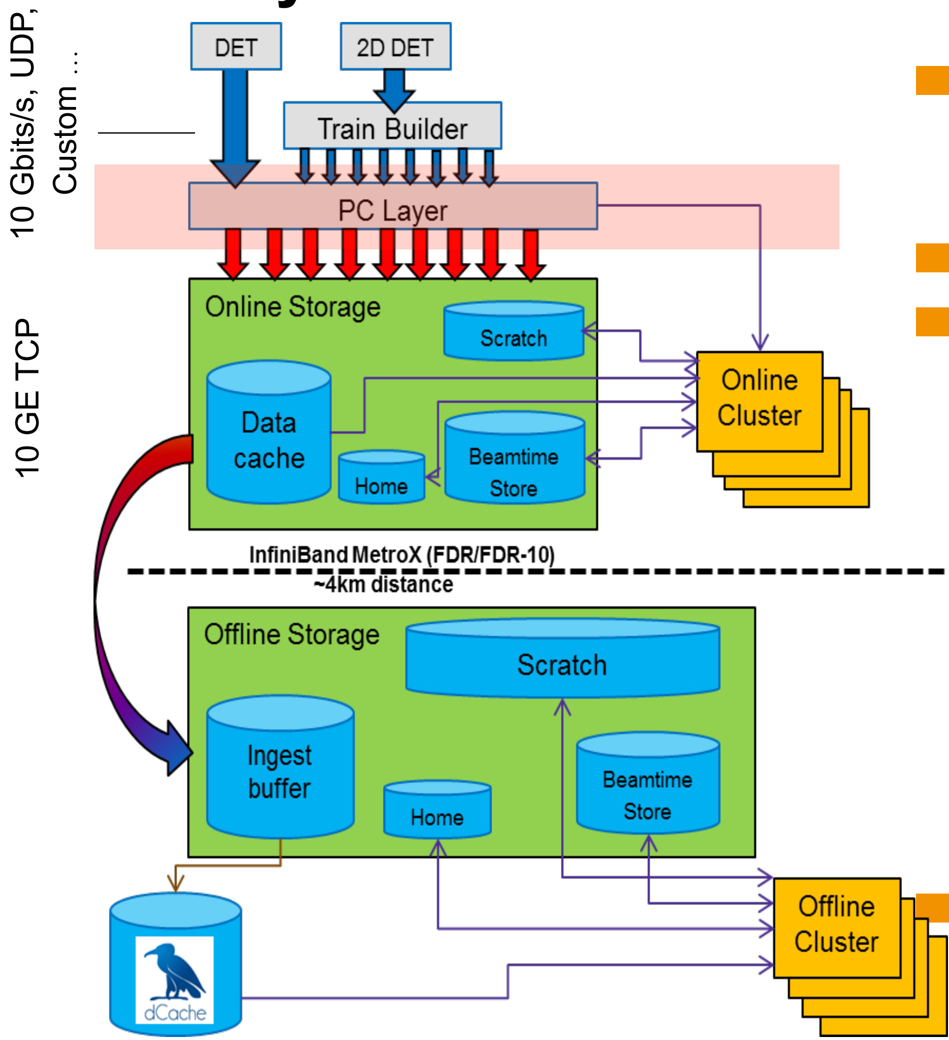
Multi Layer Design
Flexible and scalable on each layer

Detector Front End and Front End Interface



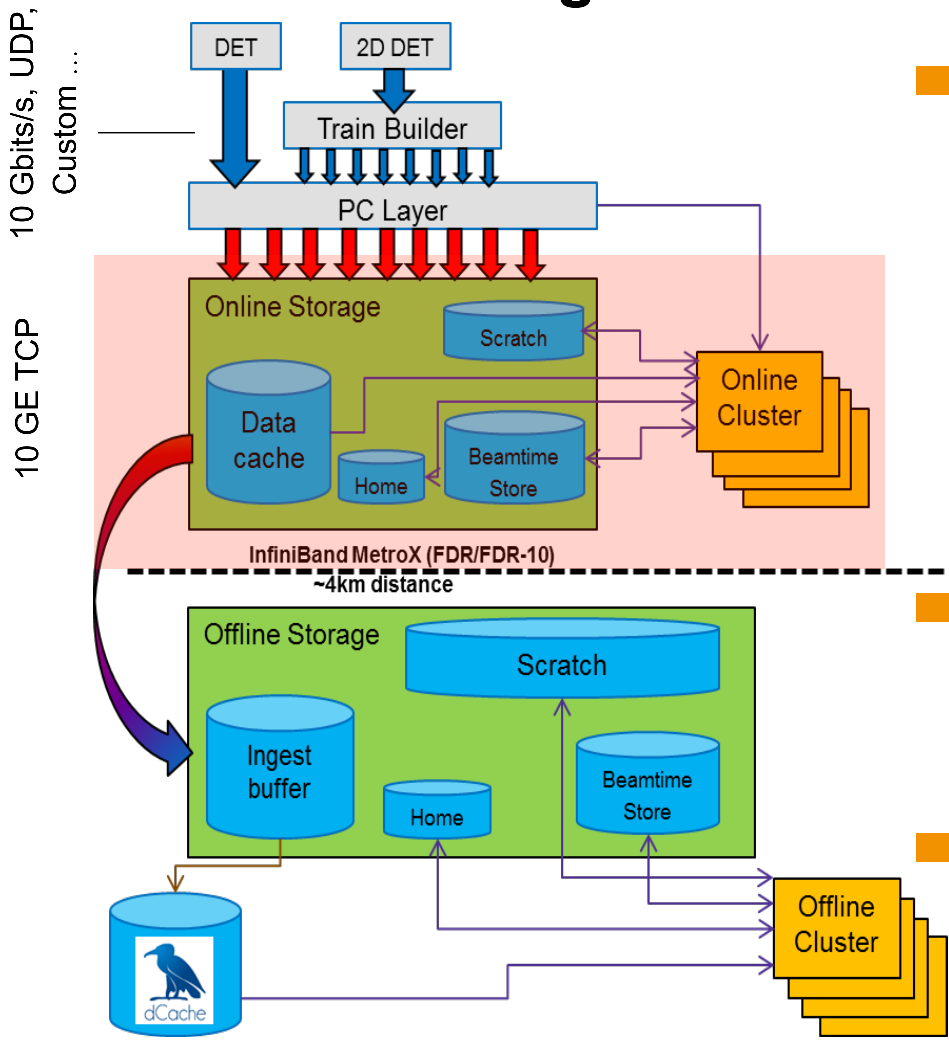
- Front End Electronics (ASIC + ADC + data link)
  - Data forwarding and standardized formatting (2D detectors)
  - Image vetoing
- Front End Electronics Interface (data readout + control)
  - Formatting, train building
  - Frame tagging
  - If possible pedestal correction, zero suppression
- Train Builder
  - Original purpose: reorganize all partial images received from different detector modules into one train
  - Exploring capabilities for data tagging and data processing

PC Layer



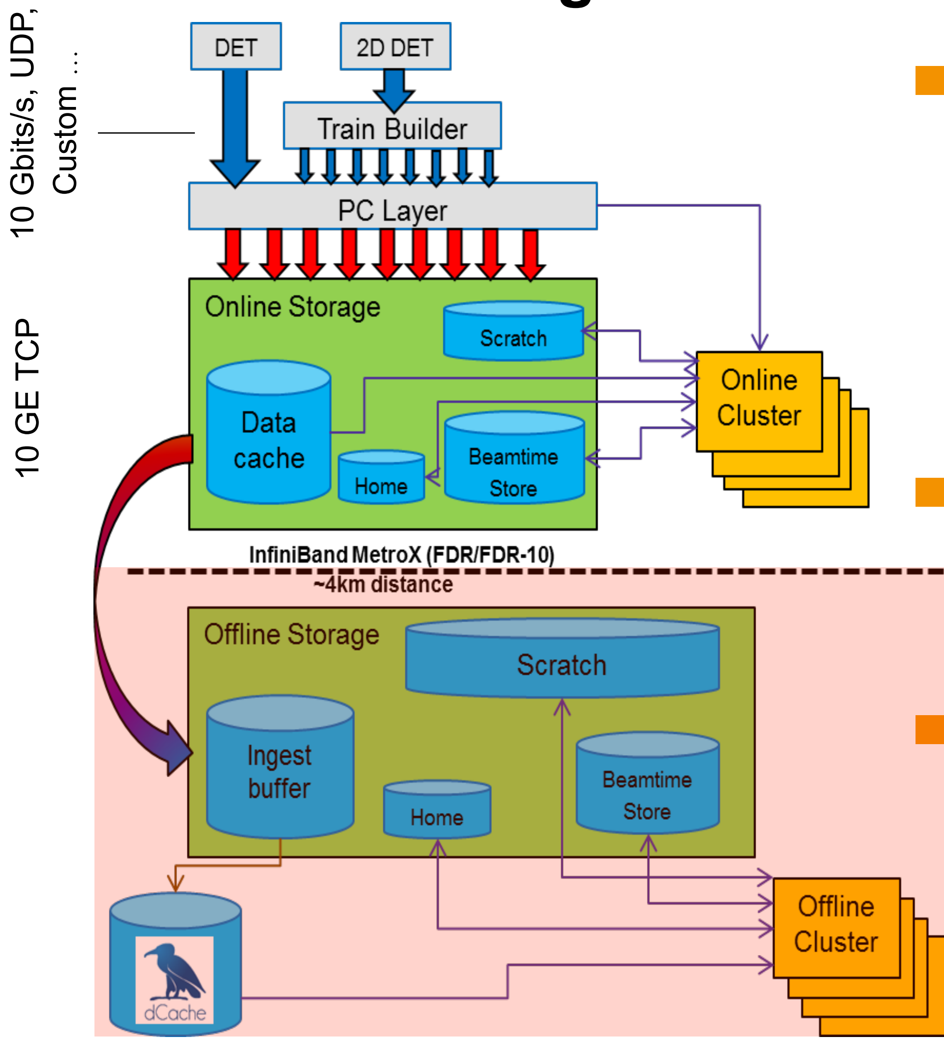
- High speed data acquisition including semi real time O(sec) data processing and formatting
- Receive data and writes it to disk
- Run Control system
  - Orchestrates PC layer activities of reading-out, monitoring and storing data generated by experiment data sources
  - Defines segments in the experiments process where generated data is simply ignored, just monitored or also recorded to data files
- Possibility to plug-in instrument or experiment class specific software directly into data acquisition chain

Data Processing Online on Site



- Online Computing Cluster for data monitoring and fast user analysis
  - Optimized access to raw data
  - Dedicated PC farm for each SASE
  - Servers for users to look at data and perform individual data processing
    - ▶ Interactive or batch processing
    - ▶ Access to scratch, proc, cal and usr folders
- Nodes running calibration pipe lines are equipped with GPUs
  - Optimized GPU code is provided by detector development group
- Beam time store
  - Used for data upload before experiment and storing results
  - e.g. 5 TB per beam time, backup

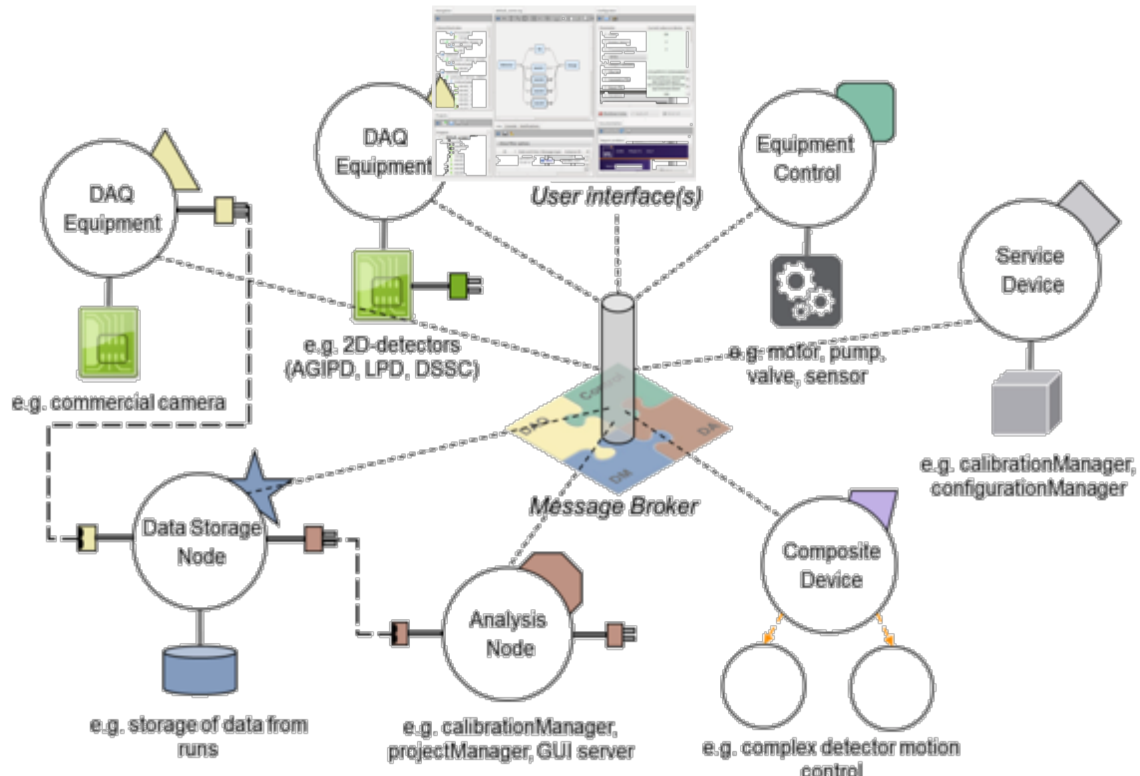
Data Processing Offline off Site



- Good quality data from the experiments (online storage) is migrated to the XFEL offline data analysis facility located at DESY Data Center
  - Ingest buffer, data archiving
  - Possibility of caching intermediate results on scratch storage
- Planned offline storage capacity:
  - ▶10 PB (2017), 56 PB (2020),
  - ▶ 96 PB (2023)
  - ▶ additional SFX 2 PB (2017)
- Export of the results or reduced/corrected datasets
  - Using ftp servers max. theoretical bandwidth 2x 5 Gbit/s shared with DESY

Karabo

- Software framework for
  - Hardware control
  - Fast data acquisition
  - Data management
  - Data analysis and scientific computing

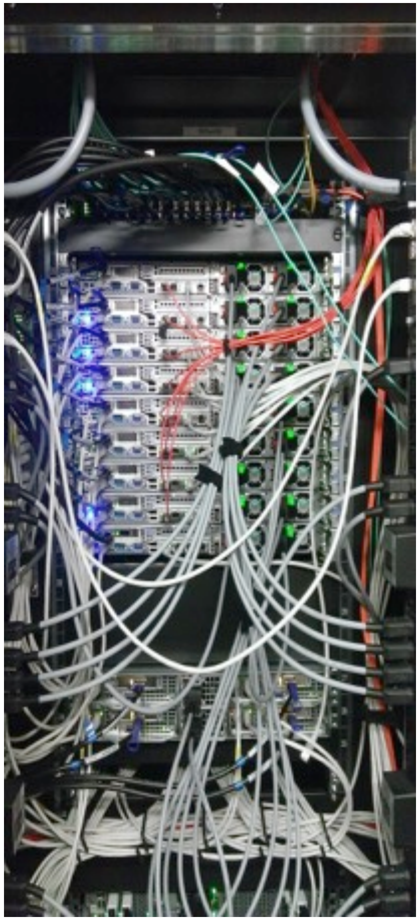


- Broker based, event based, asynchronous
- User interface to experiment control and data
- Multiple interfaces, including Python
- Developed by European XFEL

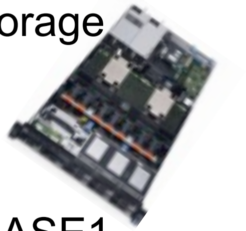
Train Builder

- Original goal
  - Reorganize all partial images into one train
  - Send the complete train via one 10 GbE line to PC Layer node
- Train builder receives 16 x 10 GbE channels
- 16 outputs exist which can be used train by train in round robin
- Pixel reordering of LPD detector is done on TB.
- Presently exploring usage for data processing and data tagging
- Throughput 512 images per train to be extended in the near future to > 800

PC Layer Implementation



- Dell Power EdgeR630
  - 10 GE SFP+ interface for data receiving from detector/train builder
  - IBM FDR 56 Gbps to online storage and computing cluster
  - Redundant power supply



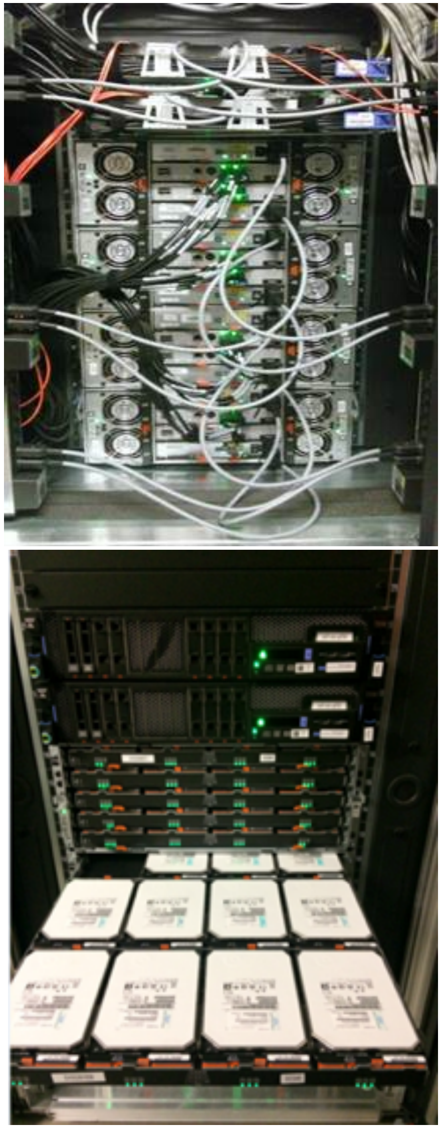
- 23 servers installed in racks for SASE1 beam line
  - ►Connected to 10GE and IB networks
- Presently ongoing tests
  - IBM Power 8 servers with dedicated FPGA board for fast on the fly gzip compression

Caches

- Data storage close to experiments
  - ▶ Hardware: IBM Elastic Storage System
  - ▶ Software: GPFS
- Offline data storage
  - Fast access
    - ▶ Hardware: IBM Elastic Storage System
    - ▶ Software: GPFS
  - Large capacity
    - ▶ Hardware: DELL Systems
    - ▶ Software: dCache

dCache Storage Nodes

IBM ESS System

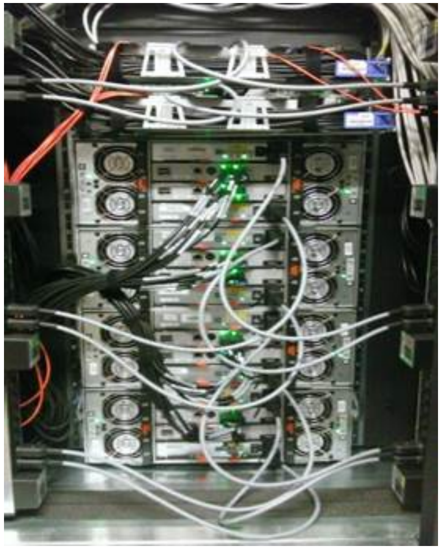


Caches

- 5.5 PB of dCache storage deployed
- Additional 5 PB of dCache storage ordered
  - 40 servers
  - 20 disk enclosures
- Total capacity will be ~10.5 PB net space.

dCache Storage Nodes

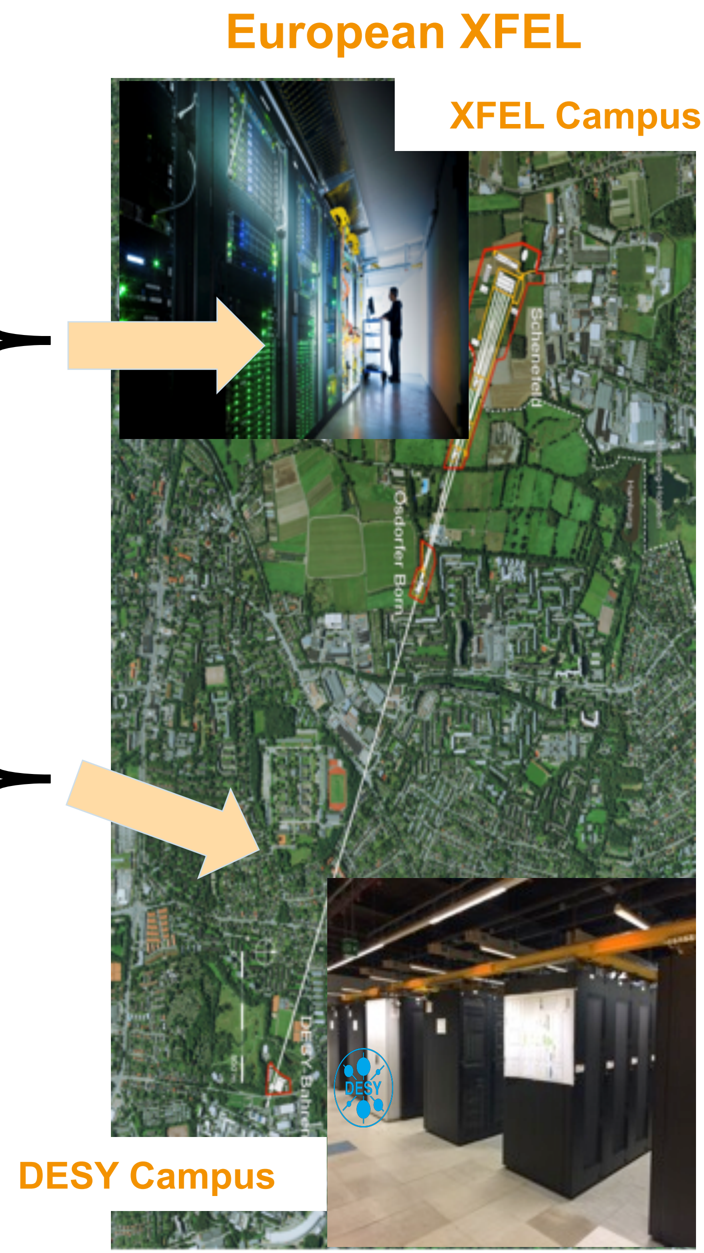
IBM ESS System



Data analysis Infrastructure

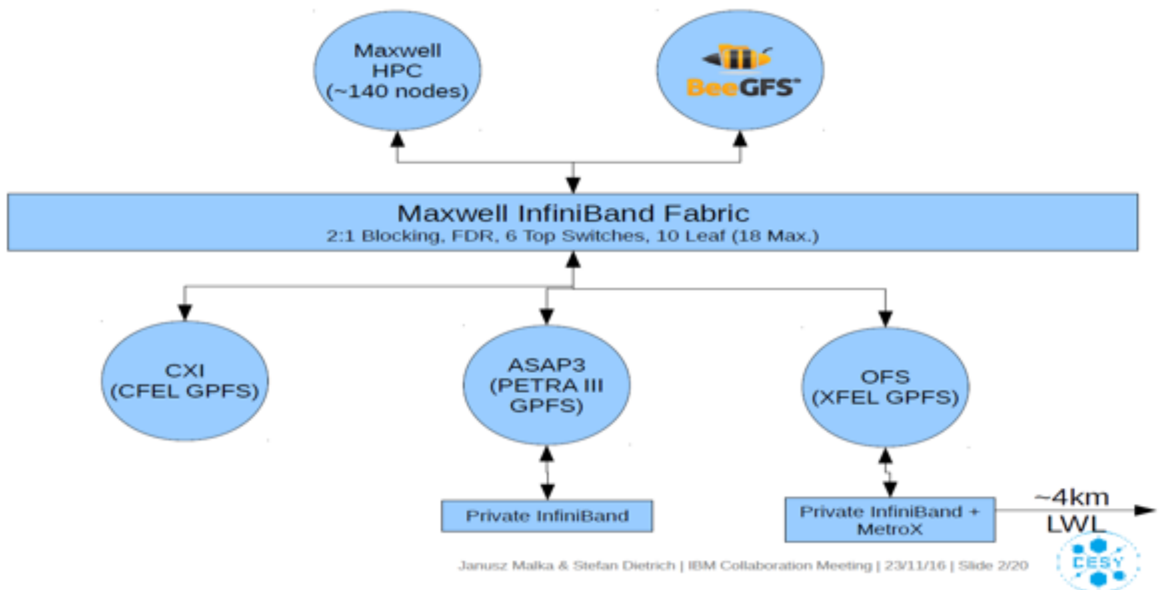
- “Online cluster” for data monitoring and fast user analysis,
  - 8 nodes x (20 cores, 256GB RAM) dedicated to users
  - Additional nodes for control and XFEL provided calibration and processing

- “Offline cluster” = Maxwell cluster (DESY)
  - Deployed XFEL resources on Maxwell
    - ►80 nodes/3200 cores (Intel Xeon E5-2698v4)
    - ►~112 TFlops
    - ►512GB RAM each node
    - ►20 cores, 2.2GHz
    - ►512 GB RAM



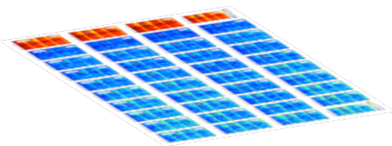
Data analysis Infrastructure

- Overall XFEL resources on Maxwell cluster
  - ►100 CPU nodes
  - ►7 nodes with GPU cards
- Upgraded end of 2017 by additional
  - ►100 CPU nodes
  - ►16 GPU nodes

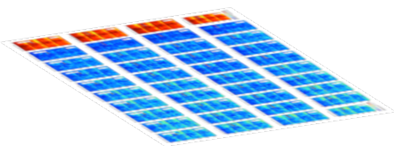


Calibration Data Base – CalDB

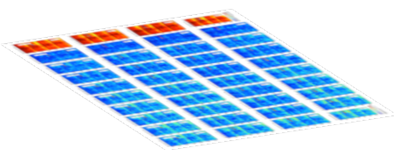
Cal. Measurement 1



Cal. Measurement 2



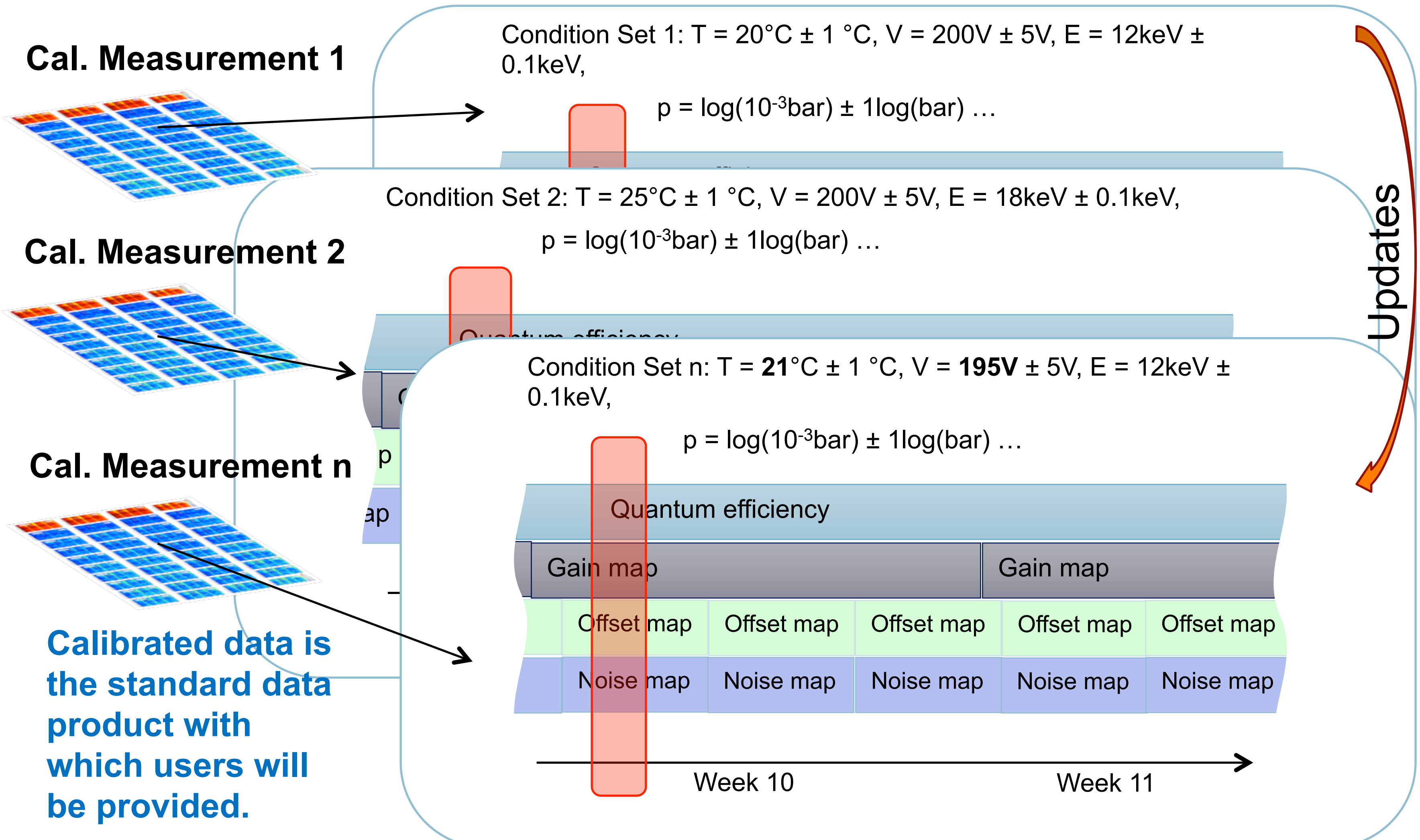
Cal. Measurement n



Calibrated data is the standard data product with which users will be provided.

- Centralized storage and management of calibration data
  - Provide up-to-date calibration
  - Provide software interface for users to calibrate data
  - Provide calibration data for specific scientific needs if required (non standard applications)
  - Provide transparent calibration algorithms (no black boxes)
- Why?
  - All information is in one place
  - Users have access to calibration data before beam time
  - Scientific data can be re-processed at any time using different versions of calibration data sets
  - Users can trust their data has been calibrated using the most up-to-date calibration data set available based on detector experts knowledge

Calibration Data Base – CalDB



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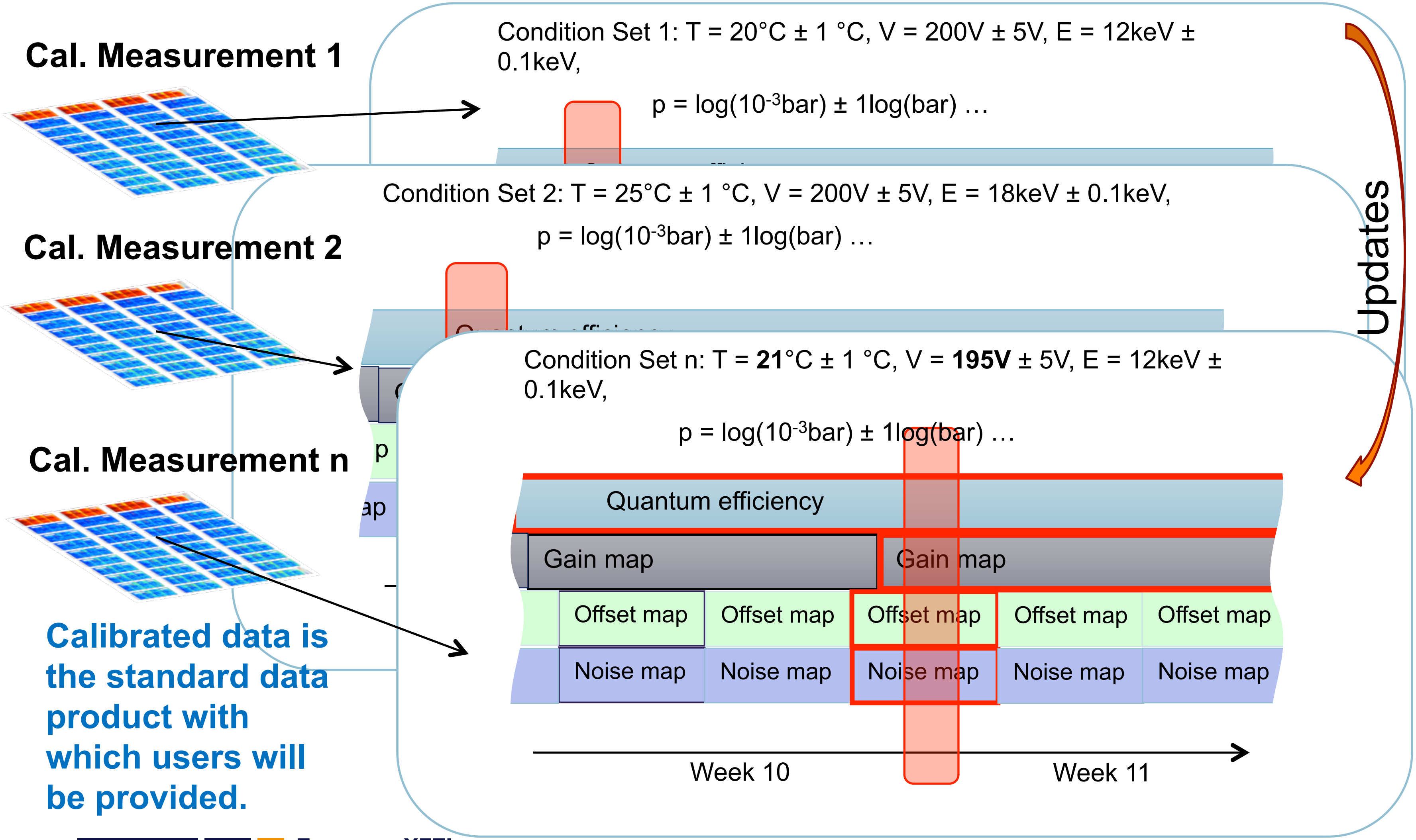
Calibration Data Base – CalDB

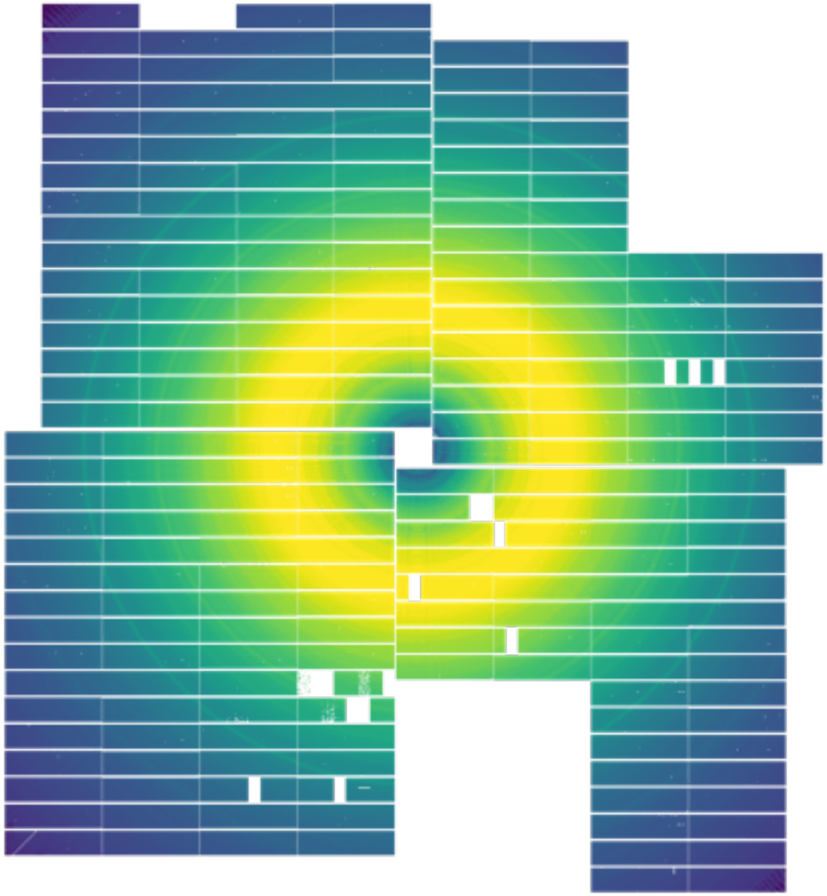


Calibrated data is the standard data product with which users will be provided.

Alignment Data

- Goal
  - Facility-side provide initial module positions off segmented detectors
    → possible refine in situ if needed
- In verification with FXE for LPD for positions up to quadrant level determined using photographic metrology data
  → precision ≈ 1/10 pixel size
- Data store in HDF5 file matching the hierarchical layout of the detector, will be made available through calibration database in the future
- Python code provided to get position of a given module in terms of top left corner pixel
- Within module lithography assumed as “perfect”

Corrected LPD Data (5 train mean) Modules Positioned

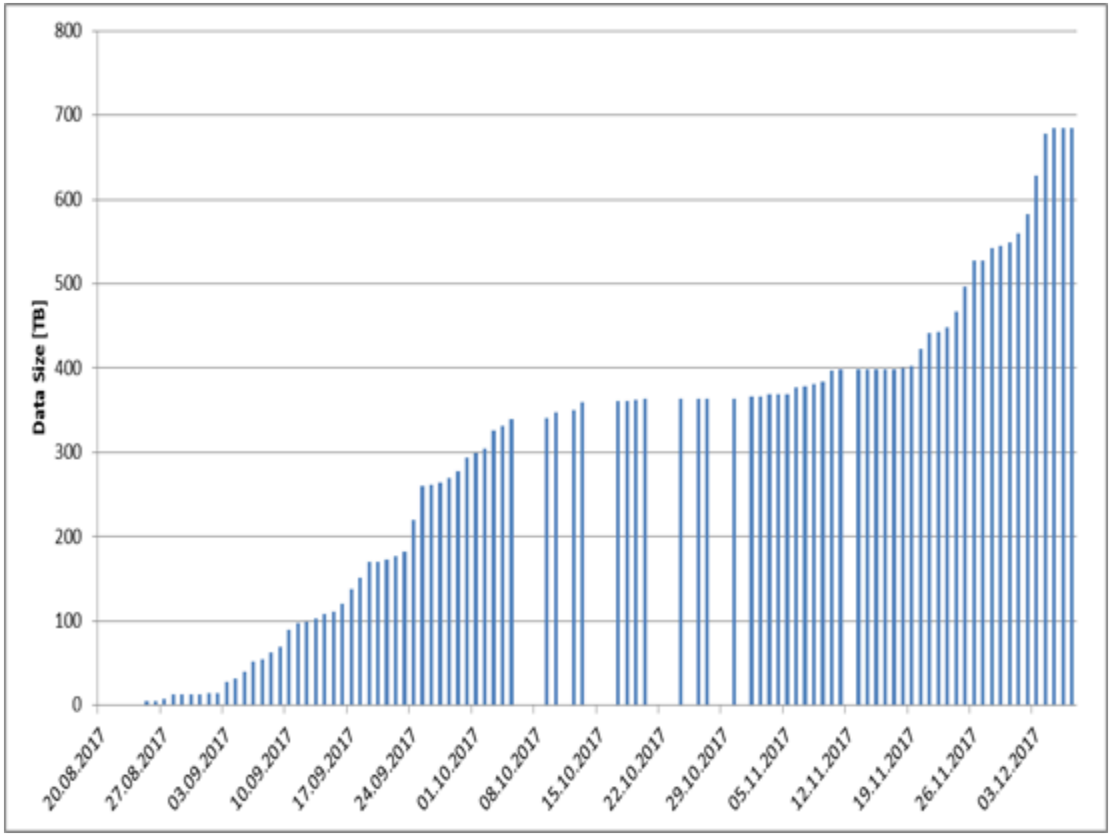


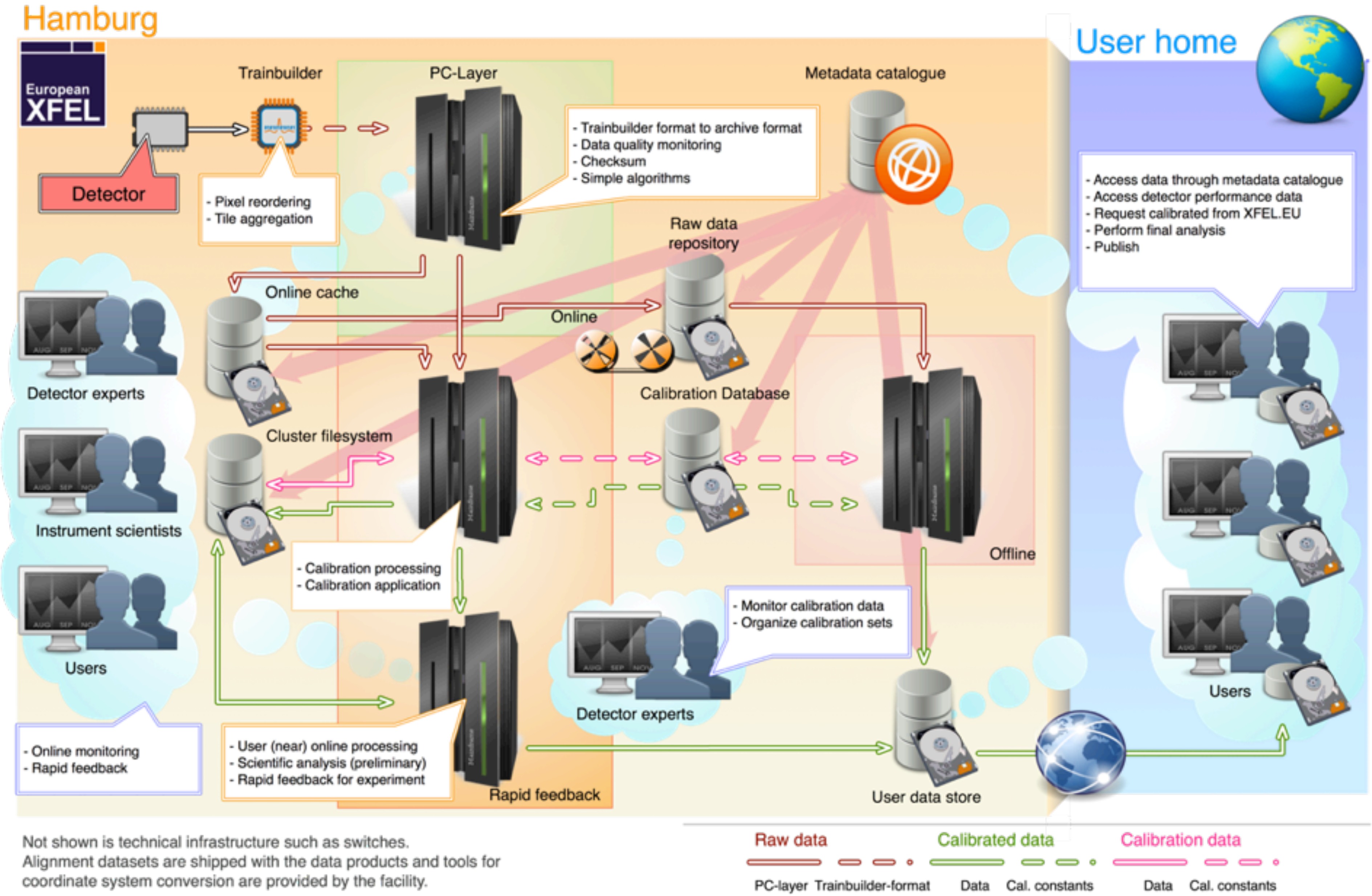
All Generated Data August 2017 – December 2017

- Includes user experiments and commissioning activities
- FXE, SPB/SFX instruments and SASE1 tunnel
  - 12 proposal

Activity	Amount of Data (TB)
FXE Commissioning	3,4
LPD Commissioning	6,6
LPD DAQ Commissioning	0,24
Tunnel DAQ commissioning	0,005
AGIPD Calibration Commissioning	0,004
First LPD commissioning	0,58
SASE1 Tunnel commissioning	0,41
SPB DAQ commissionning	15,8
SPB/SFX commissioning	191,2
DAQ tests	8,6
DAQ tests 2	0,03

Total Accumulated Data in TB

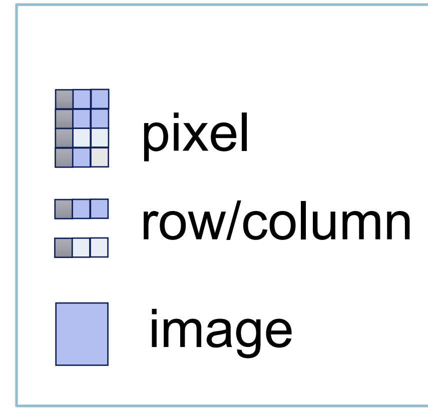




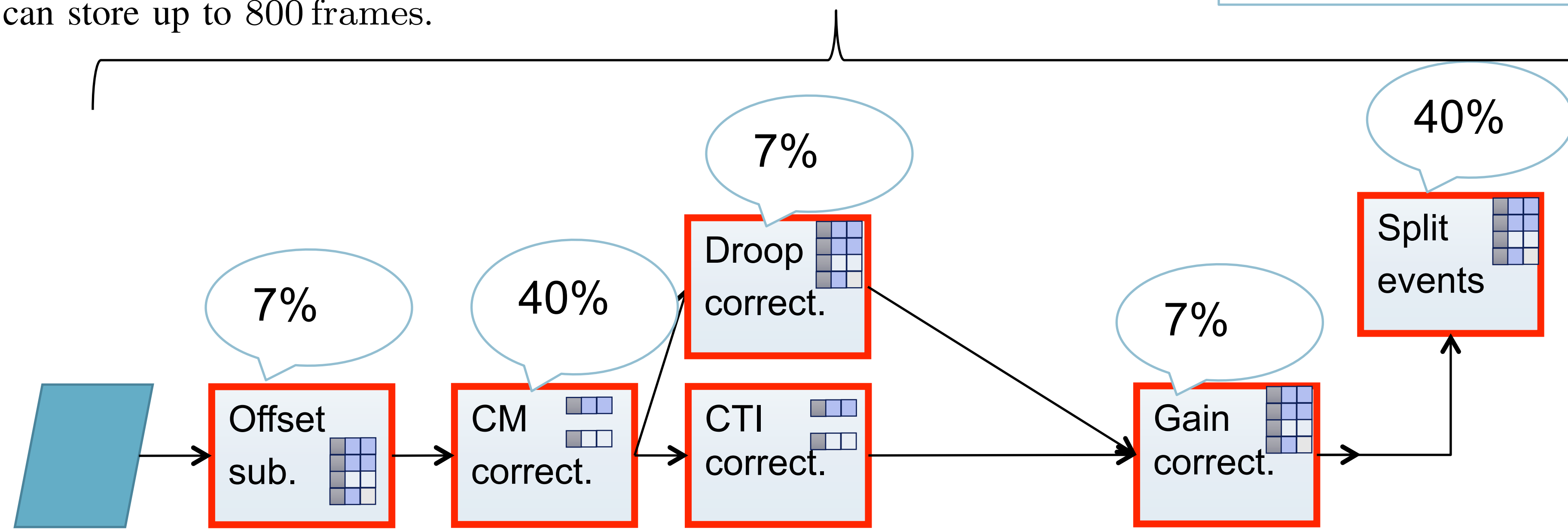
Not shown is technical infrastructure such as switches.
Alignment datasets are shipped with the data products and tools for coordinate system conversion are provided by the facility.

Data Correction Pipelines and Importance of Throughput

Detector	Data size (pixel × frames)	Processing time (ms)
AGIPD	$128 \times 512 \times 352$	76.6
DSSC	$128 \times 512 \times 512^{a}$	106.1
LPD	$256 \times 256 \times 512$	103.6



[a] Limited to 512 frames by the train–builder hardware, the detector head can store up to 800 frames.



Characterization Processing

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

Frequent updates, 5 min processing (dark image analysis)

More static, Each about 2-4 hours processing each (pulse capacitor data, current source data, flat fields)

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

Frequent updates, 5 min processing (dark image analysis)

More static, Each about 2-4 hours processing each (charge injection data, flat fields)

Acknowledgment

XFEL.EU Groups

IT and Data Management (K. Wrona)

Advanced Electronics (P. Gessler)

Control and Analysis Software Group (S. Brockhauser)

Detector Group (M. Kuster)

SPB/SFX (A.P. Mancuso)

FXE (C. Bressler)

AGIPD Consortium

Lead by DESY (H. Graafsma)

LPD Consortium

Lead by Rutherford Appleton Laboratory (M. Hart)