Data Challenges at the European XFEL

From Bytes/s to GBytes/s

Dr. Steffen Hauf, European XFEL GmbH
27.10.2020

Data Challenges and solutions at the European XFEL

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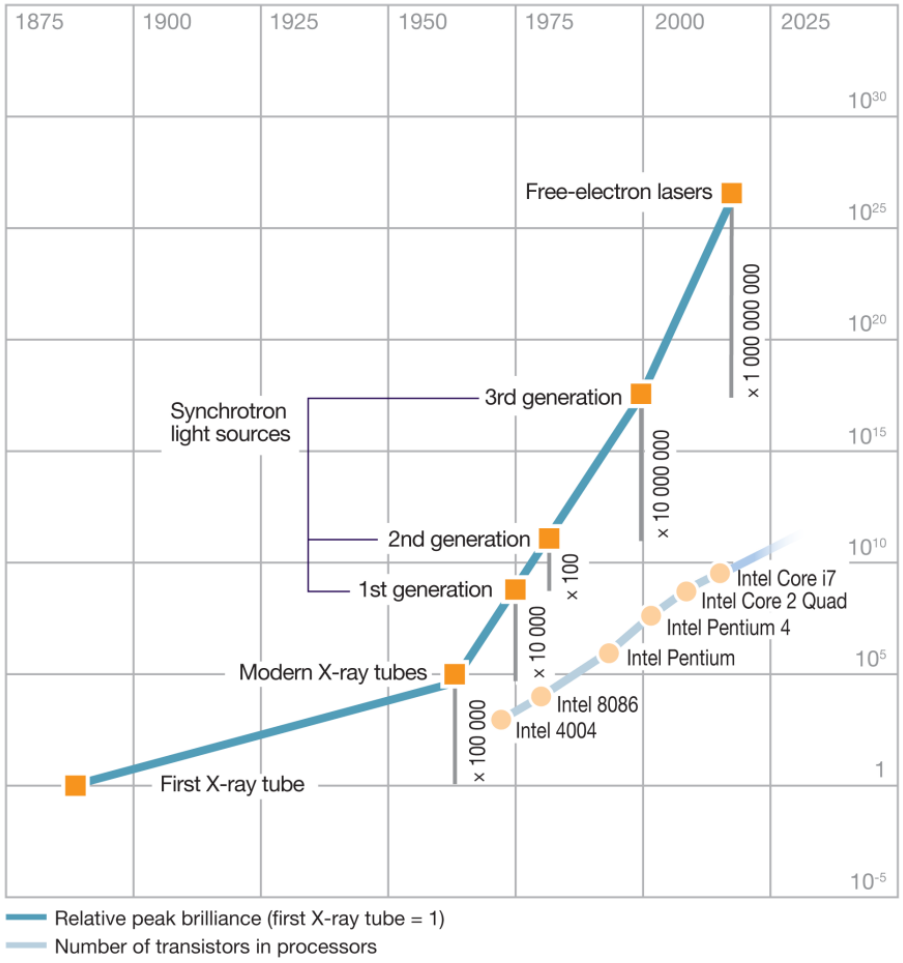
Data Challenges at the European XFEL

- The European XFEL – a (short) Introducion
- Data Challenges
- Data Drivers
- Data Solutions
- Lessons Learned and Outlook

PR Slide: Light source development



- The development of light source facilities has been faster than the increase in computer processing capacity (i.e., Moore's Law)

The European XFEL Facility

Schenefeld Campus

Experiment hall

Laboratories

Offices

Osdorfer Born

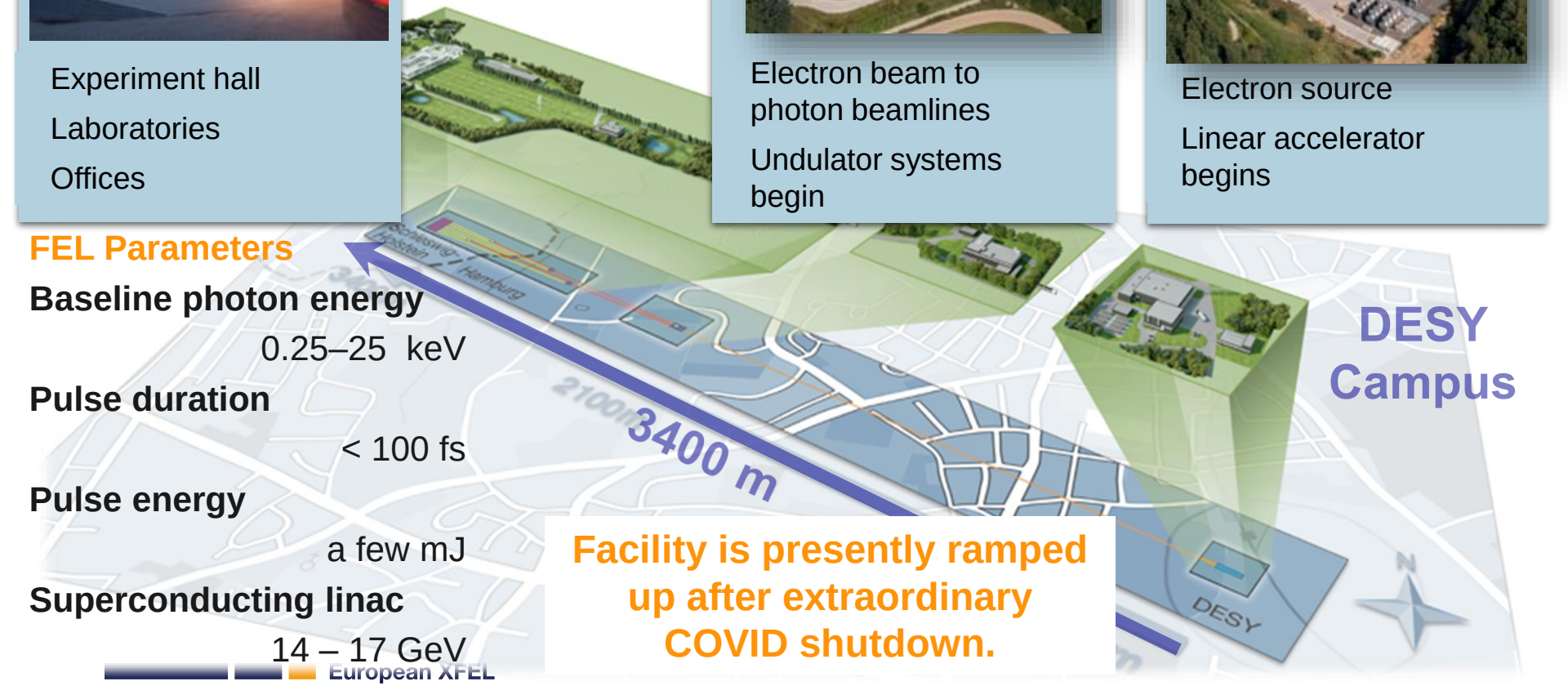
Electron beam to photon beamlines

Undulator systems begin

DESY-Bahrenfeld

Electron source

Linear accelerator begins



DESY Campus

FEL Parameters

Baseline photon energy

0.25–25 keV

Pulse duration

< 100 fs

Pulse energy

a few mJ

Superconducting linac

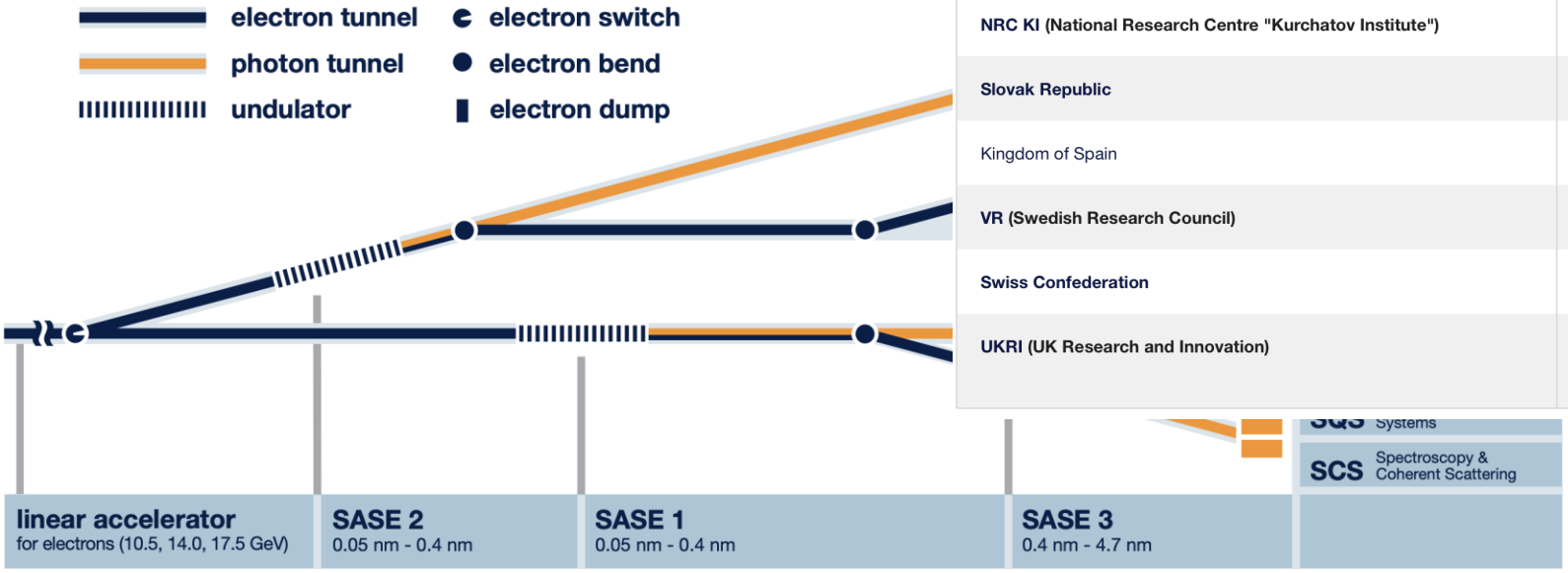
14 – 17 GeV

Facility is presently ramped up after extraordinary COVID shutdown.

The European XFEL Facility

- An international research facility
  - 12 participating countries
  - 300+ employees from 50+ different nations
- A user facility:
  - 6 scientific user experiments hosting 56 user groups in 2019
  - User groups change on a weekly schedule

Present (bold) or likely future shareholder of the European XFEL GmbH		Country
DASTI (Danish Agency for Science, Technology and Innovation)		Denmark
CEA (Commissariat à l'énergie atomique et aux énergies alternatives) **CNRS** (Centre national de la recherche scientifique)		France
DESY (Deutsches Elektronen-Synchrotron)		Germany
NRDI Office (National Research, Development and Innovation Office)		Hungary
INFN (Istituto Nazionale di Fisica Nucleare) **CNR** (Consiglio Nazionale delle Ricerche)		Italy
NCBJ (National Centre for Nuclear Research)		Poland
NRC KI (National Research Centre "Kurchatov Institute")		Russia
Slovak Republic		Slovakia
Kingdom of Spain		Spain
VR (Swedish Research Council)		Sweden
Swiss Confederation		Switzerland
UKRI (UK Research and Innovation)		United Kingdom



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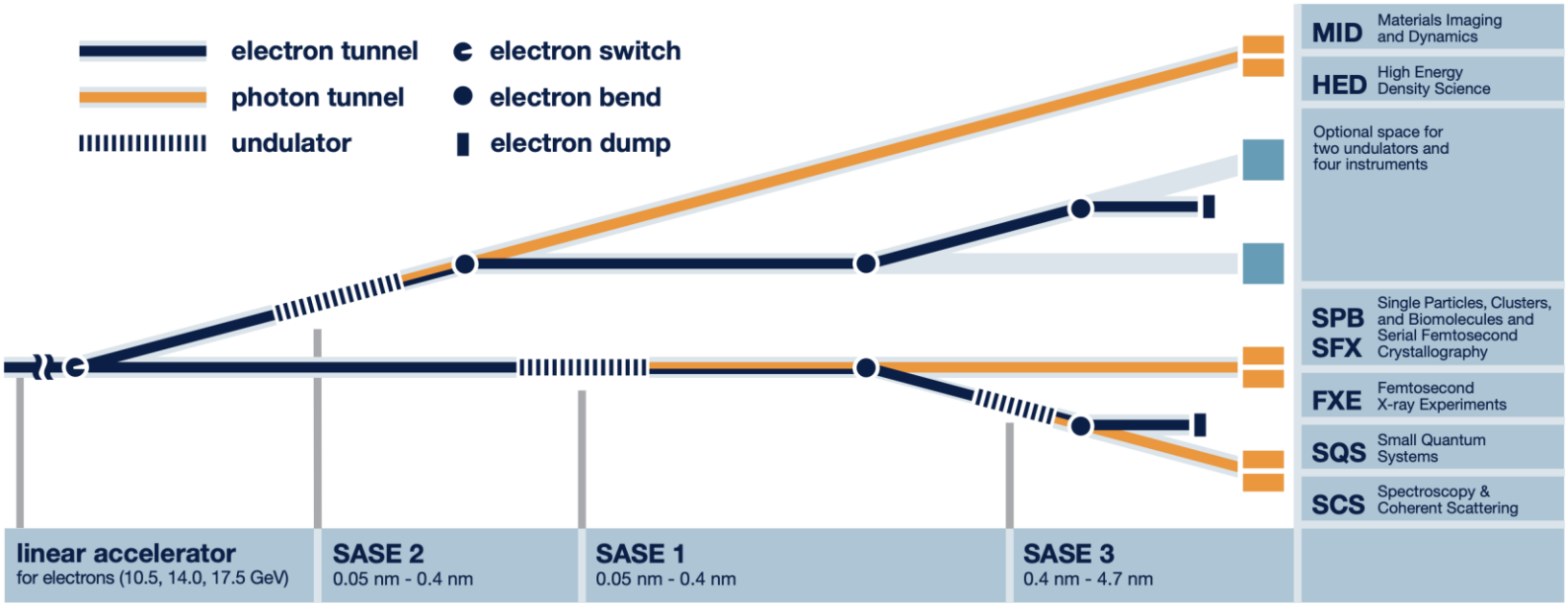
	Russia
	Slovakia
	Spain
	Sweden
	Switzerland
	United Kingdom

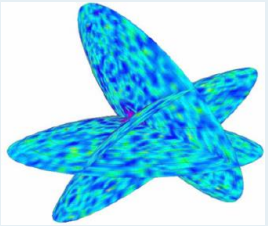


XFEL Scientific Instruments

Hard X-Rays

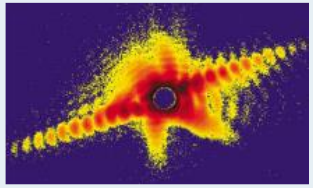
SPB **Single Particles, Clusters and Biomolecules and Serial Femtosecond Crystallography**

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



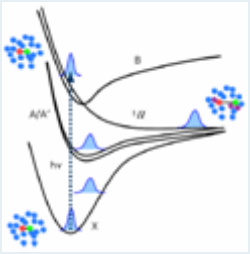
MID **Materials Imaging & Dynamics**

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



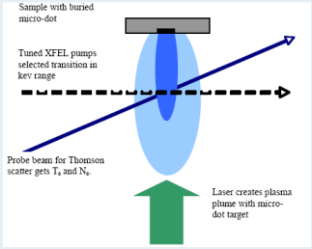
FXE **Femtosecond X-Ray Experiments**

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



HED **High Energy Density Matter**

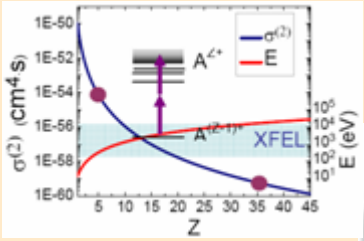
Will look into some of the most extreme states of matter in the universe, such as the conditions at the center of planets



Soft X-Rays

SQS **Small Quantum Systems**

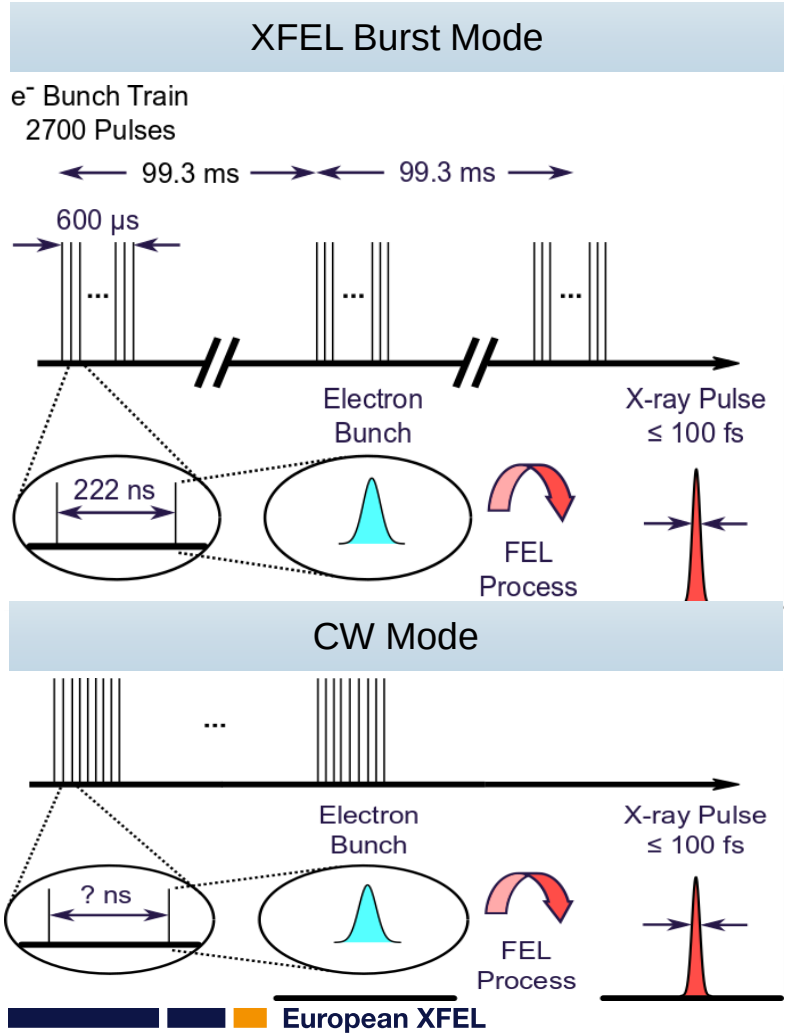
Will examine the quantum mechanical properties of atoms and molecules.



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

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

European XFEL Time Structure



The European XFEL pulse structure poses strict constraints on detectors (e.g. intensity and time structure)

Most of the time the use of commercial detectors is excluded

Most applications require 4.5 MHz repetition rate detectors

On average up to 27.000 pulses/s

Pulse duration

< 100 fs

High peak intensities

up to 10^{12} photons/pulse

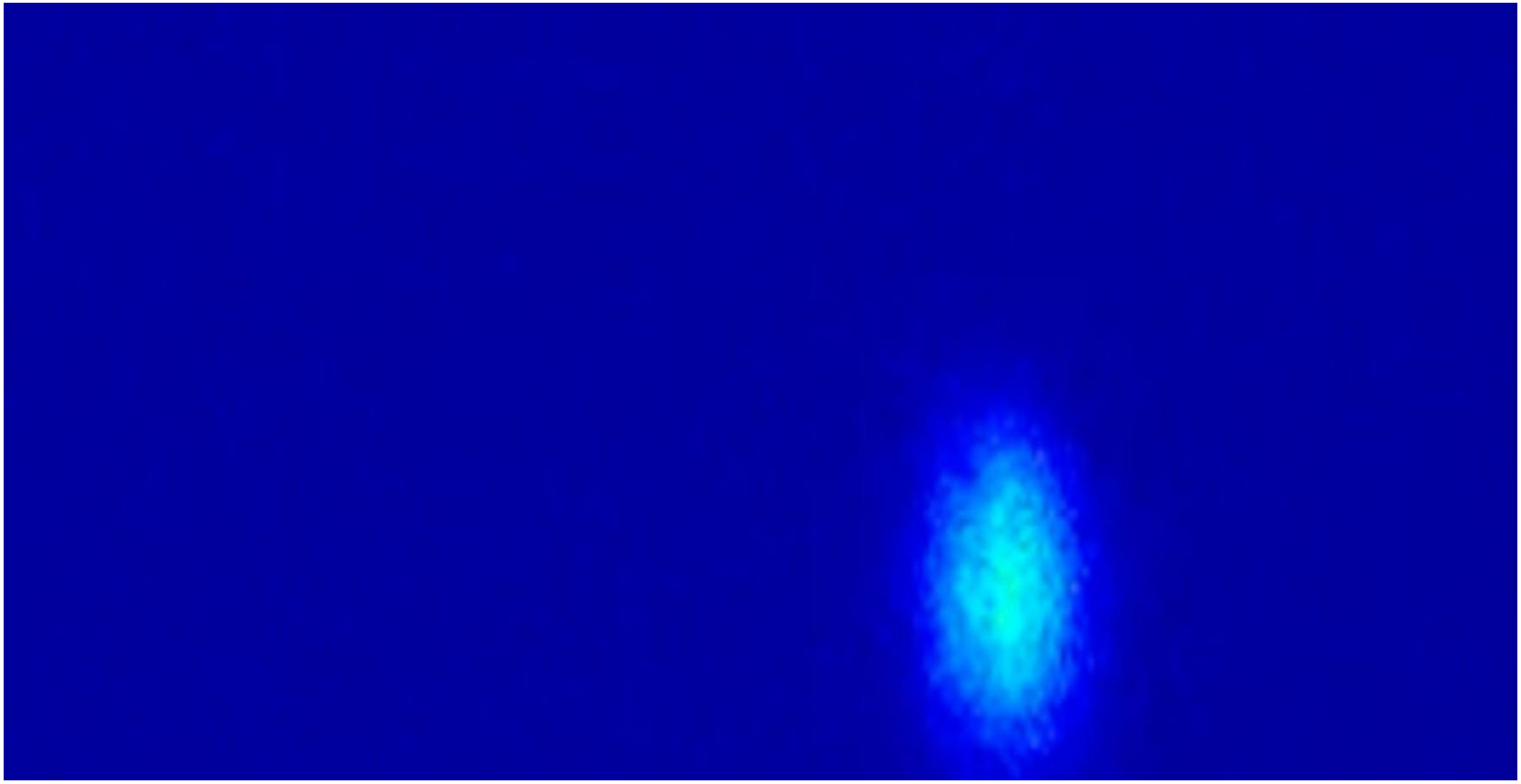
Various different pulse patterns possible

1 pulse per train

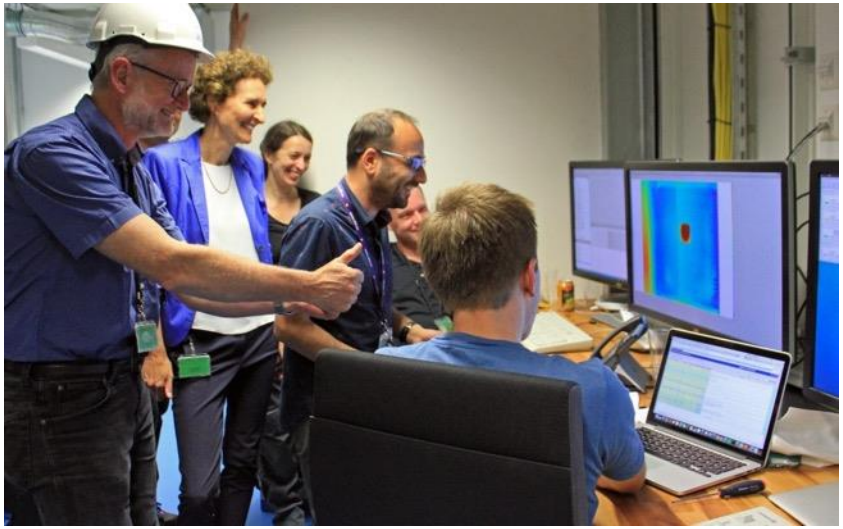
n pulses per train …

Linear, logarithmic or random distribution

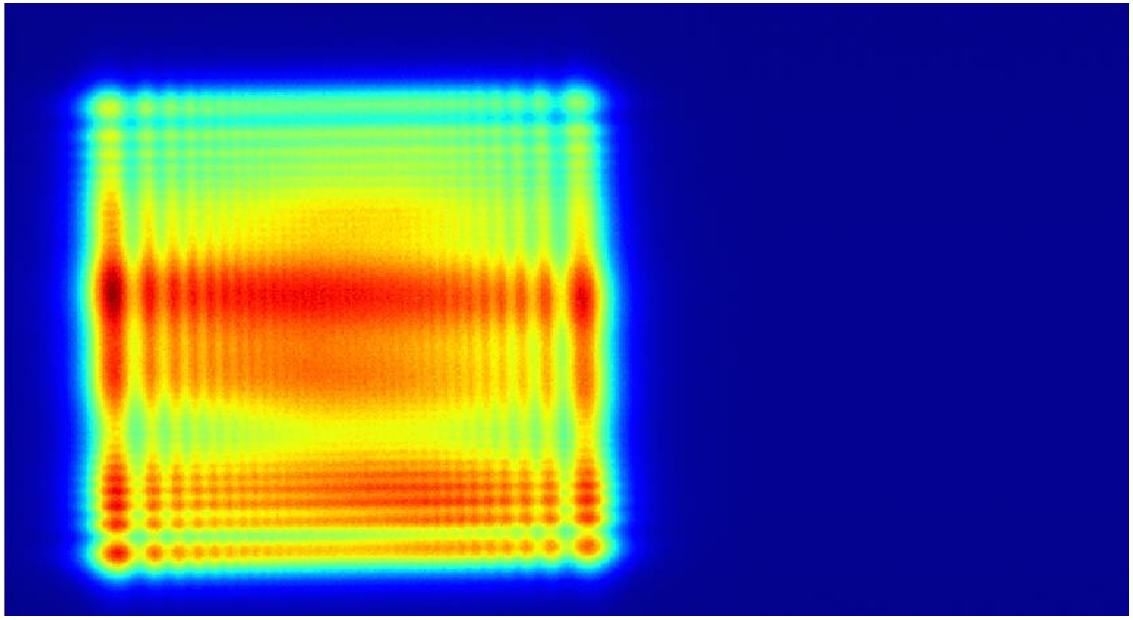
4 May 2017—first lasing!



23 June 2017—first X-rays in the experiment hall!



X-ray laser beam quality



- Fresnel pattern taken on 30 June 2017
- Diffraction pattern shows an interference pattern that is classic for high quality laser beams

1 September 2017—Inauguration and start of user operation

A strong laser from Elbphilharmonie greets European XFEL in the languges of the partner countries

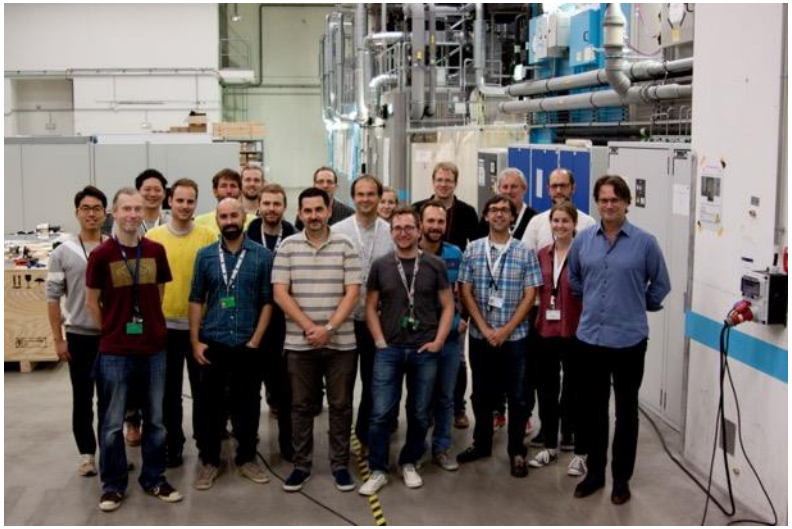
Ribbon-cutting with high-ranking representatives of the partner countries

FXE and SPB/SFX instruments: available for users since Sept 2017

FXE instrument: ultrafast chemistry studies looking into catalysts, photosensitive materials, biochemistry

SPB/SFX instrument: structural biology, studies of atomic clusters, imaging of single cells, viruses, eventually molecules

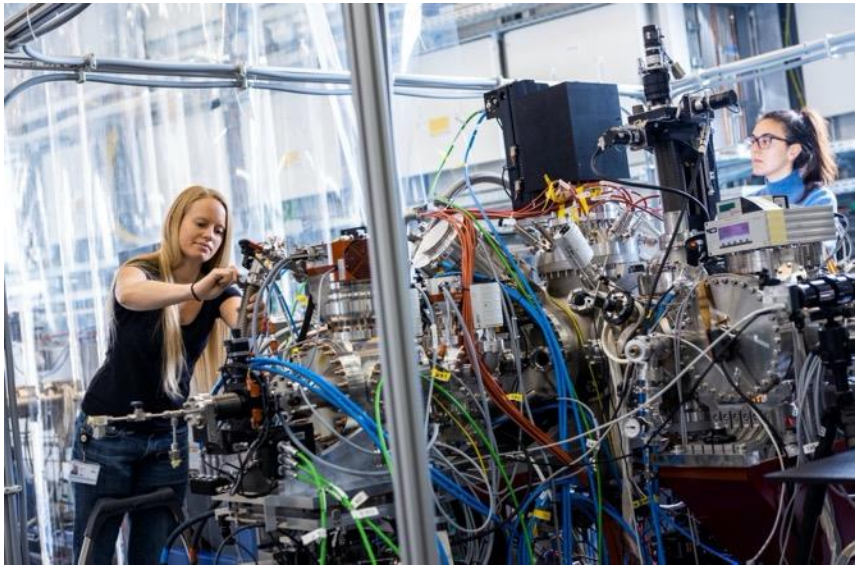
FXE and SPB/SFX instruments: available for users since Sept 2017



FXE instrument: ultrafast chemistry studies looking into catalysts, photosensitive materials, biochemistry

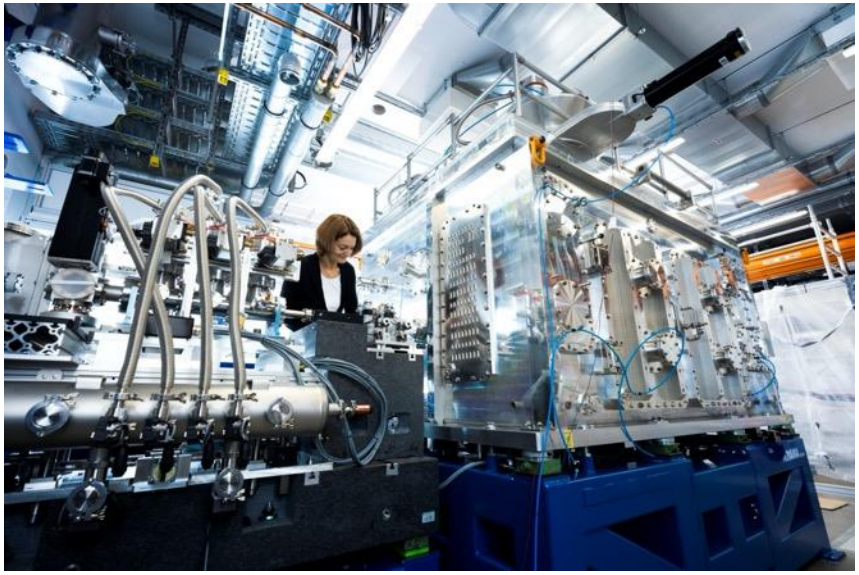
SPB/SFX instrument: structural biology, studies of atomic clusters, imaging of single cells, viruses, eventually molecules

SQS and SCS instruments: first users since late 2018



SQS and SCS instruments: first users since late 2018

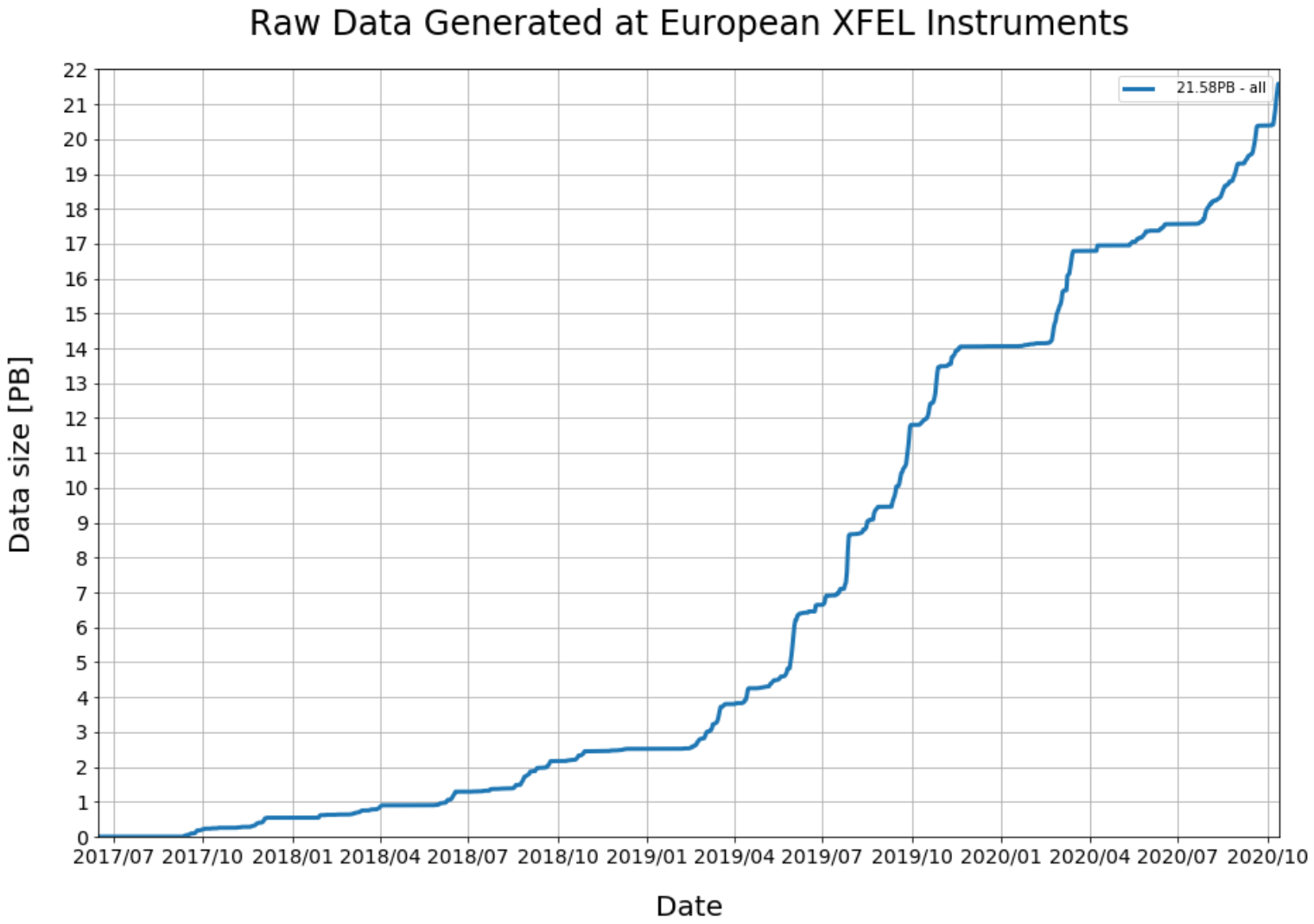
HED and MID instruments: first users in 2019



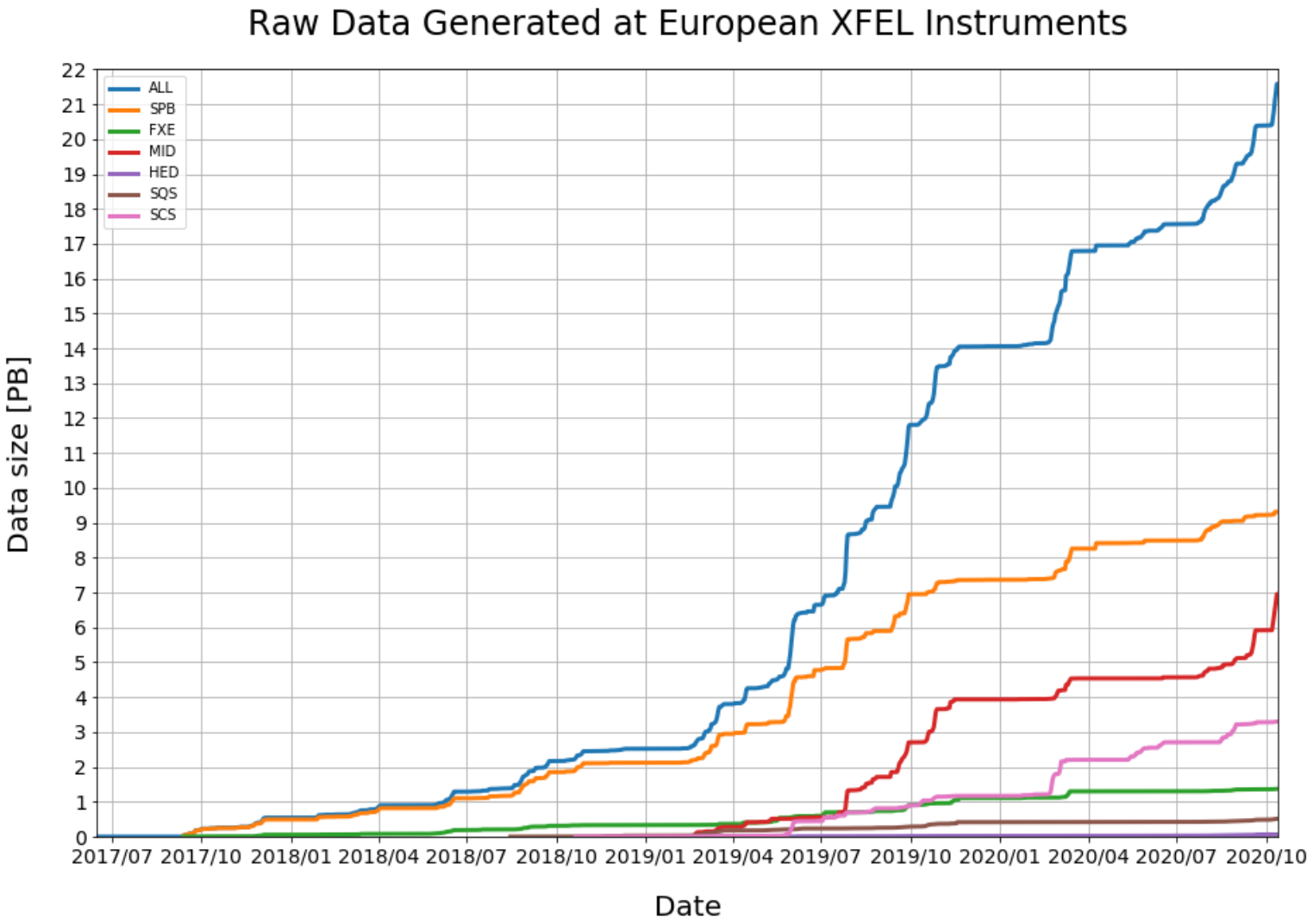
HED and MID instruments: first users in 2019

At MID no camera seems to have been around for the first experiment

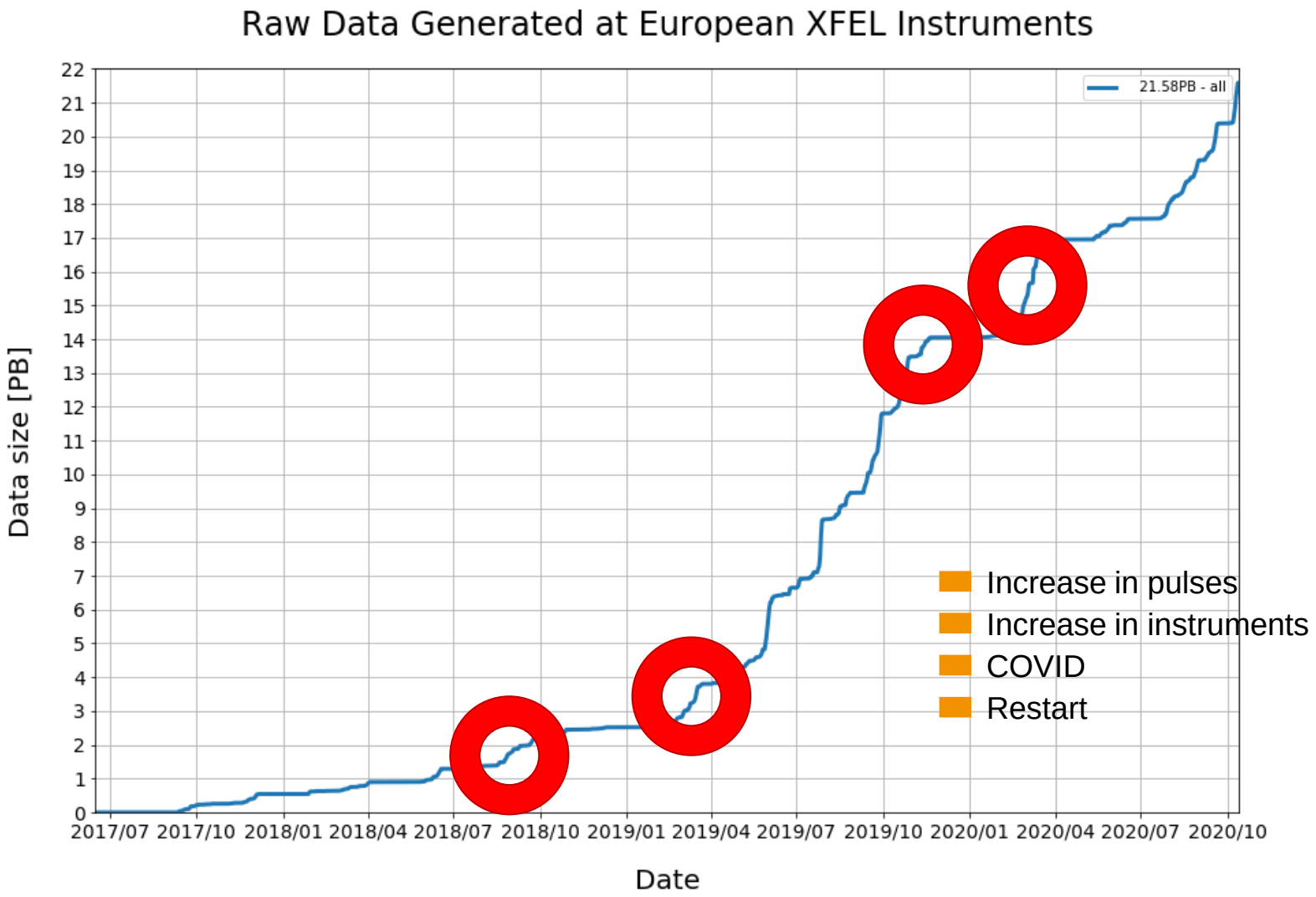
Data Challenges at the European XFEL



Data Challenges at the European XFEL

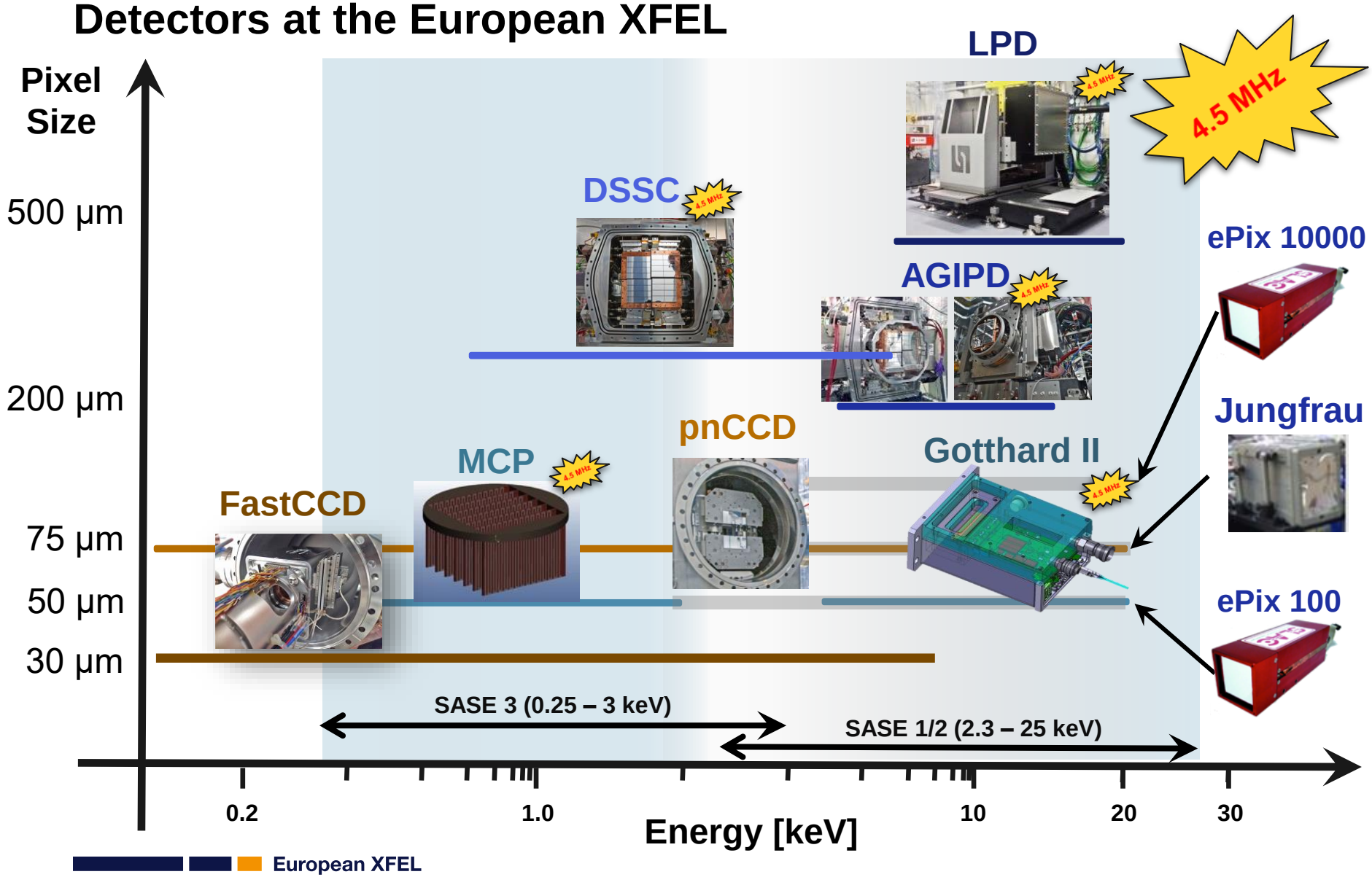


Data Challenges at the European XFEL

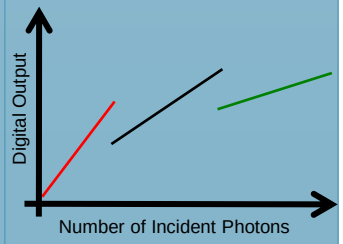
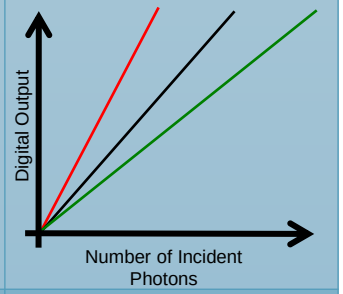
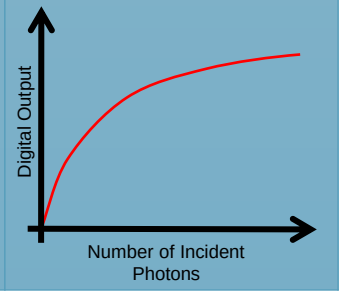


Data Challenges – Data Drivers

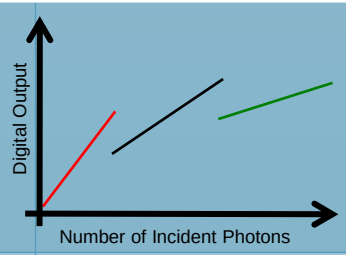
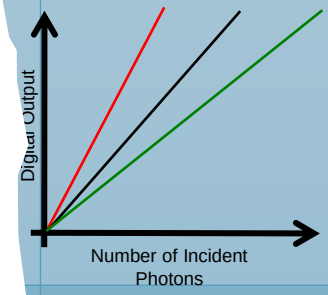
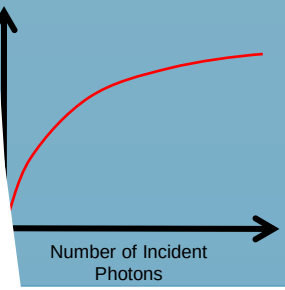
Detectors at the European XFEL



4.5 MHz High Dynamic Range Imaging Detectors

Detector	Specs	Modularity	Gain	Gain Curve
AGIPD 	1 Mpixel, 4.5 MHz 352 memory cells 200 µm 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 510 memory cells 500 µm 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 ≈236 µm hex. pixels 1-10^4 ph@ >1keV 0.5 – 6 keV	**16 modules** in 2 cols x 8 rows on 4 quadrants	Linear gain in ASIC (miniSDD) non-linear gain in sensor (DePFET)	

4.5 MHz High Dynamic Range Imaging Detectors

Detector	Specs	Gain Curve
AGIPD 	1 Mpixel, 4.5 352 memory 200 µm sq. pi 1-10^4 ph@ 12 3 – 13 keV	
LPD 	1 Mpixel, 4.5 M 510 memory ce 500 µm sq. pixe 1-10^5 ph@ 12 k 5 – 25 keV	
DSSC 	1 Mpixel, 4.5 MH 800 memory cell ≈236 µm hex. pi 1-10^4 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
- ....

4.5 MHz High Dynamic Range Imaging Detectors

Detector	Specs
AGIPD 	1 Mpixe 352 me 200 µm 1-10^4 p 3 – 13 k
LPD 	1 Mpixe 510 me 500 µm 1-10^5 ph@ 12 k 5 – 25
DSSC 	1 Mp 800 ≈236 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

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

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

Parameter Dependence

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

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

Detectors for the Scientific Instruments

SASE I / SASE II — High E	Single Particles, Clusters and Biomolecules (SPB)	AGIPD 4.5 MHz	Gotthard V1/2 4.5 MHz			Jungfrau
SASE I / SASE II — High E	Materials Imaging & Dynamics (MID)	AGIPD 4.5 MHz	Gotthard V1/2 4.5 MHz, 1 MHz	ePix		Jungfrau
SASE I / SASE II — High E	Femtosecond X-ray Experiments (FXE)	LPD 4.5 MHz	Gotthard V1/2 4.5 MHz			Jungfrau
SASE I / SASE II — High E	High Energy Density Matter (HED)	Jungfrau 1 MHz	Gotthard V1/2 4.5 MHz, 1 MHz	ePix		Jungfrau
SASE III — Low E	Small Quantum Systems (SQS)	DSSC 4.5 MHz		pnCCD		MCP
SASE III — Low E	Spectroscopy and Coherent Scattering (SCS)	DSSC 4.5 MHz	Fast CCD			MCP

Detectors for the Scientific Instruments

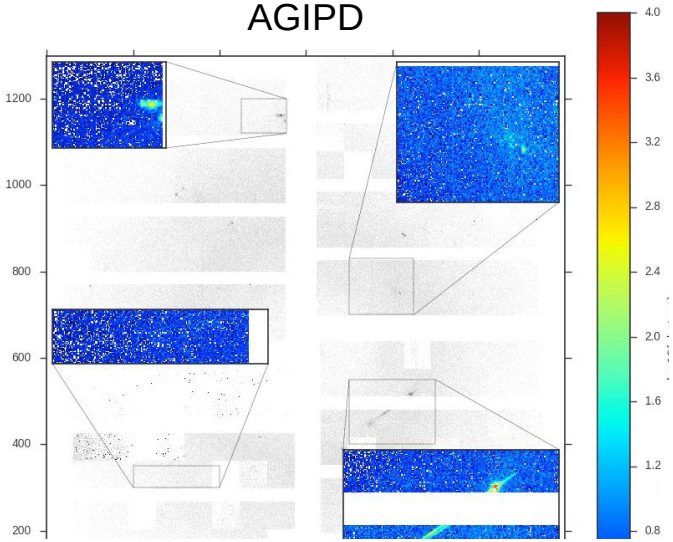
SASE I / SASE II — High E	Single Particles, Clusters and Biomolecules (SPB)	AGIPD, Gotthard V1/2, Jungfrau
SASE I / SASE II — High E	Materials Imaging & Dynamics (MID)	AGIPD, Gotthard V1/2, ePix, Jungfrau
SASE I / SASE II — High E	Femtosecond X-ray Experiments (FXE)	LPD, Gotthard V1/2, Jungfrau
SASE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

100 MB/s - 10 GB/s
10 Hz burst

Data Drivers: Data Examples from Detectors

- Data comes in a variety of „flavors“
- Not trivial to generically reduce, as very experimental context dependent
- Usefulness of data determined by calibration quality

AGIPD



LPD

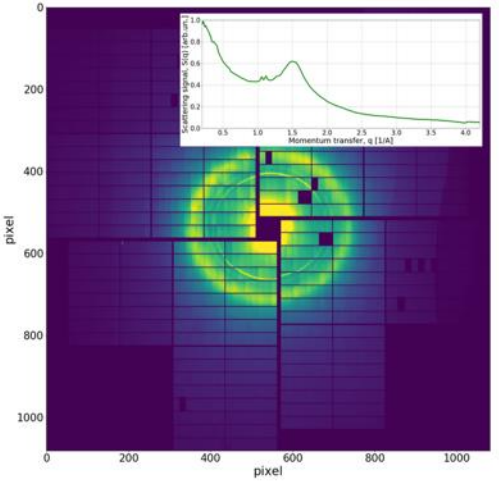
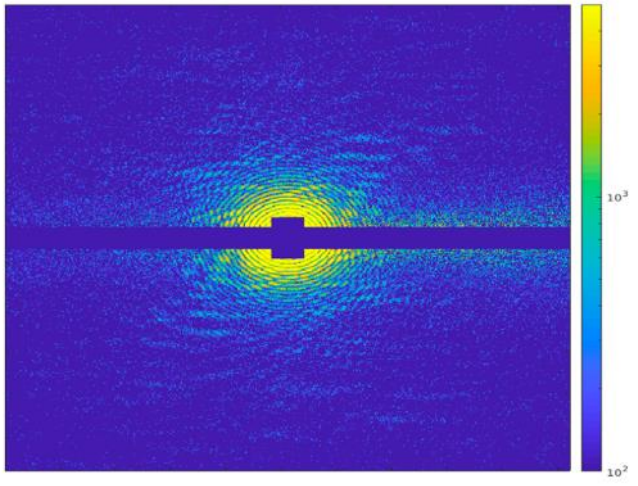


Figure 8: Liquid scattering pattern of tetrahydrofuran solution of a Cu complex collected with the LPD detector [23,24] at scientific instrument FXE [25](corrected for dark offset). Inset: Average of the azimuthally integrated set of 150 image.

Doped He nanodroplets imaging
PI: R. Tanyag, D. Rupp (TU/MBI Berlin)



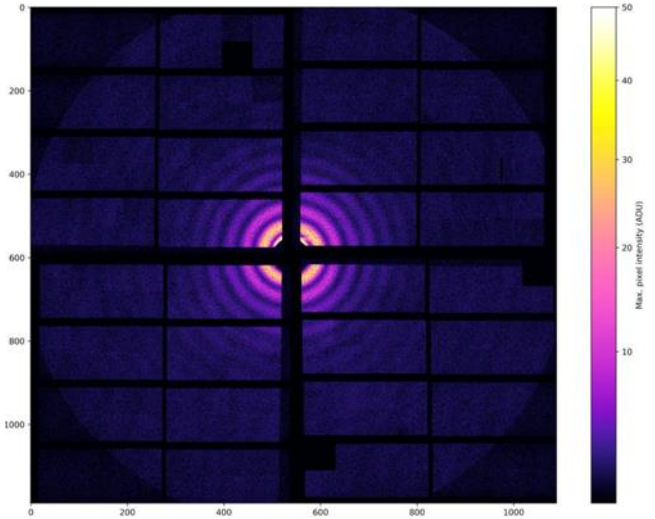
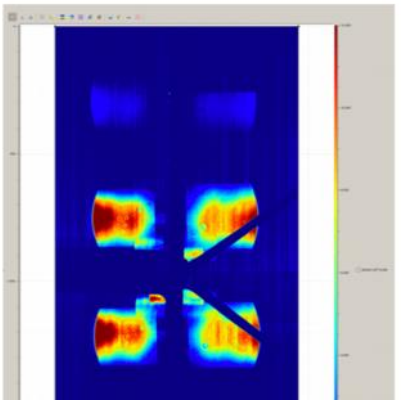


image of pinholes with 707 eV photons, acquired by DSSC detector during commissioning at the SCS experiment. The DSSC detector readout

FastCCD



Data Drivers: Digitizers & FPGAs

MicroTCA Crates

Large 12 slot 9U and small 6 slot 2U (including MCH, Power Supply and CPU)

X2Timer

XFEL Timing System module for synchronization (clocks and triggers) and pulse parameters from NAT

DAMC2

Required for Clock & Control system for fast 2D detectors, VETO System, Machine Protection System and photon beam loss monitors from DESY

SIS8300

Fast 125MSPS ADC with 10 channels and 16bit resolution for diagnostics and detectors from Struck Innovative Systeme

ADQ412/ADQ14/ADQ7

High-speed digitizers from 1.8GSPS to 10GSPS with 12 to 14 bit resolution from Teledyne SP Devices

Data Drivers: Digitizers & FPGAs

MicroTCA Crates

Large 12 slot 9U and small 6 slot 2U (including MCH, Power Supply and CPU)

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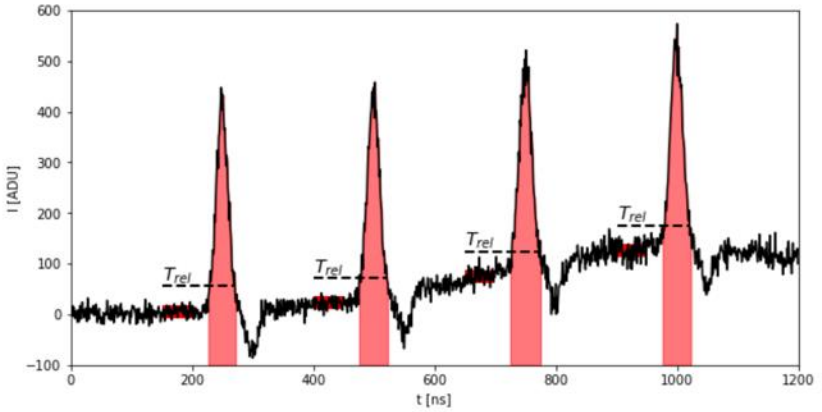
High- d digitizers GSPS to 2 to 14 ces

1 MB/s - 1 GB/s
10 Hz burst

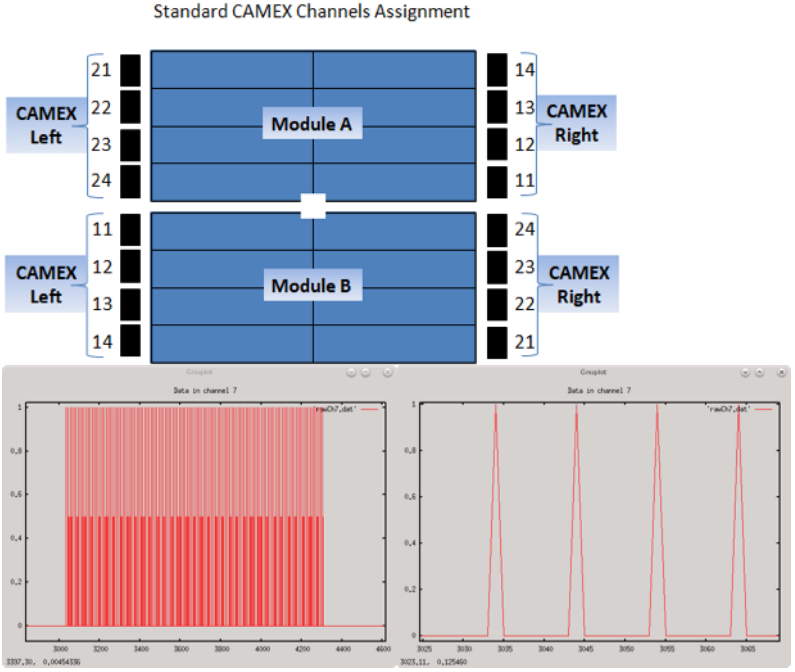
Data Drivers: Data Examples from Digitizers & FPGAs

- Raw data to very condensed derived data
- Processing on FPGA
- Processing in software
- Often diagnostics → more fixed in content than detectors



ROI sampling, e.g. from MCP data

pnCCD sampling at pixel clock



Joakim Laksman *et al.* • EuXFEL photoelectron spectrometer

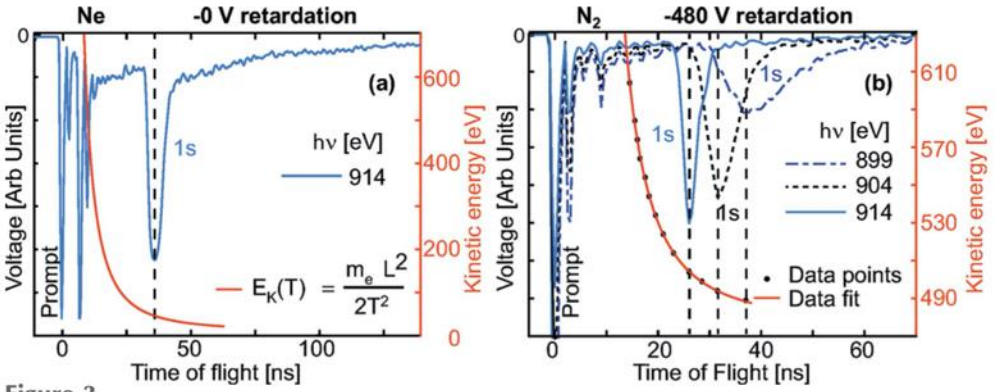
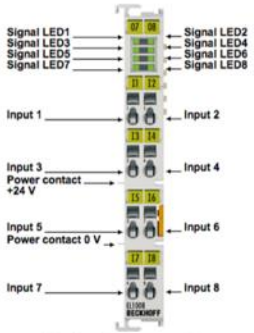


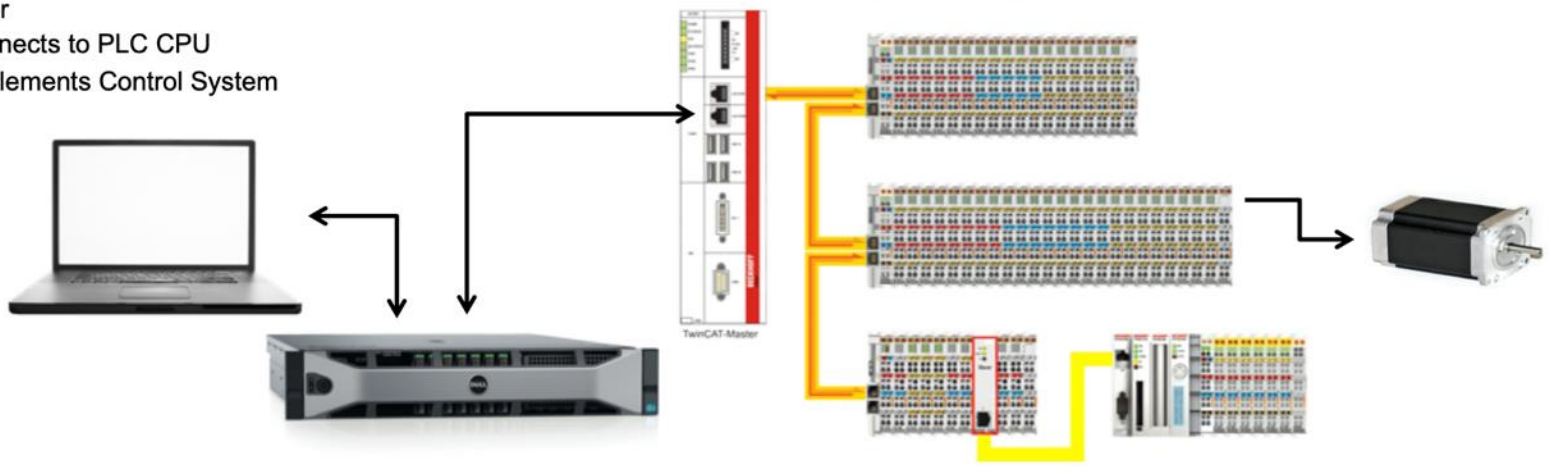
Figure 3
(*a*) 0 V retardation. Electron TOF spectrum after Ne 1*s* ionization at 914 eV. TOF is 36.25 ns which corresponds to a kinetic energy of 44.2 eV according to equation (1) (red curve). (*b*) −480 V retardation. Electron TOF spectrum after N_2 1*s* ionization at different photon energies. Peak center (black dots) fitted to equation (2) (red curve). Spectra are averaged over 100 pulses for higher statistics.

Data Drivers: PLCs and other “slow“ Data

- **P**rogrammable **L**ogic **C**ontroller
- Terminals as interface to h/w
- Terminals are connected together
- PLC CPU
  - Connects via cables to Terminals
  - Implements programs for control
- Computer
  - connects to PLC CPU
  - Implements Control System

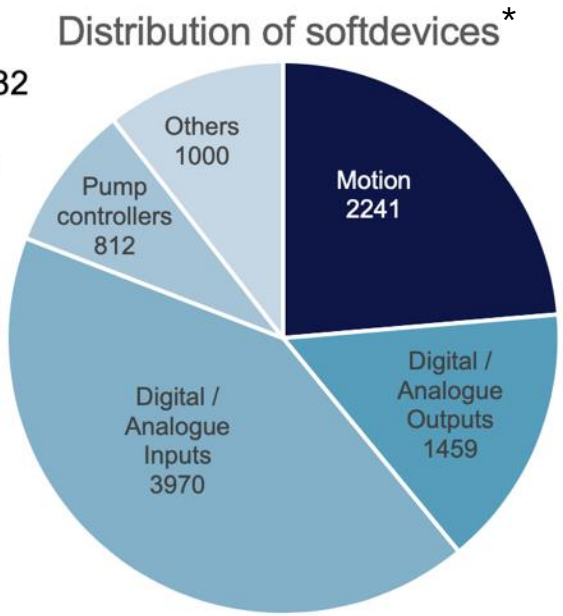


Terminals (i.e. digital input)



Data Drivers: PLCs and other “slow“ Data

- Softdevices/Equipment: 9.482
- Number of Terminals: 8.452
- PLC Loops / CPUs: 120
- PLC Modules / crates: >500
- MicroTCA Systems: 35
- Digitizer channels: >280



*Status Sept. 2019

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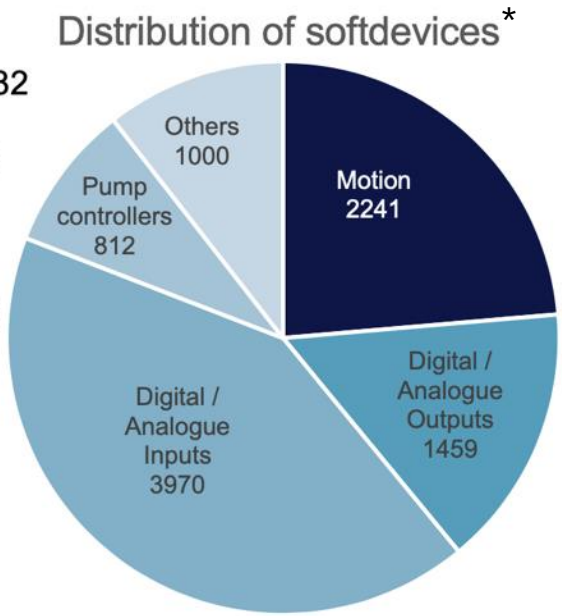
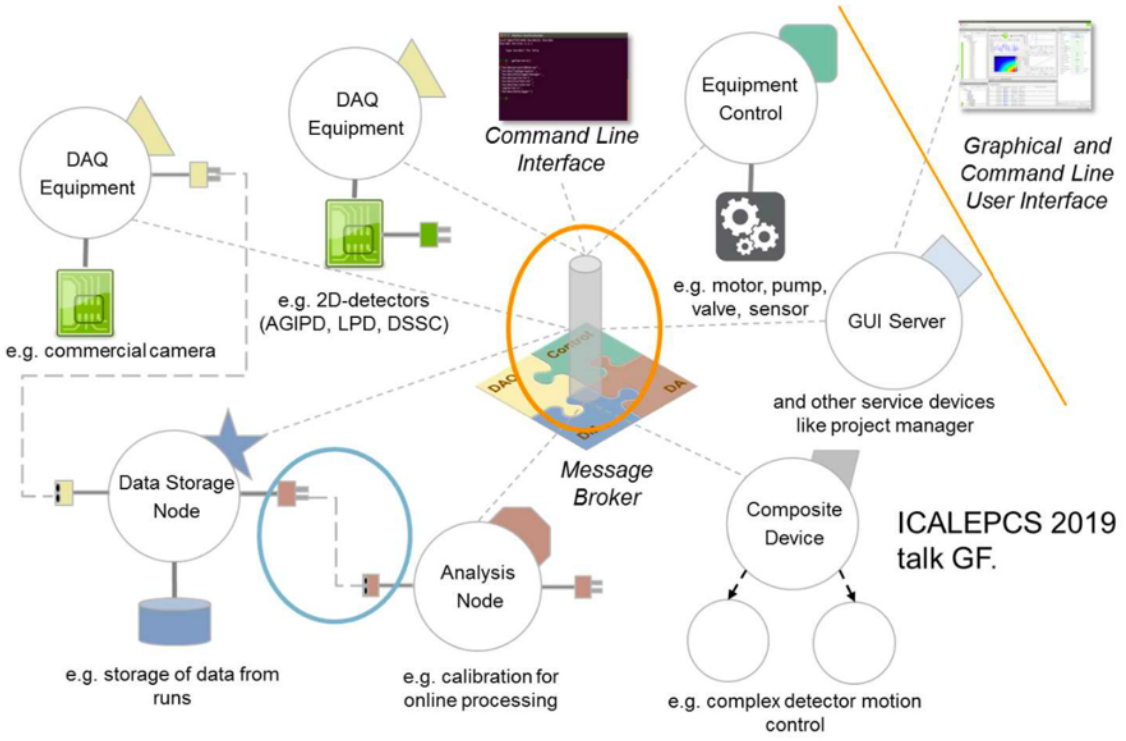


*Status Sept. 2019

Data Drivers: Karabo, the XFEL.EU SCADA Framework

- **Communication**
  - Broker: cmds, values, schemas
    - ► Partitioning: topics SA1, SA2, SPB…
  - Data: p2p TCP
- **Apis**
  - cpp (c++, boost)
  - bound (Py 3.6 bound on cpp)
  - middlelayer (Py 3.6)
- **Devices – everything's a device**
  - reflect h/w (tight for Beckhoff)
  - control few to many other devices
  - interface to other services
- **Device servers – run devices**
  - Multi-thread + event loop + GIL handling
- **User interfaces**
  - Gui-client
  - CLI



- Photon systems + Experiments: Karabo
- Accelerator: DOOCs
- Any some EPIX, TINE, Tango niches

Data Drivers: Karabo, the XFEL.EU SCADA Framework

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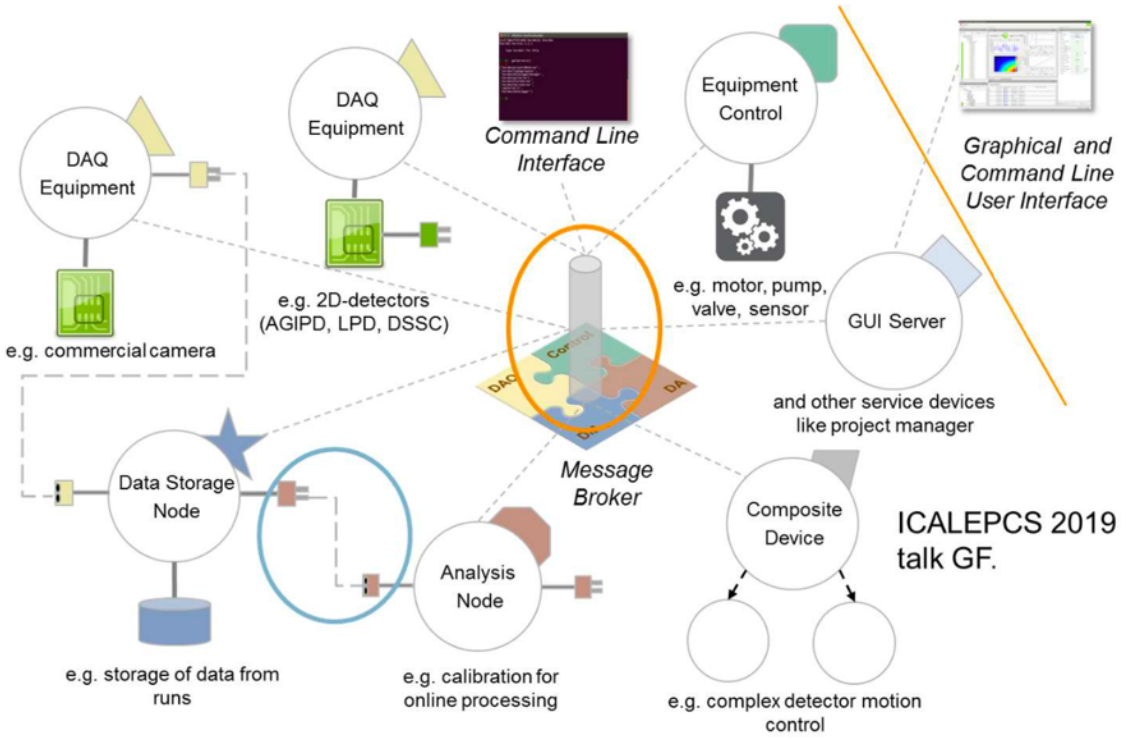
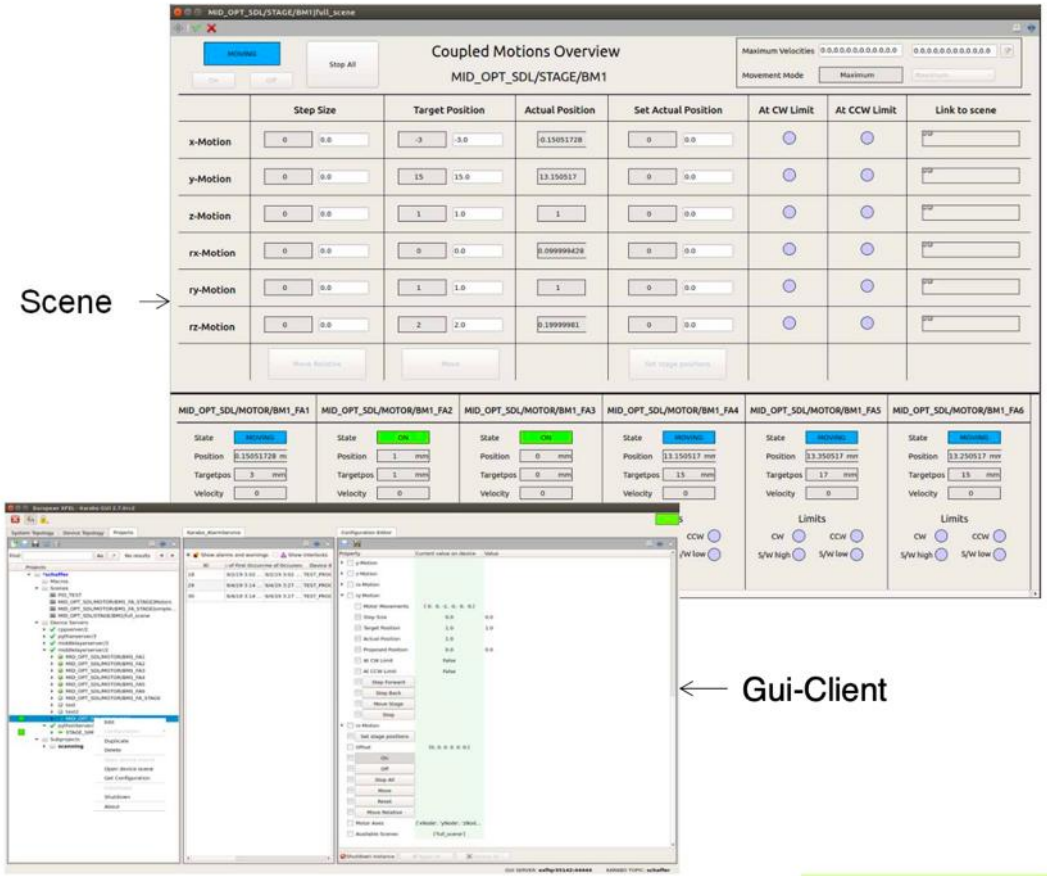


- SPB Instrument: 104 device servers and 1452 devices on 28 ITDM control servers
- Facility total (Sept. 2019): ~14000 devices, 1.7 million control parameters
- ~30 GB/day → to InfluxDB

Data Drivers: Karabo, the XFEL.EU SCADA Framework



- **Gui-client user interface**
  - device instantiate and shutdown
  - single device command and configuration
  - interface to Project navigation
  - …
- **Projects**
  - scene and macro interface
  - allows group actions
  - …
- **Scenes**
  - customizable, cuts away all but needed
  - drag & drop dynamic creation
  - …

Gui-client primary tool used by experiments

European XFEL

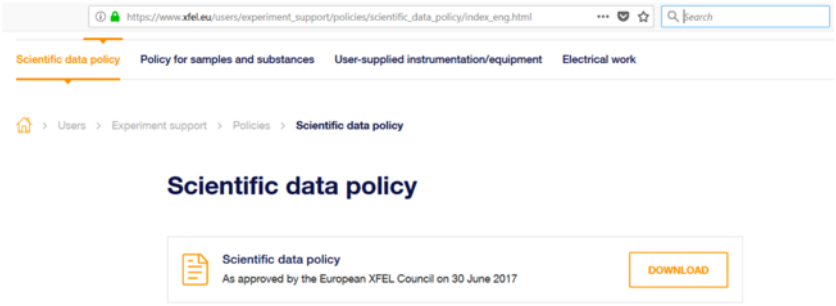
Data Drivers: Infrastructure

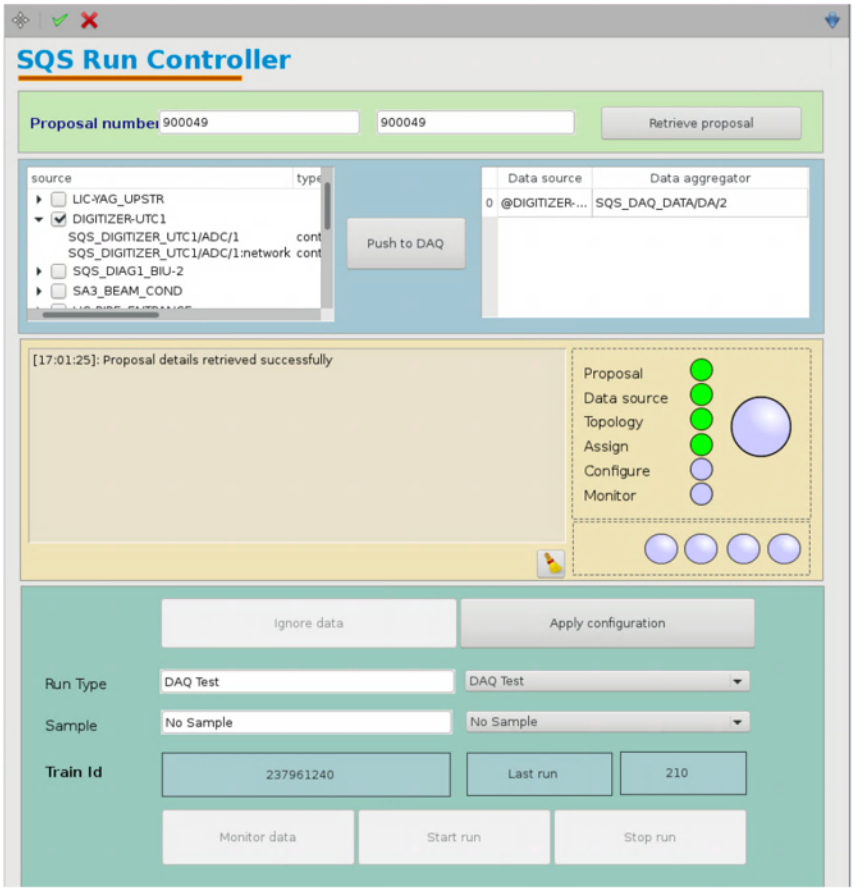
See talk by Janusz Malka (14:00)

Data Solutions

Data Solutions: Data Acquisition

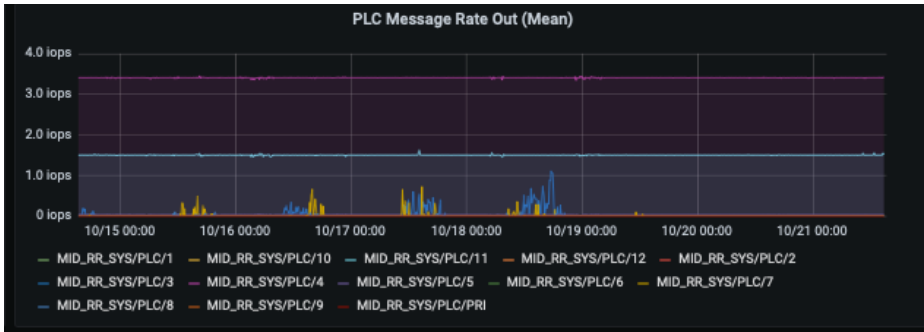
- Destinguish between **user** data acquisition and **facility** “housekeeping“ data
  - User data, needs to conform to *Scientifc Data Policy*
    - ► Long term data curation
    - ► Open access
    - ► Embargo period with restricted access
    - ► Data accessible by European XFEL staff during embargo period
    - ► All users need to agree to the policy as part of beamtime application
  - Facility data, only used for facility purposes, not tied to individual experiments

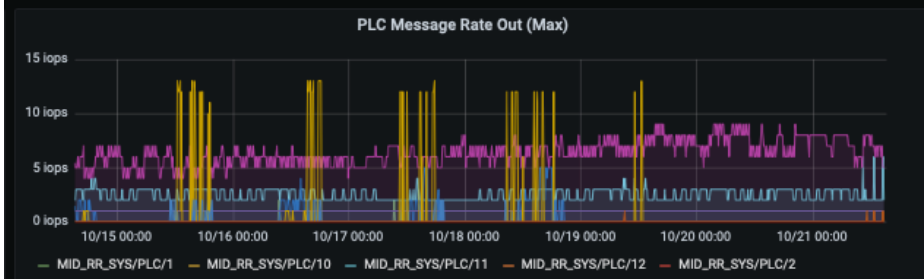




Data Solutions: Data Logging in InfluxDB

- In the last month rolled out logging service based on a community leading timeseries DB: InfluxDB
  - Coporate solution with input from InfluxData, failover and load balancing for high availabity
  - Enables use of community tools such as Grafana for all our slow control data
  - Train Ids are stored in the DB, so data can be correlated with DAQ (fast) data as well on a per train basis
  - Still at the beginning of exploring the options, but already
    - ► Significant benefits for understanding incidents and problems
    - ► Many more options in data exploration
  - Exploring if it could supplement DAQ as user avaialbe data source in the future





Data Solutions: Calibration and Correction (2D Detectors)

- ***Retrieve parameters for correction:*** resolve detector conditions, point in time leading to most appropriate *parameters*
- ***Corrected and calibrated data is main data product:*** needs to be available as soon as possible and reliable
- ***Produce correction parameters:*** characterize detector and select necessary subset of information. Perform quality assessment
- ***Manage correction parameters:*** centrally persist, categorize, select parameters
- **Optimize corrections according to specific scientific needs** e.g. real vs integer photon numbers, split event corrections
- ***Agility:*** support short cycles from prototyping, testing to production deployment where ever possible

Python: fast development cycles, good data analysis capabilities

Data Solutions: Community Tools

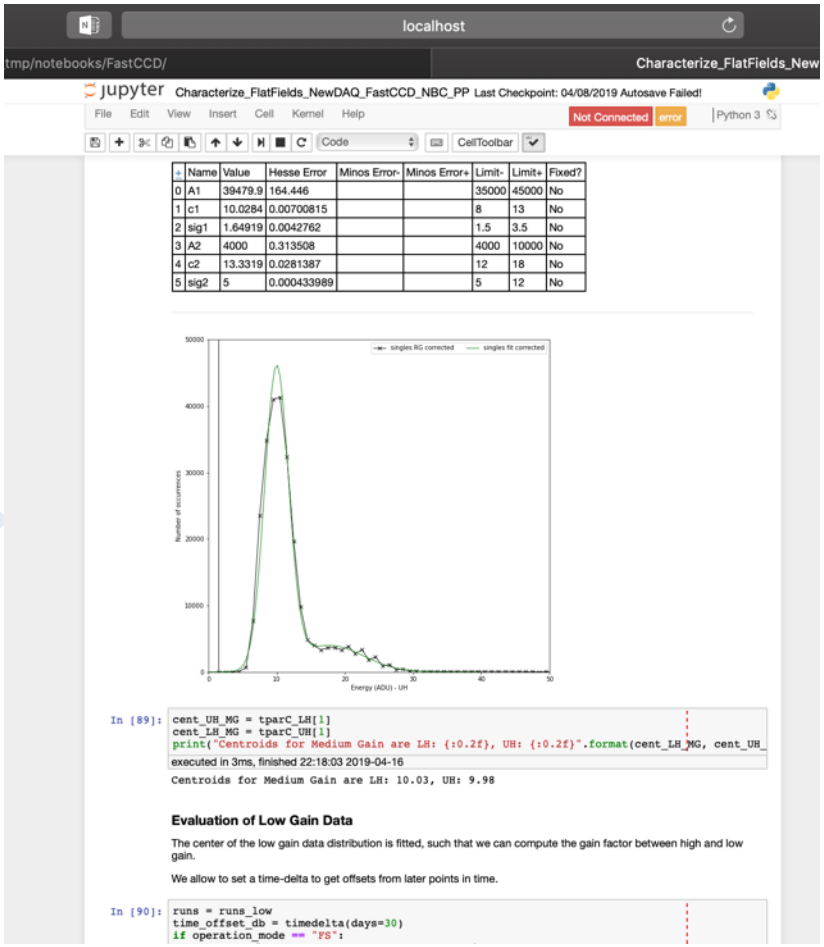
jupyter

Python

NumPy

matplotlib

SciPy



Rapid, interactive development in Jupyter Notebook

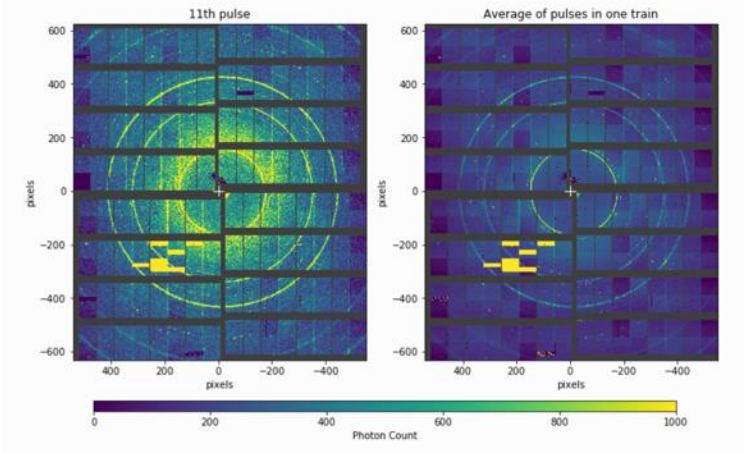
Data Solutions: Simplifying Data Access and Correlation

- extra-data:
  - Python library for iterating over XFEL run data on a train-wise basis
  - Select data sources by name, filter by index, trainId, ...
  - Abstracts away indexing needed within files for time correlation
  - https://extra-data.readthedocs.io/en/latest/
- extra-geom
  - Geometry handling of segmented detectors
- extra-data-validate
  - Validy check for data contents
- **See talk by Philipp Schmitt (16:15)**

```python
from extra_data import open_run, RunDirectory, H5File

# Find a run on the Maxwell cluster
run = open_run(proposal=700000, run=1)

# Open a run with a directory path
run = RunDirectory("/gpfs/exfel/exp/XMPL/201750/p700000/raw/r0001")

# Open an individual file
file = H5File("RAW-R0017-DA01-S00000.h5")
```

```python
for train_id, data in run.select("*/DET/*", "image.data").trains():
    mod0 = data["FXE_DET_LPD1M-1/DET/0CH0:xtdf"]["image.data"]
```

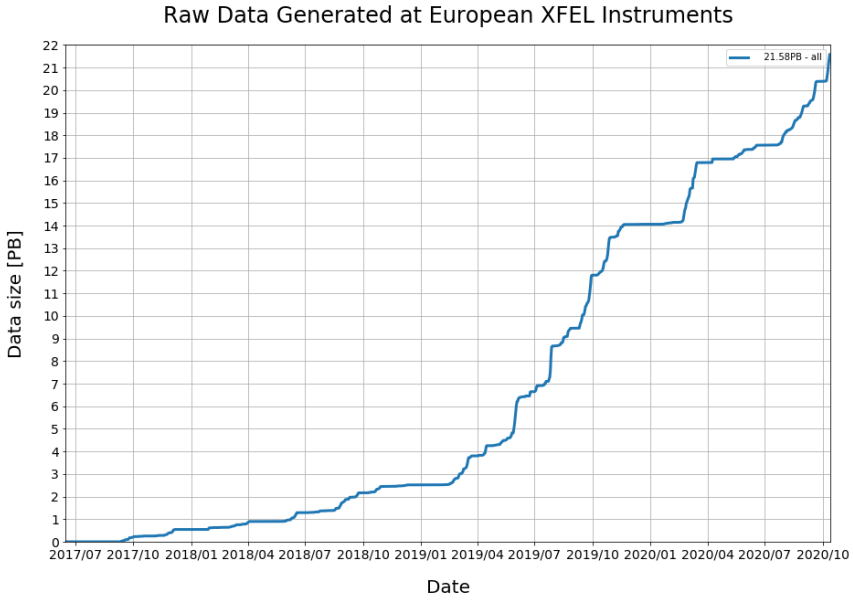
```python
geom.plot_data_fast(stacked_pulse, vmin=0, vmax=1000)
```



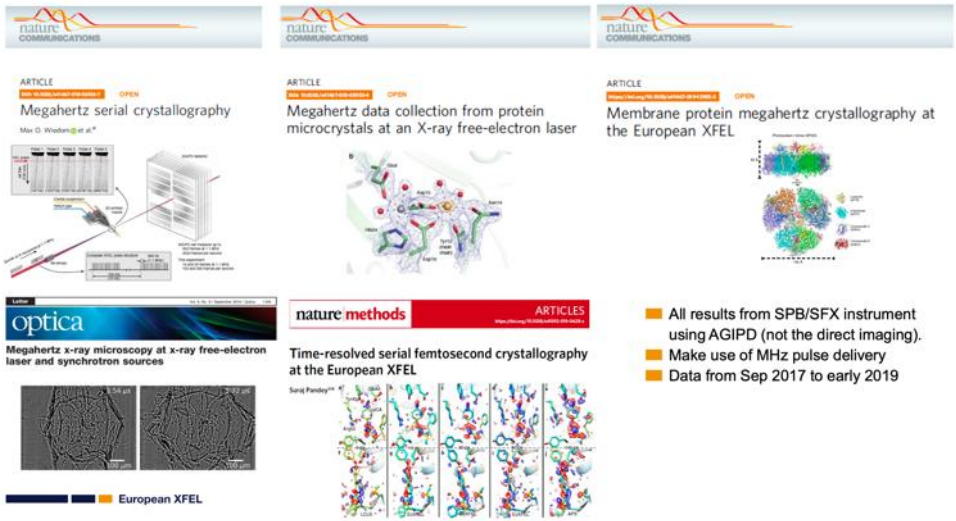
Data Challenges and Lessons Learned

Challenges: Data Reduction

- **When running smoothly, single experiments can produce ~1PB per week**
  - Not all data contains sample hits
  - Data is reduced during analysis, but not upon storage
- Mid- and long-term running XFEL is only feasible if data is reduced as early as possible
  - More efficient storage
  - Faster analysis on actually interesting data
  - Better online monitoring
  - Requires very good understanding of our detectors



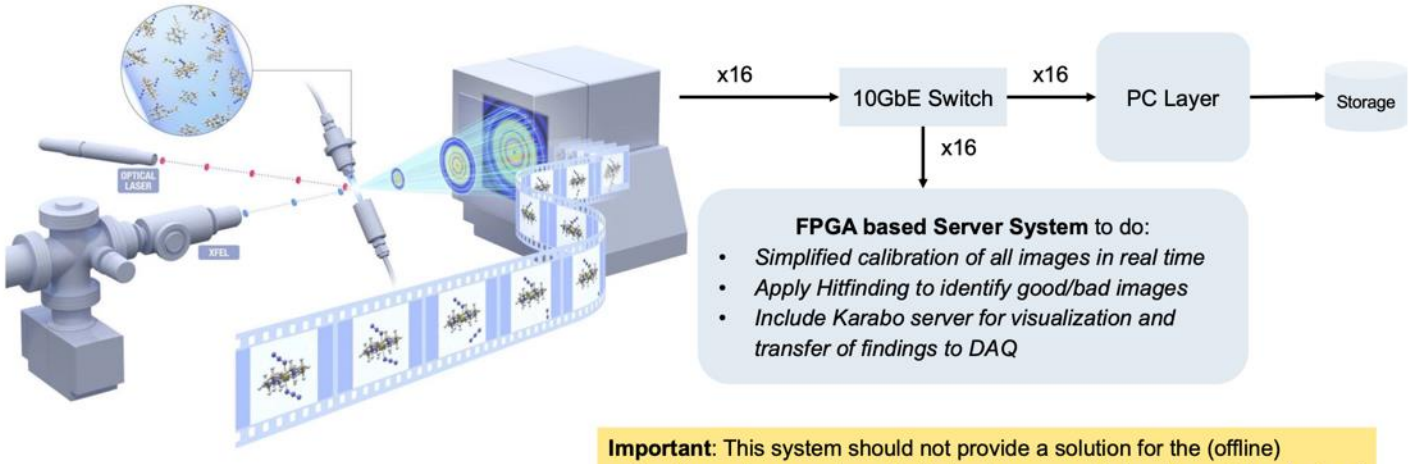
First publications



Challenges: Context Specific Reductions

- First step, filtering known empty pulses
  - Arrises from detector characterization observations
- Solutions which take context into account, e.g. experiment is interested in Bragg peaks
  - Software or FPGA solutions are being investigated
  - Start with only tagging data, then get user feedback on our filters
  - Final solution: filter most, but pass through some data which would otherwise be filtered for verification purposes

Planned demonstrator project for AGIPD at SPB



Important: This system should not provide a solution for the (offline) calibration and processing with highest accuracy. It should provide a fast and low-latency online monitoring solution to provide valuable feedback to the users in real-time! It could also provide classification information of the images for later decisions for processing or data reduction.

Powerful commercial off-the-shelf technology used for the implementation

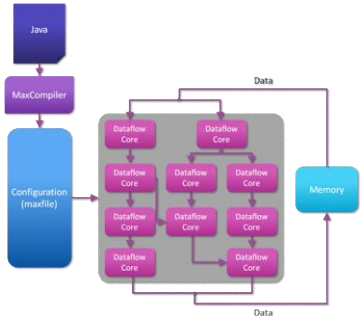
4x Xilinx Alveo U250 Accelerator Cards
High-end FPGA (Xilinx UltraScale) based accelerator card with 2x QSFP28, PCIe Gen3 x16, 64GB DRAM@77GB/s, 57MB SRAM@47TB/s per card

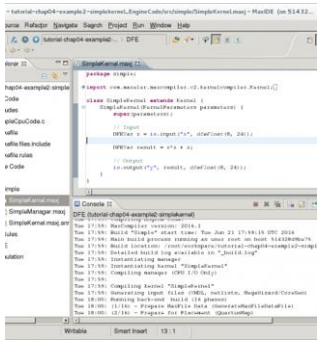
DELL PowerEdge R940xa Rack Server
Powerful computing server as host system compatible to ITDM / EuXFEL environment, which allows native Karabo integration and resources for further processing if required.

Development of the implementation on high-level language MaxJ

- The R&D project includes the implementation service with the company Maxeler
- They provide a proprietary high-level Java like programming language with optimized libraries (e.g. for network, image processing and more)
- Investigations were done in past about how efficient the programming language is
- The project started in April 2020 and is to conclude in November 2020

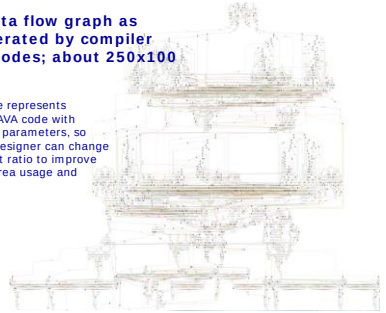
MAXELER
Technologies
Maximum Performance Computing





Data flow graph as generated by compiler 4866 nodes; about 250x100

Each node represents a line of JAVA code with area time parameters, so that the designer can change the aspect ratio to improve pin BW, area usage and speedup



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  - Start with only tagging data, then get user feedback on our filters
  - Final solution: filter most, but pass through some data which would otherwise be filtered for verification purposes
- Other facilities face the same challenges:
  - LCLSII mandatory reduction by factor 10x early on
    - ► Users can provide algorithm specific to experiment
    - ► Facility “hard“ filter will take care of anything above 10% input if the user algorithm didn‘t
    - ► XFEL is looking into collaboration here, e.g. in the context of HIR3X
  - Multiple „power“ user groups have experience and knowledge that can help

Data lessons learned in the first two years of operation

- Well running experiments can produce up to 1PB of data in a single beamtime
  - Since we are a user facility, how such an experiment may look like can change on a daily basis → contrasts to HEP or AstroPhys.

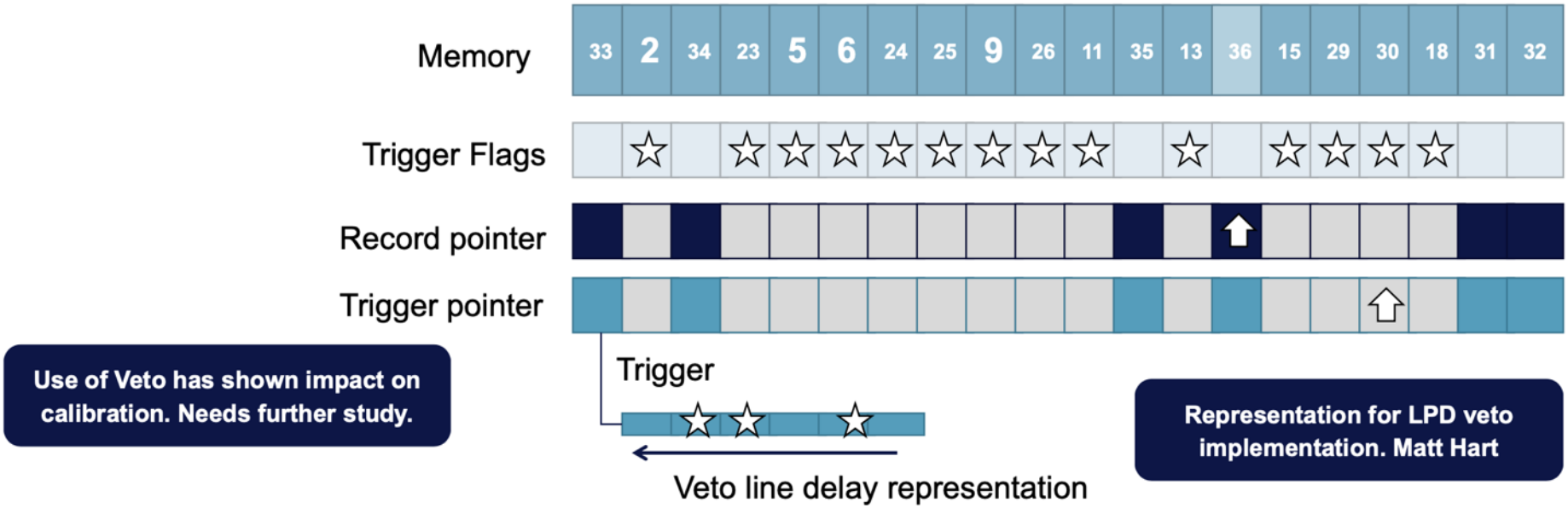
- Reducing this data in an efficient and appropriate way is one of the key challenges
  - Users will not care so much about our storage costs but be interested in maximing useful feedback and speeding up analysis
  - We observe two user flavors:
    - ► Power users who are accustomed to handling such data amounts and often are willing to contribute with solutions
    - ► Non-power users, who ideally only want a very reduced data product. Getting there should be as transparent to them as possible.
  - Frequently, users have synchrotron experience where data rates in the past have not been such an issue. There is a “pyschological“ componenent in raising awareness into the challenges that facilities like XFEL entail.

Outlook

- More detectors will be installed at the European XFEL in the next months and years
  - AGIPD4M
  - HiBEF AGIPD
  - Second DSSC (DePFET)
  - More Jungfrau detectors
- Next generation of detectors is in definition phase. Wishlist includes:
  - More and smaller pixels
  - More memory cells
  - CW operation
  - Generally, more data
- The need for efficient data management, provenence and reduction will become even more pressing
  - Other user facilities are facing similiar challenges: LCLS II, many synchrotrons
  - Internal R&D projects have been started: FPGA, Software filtering
  - There are chances for collaboration
    - ► Among facilities
    - ► With user groups

Challenges: Vetoing on Detector is not a Reduction Solution

- Designed to reuse memory cells during a train, i.e. increase the yield of meaning data
- No need to reject data within micro seconds with less data, when you could **do it with more data, later**
- Data reduction using the Veto would only become necessary to reduce the data load on the DAQ, though is this currently not the problem (exception 4M AGIPD)



- **At 2700 pulses nominal, XFEL.EU oversamples the detector memory**
- Not less data, but same amount of data with more useful content