Big Data at European XFEL



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European XFEL — a leading new research facility



Location: Schenefeld and Hamburg, Germany

European XFEL



Schenefeld site at the start of user operation

The European XFEL (X-Ray Free-Electron Laser) is a research facility under construction which will use high intensity X-ray light to help scientists better understand the nature of matter.

User facility with 280 staff (+ 230 from DESY)

2017 start of user operation

About European XFEL



Organized as a non-profit corporation in 2009 with the mission of design, construction, operation, and development of the free-electron laser

- Supported by 11 partner countries
 - Germany covers 58% of the costs
 - Russia contributes 27%
 - Each of the other international shareholders 1–3%

Total budget for construction (including commissioning)

1.22 billion € at 2005 prices

600 M€ contributed in cash, over 550 M€ as in-kind contributions (mainly manufacture of parts for the facility)

K.Wrona, 2017-02-15

In-kind contributions

Many in-kind contributions to the European XFEL project come from Russian Federation



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A big facility for studying tiny objects...





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- High intensity X-rays show structures in greater detail
- Molecular movies reveal biochemical processes
- New details of physical processes
- Quantum world in action
- Extreme states of matter





European XFEL in commissioning phase

Superconductive Accelerator



Scientific instruments

FXE instrument

Pump-probe laser laboratory

European XFEL

Femtosecond X-ray experiments: time-resolved investigations of the dynamics of solids, liquids, gases

Detectors

AGIPD Adaptive Gain Integrating Pixel Detector (AGIPD) 2017



Energy range 3 - 13 keV ^(25 keV) Dynamic range 10⁴@12 keV Single Photon Sens. Storage Cells ≈ 360 ^{128 × 256 Pixel Sensor} Heat Spreader Pixel Size 200 x 200 µm²

DEPFET Sensor with Signal Compression (DSSC) 2018



Large Pixel Detector (LPD) 2017



Energy range 5 (1) - 20 keV (25 keV) Dynamic range 10⁵@12 keV Single Photon Sens. Storage Cells ≈ 512 Pixel Size 500 x 500 µm²

Other Detectors

- 1D detectors for high repetition rate applications (e.g. dispersive spectrometers)
- Small areas, low rep. rate, low energy 2D imaging detectors
- CCDs for low speed imaging
- OD detectors (veto) coming soon

2D Detector Camera

A high data rate experiment setup

2,700 light pulses 10 times per Second



Typical camera 1-4 mln pixels

- Up to 27000 pulses per second delivered
- 4.5MHz at 220ns pulse to pulse distance
- Results in 10-30GB/sec max data rates due to the limitation of detectors

DAQ Challenges

- Readout rate driven by bunch structure
 - 10 Hz train of pulses
 - 4.5 MHz pulses in train
- Data volume driven by detector type





Detector type	Sampling	Data/pulse	Data/train	Data/sec
1 channel digitizer	5 GS/s	~2 kB	~6 MB	~60 MB
1 Mpxl 2D camera	4.5 MHz	~2 MB	~1 GB	~10 GB
4 Mpxl 2D camera	4.5 MHz	~8 MB	~3 GB	~30 GB*

 In 2017 start of the user operation with 60 pulses/train
 10GB/sec -> 1GB/sec
 Expecting full rate in 2018

* Limited by AGIPD detector internal pipeline depth (352 img/sec), hence factor 3 compare to LPD 1MPx

Data Management Challenges

- Aggregate and record large volumes of data during experiments
- Provide deep insight into the data during experiment
- Organize and manage data in a coherent way
- Enable users to analyze experiment data when back at home institute







Data processing On 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
- Computing Cluster for data analysis
 Computing Cluster ~300TFlops
 Optimized access to raw data
 Possibility of caching intermediate results on scratch storage
 - Export of the results or reduced/corrected datasets



Offline data storage

Offline data storage classes

- Raw and calibration data repositories
 - commodity storage, distributed system (dCache) with pNFS access protocol
 - Raw data files organized according to experiment runs with appropriate ACL (access control list) defined using NFS4.1 ACL
 - Planned capacity: 10PB (2017), 50PB (2020), 100PB (2023)
 - <u>Archive</u>
 - tape backend for data repositories
- Ingest buffer
 - receives data from online cache
- Scratch space
- ~3PB provided by XFEL
- used for hot data processing, export of calibrated data, no backup, fast access
- Beamtime store,
- Used for data upload before experiment and storing results
- ► e.g. 5TB per beamtime, backup

User access to XFEL analysis facility

- Each user listed in a successful proposal will be granted access to the analysis facility through the standard LDAP account
- The account will be valid for a limited time after the last beamtime e.g. one year.
 - Can be extended by the request of PI
 - Will be automatically extended upon the new successful proposal
- Resources given to users
 - Access to HPC cluster
 - Access to beamtime store, data repository and scratch space
 - Access to web based tools





Offline analysis cluster

XFEL computing resources integrated into Maxwell HPC and connected to DESY IB fabric

- Planning for quick expansion
 - Space for 50 racks reserved
 - Power and cooling infrastructure DESY upgrade power and cooling to 1.5MW





Beyond classical computing model

- Possibility to enlarge the computing model of the European XFEL by including external computing centers, located in partner countries and connected to the data center located at DESY via high speed data links.
- A strong data link from Germany to Russia is crucial to tie these two powerful Partners
- We need to prove that the distributed computing model can be adopted by the XFEL users communities
- A pilot project would allow us to test whether this approach is useful for the likely increased needs in the operation phase of the facility
- The location of a European XFEL computing facility in Russia will help increasing the Russian user base for the European XFEL and DESY and will serve as a focus point in Russia

THE END