PSI Center for Photon Science

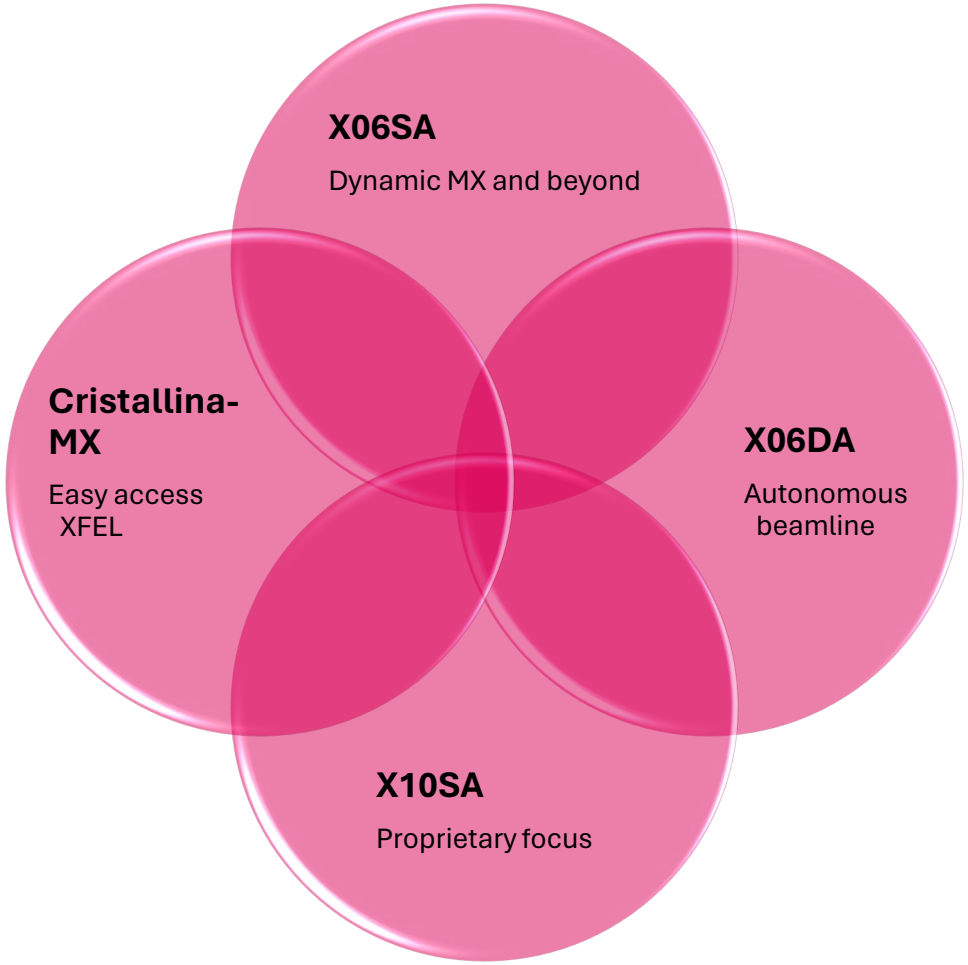
Big data @ PSI

HDR MX Online Meeting

Filip Leonarski
Zoom, 19 Mar 2025

Macromolecular crystallography @ SLS 2.0 and SwissFEL

Swiss Light Source 2.0 is back with beam, first X-ray light expected in the coming **days**!



X06SA (PXI)

A versatile MX beamline for

- Dynamic MX studies
- Spectroscopy
- Chemical crystallography
- Small angle scattering tensor tomography (SAS-TT)

Cristallina-MX

- SwissFEL endstation for serial femtosecond crystallography

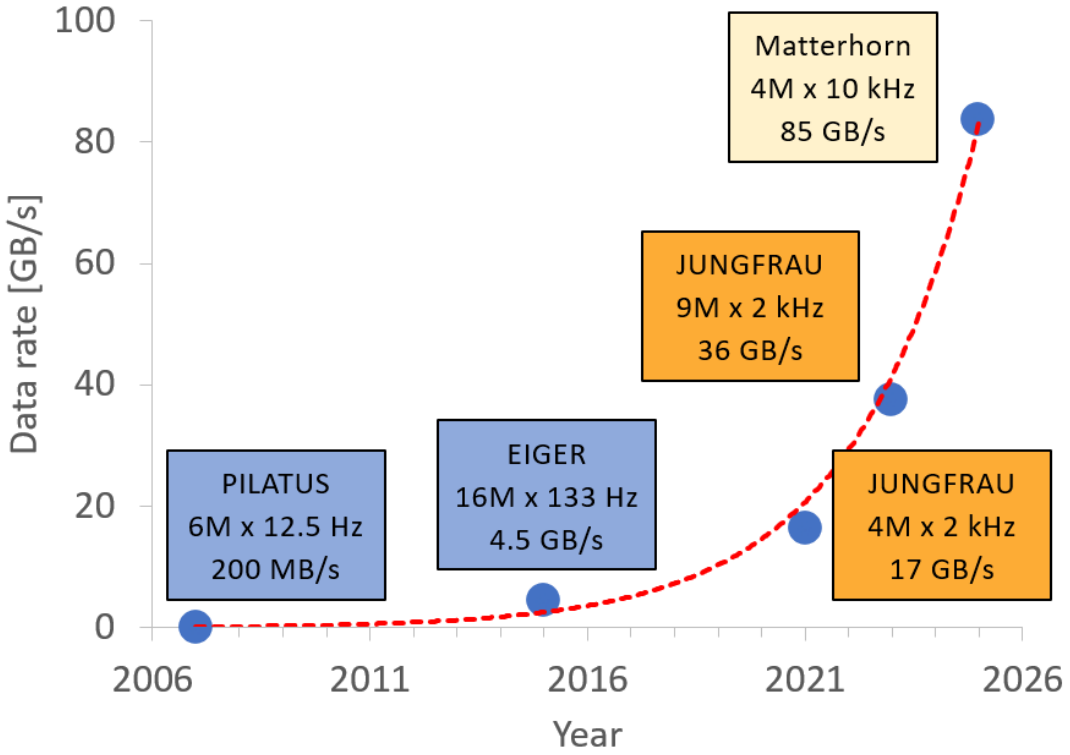
X10SA (PXII) – Industry

- Tailored to the needs of our proprietary beamline partners
- Manual & automated data collections

X06DA

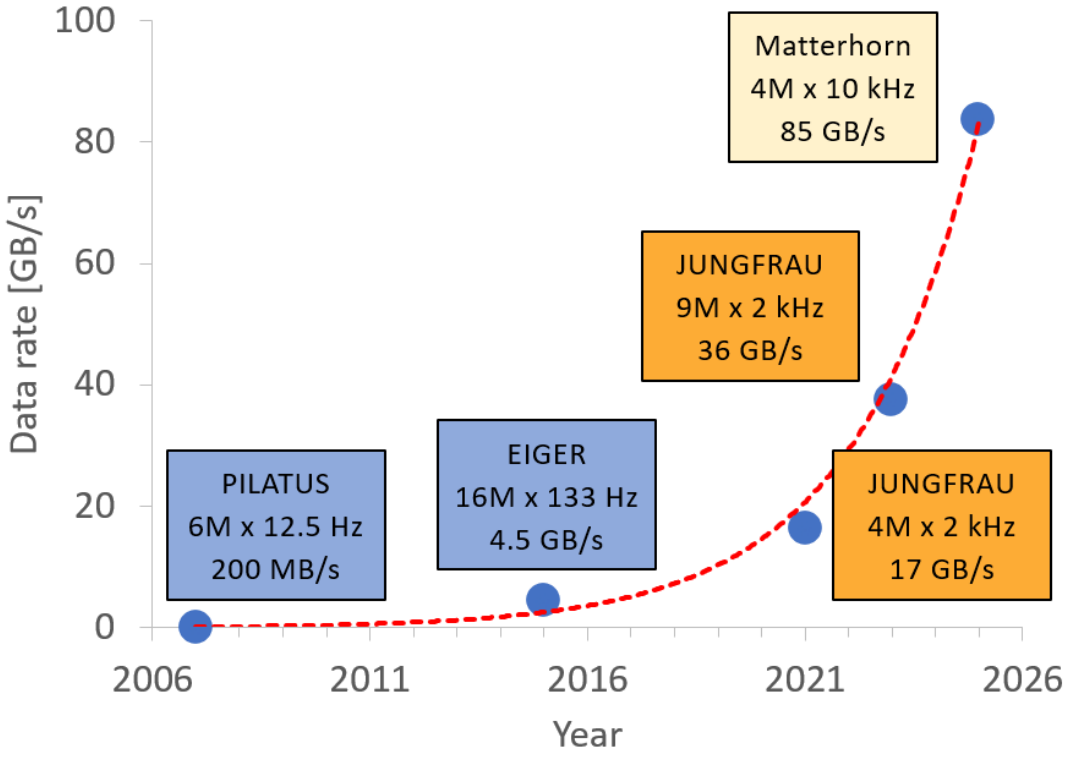
- Autonomous beamline (queued mode)
- Room-temperature experiments

How big are the data we need to handle?



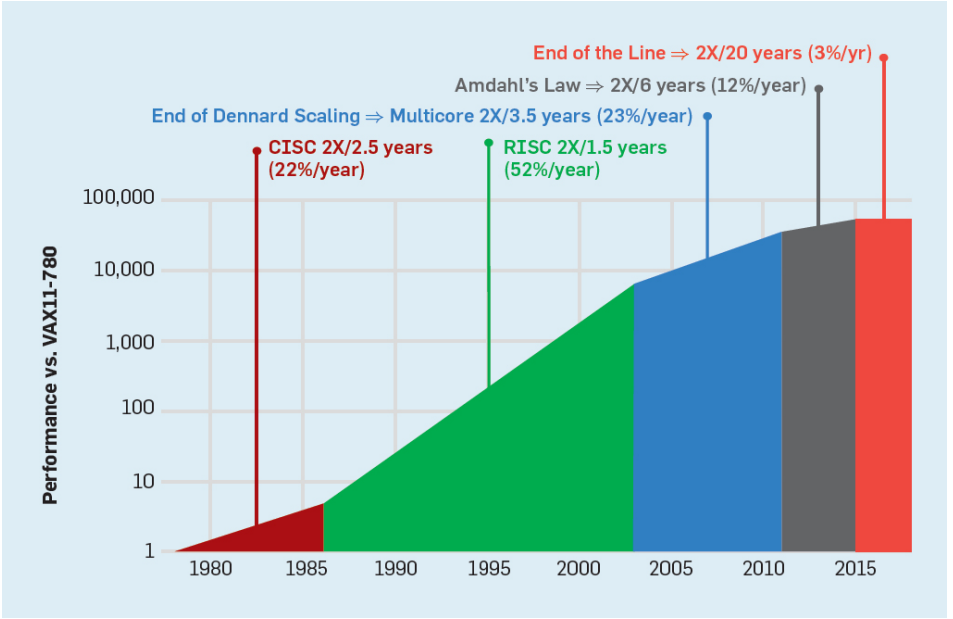
Macromolecular crystallography data rates at SLS double every two years

Why it is difficult to handle them in the future?



Macromolecular crystallography data rates at SLS double every two years

CPU performance increase is no match for such a growth



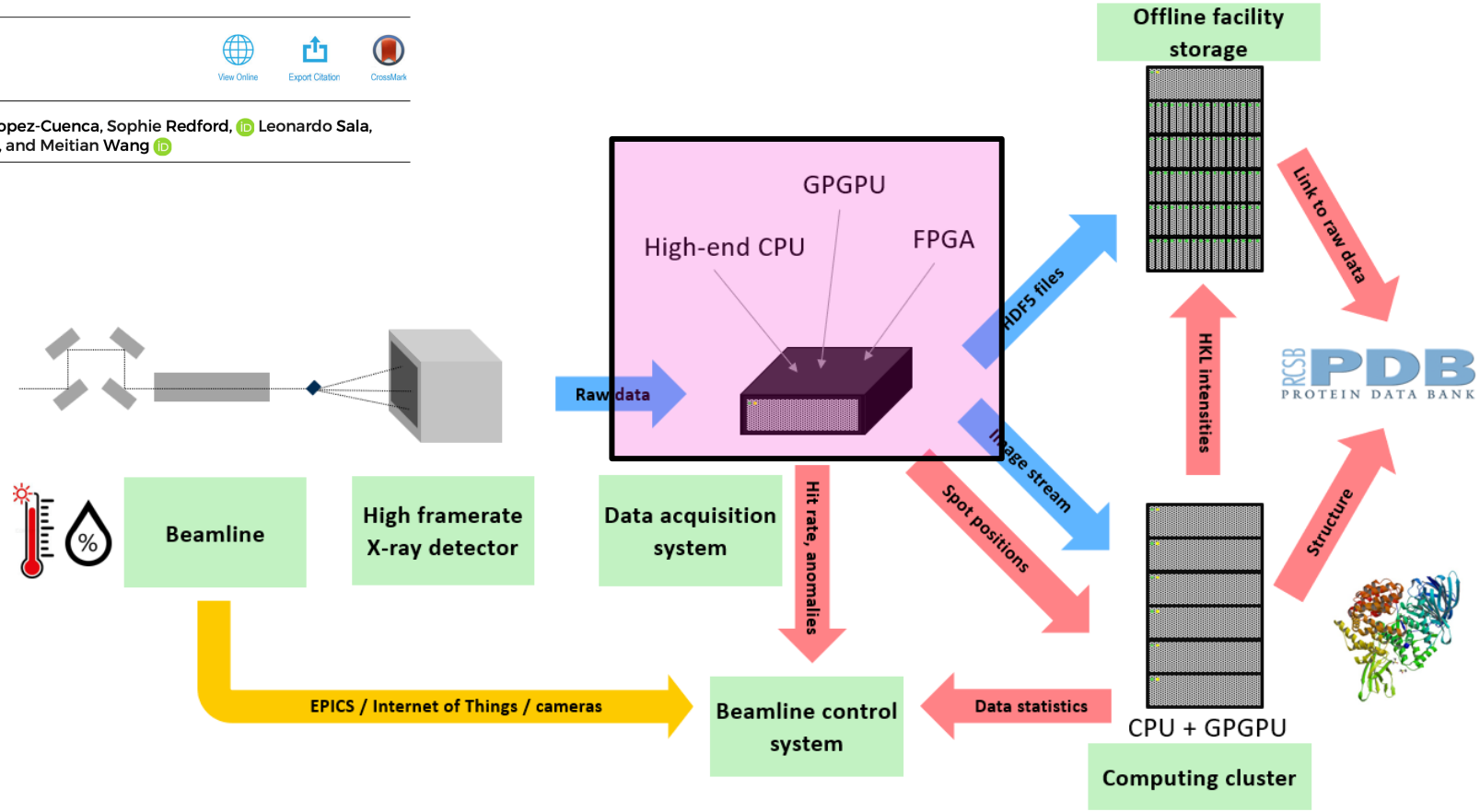
Hennessy & Patterson
"A New Golden Age for Computer Architecture"
Communications of the ACM

Jungfraujoch: edge system connecting detector and facility IT infrastructure

JUNGFRAU detector for brighter x-ray sources: Solutions for IT and data science challenges in macromolecular crystallography

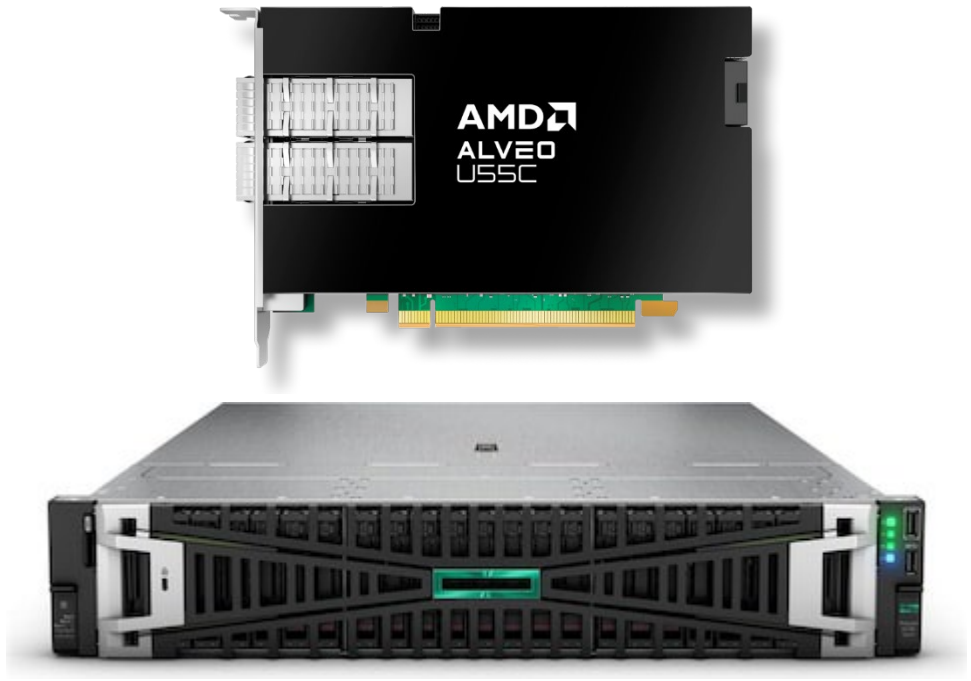
Cite as: Struct. Dyn. **7**, 014305 (2020); doi: 10.1063/1.5143480
Submitted: 27 December 2019 · Accepted: 4 February 2020 ·
Published Online: 26 February 2020

Filip Leonarski,[a] Aldo Mozzanica, Martin Brückner, Carlos Lopez-Cuenca, Sophie Redford, Leonardo Sala, Andrej Babic, Heinrich Billich,[b] Oliver Bunk, Bernd Schmitt, and Meitian Wang



PSI Jungfraujoch

- **Edge computing**
  - Reduce data close to the detector
  - Limit data transfer
- **Accelerated computing**
  - Field programmable gate array (FPGA)
  - Graphic processing unit (GPU)



JSR Synchrotron
JOURNAL OF SYNCHROTRON RADIATION
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Jungfraujoch: hardware-accelerated data-acquisition system for kilohertz pixel-array X-ray detectors

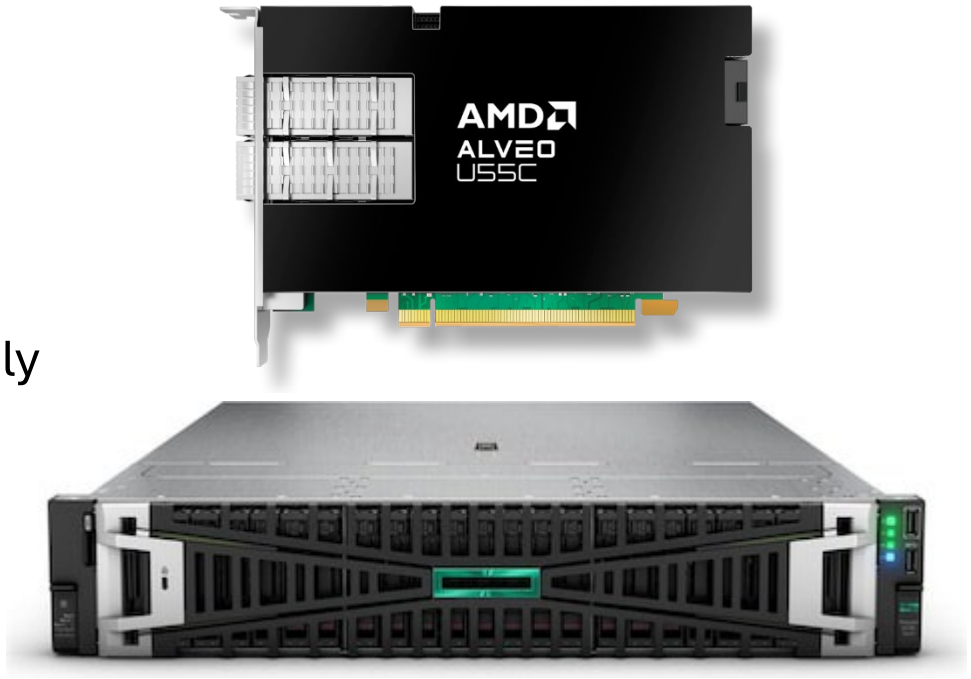
Filip Leonarski,[a]* Martin Brückner,[a] Carlos Lopez-Cuenca,[a] Aldo Mozzanica,[a] Hans-Christian Stadler,[b] Zdeněk Matěj,[c] Alexandre Castellane,[d] Bruno Mesnet,[d] Justyna Aleksandra Wojdyla,[a] Bernd Schmitt[a] and Meitian Wang[a]

Received 23 June 2022

PSI Jungfraujoch

- Development started in 2019
- **First test in Photon Factory (KEK, Japan) in 2020** remotely

- First iteration: **specialized IBM hardware**
- Now: **off-the-shelf x86 server**



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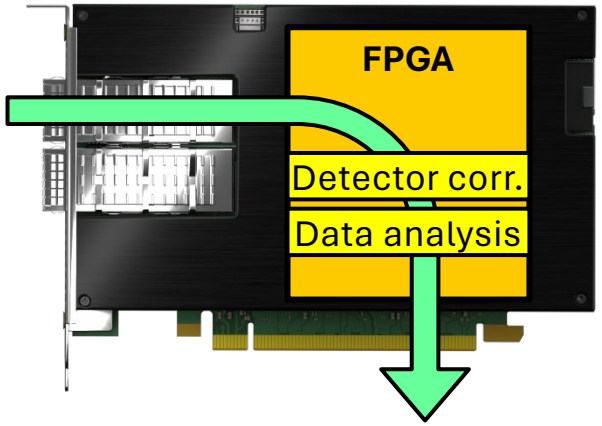
Jungfraujoch: FPGA smart network card

Off-the-shelf AMD Alveo U55C card

Data acquisition: receive network and sort them according to frame number (pulse ID) and module

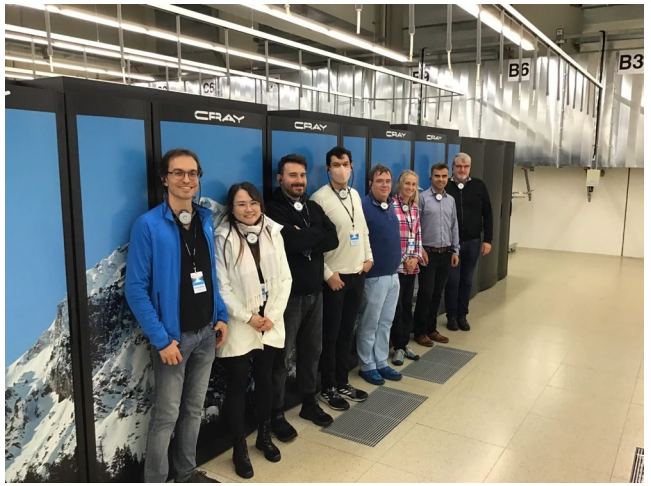
Detector corrections: bring JUNGFRAU read-out format to energy/photon counts
(a prerequisite for further analysis and compression)

Data analysis: spot finding, azimuthal integration, ROI integration and thresholding at full frame-rate



Jungfraujoch: GPU indexing

- For SFX/SSX distinguishing hits based only on spot finding results is tricky
- Need indexing to **keep up** with **kilohertz** data acquisition
- Collaborative project with Swiss Data Science Center
- Our new GPU implementation: >**1 kHz / L4 GPU**
- Just integrated in **CrystFEL** and **DIALS**
- Lead developer: **Hans-Christan Stadler**



SDSC CSCS Centro Svizzero di Calcolo Scientifico Swiss National Supercomputing Centre

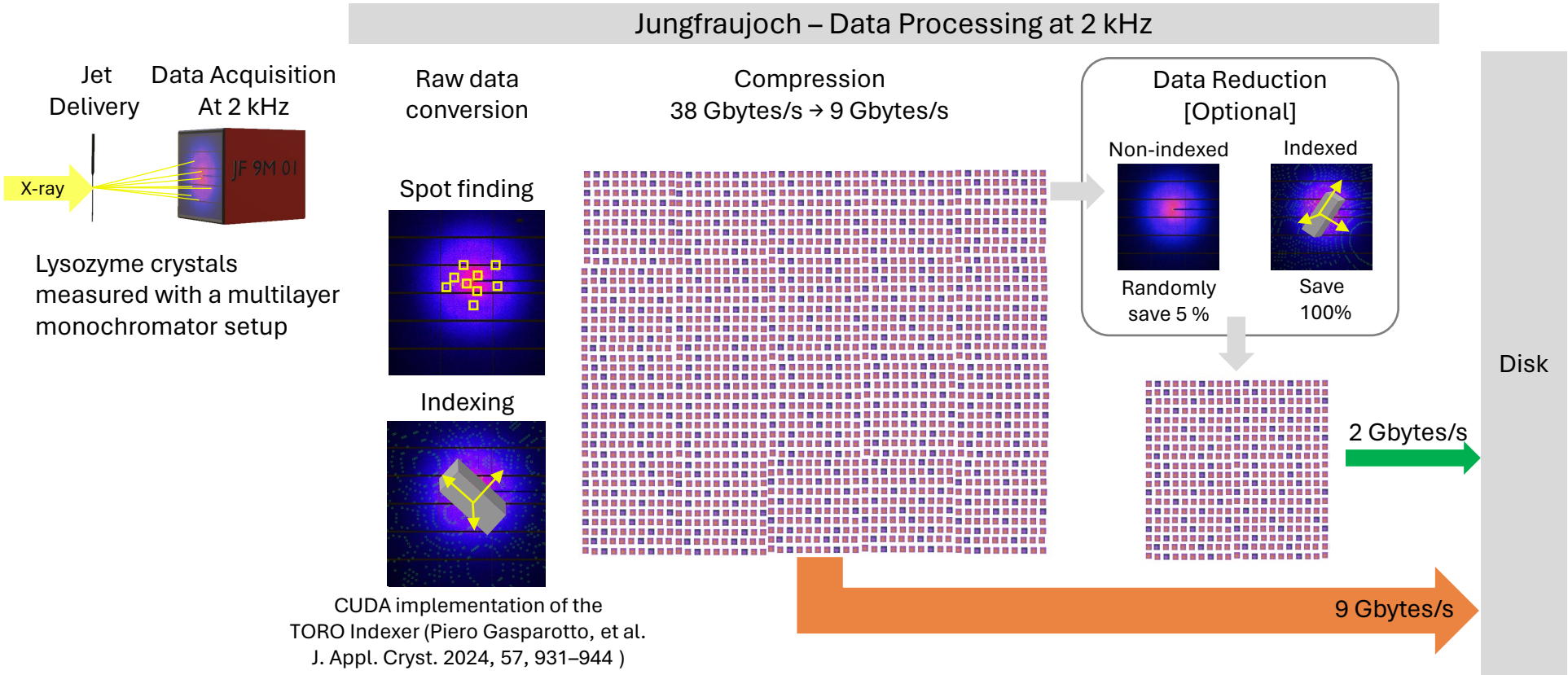
JAC JOURNAL OF APPLIED CRYSTALLOGRAPHY
ISSN 1600-5767

***TORO Indexer*: a *PyTorch*-based indexing algorithm for kilohertz serial crystallography**

Piero Gasparotto,[a]* Luis Barba,[b] Hans-Christian Stadler,[a] Greta Assmann,[a,c] Henrique Mendonça,[d] Alun W. Ashton,[a] Markus Janousch,[a] Filip Leonarski[c] and Benjamín Béjar[b]

https://github.com/paulscherrerinstitute/fast-feedback-indexer

Milestone (2024)
Jungfraujoch with 38 GB/s detector at MicroMAX



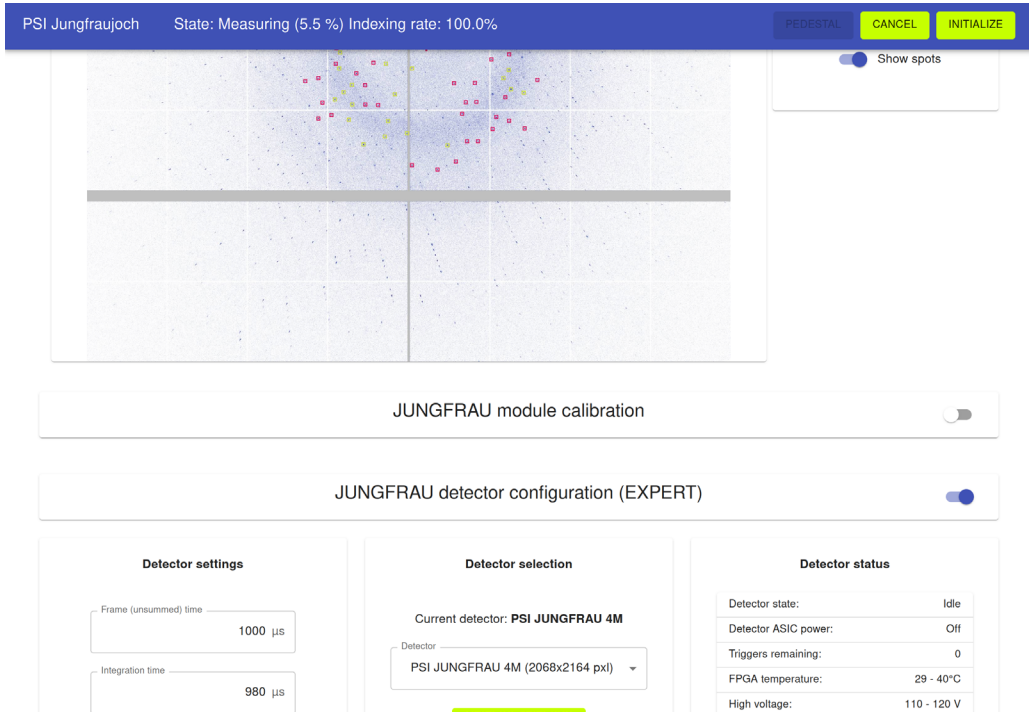
Jungfraujoch: user interface

- Web interface to configure Jungfraujoch
- All data analysis, correction, reduction can be configured on/off

- Live view of the detector image
- Live plot of auto-processing
  - Azimuthal integration (background estimation)
  - Spot number
  - Indexing rate

- All the above can be accessed via APIs (REST/ZeroMQ)

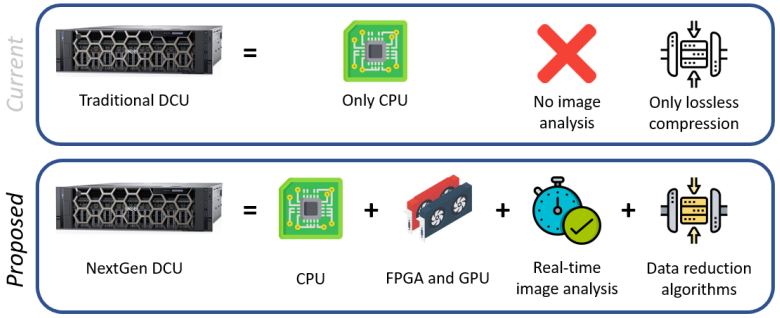
- Built-in simulator – internally generate detector packets (same data rate as real JUNGFRAU)



PSI Jungfraujoch -> DECTRIS NextGenDCU

PSI

- Academic projects focus on **novelty** and **performance**, rather than **long-term sustainability** and **serviceability**
- Many serial crystallography beamlines use **photon counters** (e.g., DECTRIS EIGER2)
- Innosuisse project to develop **NextGen Detector Control Unit** for the current and future **DECTRIS X-ray detectors**
- We will continue to **support PSI detectors with Jungfraujoch**



DECTRIS
detecting the future

Innovation project supported by

Schweizerische Eidgenossenschaft
Confédération suisse
Confederazione Svizzera
Confederaziun svizra

Swiss Confederation

Innosuisse – Swiss Innovation Agency

Outlook

- We explore DECTRIS Cloud operation:
  successful test with JUNGFRAU 9M + Jungfraujoch + DECTRIS Cloud (MAX IV)
- System deployed at few facilities (SwissFEL, MAX IV, ELI, Uni Wien)
- Getting ready for 1.0.0 release of Jungfraujoch and making the code available
- Challenge for NXmx: no definitions for on-the-fly generated results
- Open project on diffraction viewer compatible with Jungfraujoch data

Acknowledgements

- **MX Group (PSI)**
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  - Zdeněk Matěj
  - Thomas Ursby

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  - Open Research Data (ETH Domain)
  - Swiss Data Science Center