Serial crystallography at the EMBL–ESRF

Shibom Basu

Staff scientist

On behalf of Daniele de Sanctis, ESRF

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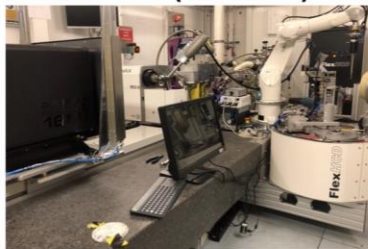
The EMBL-ESRF joint structural biology group beamlines post-EBS
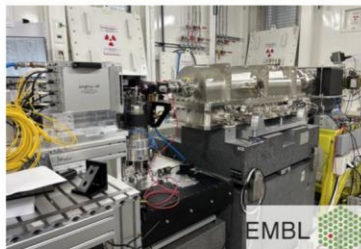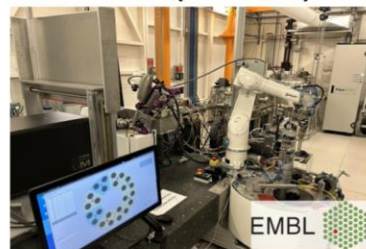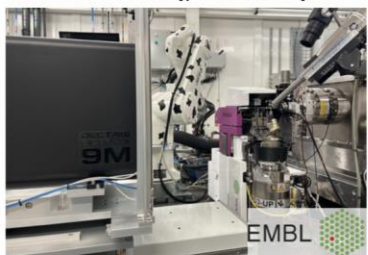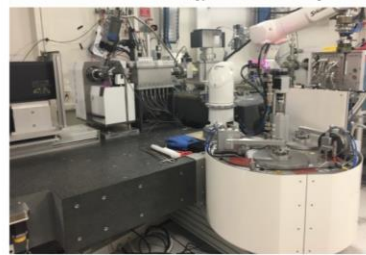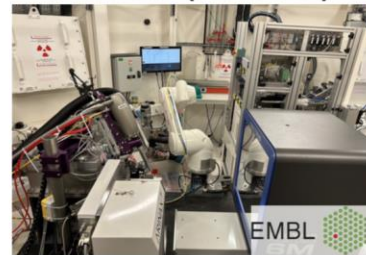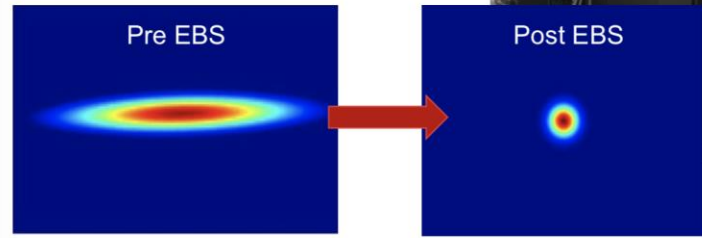
Science @ ID29
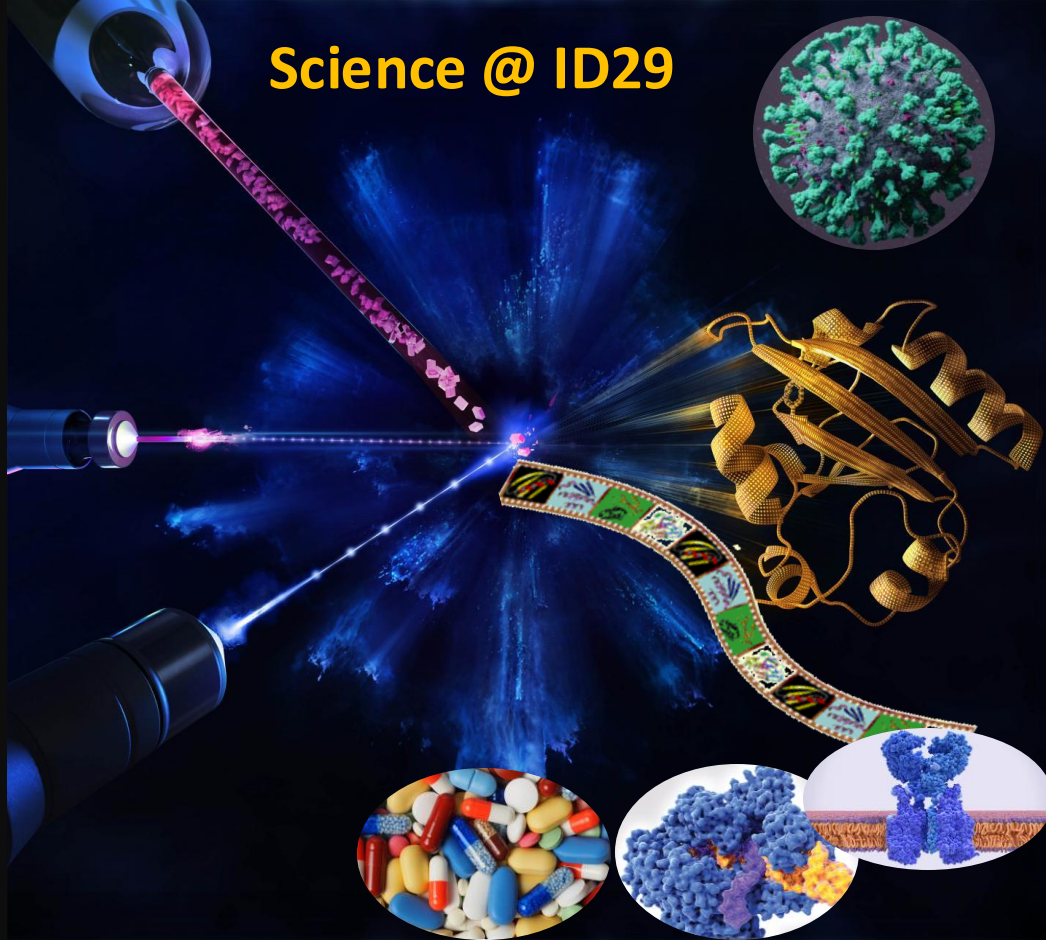
DRUG BINDING

pH/T—JUMP

PROTEIN DYNAMICS @ μS—SEC

ENZYMOLOGY

PHOTOACTIVATABLE PROTEINS

PHOTOACTIVATABLE LIGANDS

PHOTO-SWITCHES

PHOTOCAGES

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ID29 – experimental setup for serial microsecond crystallography (SµX)

Compact and versatile MD3-Up-SSX diffractometer

Jungfrau 4M detector

RINAX

Jungfrau 4M PSI

90 µs pulsed X-ray beam frequency – 231.25 Hz

Heat-load chopper

Multi-layer monochromator Δ E/E = 1 %

ESRF–EBS Storage Ring

X-rays

1% Bandwidth ensures "fuller" Bragg
90 µs pulsed X-ray beam ensures low-background

Diffraction data acquired at 240,000 frames / 20 min on Jungfrau 4M

Example diffraction pattern from serial microsecond crystallography (SµX)
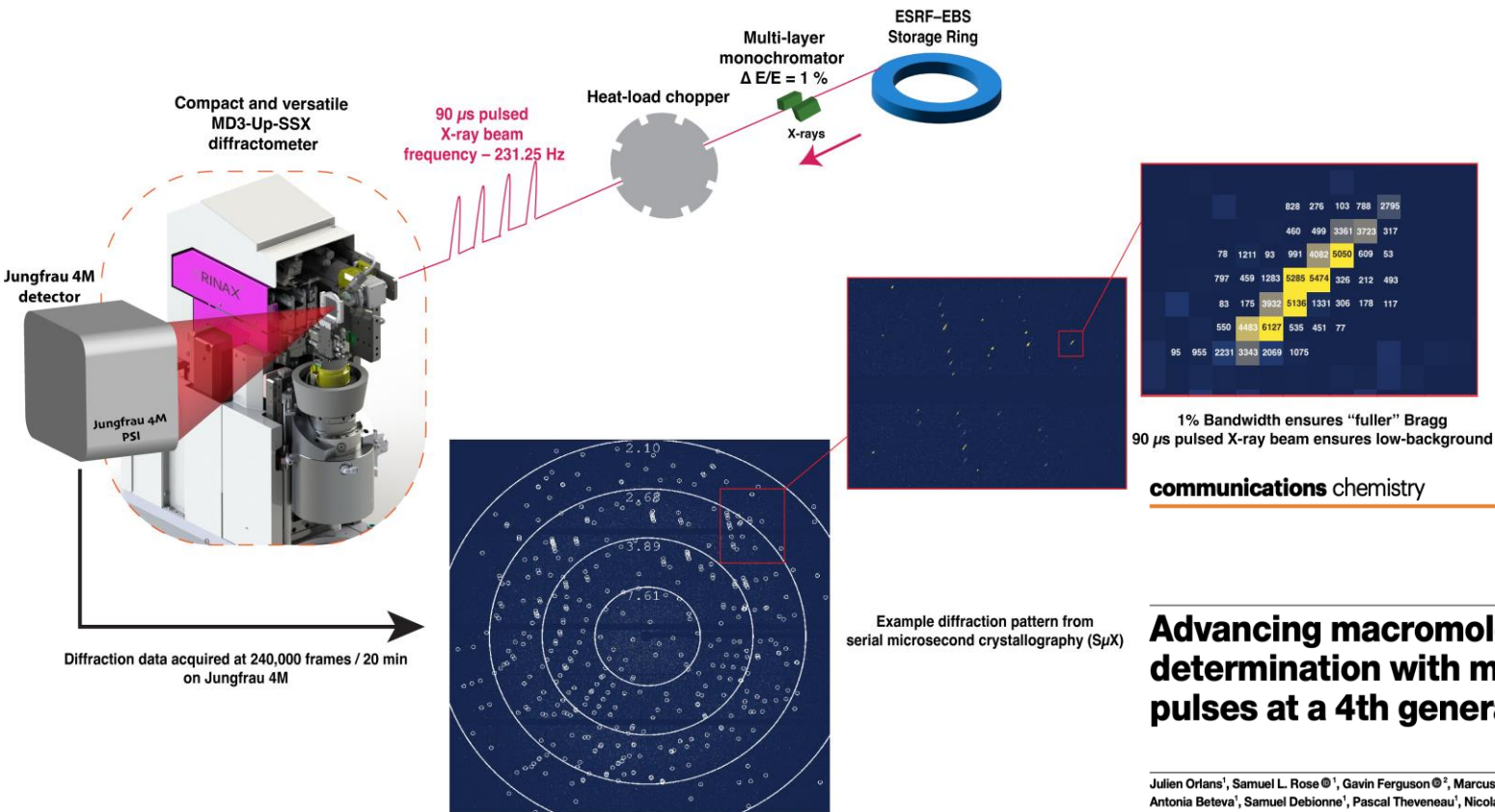
Advancing macromolecular structure determination with microsecond X-ray pulses at a 4th generation synchrotron

Check for updates

Julien Orlans[1], Samuel L. Rose [1], Gavin Ferguson [2], Marcus Oscarsson[1], Alejandro Homs Puron[1],
Antonia Beteva[1], Samuel Debionne[1], Pascal Theveneau[1], Nicolas Coquelle[1], Jerome Kieffer [1],
Paolo Busca[1], Jeremy Sinoir[2], Victor Armijo [3], Marcos Lopez Marrero[3], Franck Felisaz[3],
Gergely Papp [3], Herve Gonzalez[1], Hugo Caserotto[1], Fabien Dobias[1], Jonathan Gigmes[1],
Guillaume Lebon [2], Shibom Basu [3] & Daniele de Sanctis [1]

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ID29 fixed target setup
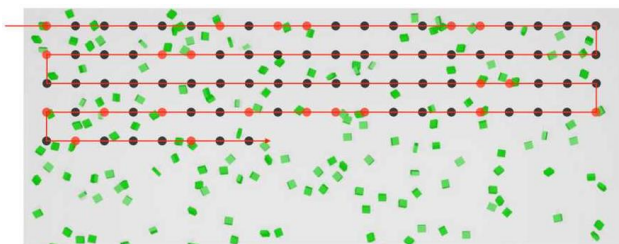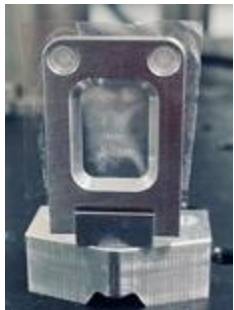
Carrillo *et al.*, IUCrJ (2023)
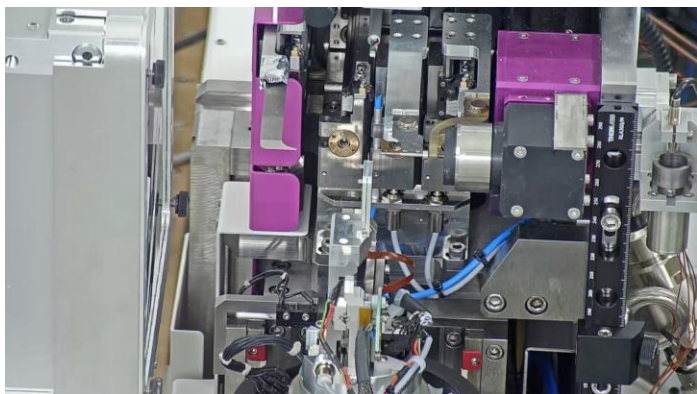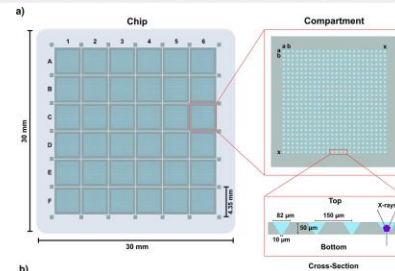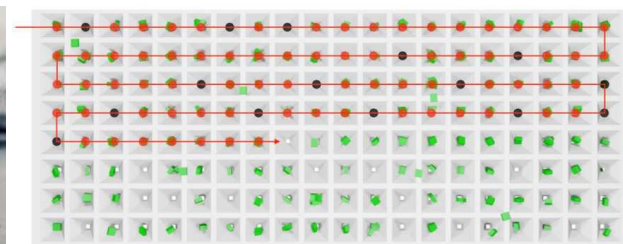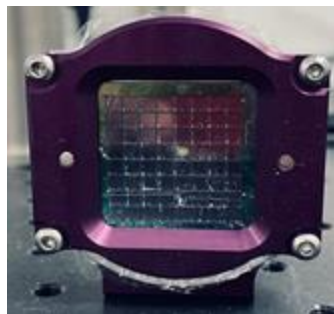
- **Fixed target – foils, silicon chips or customized devices**

- For foils –
  - ➢ **Best for sample pre-characterisation (3-5 µL)**
  - ➢ **240K images / 20 min**

- 1000 indexed images may be sufficient to get high quality maps

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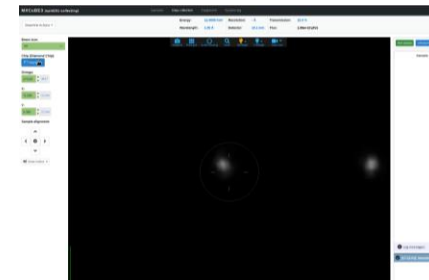
ID29–TRSX data deluge
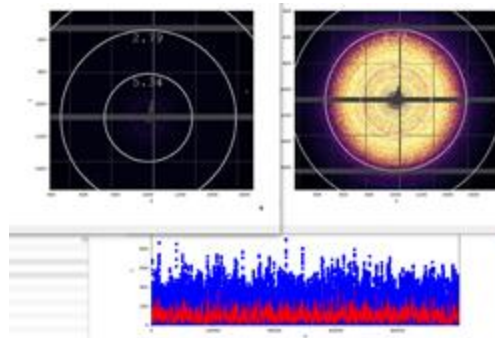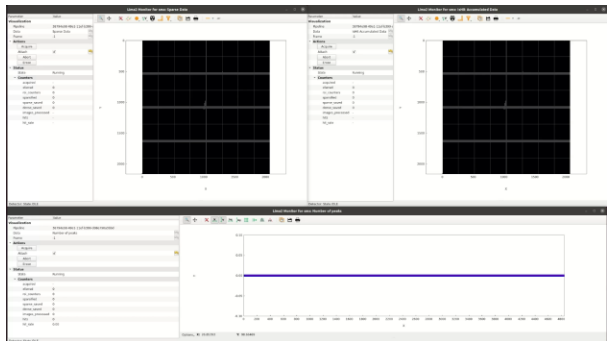
- The data acquisition system (LImA2) identifies and flags frames that contains diffraction (int32 type), facilitating the downstream data processing

EDNA2 0.1 documentation »

Next topic
Project overview

EDNA2 version 0.1

SX visualization on ICAT
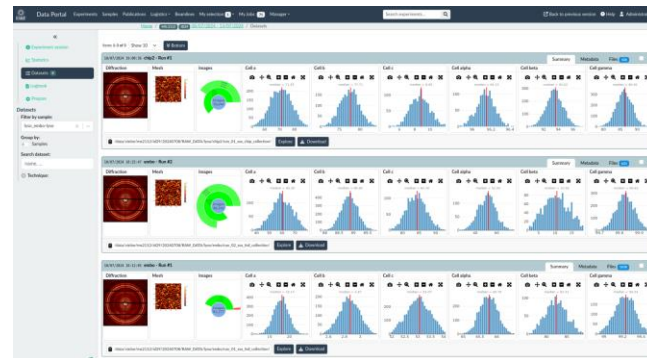
TB per session vs cumulative TB
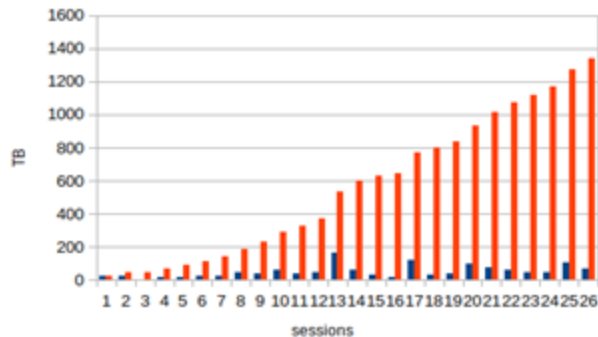
- Data reduction protocols in place to reduce the amount of data produced: ~10% of all images

- Automatic data processing pipeline soon to be deployed, together with ICAT upload

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Legacy of Lima and motivation for Lima2

Legacy of Lima

- ESRF designed a dedicated and unified software to support 2D detector control and image processing
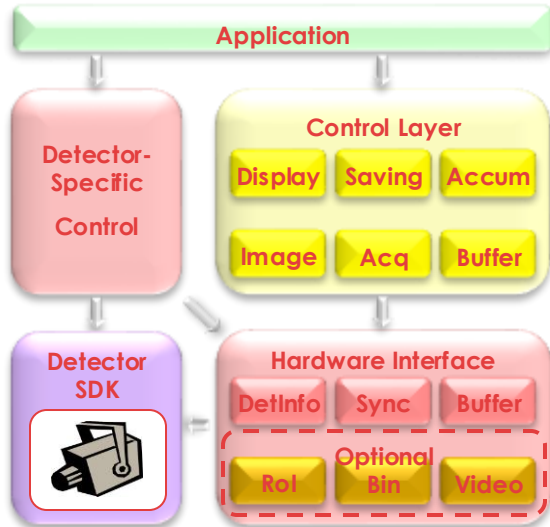
Motivation for Lima2

- Improve Scalability – Faster frame rate detectors
- Ability to perform real-time data processing
- Provides a high-level API to experiment controls (e.g. BLISS)

Alejandro Homs, Samuel Debionne
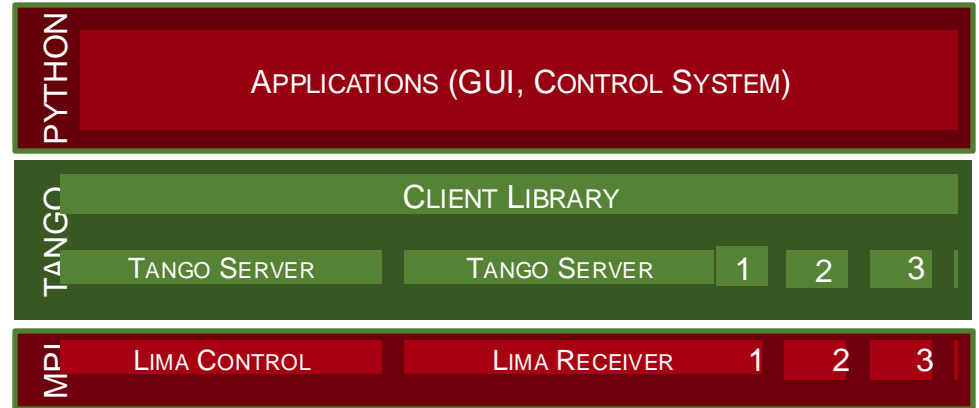
Computing infrastructure for JungFrau 4M

- PSI JungFrau – a charge integrating, 2D pixel detector
- Challenging packet stream rate of 8GB/s at 1 kHz frame rate
- Use Multiple computers, each running two receivers and transfer frames using a Load balancer

09/04/2025

Alejandro Homs, Samuel Debionne
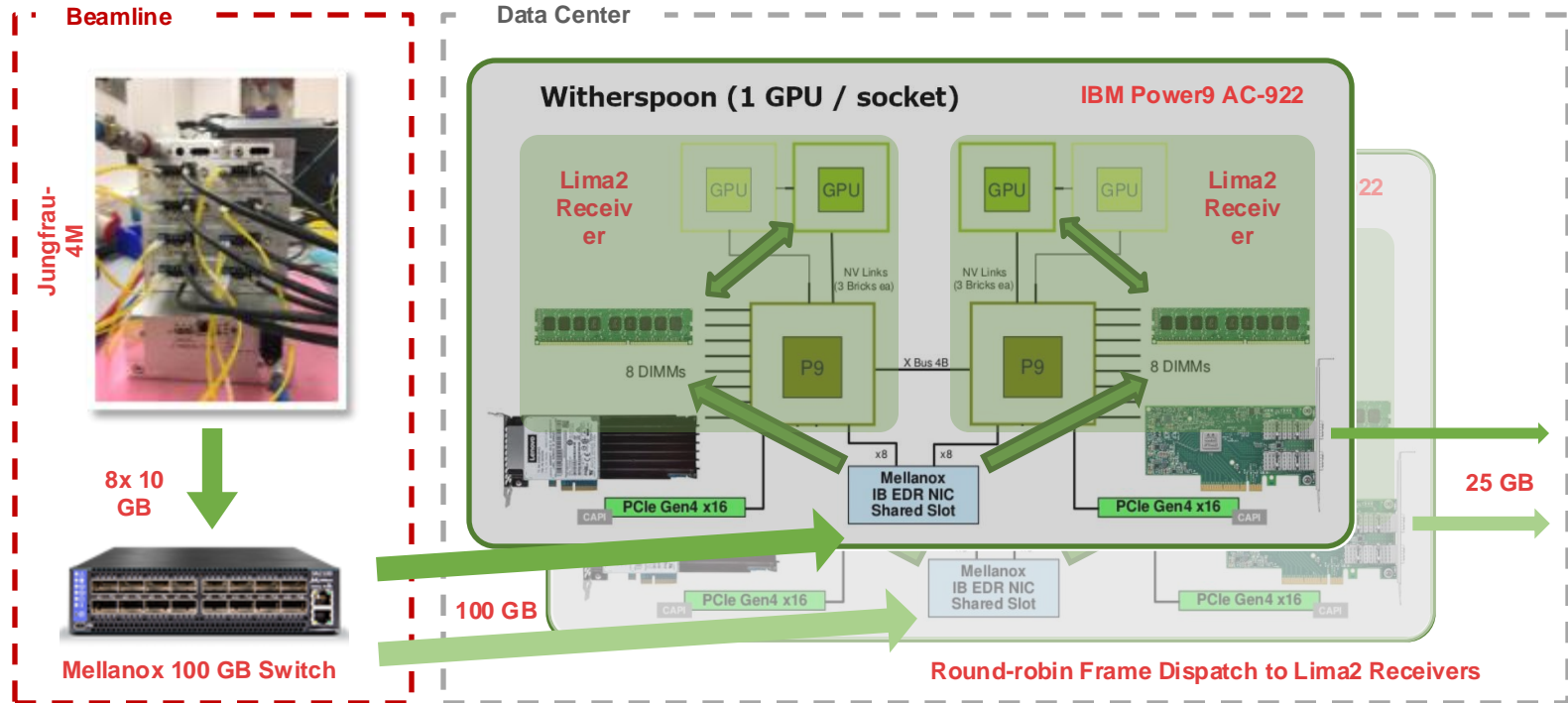
Saving of data together with analysis

Image Reconstruction

UDP packets data from detector are geometrically assembled (CPU)

Background & GainCorrection

Per pixel & per frame gain selection: 3 pedestal + 3 gain maps (Power9 GPU)

pyFAI-based Data Reduction

Peak finding and background extraction using Sigma Clipping on Power9 GPU

Sparse Data Saving

Radius

Scattering

Frame

Time Frame

0 1 2 3 4 5 6 7 8 9

Peak pixel position & intensity per frame

Offline re-densification

Performed to feed downstream SSX processing

Jerome Kieffer, Alejandro Homs

Thanks to…

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  - Marcus Oscarsson
  - Antonia Beteva
  - Nicolas Coquelle
  - Nicolas Caramello
  - Thierry Giraud
  - Montserrat Soler Lopez
  - Didier Nurizzo
  - Anton Popov
  - Antoine Royant
  - Sylvain Engilberge
  - Peter van der Linden

- Philippe Carpentier
- Fabien Dobias
- Hugo Caserotto
- Jonathan Gigmes
- Pascal Theveneau
- **Samuel Debionne**
- **Alejandro Homs**
- **Jêrome Kieffer**
- Mael Goanach
- Andy Goetz
- Paolo Busca
- Nicolas Janvier
- Herve Gonzalez
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  - Franck Felisaz
  - Christopher Rossi