Processing data in serial crystallography on-the-fly: what kind of raw data do we want to store?

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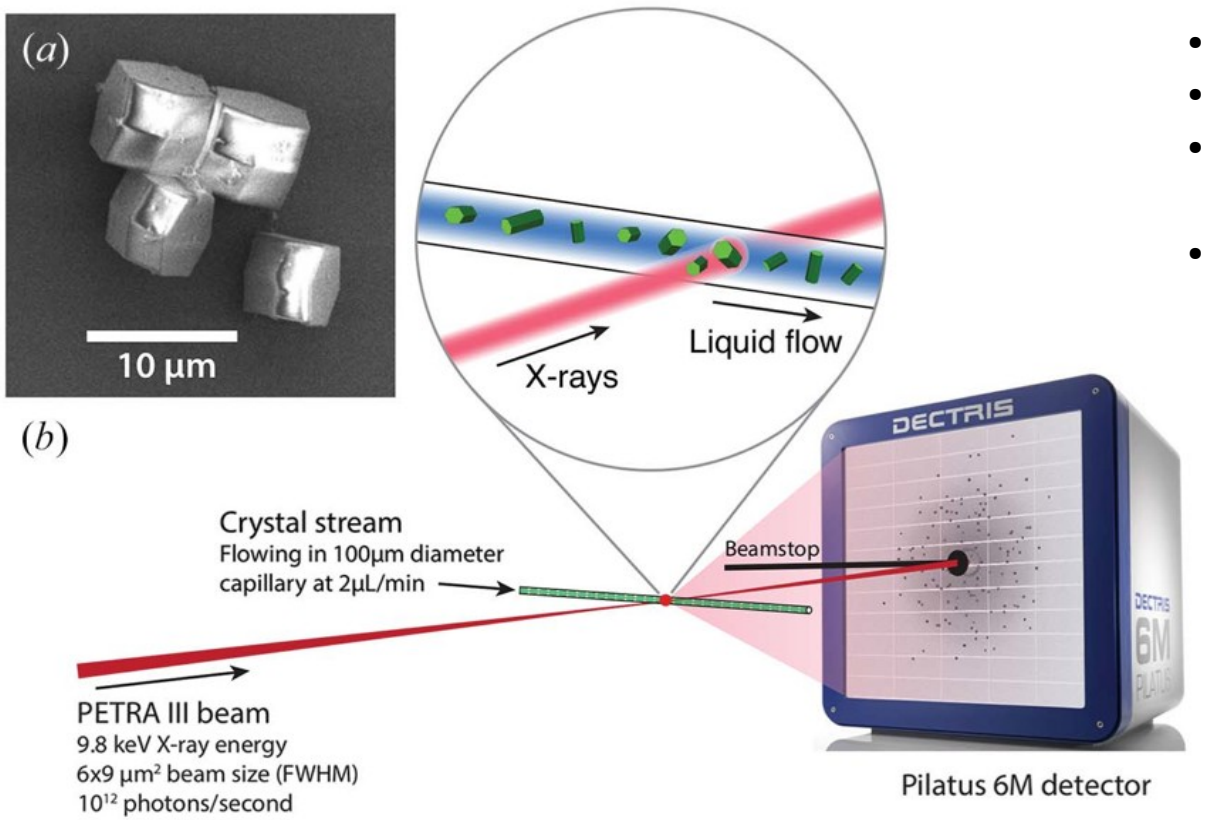
Workshop on “Raw diffraction data reuse: the good, the bad and the challenging”

IUCr 2023 Congress

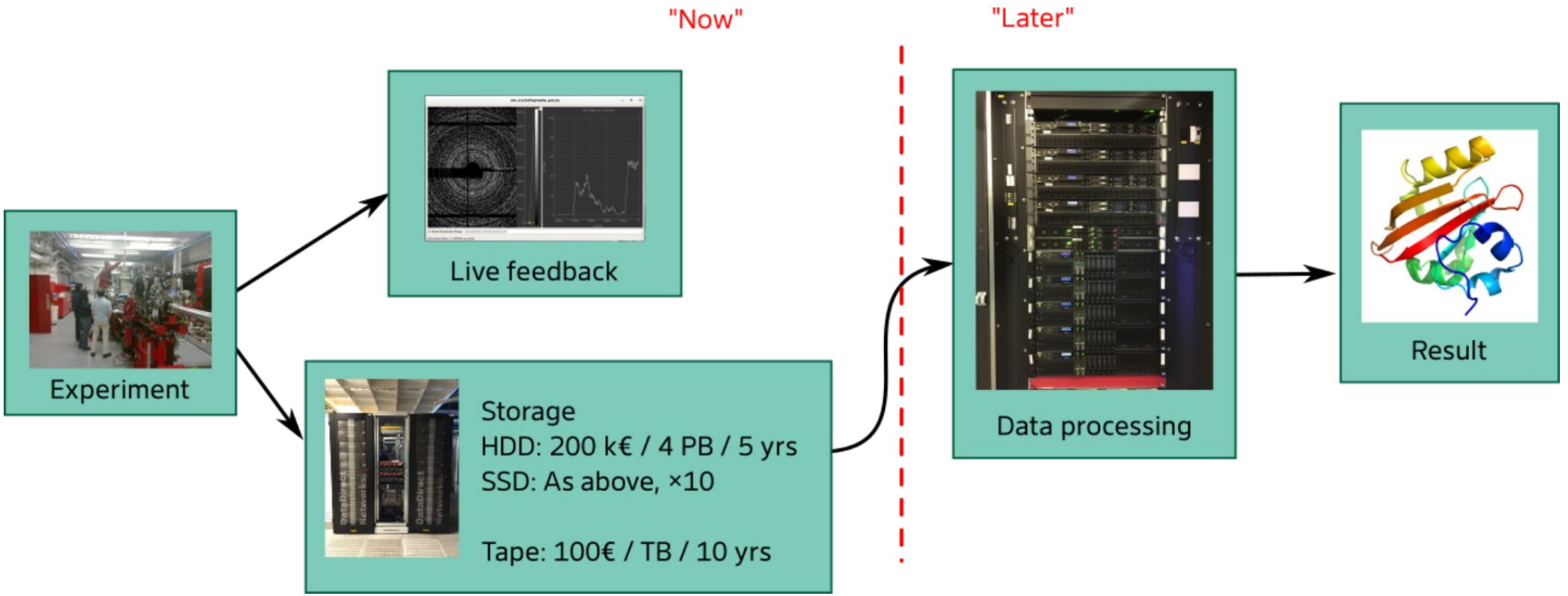
Serial crystallography



- One exposure per crystal
- Steady stream of crystals
- Each image processed independently
- A lot of images (millions)
  (5GB/s, 100TB per experiment)
- Data processing after experiment
  (month, even years)

Figure: Stellato et al.,IUCrJ 1 (2014) p204–212

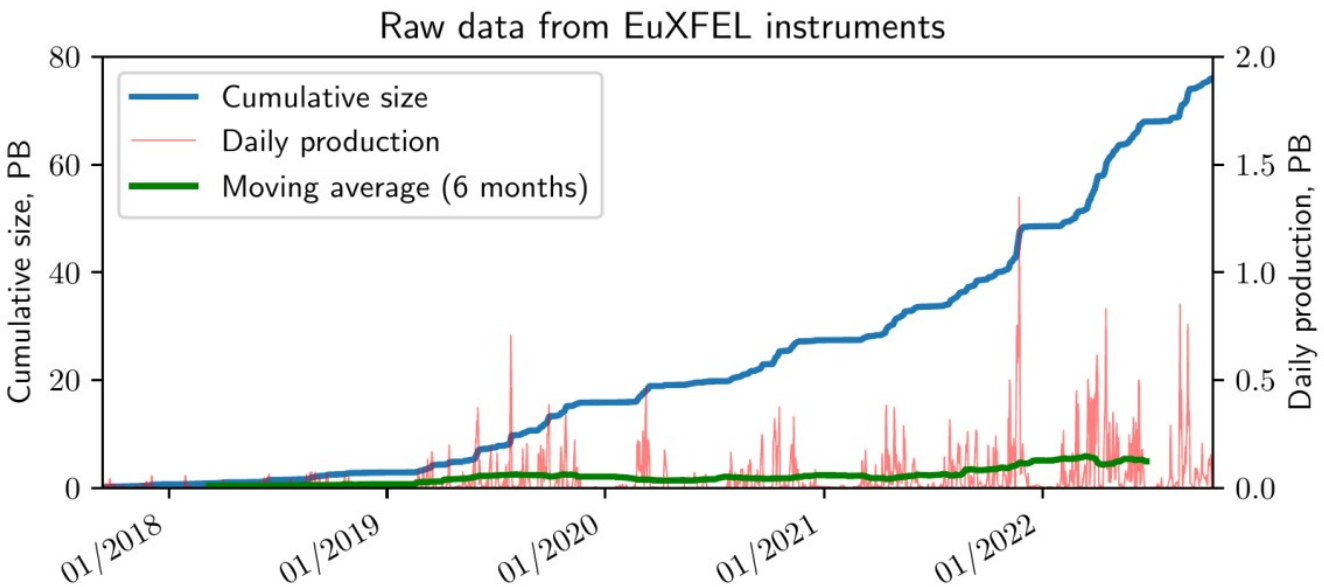
Data processing in SX



Data processing in SX – storage costs

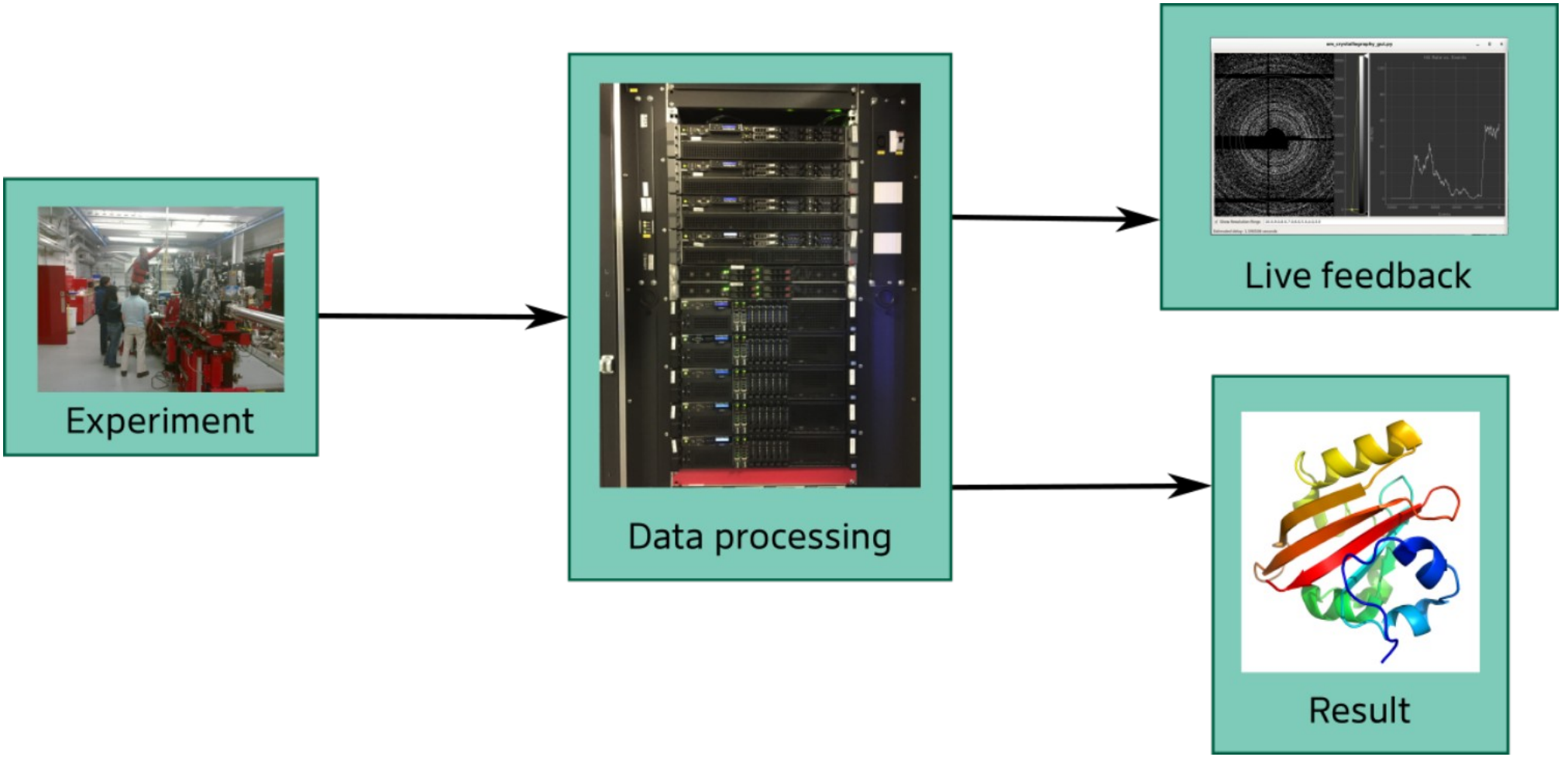
HDD: 200k€ / 4 PB / 5 yrs
SSD: as above x10

Tape: 100€ / TB / 10 yrs



2 PB of storage ↑

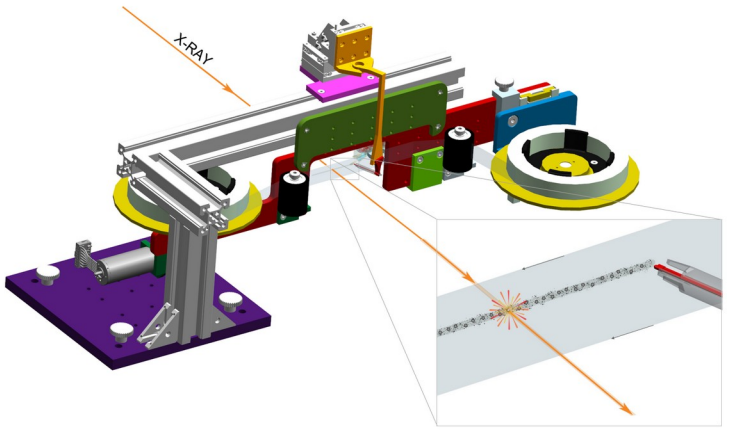
Data processing in SX



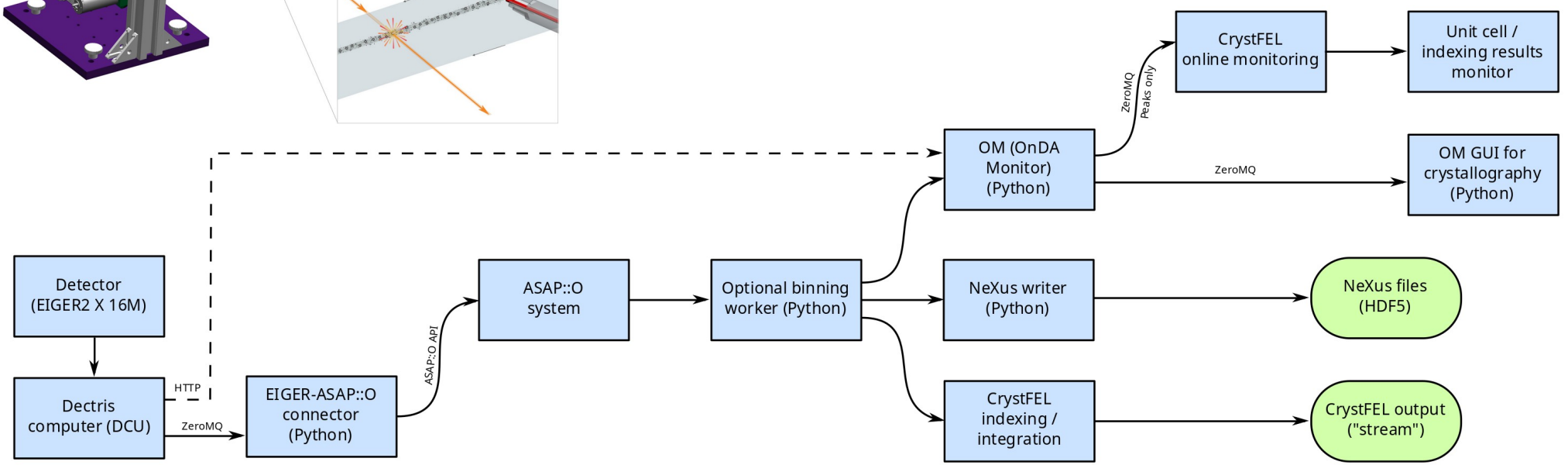
Benefits of real-time data processing

- Faster results and publication
- No need to store raw data
- Better situational awareness during experiment
- Faster diagnosis of experiment problems
- Less scope for self-delusion
- Energy efficiency – processing data only once

Real-time data processing pipeline at P11



- 133 frames/sec, 16 megapixel, 16 bits/pixel
- all frames processed with below 1s latency



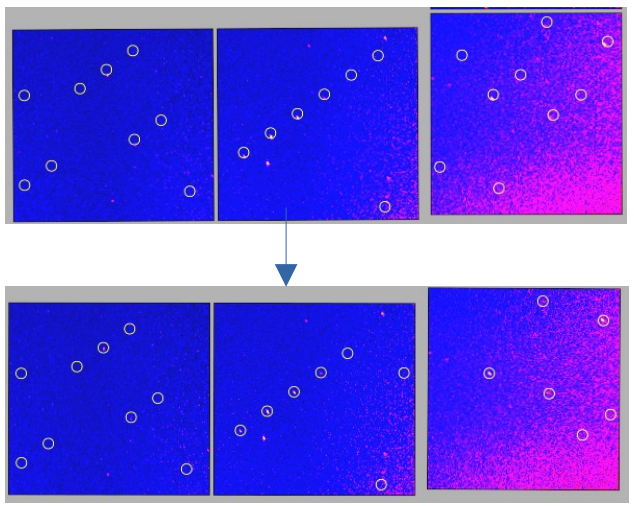
CrystFEL: https://www.desy.de/~twhite/crystfel
OM: https://www.ondamonitor.com
ASAP::O: https://asapo.pages.desy.de/asapo

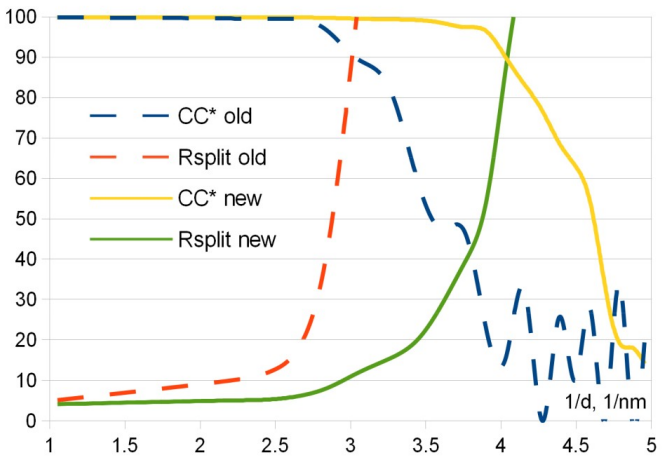
Project led by Thomas White

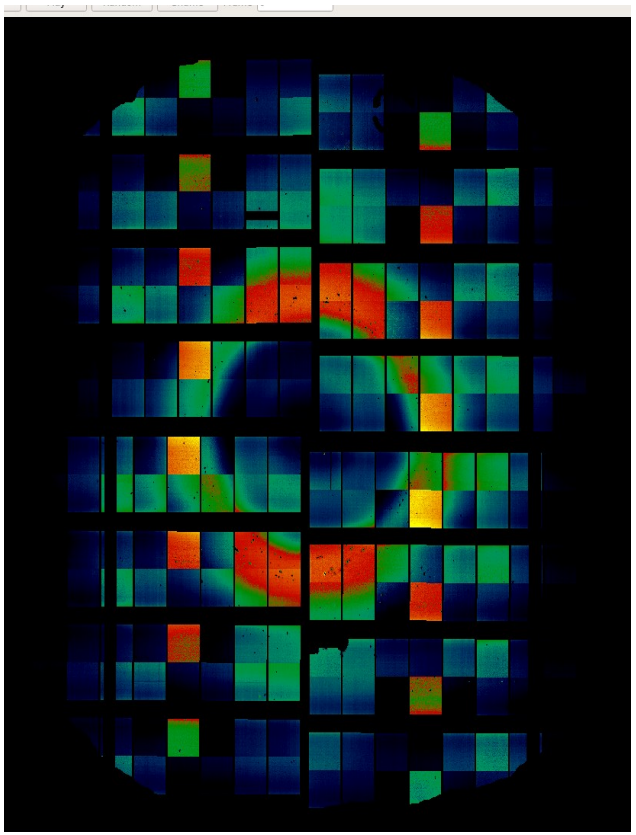
Requirements for real-time processing: detector calibration

We must get the data processing right first time.

Yefanov et al., Optics Express 28459 (2015)



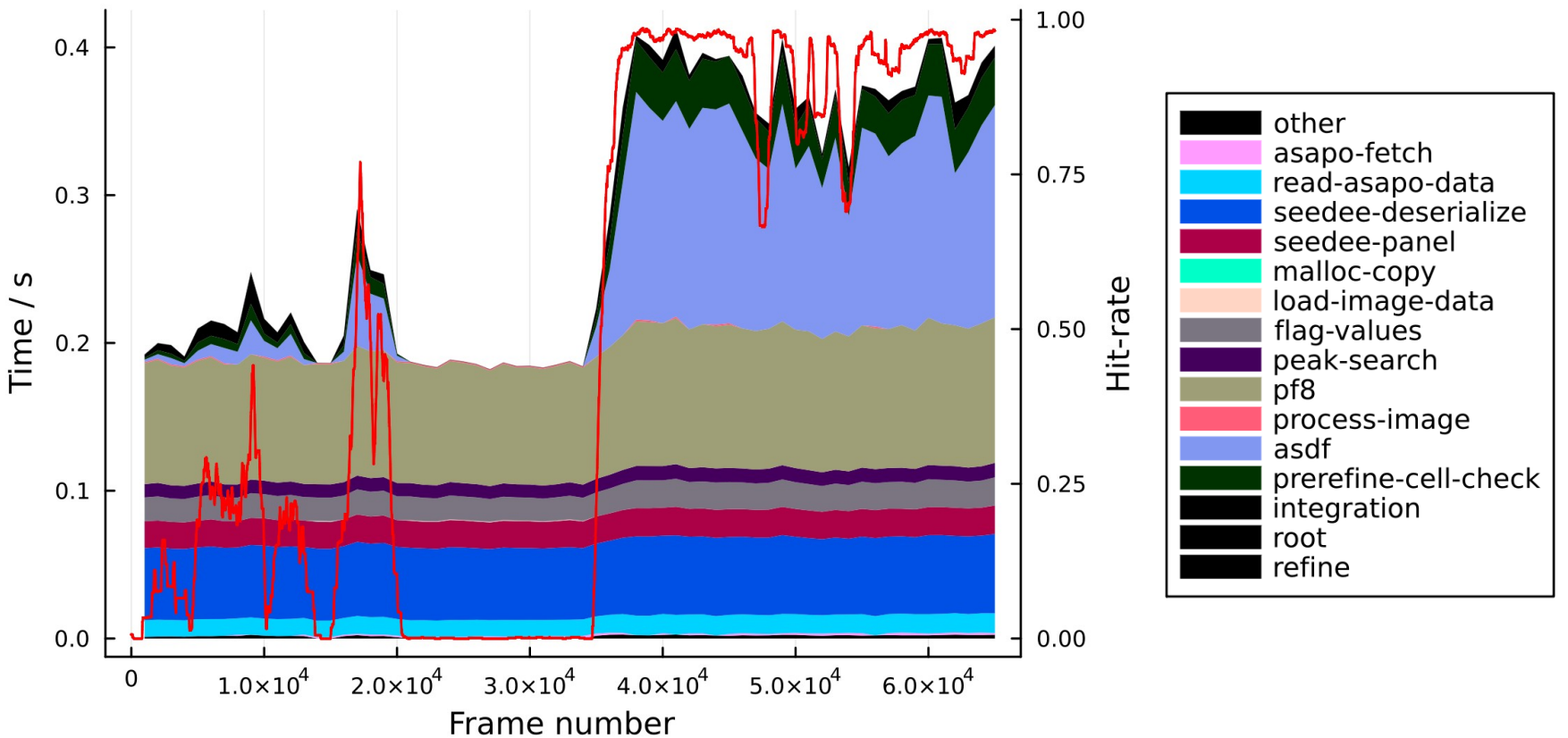




Automated real-time geometry calibration is currently under development.

Requirements for real-time processing: computing resources

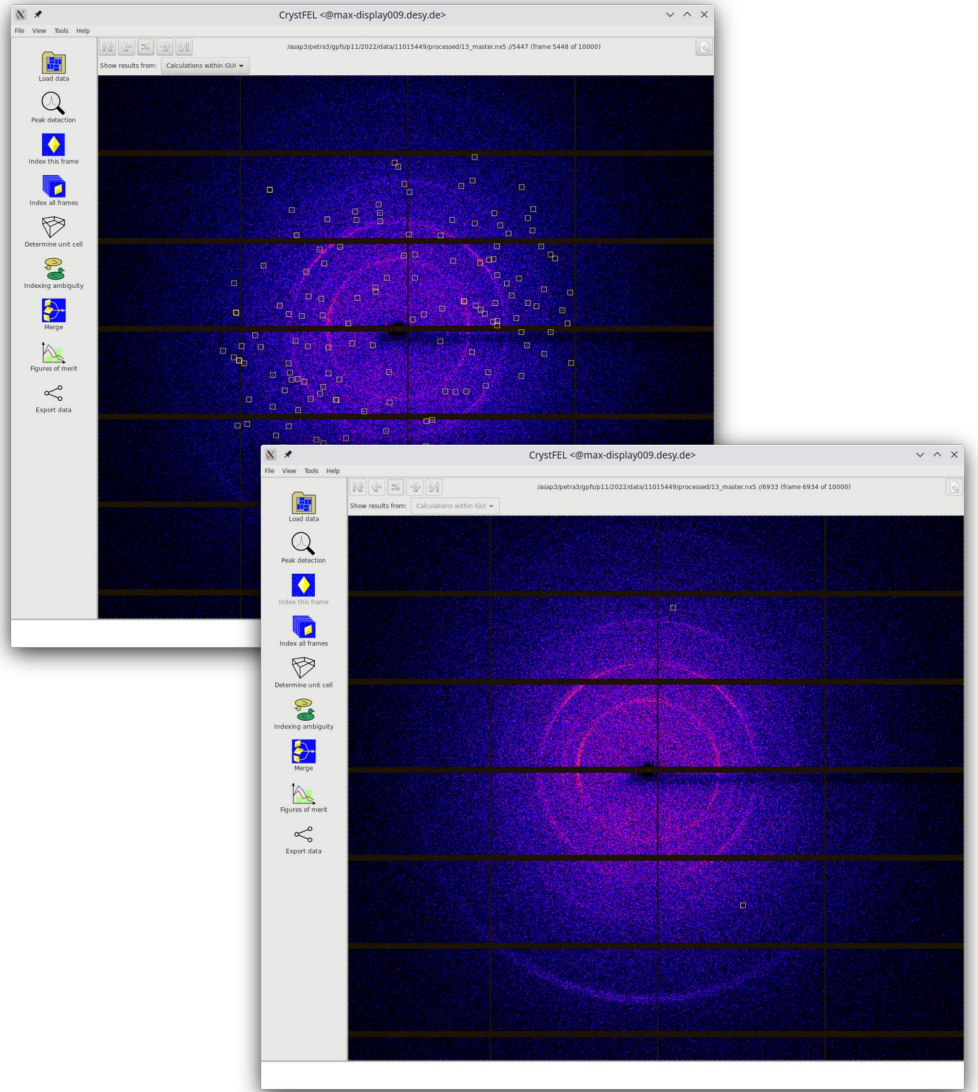
- A lot of performance improvements in CrystFEL since the start of the project
- 133 frames/sec, 16 megapixel – 32 CPUs on one node (at 40% hit-rate)



What kind of data do we want to store?

What kind of data can we store?

- All raw data
- Calibrated data (converted to photons)
- Only hits
- Only indexed frames
- Unmerged intensities
- Final result – merged intensities



Reasons to store data

- Fraud prevention
- Hope for a better software/analysis methods
- "Unobtainium" sample

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Storage costs:

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Is it **really** cheaper to store the data, compared to re-running experiment?
What if you (as a user) have to pay for it?

Possible compromise solutions

- Store hits only
- Store indexed frames only
- Lossy compression:
  pixel binning (2x2, 3x3, 4x4...)
  peaks only?
  other methods*
- Store data only when it yields result
- Store random sample of the data
- Send data straight to archive (tape)

*Talk by O. Yefanov (Session A118, Wed 23 Aug)

Acknowledgments

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P11: Johanna Hakanpää, Helena Taberman, Guillaume Pompidor
IT: Martin Gasthuber, Juergen Hannappel, Sergey Yakubov
LCLS: Valerio Mariani

Want to try it?

ZeroMQ data interface: already in CrystFEL 0.10.0
ASAP::O interface: in CrystFEL 0.10.2
See **doc/articles/online.rst** and **doc/articles/speed.rst** in CrystFEL directory

Want to hear more?

Novel Data Methods Workshop tomorrow, Wed 23 Aug @ 14:00
https://sites.google.com/view/newdatamethods-iucr2023