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Lossless and Lossy Compression for Photon Science

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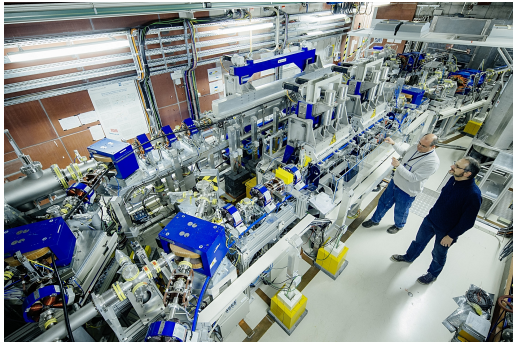
Introduction: Photon Science

Free Electron Laser at ELBE



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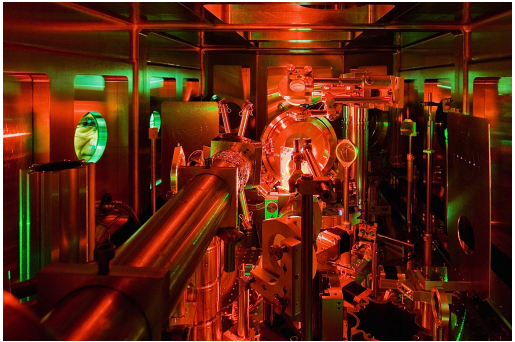
Experimental Chamber of DRACO laser



(Copyright HZDR/Jürgen Lösel)

high fidelity experiments, vast topic reach (physics, materials, life sciences, chemistry), diverse science community

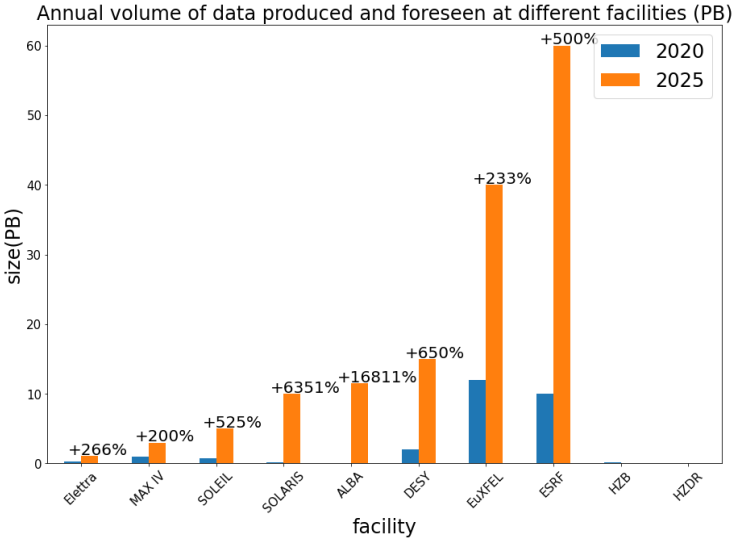
Photon Science in Europe

- 356 beamlines in 24 facilities (see wayforlight.eu)
- mode of operation at beamlines:

1. scientists apply for (limited) beamtime
2. plan/prototype for experiments (custom, standardized)
3. intense research during beamtime (24/7)
4. analysis period afterwards

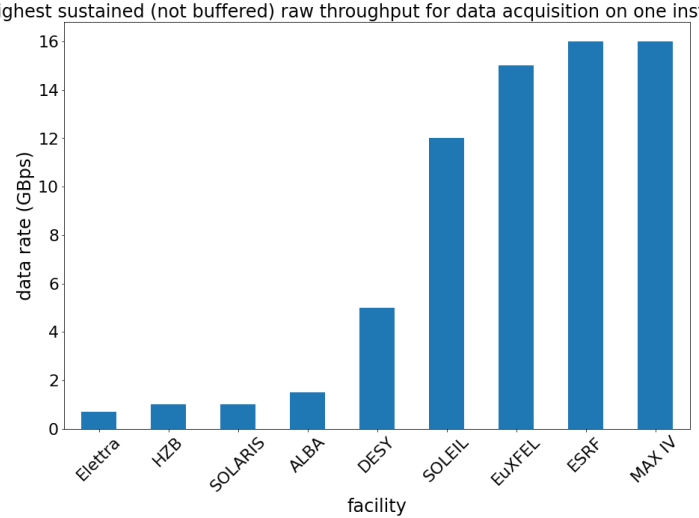
SESAME LENS Canadian Light Source Centre canadien de rayonnement synchrotron ESUO EUROPEAN SYNCHROTRON AND FEL USER ORGANISATION

Data Volumes in Photon Science



(source: LEAPS-INNOV WP7.2 report, survey among participating centers, 2020)

Data Rates in Photon Science



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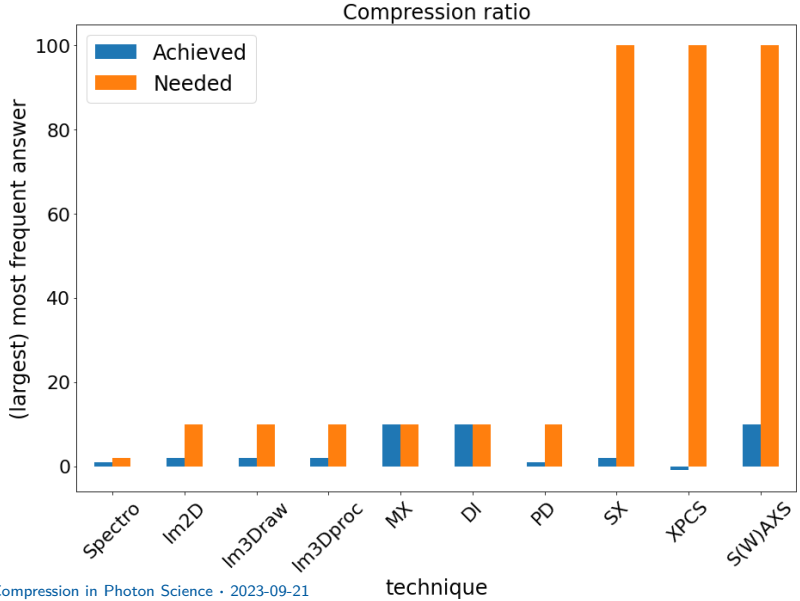
Present and Future



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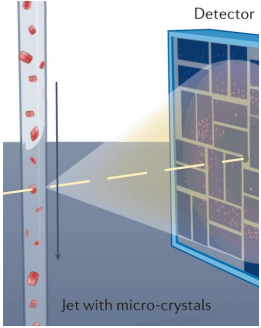
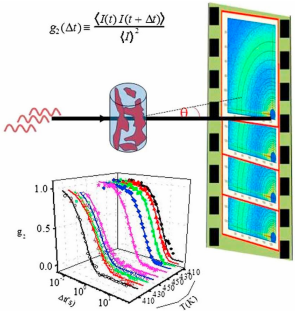
The Diabolic Three

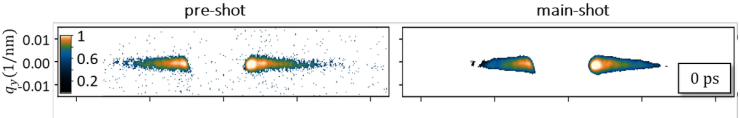
Serial Crystolography
(SX, [Barends et al., 2022])



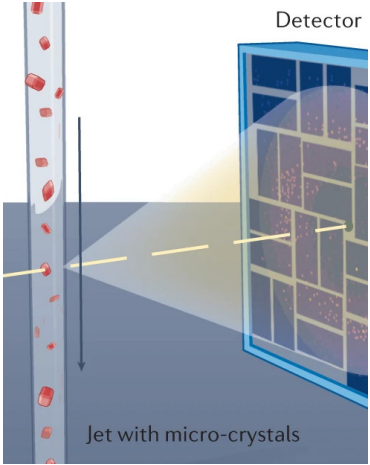
X Ray Photon Correlation Spectroscopy
(XPCS, [Nogales and Fluerasu, 2016])



Small-Angle X-Ray Scattering
(SAXS, [Kluge et al., 2023])



Common Observations



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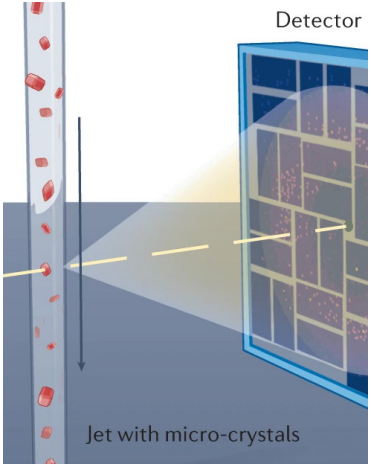

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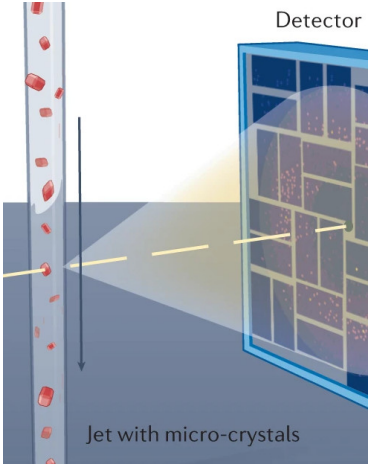

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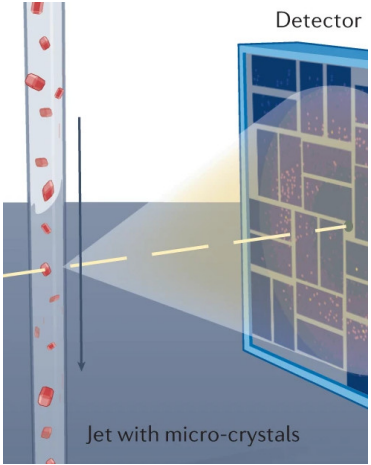

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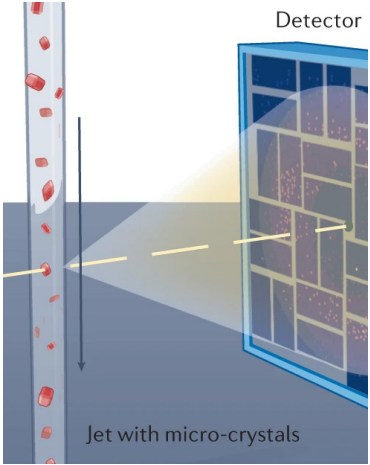

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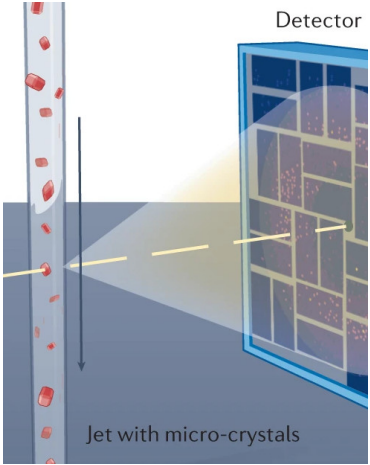

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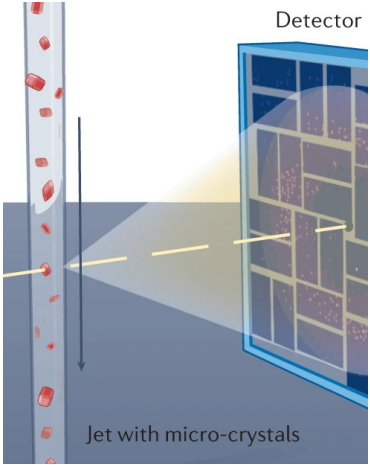

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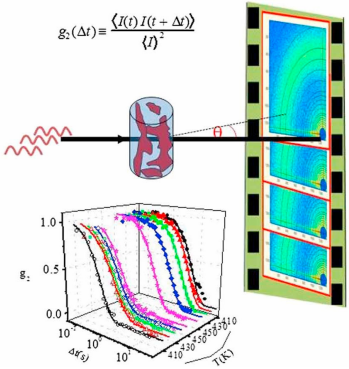
- pipelines are experiment specific:
  - veto as early as possible
  - denoise + compress
  - reconstruct as early as possible

Uncommon Observations



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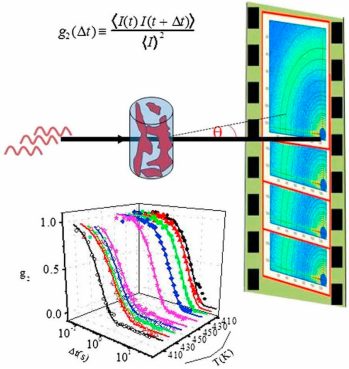

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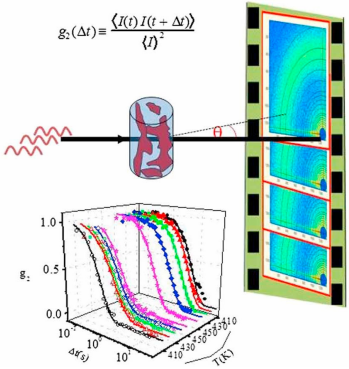
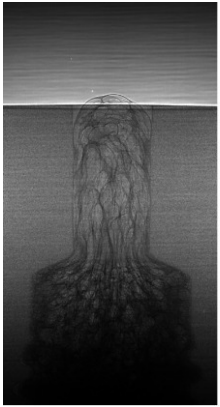
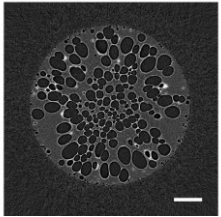


- signal processing before compression can become key
  (denoising with AI, quantisation, blocking, etc)
- lossless compression has limits $c_r = 2 - 2.5$
  (with btune possibly $c_r = 3 - 4$)
- sometimes simple filters help
  (dictionary coding when only unique values are stored, currently missing from hdf5 plugins)

Lossy Compression: Are metrics enough?

X-Ray Tomography dataset on evolving magma
[Pistone et al., 2021]





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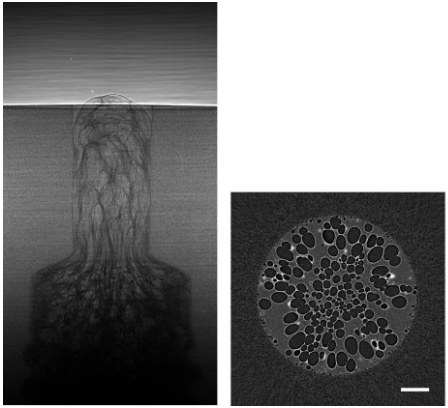
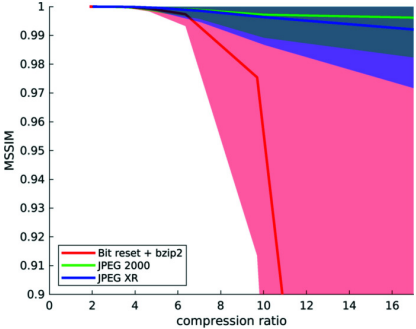


Compression Working Point Scan
[Marone et al., 2020]



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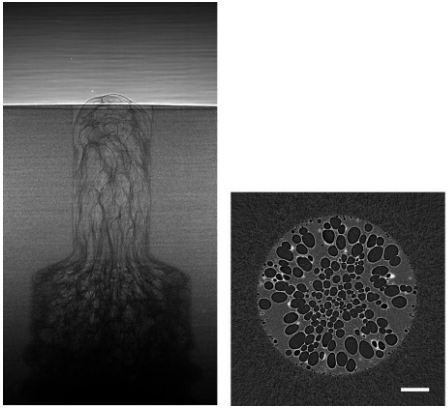

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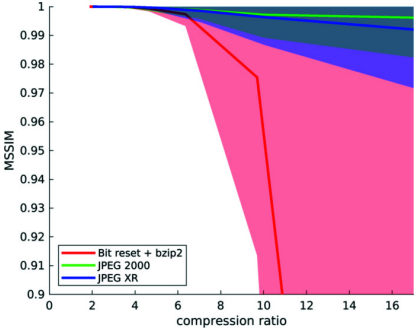
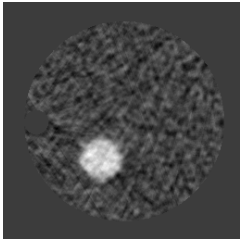


Which working point to choose? What is the impact on (downstream) science?

End-to-End Lossy Compression Workflow



X-Ray Tomography ROFEX,
1 timepoit $= 15000 \times 256 \times 256$,
`float32`, 3750 MB

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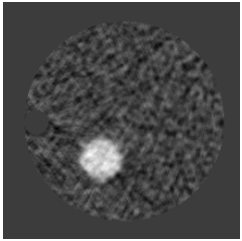

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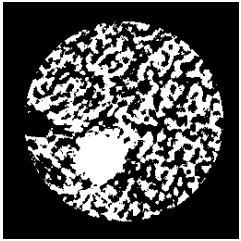
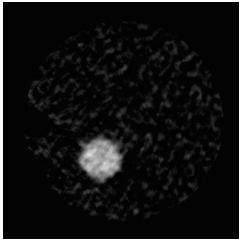
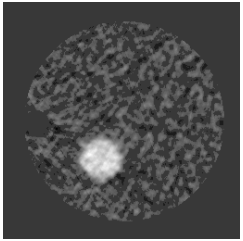


Otsu-Thresholding



Quantise `float32` to `uint8`



zip compress, 214 MB, $c_r \approx 17.5$

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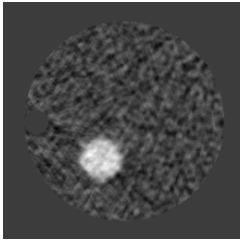

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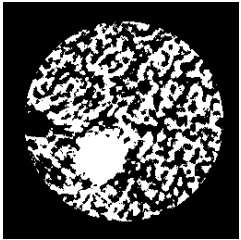

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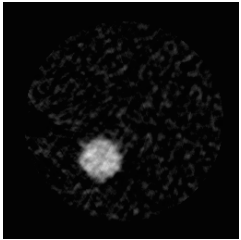

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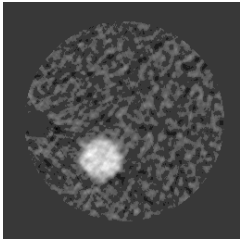

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Does lossy compression impact science output?

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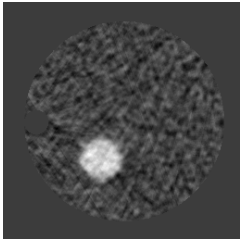

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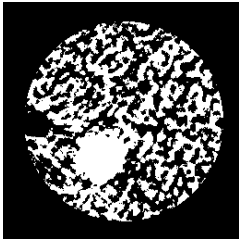

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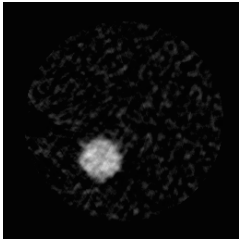

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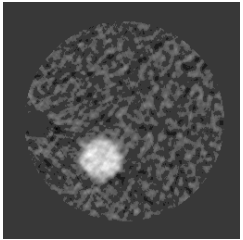

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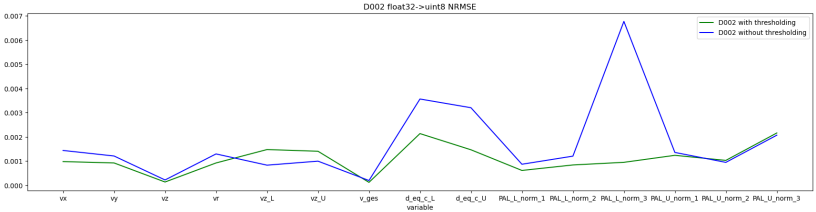
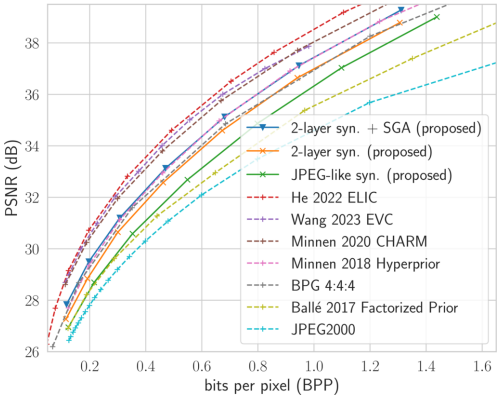
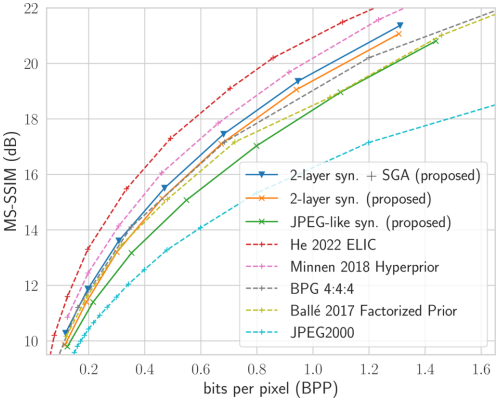


New Kids on the Block: Neural Compressors

Rate-Distortion performance on Kodak [Yang and Mandt, 2023]





New challenges: Store model, sampling distribution and encoded data!

Summary

- high bandwidth detectors and simulations proliferate
- photon science is a diverse field with respect to data generation bandwidths
- lossless compression remains a first solid choice
  (albeit with humble compression ratios)
- scalable and reproducbile signal processing pipelines required for lossy compression
  (important: end-to-end quality assurance to sustain scientific outputs)

Thank you for your attention!
Happy to hear your thoughts, feedback, questions and concerns!
Or reach out by , , !

References (I)

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