HPC & AI ENABLED SCIENCE AT THE ADVANCED PHOTON SOURCE

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https://cai.xray.aps.anl.gov/

Argonne NATIONAL LABORATORY 75 1946–2021

HPC+AI unlocks new scientific capability from existing instruments

WE BUILD AS A TEAM

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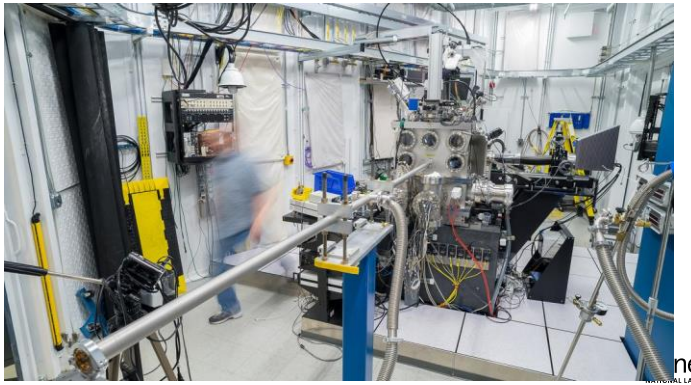
Zichao Di

And many others…

THE ADVANCED PHOTON SOURCE @ ARGONNE



ADVANCED PHOTON SOURCE

68
X-ray beamlines

5,500
Unique users
in a typical year

6,000
Experiments
per year

2,000
Publications
per year

Countless
Societal impacts

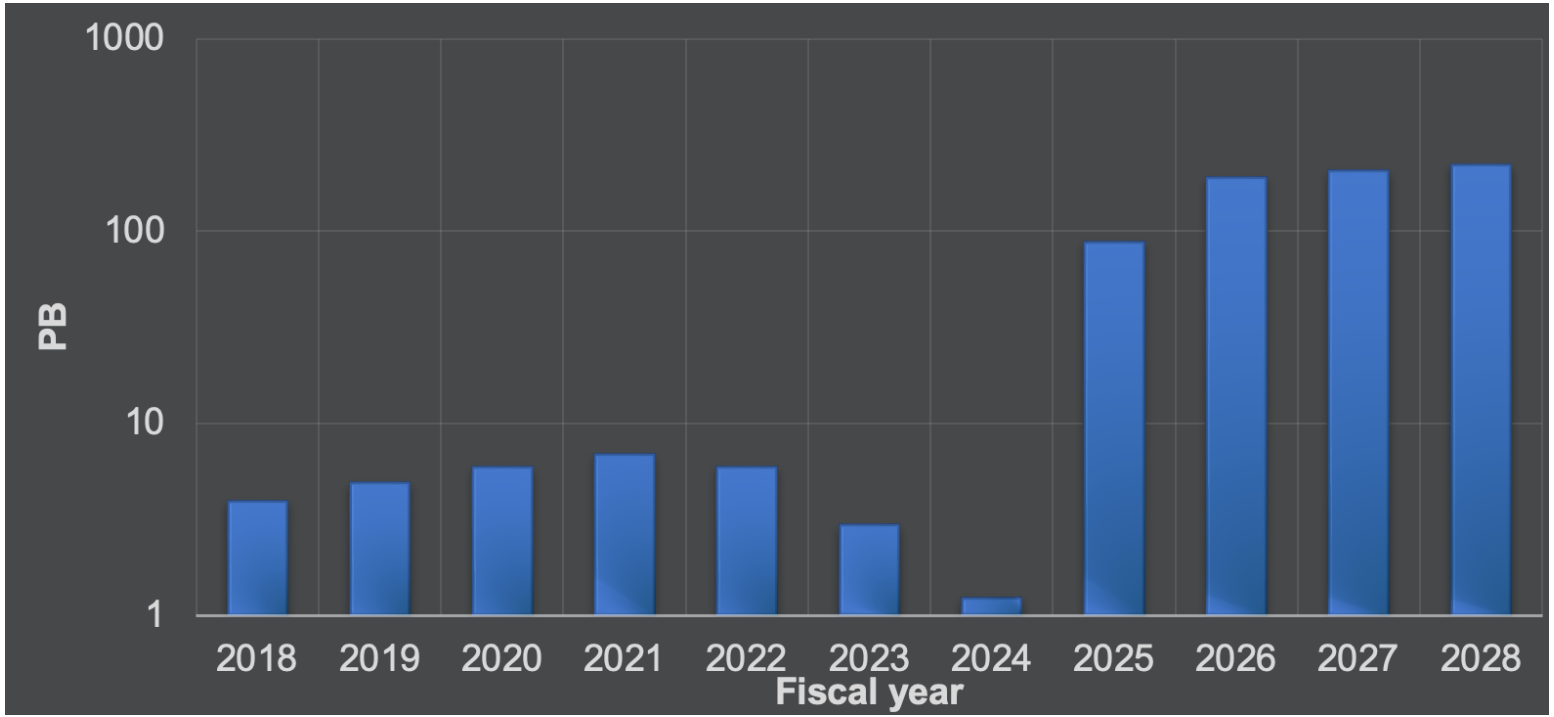
X-RAY LIGHT SOURCES OF THE WORLD

- >50 across the world
- Current and future upgrades to increase brightness and coherence
- Enable scale-bridging, multi-modal view of materials operando
- **APSU >500X coherent flux**

Source: Xu, W., et al. "The complexity of thermoelectric materials: why we need powerful and brilliant synchrotron radiation sources?." Materials Today Physics 6 (2018): 68-82.

Introduction

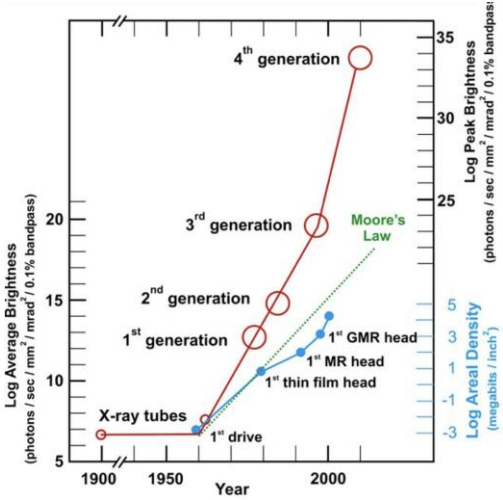
The APS anticipates collecting 100s of petabytes of raw data per year requiring 10s of petaflops of on-demand computing power per year



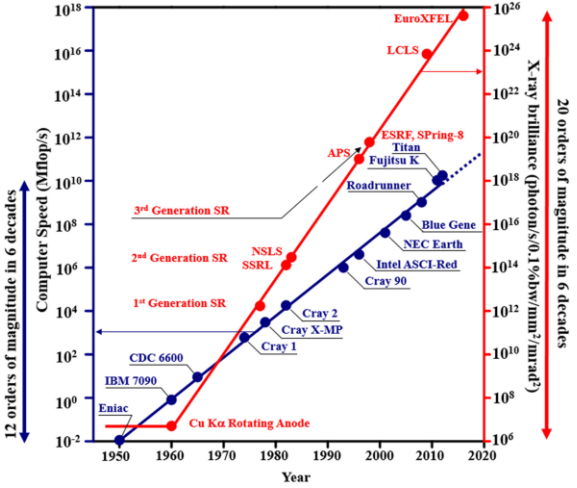
Slide from Nicholas Schwarz, APS, ANL

WHY HPC+AI?

Light source Compute needs outpace Moore's law



http://archive.synchrotron.org.au/images/AOF2017/Boland---AOF---Future-light-sources-2017-05-29.pdf



https://www.physics.ucla.edu/research/imaging/research_CDI.html

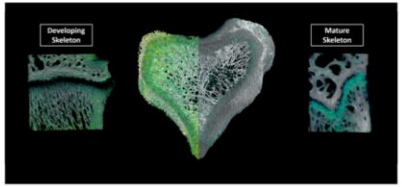
Oleg Shpyrko Ph.D thesis: https://arxiv.org/abs/cond-mat/0407333

We need to rethink *how* we do data analysis → NN models 100-1000X faster than conventional methods

INVERSE PROBLEMS IN MATERIALS CHARACTERIZATION

1 **IMAGING** TAKING A SNAPSHOT

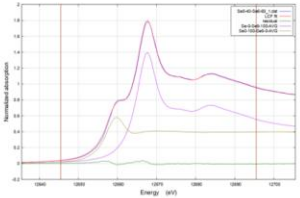
Synchrotron X-rays allow us to take an image of a sample. By studying the interaction of light with an object, we are able to get information about the structure or the function of whatever we are imaging. Our beamlines can take a picture of the tiny airways in a lung or get a three-dimensional image of materials like steel pipelines.



E.g.: Projections -> 3D image

2 **SPECTROSCOPY**
ANALYZING THE CHEMISTRY

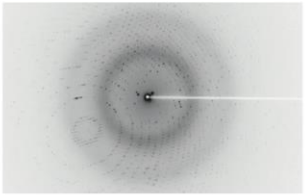
We can see how different wavelengths of light interact with matter, allowing us to analyze what the sample is made of. With spectroscopy we can look at the matter inside of a lentil or model the molecules that exist in space.



Spectra -> chemical composition

3 **DIFFRACTION AND SCATTERING**
UNDERSTANDING THE STRUCTURE

Sometimes light can bounce off a sample and create a unique pattern. This pattern allows us to gain insight into the structure of the object. With diffraction and scattering we are able to understand the shapes of proteins inside of living things or visualize the structure of crystalized materials.



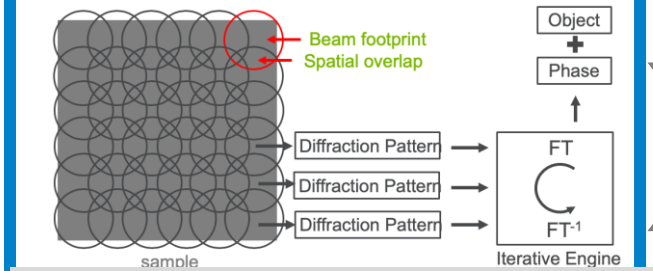
Diffraction -> atomic structure

Source: https://www.lightsource.ca/public/images-pdfs-tour-posters/2020.light.pdf

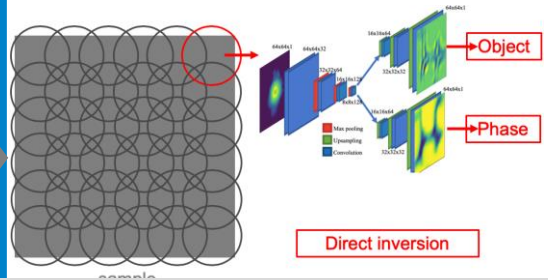
REINVENTING X-RAY DATA ANALYSIS WITH AI

AI4Analysis

Iterative



Single-shot



Cherukara, M. J., Zhou, T., Nashed, Y., Enfedaque, P., Hexemer, A., Harder, R.J., and Holt., M.V "AI-enabled high-resolution scanning coherent diffraction imaging." *Applied Physics Letters* 117, no. 4 (2020): 044103.

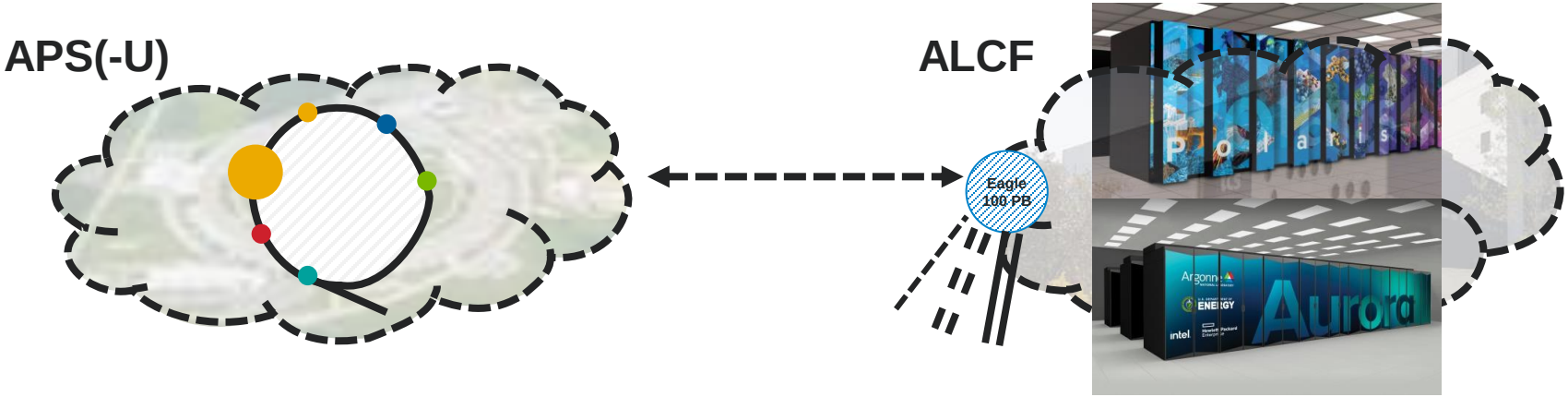
Sinogram
Diffraction
Spectra

3D image
Structure
Composition, Oxidation state etc.

PtychoNN is >100X faster
Needs 25X less data

POLARIS – INSTRUMENT 2 EDGE (I2E)

Tightly coupling APS instruments with ALCF supercomputers

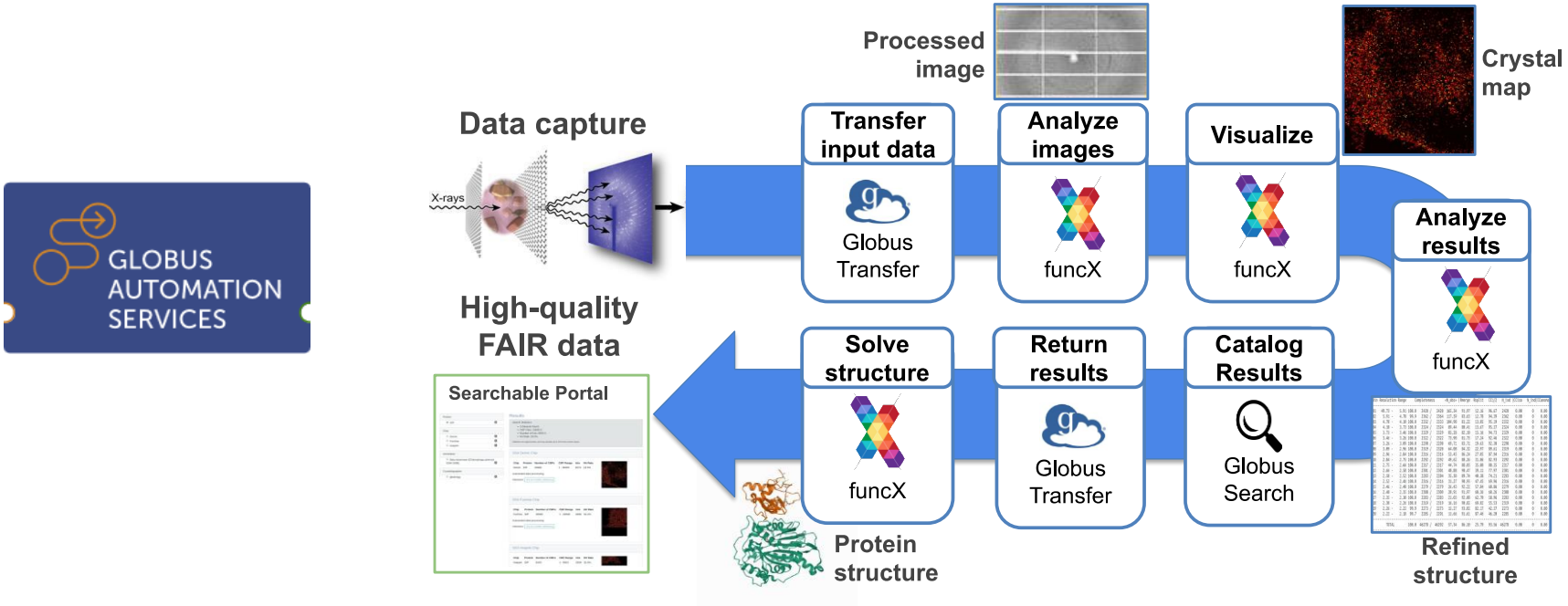


Workflows:

- Scalable software solutions for inverse problems
- Online and offline AI model training at scale
  - Deploy at edge
- 50+ people working across divisions

Data Management

Leveraging Globus as a computational fabric to enable computing



AI4Analysis

HPC + AI@EDGE ENABLES REAL-TIME PTYCHOGRAPHY

Train AI @ ALCF, deploy AI @ beamline

SCAN ME

Real-time imaging: >100X faster than phase retrieval

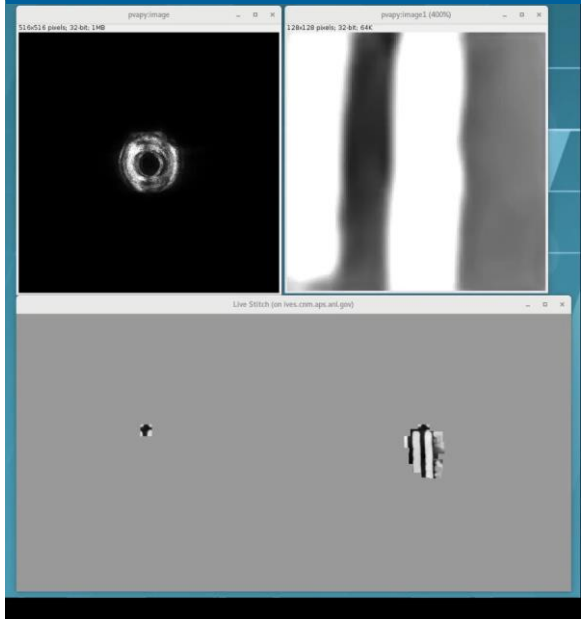
*Live inference at **8 KHz** on 128x128 detector images (8 Gb/s)*

A. V. Babu, T. Zhou, S. Kandel, T. Bicer, Z. Liu, W. Judge, D. Ching, Y. Jiang, S. Veseli, S. Henke, R. Chard, Y. Yao, E. Sirazitdinova, G. Gupta, M. V. Holt, I.T. Foster, A. Miceli and M. J. Cherukara, “Deep learning at the edge enables real-time, streaming ptychography”, *Nature Communications*, 14, 7059 (2023).

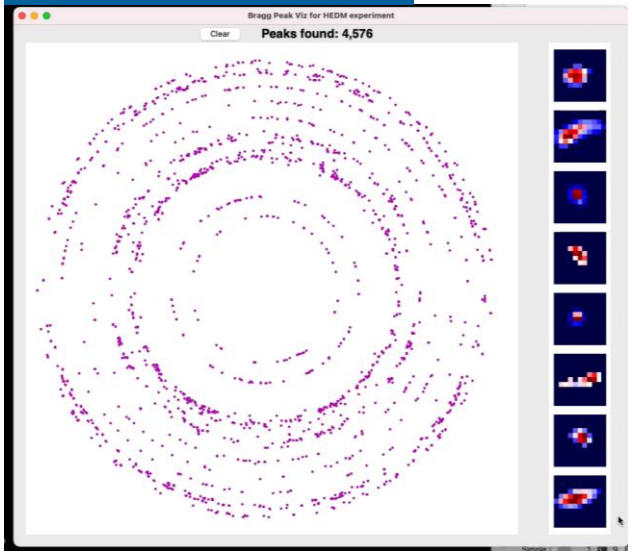
AI@EDGE ENABLES REAL-TIME ANALYSIS

Train AI @ ALCF, deploy AI @ beamline

PtychoNN: Ptychography



BraggNN : HEDM



A. V. Babu, T. Zhou, S. Kandel, T. Bicer, Z. Liu, W. Judge, D. Ching, Y. Jiang, S. Veseli, S. Henke, R. Chard, Y. Yao, E. Sirazitdinova, G. Gupta, M. V. Holt, I.T. Foster, A. Miceli and M. J. Cherukara, “Deep learning at the edge enables real-time, streaming ptychography”, *Nature Communications*, 14, 7059 (2023).

Liu, Z., Sharma, H., Park, J.S., Kenesei, P., Miceli, A., Almer, J., Kettimuthu, R. and Foster, I., BraggNN: fast X-ray Bragg peak analysis using deep learning. *IUCrJ, 9(1), pp.104-113. (2022)*

AI4Analysis

HPC+AI@EDGE TRANSFORMS EXPERIMENTAL SCIENCE

No HPC

- Reconstruction time: days-weeks
- Data needed: full

HPC

- Reconstruction time: minutes-hours
- Data needed: full

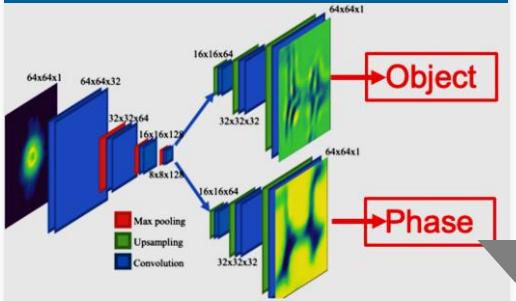
HPC+AI@Edge

- Reconstruction time: **milliseconds**
- Data needed: >25X less

A. V. Babu, T. Zhou, S. Kandel, T. Bicer, Z. Liu, W. Judge, D. Ching, Y. Jiang, S. Veseli, S. Henke, R. Chard, Y. Yao, E. Sirazitdinova, G. Gupta, M. V. Holt, I.T. Foster, A. Miceli and M. J. Cherukara, “Deep learning at the edge enables real-time, streaming ptychography”, *Nature Communications*, 14, 7059 (2023).

END-TO-END HPC+AI-POWERED X-RAY SCIENCE

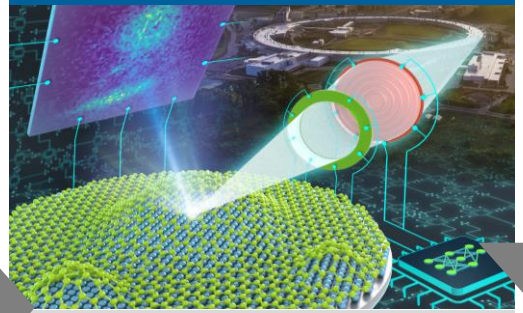
AI4Analysis



- AI@Edge: >100X faster & (sometimes) more accurate analysis
- Enables real-time analysis on Gb/s data streams

A. Babu, T. Zhou et al., *Nature Comm., 14, 7059 (2023)*

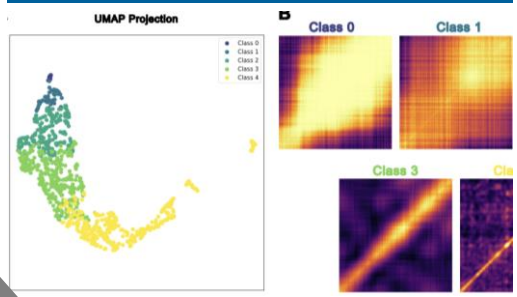
AI4Steering



- AI@Edge: Self-driving experiments and instruments: maximize info gain in minimal time

S. Kandel et al., *Nature Comm., 14(1), p.5501 (2023)*

AI4Knowledge



- Learn material physics directly from measurements

Horwath, J.P., et al. *Nature Comm.*, 15, 5945 (2024)

CALMS: Retrieval & Tool Augmented LLM