ARGONNE-ILLINOIS TECH RESEARCH SEMINAR SERIES

Argonne NATIONAL LABORATORY

SCIENTIFIC COMPUTING AND WORKFLOWS AT THE EDGE (AND BEYOND)

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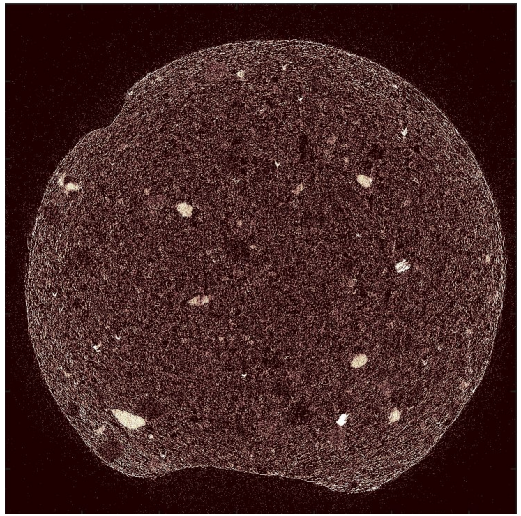
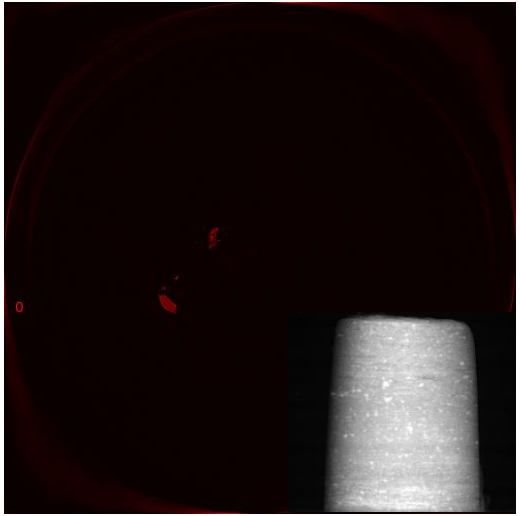
RESEARCH & DEVELOPMENT ACTIVITIES

- High-performance, parallel and distributed computing; scientific computing runtime systems; Application of AI/ML to X-ray
- (Large-scale) X-ray image analysis problems
  - Inverse problems
- Scientific workflows
  - Edge to Supercomputers
  - Federated facilities: Leadership Computing



Charcoal Reconstruction (mCT)
200-250 GB

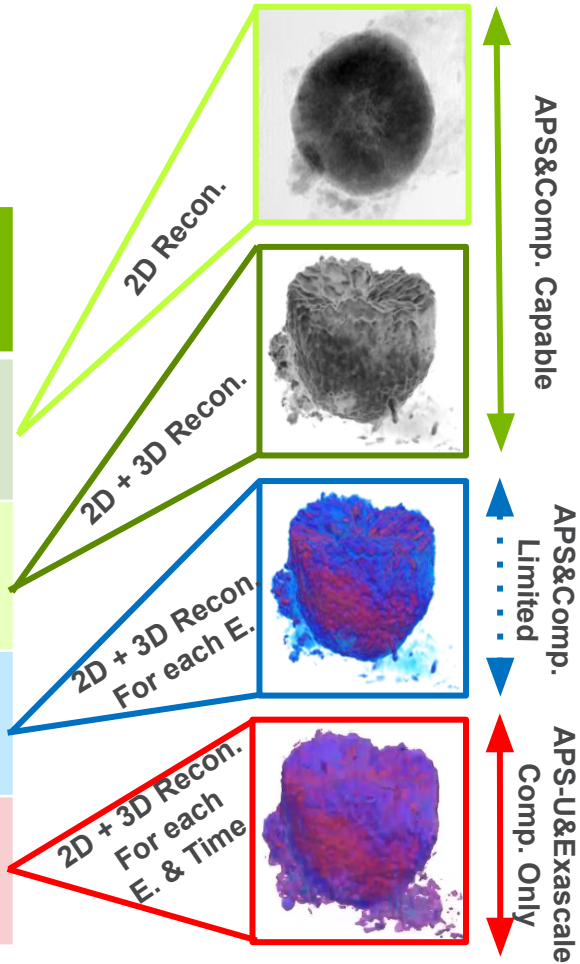


Shale Reconstruction (mCT)
10-15 GB
2-3 days of processing

EXPERIMENTAL AND COMP. CHALLENGES IN MULTI-DIMENSIONAL PTYCHOGRAPHY

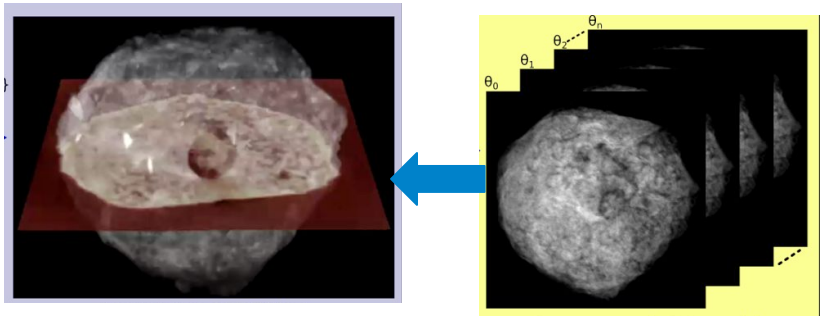
Experimental Configuration	Experiment Time	Dataset Size	Analysis Times*
2D Single View	2 mins	5 GB	~2 mins
3D Mult. Views (MV)	12 hours (360 Views)	1.8 TB	12 hours
4D MV + Mult.E. (ME)	25 days (+ 50 E.)	90 TB	1 month
5D MV + ME + Time	1250 days (50 Time)	4.5 PB	3.5 years

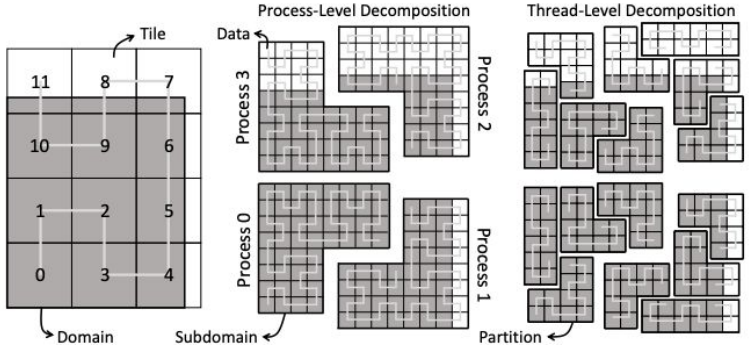
* (estimation) based on 10 GPUs

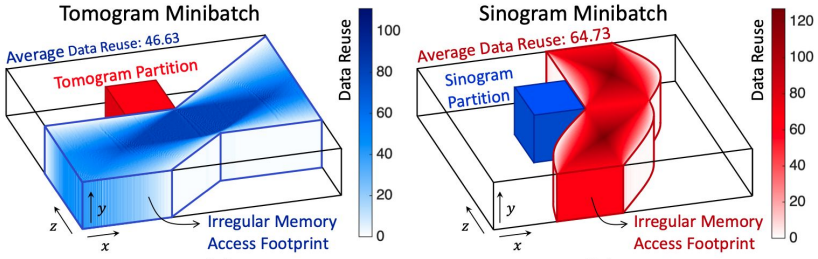


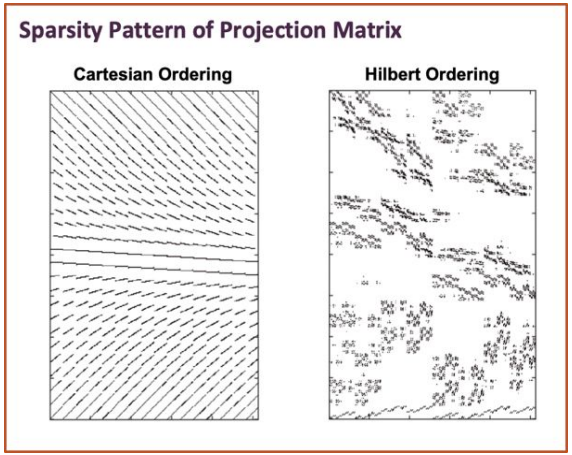
(IRREGULAR) DATA ACCESS PATTERN

Optimization with Hilbert Ordering



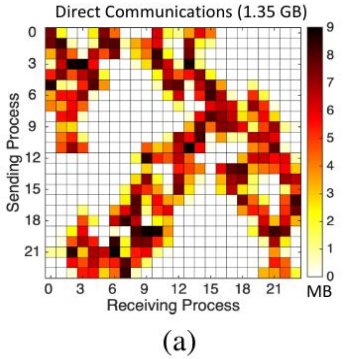






COMMUNICATION PATTERN IN 3D RECONS.

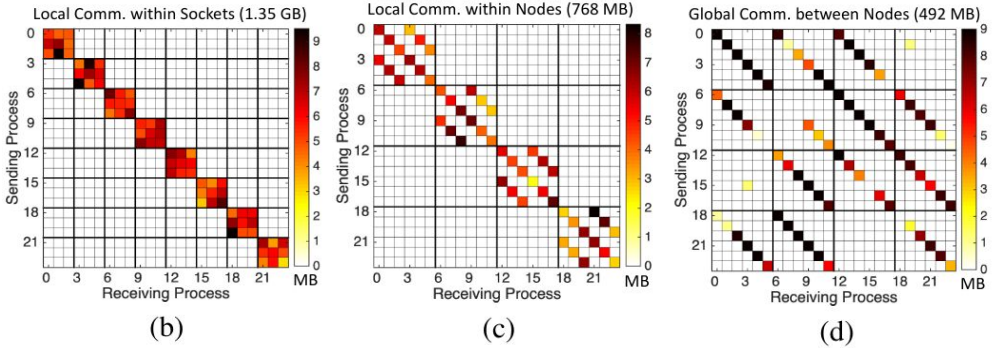
Multi-level Hierarchical Communication

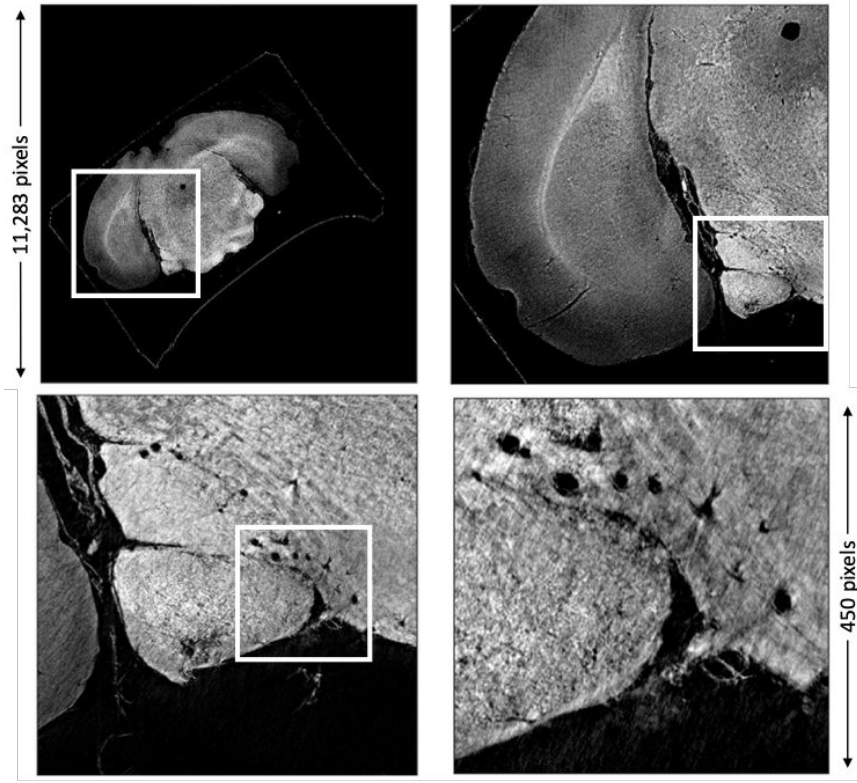


- 3-level of communication and reduction
- Overlapping communication
- Mixed-precision implementation

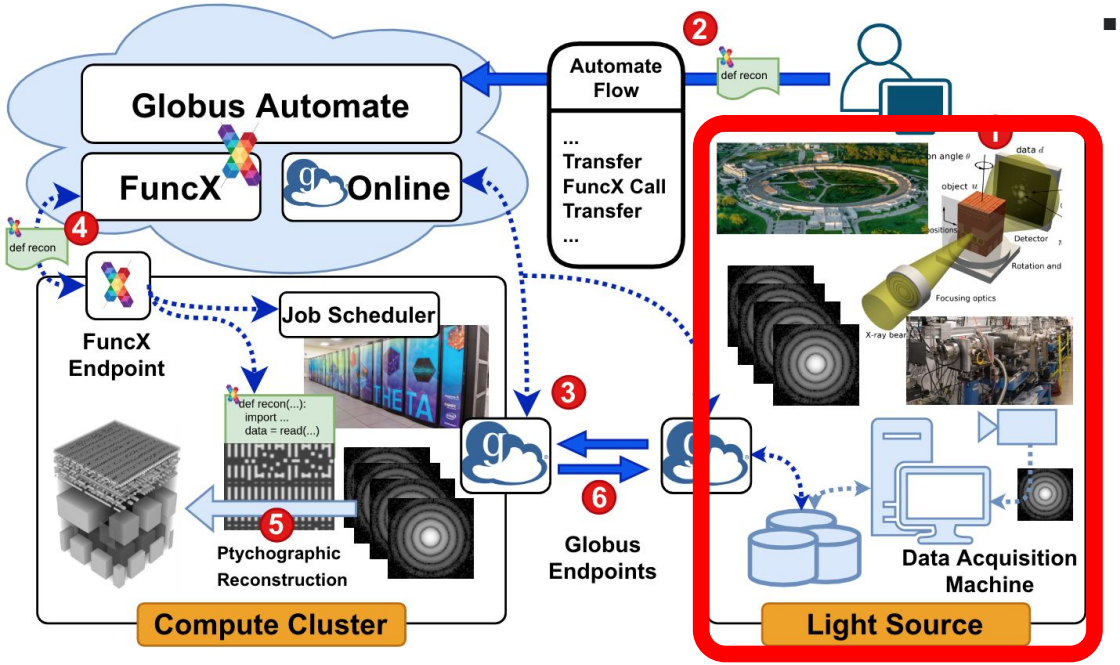
- 24K GPUs, >65PFLOPS; <3 mins.

Supercomputer

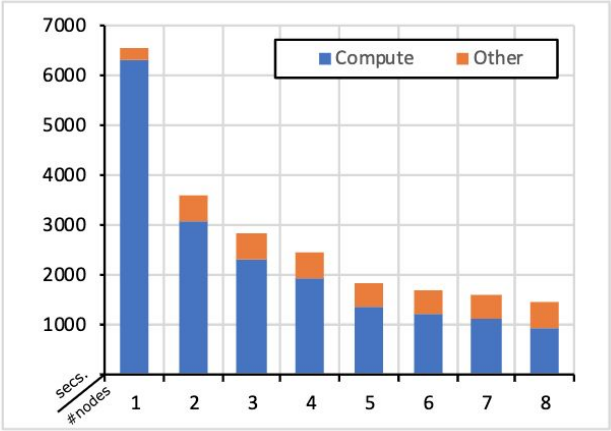




WORKFLOW SYSTEM FOR IMAGE DATA ANALYSIS



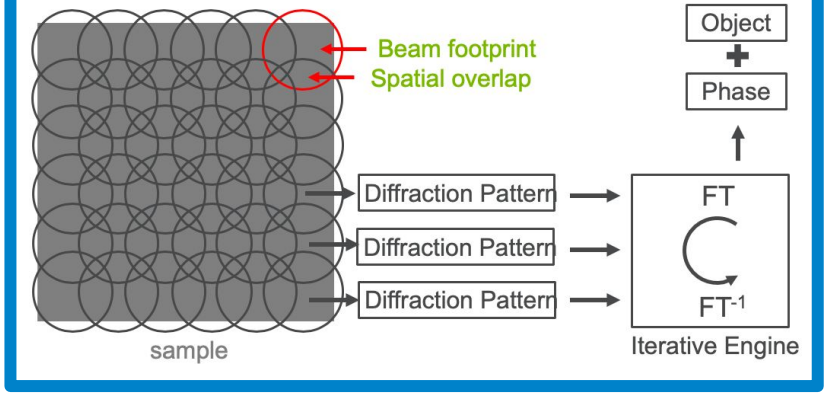
- System components
  - Globus Automate
  - FuncX
  - Globus Transfer
  - Globus Auth



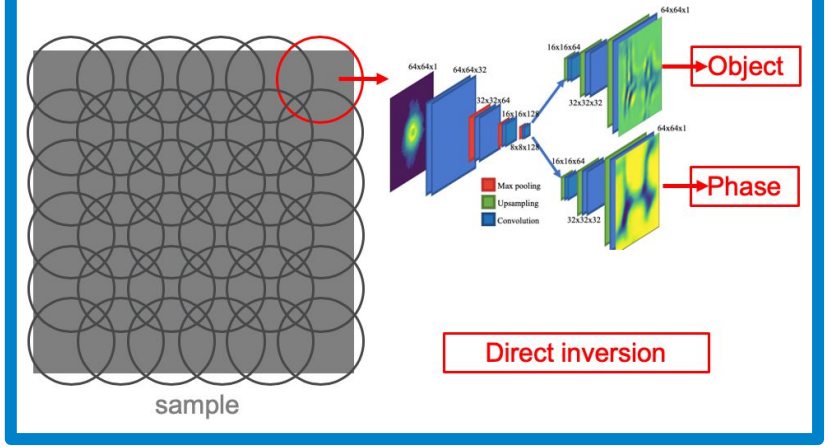
Tekin Bicer et al., "High-Performance Ptychographic Reconstruction with Federated Facilities," Smokey Mountain Conference 2021

REINVENTING COHERENT IMAGING DATA INVERSION

Ptychographic recon.



AI-driven

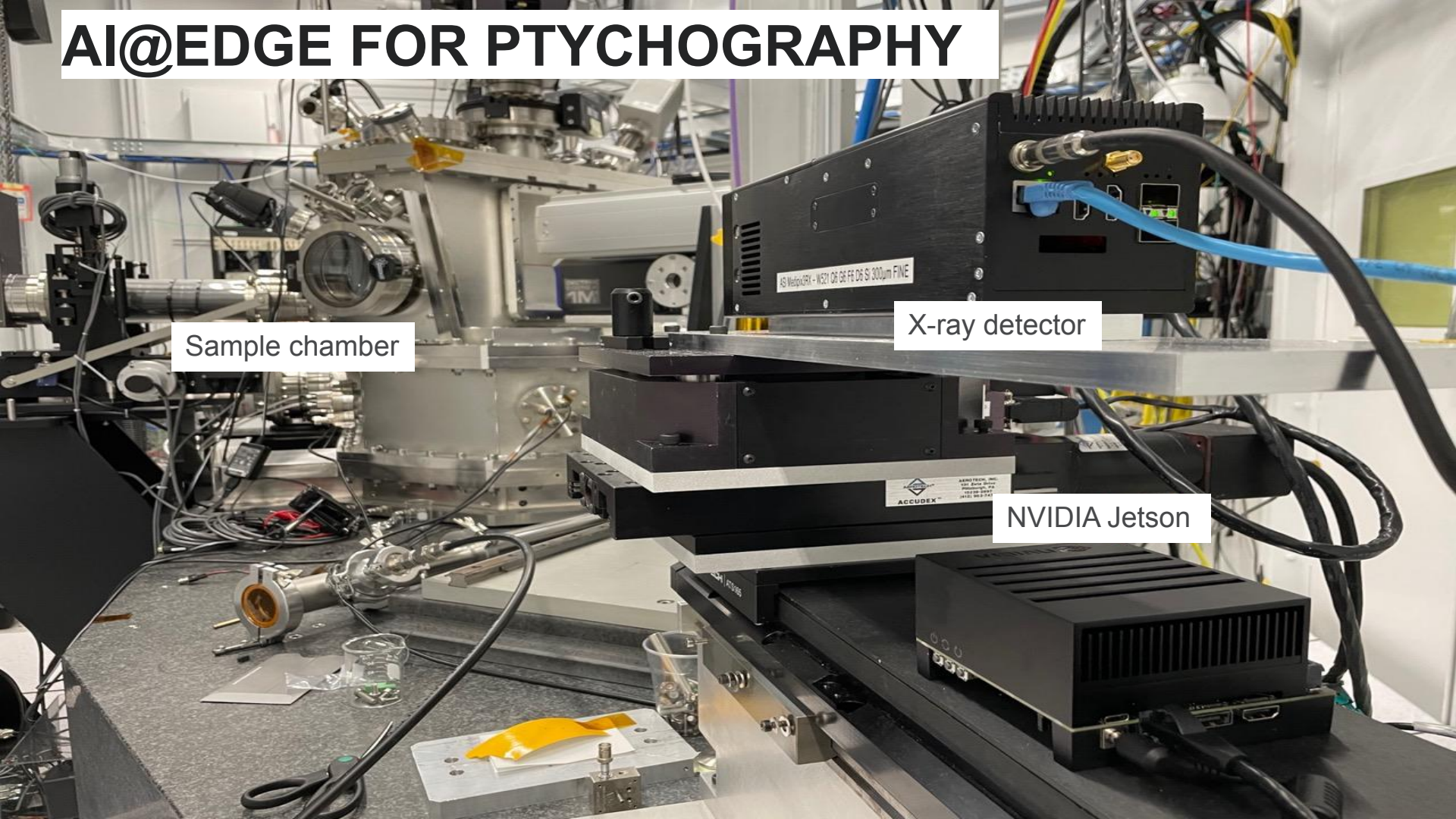


Requires >PFLOPs of on-demand to keep up with experiments

PtychoNN is >100X faster
Requires 25X less data

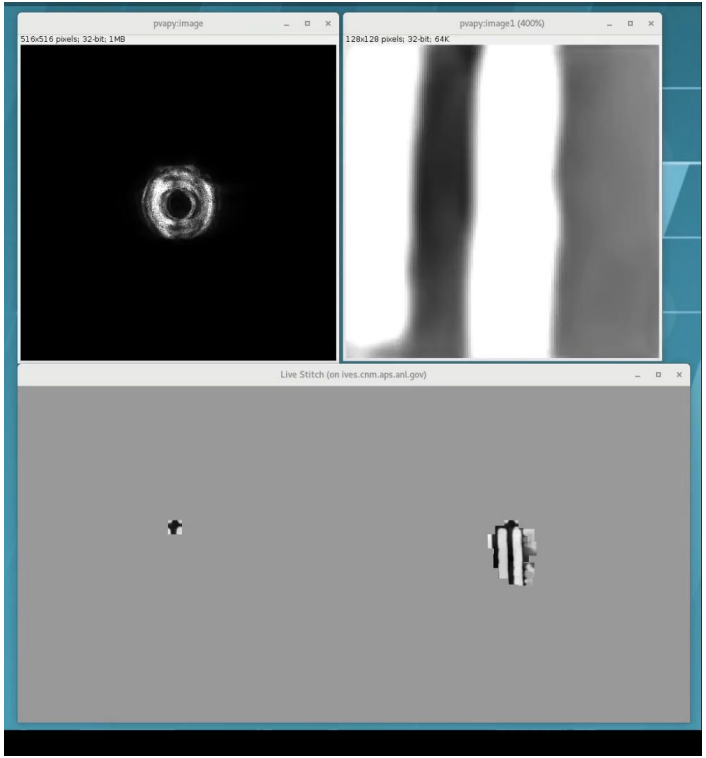
Cherukara, Mathew J., Tao Zhou, Youssef Nashed, Pablo Enfedaque, Alex Hexemer, Ross J. Harder, and Martin V. Holt. "AI-enabled high-resolution scanning coherent diffraction imaging." *Applied Physics Letters* 117, no. 4 (2020): 044103.

AI@EDGE FOR PTYCHOGRAPHY



AI-Accelerated Ptychography Workflows

Train AI @ ALCF, deploy AI @ beamline



- Real-time imaging: >100X faster than phase retrieval
  - Live inference at 100 Hz on 512x512 detector images (1 Gb/s)
- Lower-dose imaging : 25X less data than phase retrieval
- Future work: other techniques, closed-loop experimental steering

Anakha V. Babu, Tao Zhou, Saugat Kandel, Yi Jiang, Yudong Yao, Sinisa Veselli, Zhengchun Liu, Tekin Bicer, Francesco deCarlo, Ekaterina Sirazitdinova, Geetika Gupta, Martin V. Holt, Antonino Miceli and Mathew J. Cherukara, "Real-time nanoscale ptychographic X-ray imaging using deep learning at the edge"

PtychoNN: Mathew J. Cherukara, Tao Zhou, Youssef Nashed, Pablo Enfedaque, Alex Hexemer, Ross J. Harder, and Martin V. Holt. "AI-enabled high-resolution scanning coherent diffraction imaging." *Applied Physics Letters* 117, no. 4 (2020): 044103.

TAKE-AWAY MESSAGES

- Collaboration opportunities
  - HPC for large-scale data analysis
  - Runtime and workflow systems
  - AI/ML accelerated data analysis
  - Experimentation steering
- Focus on synchrotron radiation (X-ray) imaging problems
- Very diverse set of collaborators
  - Computer, computational, beamline scientists and experts

- APS: Anakha V. Babu, Tao Zhou, Saugat Kandel, Yi Jiang, Yudong Yao, Junjing Deng, Daniel Ching, Jeff Klug, Doga Gursoy, Sinisa Veselli, Francesco de Carlo, Martin V. Holt, Antonino Miceli, Nicholas Schwarz, Stefan Vogt and Mathew J. Cherukara
- DSL: Zhengchu Liu, Joaquin Chung, Xiaodong Yu, Rajkumar Kettimuthu, Ian T. Foster
- Mert Hidayetoglu (UIUC), Wen-mei W. Hwu (UIUC), Bin Ren (W&M), Simon Garcia de Gonzalo (BSC)
- Argonne Leadership Computing Facility
- and many others!