Argonne NATIONAL LABORATORY | APS

HIGH PERFORMANCE COMPUTING AND ARTIFICIAL INTELLIGENCE-ENABLED SCIENCE AT THE APS

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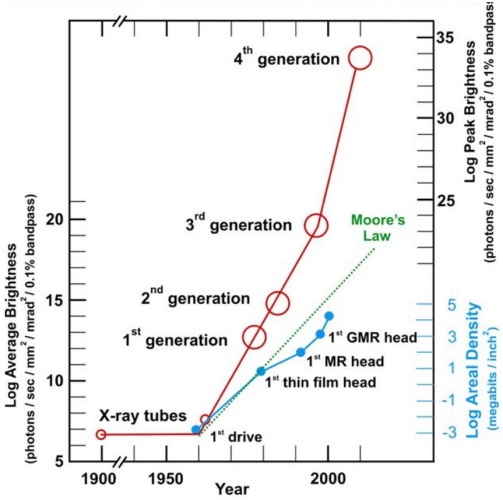
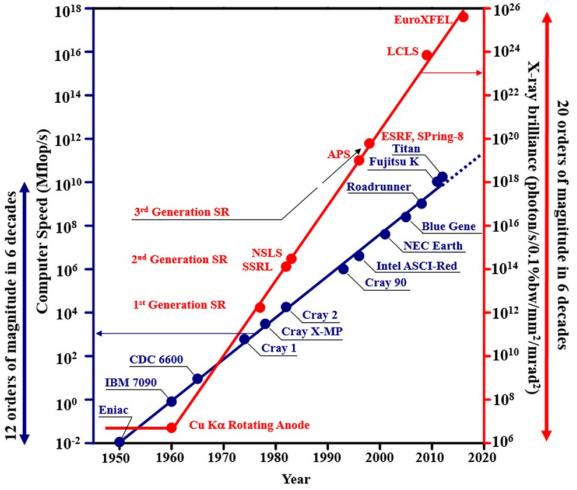
X-ray Science Division

LIGHT SOURCE COMPUTE NEEDS OUTPACE MOORE'S LAW

Why HPC + AI?



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

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**

HPC:

- Polaris: top 20 supercomputer
- Aurora: coming soon

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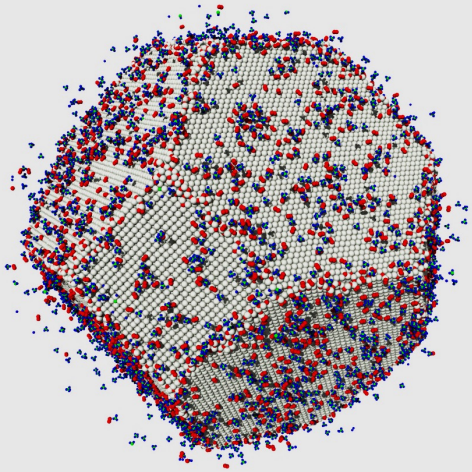
NOVEL SCIENTIFIC INSTRUMENTS ENABLED BY HPC AND AI

16 nm IC, scan field of view 50 um

J. Klug, Y. Jiang, D. Sherrell et al, ANL/LANL collaboration

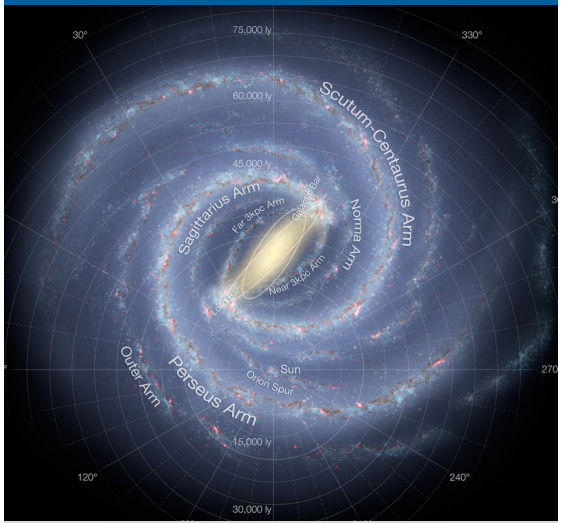
COSMIC SCALE NAVIGATION AT THE NANOSCALE

3D ATOMIC imaging



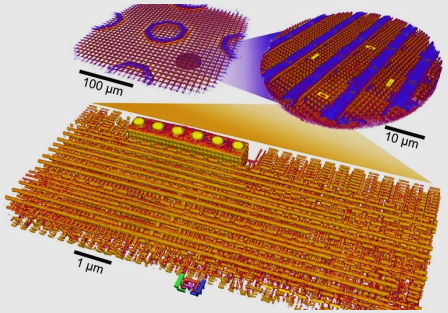
~10^9 atoms

Milky Way



~10^{11} stars

Full component imaging



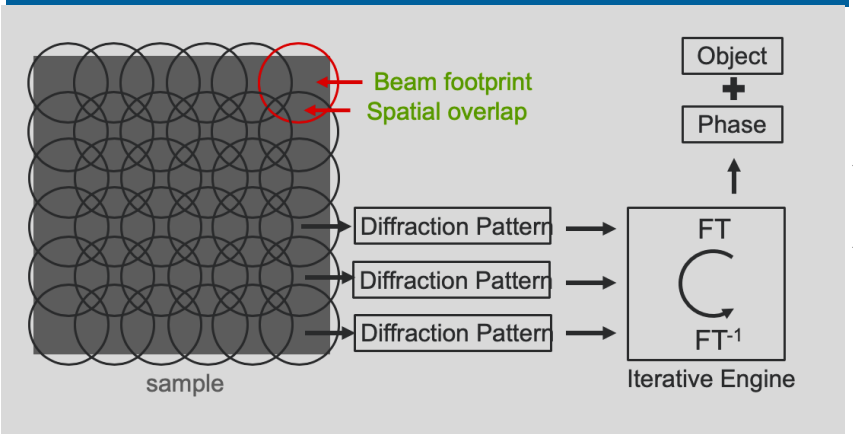
https://www.nature.com/articles/nature21698
https://spectrum.ieee.org/xray-tech-lays-chip-secrets-bare

>10^{12} voxels

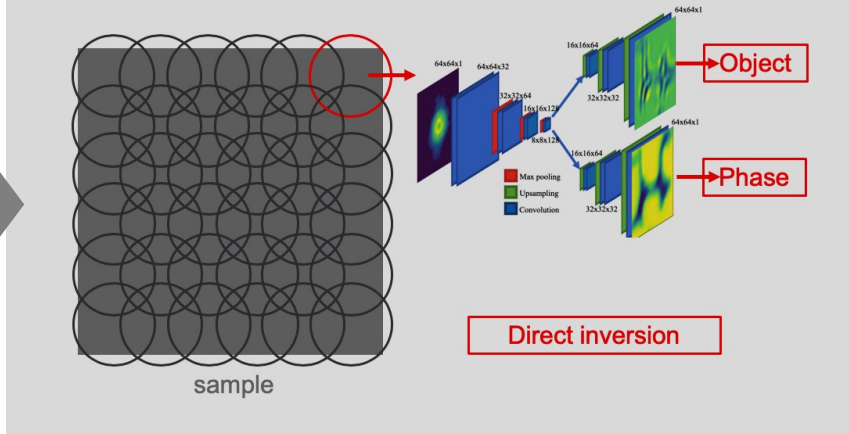
REINVENTING X-RAY DATA ANALYSIS WITH AI

AI4Analysis

Phase retrieval



AI driven



PtychoNN is >100X faster
Needs 25X less data

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.

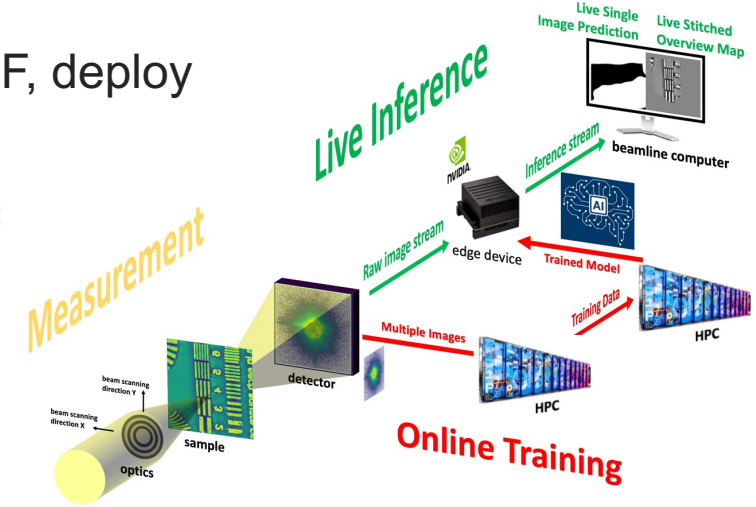
HPC + AI@EDGE ENABLES REAL-TIME PTYCHOGRAPHY

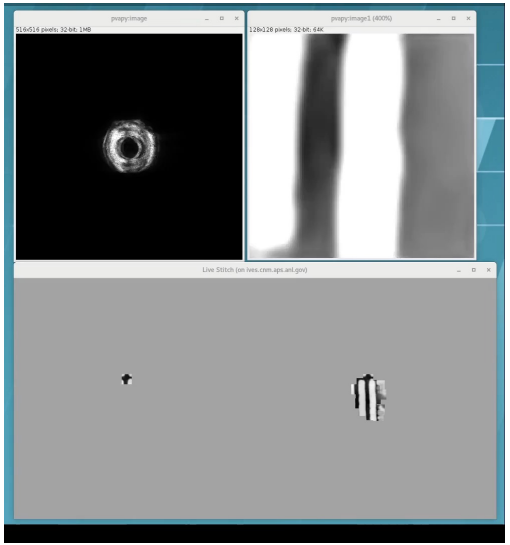
AI4Analysis

Train AI @ ALCF, deploy AI @ beamline

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).

HPC+AI@EDGE TRANSFORMS EXPERIMENTAL SCIENCE

AI4Analysis

No HPC

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

HPC

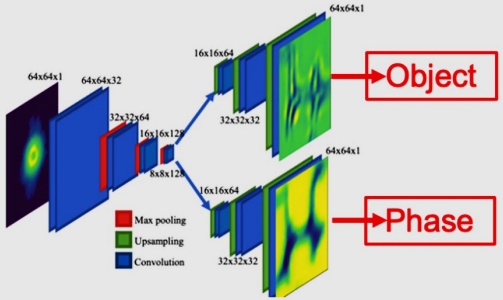
- Reconstruction time: minutes-hours
- Data needed: full

HPC+AI@Edge

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

REAL-TIME ANALYSIS ENABLES SMARTER EXPERIMENTS

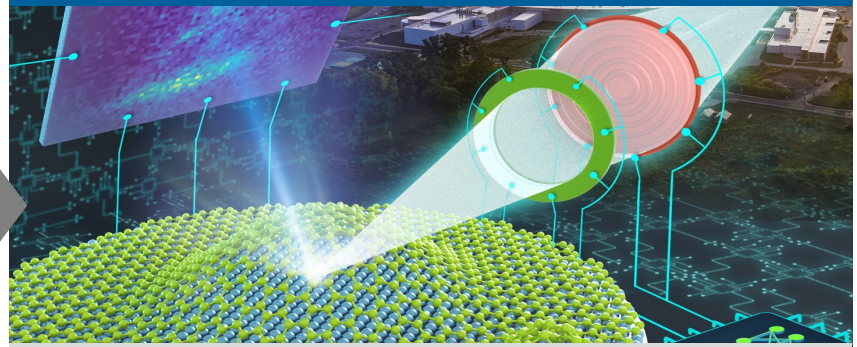
AI4Analysis



- AI@Edge: >100X faster and (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)*

UNDERSTAND HOW AND WHY MATERIALS FAIL

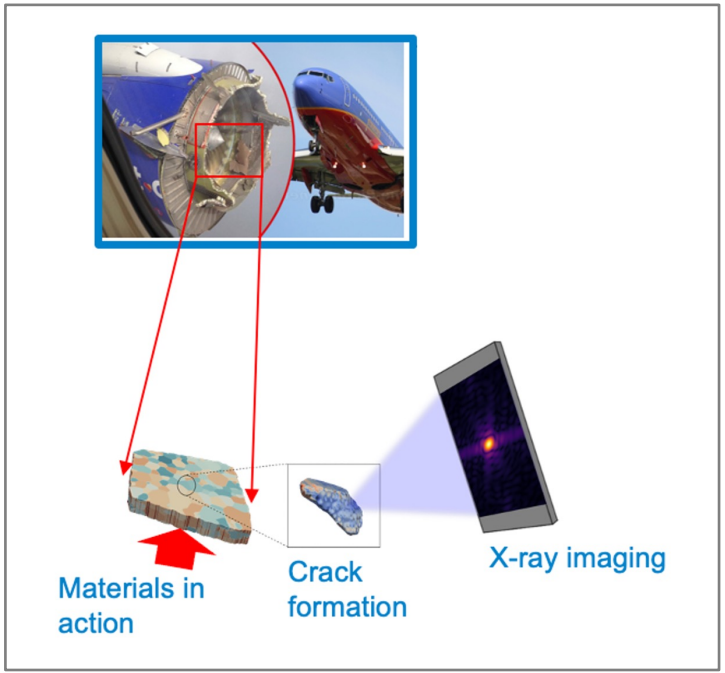


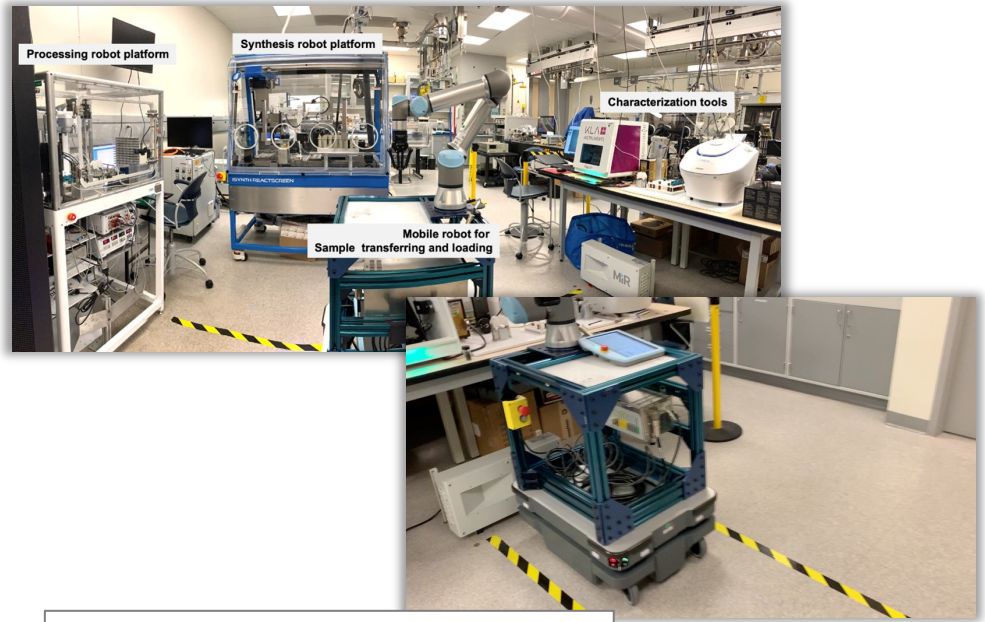
Image adapted from: Jon Almer, Stephan Hruszkewycz et al., ANL

APS-U beamlines will have the *potential* to answer these questions

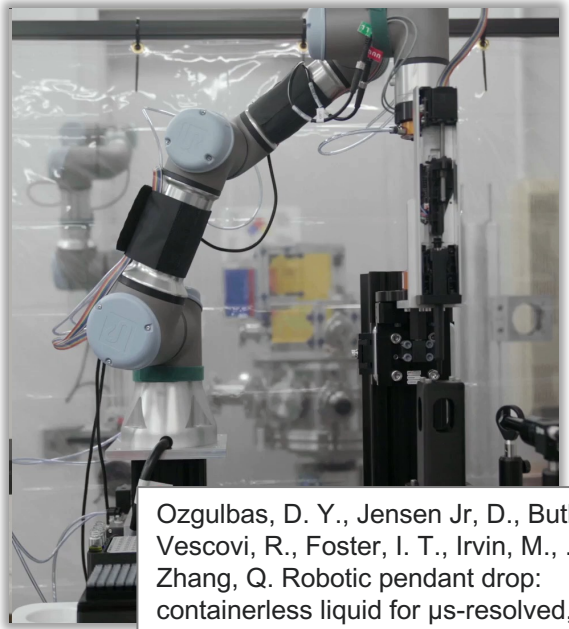
How do you *effectively* target the instrument across >10^{12} voxels?

AI-steering of experiments to prioritize relevant data

AUTONOMOUS DISCOVERY EXPANDS THE SPACE OF POSSIBLE SAMPLES



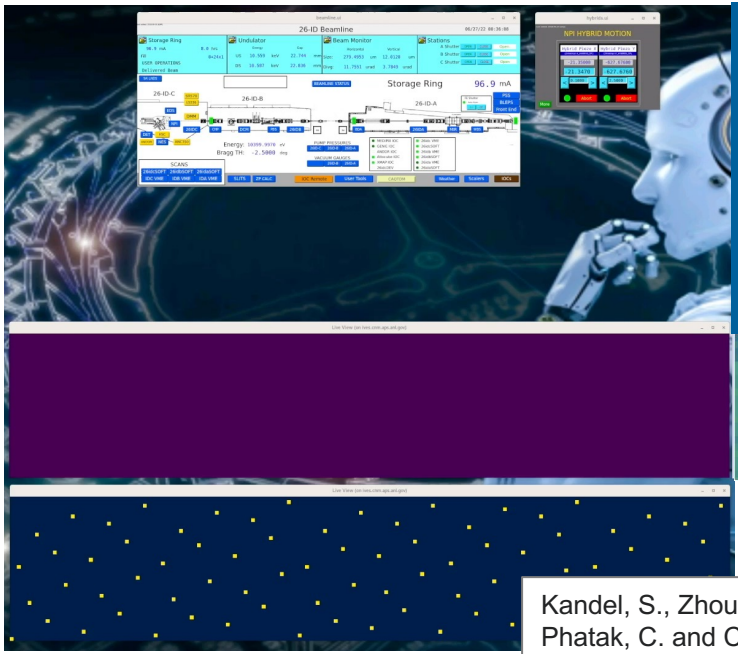
Jie Xu et al: https://www.anl.gov/cnm/polybot



Ozgulbas, D. Y., Jensen Jr, D., Butler, R., Vescovi, R., Foster, I. T., Irvin, M., ... & Zhang, Q. Robotic pendant drop: containerless liquid for μs-resolved, AI-executable XPCS. *Light: Science & Applications,* 12(1), 196. (2023).

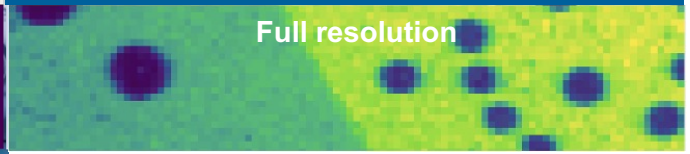
AI@EDGE DRIVES EXPERIMENTS

AI4Steering



FAST

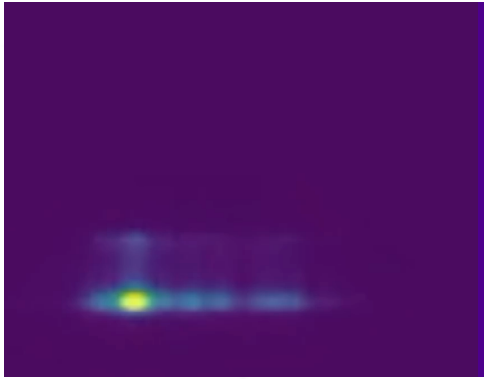
- Fast Autonomous Scanning Toolkit
- Beamline control turned over to NN
- **4.3X less time/dose**



Kandel, S., Zhou, T., Babu, A.V., Di, Z., Li, X., Ma, X., Holt, M., Miceli, A., Phatak, C. and Cherukara, M., Demonstration of an AI-driven workflow for autonomous high-resolution scanning microscopy, *Nature Communications*, 14(1), p.5501 (2023)

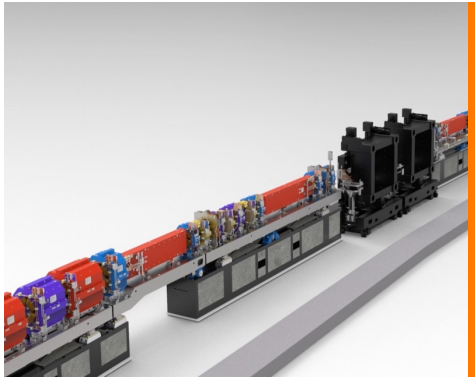
AI@EDGE CREATES BETTER INSTRUMENTS

AI4Steering



AutoFocus

- Online tuning of KB mirror focusing



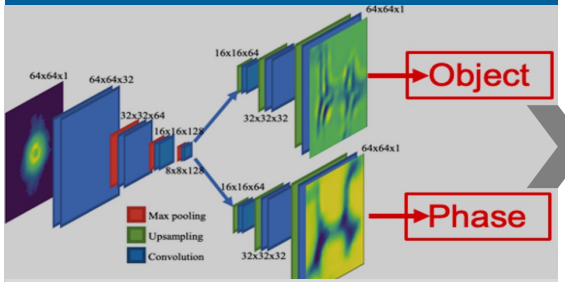
Accelerator Steering

- Efficient power operation
- Predicting power trips

Rebuffi, L., Kandel, S., Shi, X., Zhang, R., Harder, R.J., Cha, W., Highland, M.J., Frith, M.G., Assoufid, L. and Cherukara, M.J., AutoFocus: AI-driven alignment of nanofocusing X-ray mirror systems. *Optics Express*, 31(24), pp.39514-39527 (2023)

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

AI4Analysis



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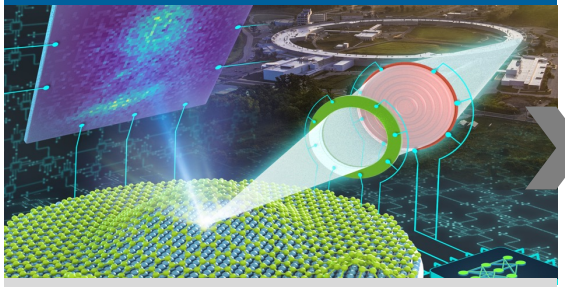

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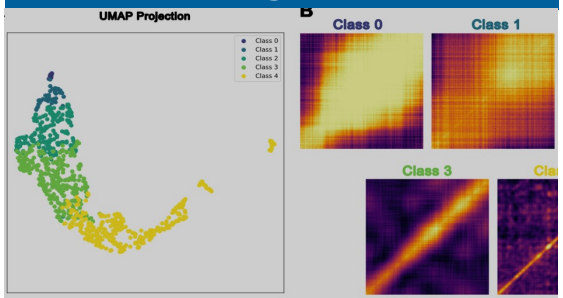
  - maximize info gain in minimal time

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

AI4Knowledge



- Learn material physics directly from measurements

Horwath, James P., et al. arXiv preprint arXiv:2212.03984 (2022).
N. Andrejevic et al. arXiv preprint arXiv:2311.14196 (2023)

OUR CODE + DATA + TRAINED MODELS ALWAYS FREE AND OPEN-SOURCE

WE BUILD AS A TEAM

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Hemant Sharma
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Henry Chan
Howard Yanxon
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Ti Leggett
Tim Mooney
Todd Munson
Tomas Walsh
William Allcock
Xianbo Shi
Xuli Wu
Yi Jiang
Yudong Yao
Zhengchun Liu
Zichao Di

And many others…