HPC & AI ENABLED MATERIALS CHARACTERIZATION AND EXPERIMENTAL AUTOMATION

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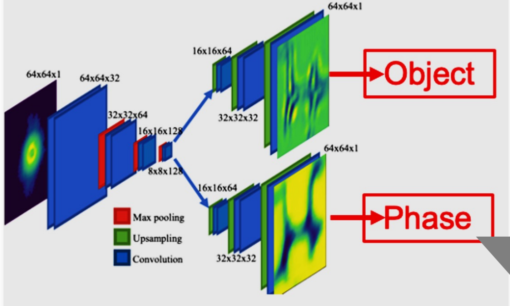
CAI https://cai.xray.aps.anl.gov/

Argonne NATIONAL LABORATORY 75 1946–2021

HPC+AI unlocks new scientific capability from existing instruments

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

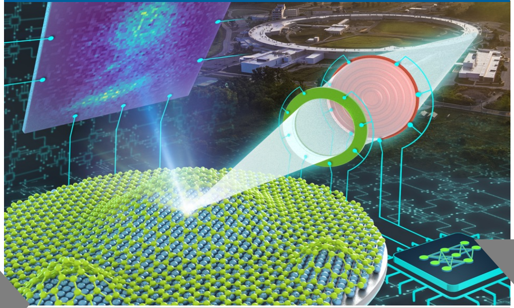
AI4Analysis



- 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)*

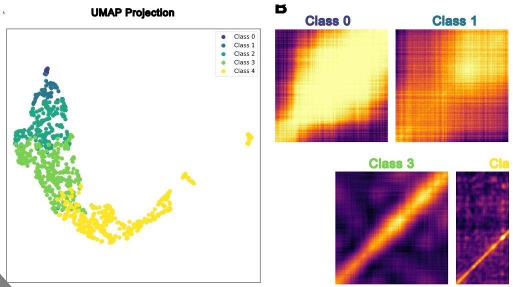
AI4Steering



- 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

ACKNOWLEDGEMENTS

APS@ANL: Antonino Miceli, Barbara Frosik, Yi Jiang, Steven Henke, Sinisa Veseli, Daniel Ching, Ross Harder, Jay Horwath, Zichao Di (also MCS), Hemant Sharma, Xianbo Shi, Luca Rebuffi


Anakha Babu (now KLA)


Saugat Kandel (now C-Z Imaging)


Yudong Yao (now ShanghaiTech)


Tekin Bicer (also DSL)


Michael Prince

MCS@ANL: Prasanna Balaprakash (now ORNL)

DSL@ANL: Zhengchun Liu (now AWS), Ryan Chard, Varuni Sastry

CNM@ANL: Subbu Sankaranarayanan, Martin Holt, Aikaterini Vriza


Tao Zhou


Henry Chan

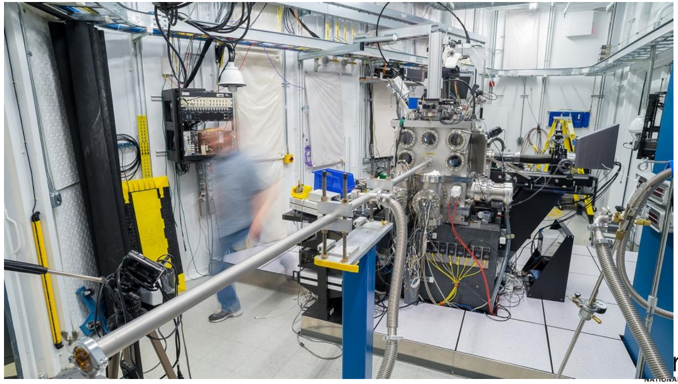
ORNL : Rama Vasudevan

LBNL: Pablo Enfedaque, Alex Hexemer

NVIDIA: Ekaterina Sirazitdinova, Geetika Gupta

FUNDING:
Argonne LDRDs: AICDI, AutoPtycho
DOE AI SUF: Digital Twin for In-Silico Experiments

THE ADVANCED PHOTON SOURCE @ ARGONNE



ADVANCED PHOTON SOURCE

68
X-ray beamlines

6,000
Experiments
per year

2,000
Publications
per year

5,500
Unique users
in a typical year

Countless
Societal impacts

X-RAY LIGHT SOURCES OF THE WORLD

- >50 across the world
- Current and future upgrades to increase brightness and coherence

- **APSU >500X coherent flux**

Enable scale-bridging, multi-modal view of materials *operando*

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.

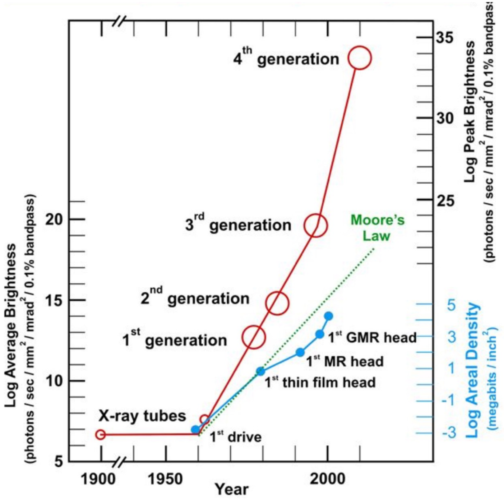
2 days to acquire, 2 months to reconstruct

16 nm IC, scan field of view 50 um

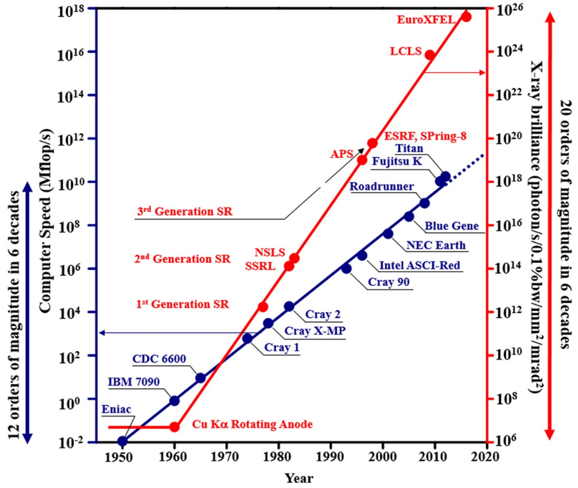
J. Klug, Y. Jiang, D. Sherrell et al, ANL/LANL collaboration

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

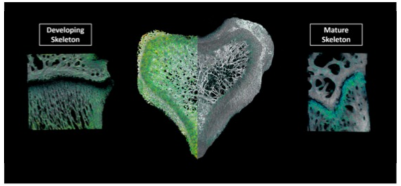
Oleg Shpyrko Ph.D thesis: https://arxiv.org/abs/cond-mat/0407333

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

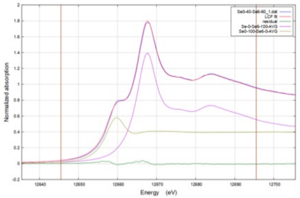
Synchrotron X-rays allow us to take an image of a sample. By studying the interaction of light with an object, we are able to get information about the structure or the function of whatever we are imaging. Our beamlines can take a picture of the tiny airways in a lung or get a three-dimensional image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



E.g.: Projections -> 3D image

2 SPECTROSCOPY ANALYZING THE CHEMISTRY

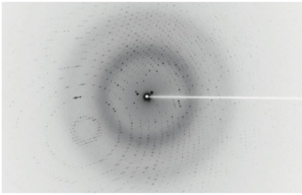
We can see how different wavelengths of light interact with matter, allowing us to analyze what the sample is made of. With spectroscopy we can look at the matter inside of a lentil or model the molecules that exist in space.



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

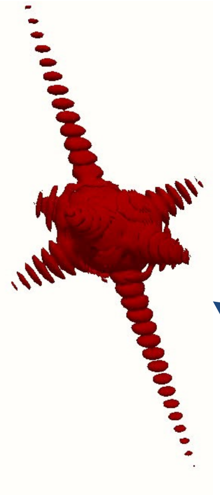
CURRENT STATE: ITERATIVE METHODS

FFT

$\tau^{(n)}$

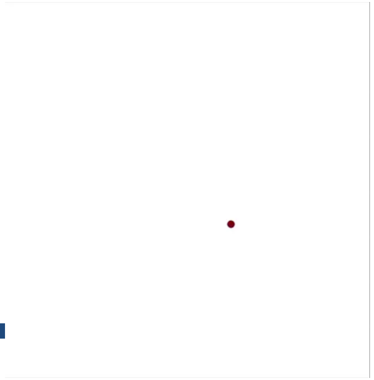
Reciprocal Space Constraints

Experimental Amplitudes
Oversampled, Thresholded, ZeroPadded



Direct Space Constraints

Evolving Support
Mixing old and new iterates.



$u^{(n)}$

FFT^{-1}

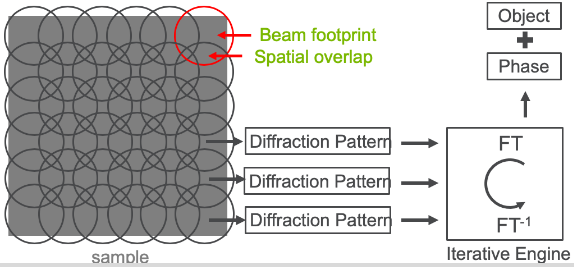
100-1000's of iterations and multiple random starts required for high fidelity data!

- Sensitive to choice of parameters: need multiple tries and expert input

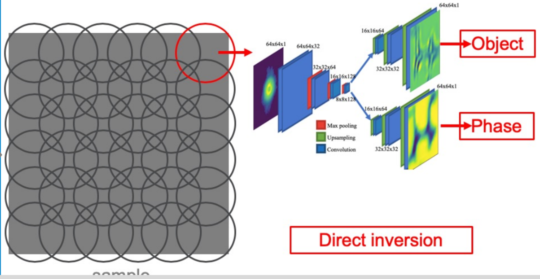
REINVENTING X-RAY DATA ANALYSIS WITH AI

AI4Analysis

Iterative



Single-shot



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.

Sinogram
Diffraction
Spectra

3D image
Structure
Composition, Oxidation state etc.

GENERALIZABILITY VS THROUGHPUT

AI4Analysis

Application Specific

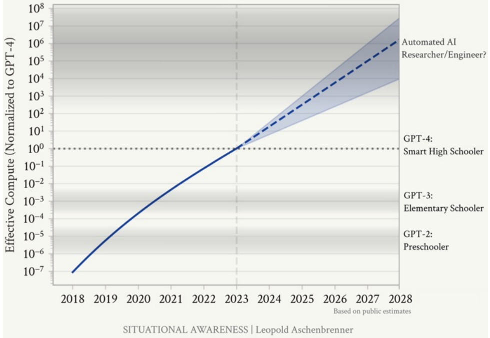
- < 1 million parameters
- Fast inference: > 1000 fps
- Poor generalizability
- Trained *online* on experiment specific data

"It shouldn't take quadrillions of operations to compute 2 + 2"

Illia Polosukhin, Co-author of "Attention is all you need" paper

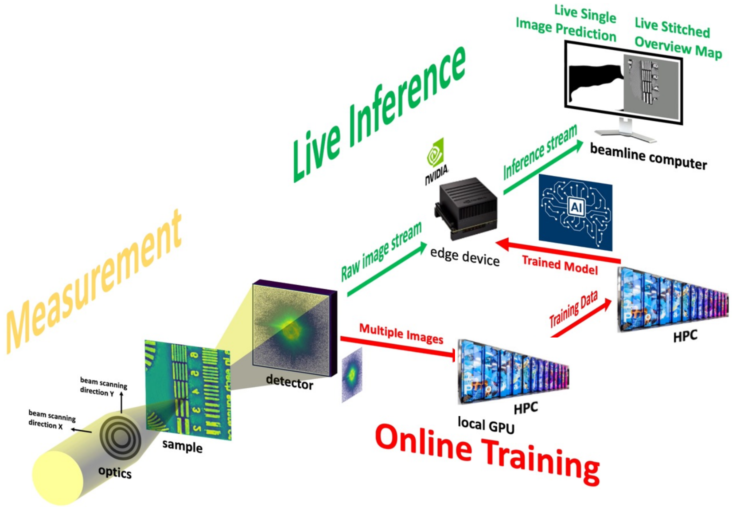
'Foundation'-like

- > 1 billion parameters
- Slow inference
- Generalizes across experiments
- Pre-trained (often unsupervised) on large corpus of simulated or experimental data

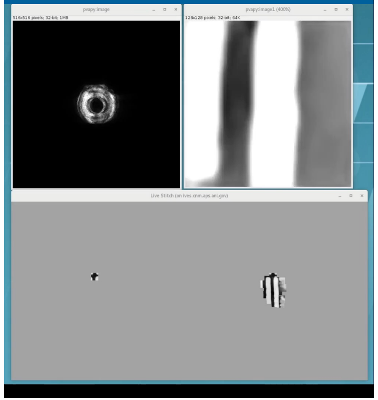


AI@EDGE ENABLES REAL-TIME ANALYSIS

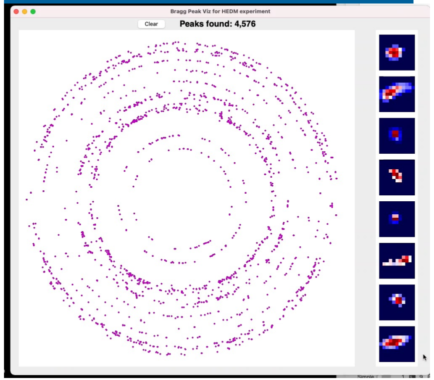
Train AI @ ALCF, deploy AI @ beamline



PtychoNN: Ptychography



BraggNN : HEDM



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).

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)*

HPC+AI@EDGE TRANSFORMS EXPERIMENTAL SCIENCE

No HPC

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

HPC

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

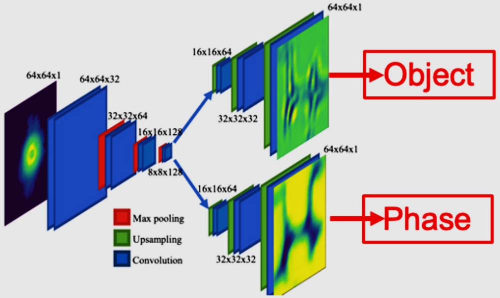
HPC+AI@Edge

- **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).

REAL-TIME ANALYSIS ENABLES SMARTER EXPERIMENTS

AI4Analysis



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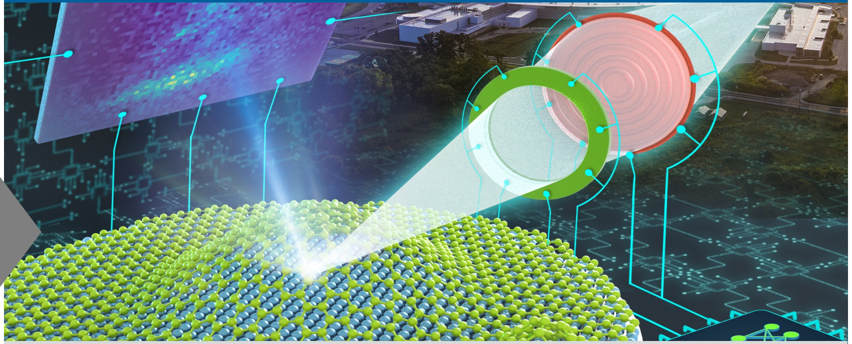

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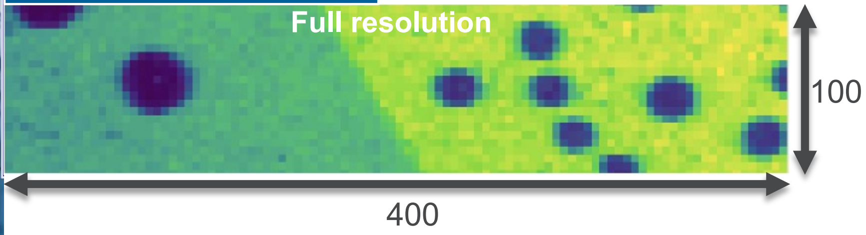
AI@EDGE DRIVES EXPERIMENTS

FAST: Fast Autonomous Scanning Toolkit

FAST

- Beamline control turned over to NN
- Decision time < 1 s
- 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)

Zhang, Y., Godaliyadda, G. M., Ferrier, N., Gulsoy, E. B., Bouman, C. A., & Phatak, C. (2018). Slads-net: supervised learning approach for dynamic sampling using deep neural networks. *Electronic Imaging*, 2018(15), 131-1.

Early experiments with LLMs as scientific co-pilots

TOWARDS A COMPLETE SCIENTIFIC AI ASSISTANT

Experiment planning

User input: What technique has been used at the APS to study butterfly wings?

LLM: The pinhole small-angle x-ray scattering technique has been used at the X-ray Science Division 8-ID-I beamline at the APS to determine the three-dimensional internal structure of scales in the wings of five butterfly species. Additionally, researchers used a powerful x-ray microscope at the APS to study the organization of the photonic crystals in the scale of the Kaiser-i-Hind butterfly, Teinopalpus imperialis, at the X-ray Science Division 2-ID-B beamline.

Experiment guidance

User input: How do I start a tomography scan?

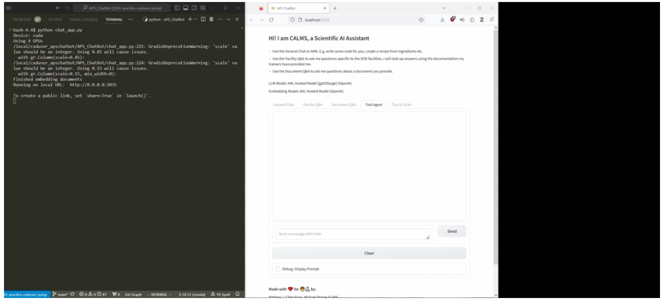
LLM: To start a tomography scan, you can enter the acquisition parameters in the tomoScan screen and press the green "Start Scan" button. Alternatively, you can run a single scan from the command line interface with the command "tomoscan single". If you want to do a vertical, horizontal, or mosaic scan, you can use the commands "tomoscan vertical", "tomoscan horizontal", or "tomoscan mosaic" respectively. You can find more details about each of these commands in the tomoScan documentation.

Operation

User input: Get the lattice parameters of WSe_2 and set the instrument peak to 012

LLM:

1. Recognizes material (WSe_2) and Bragg peak (012)
2. Calls Materials Project to get lattice parameters for WSe_2
3. Calls instrument control (Spec) and sets the diffractometer to the right location for the 012 peak.

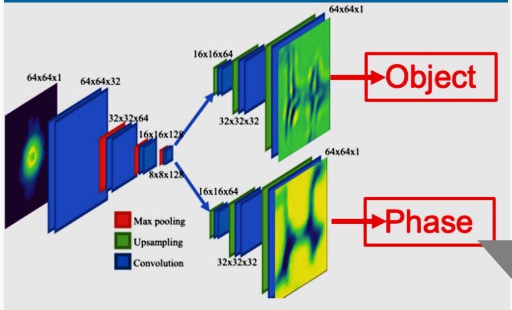


Prince, M.H., Chan, H., Vriza, A., Zhou, T., Sastry, V.K., Dearing, M.T., Harder, R.J., Vasudevan, R.K. and Cherukara, M.J., 2023. Opportunities for retrieval and tool augmented large language models in scientific facilities. *arXiv preprint arXiv:2312.01291*.

APS

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

AI4Analysis



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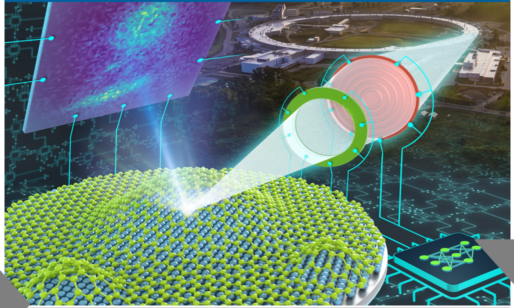

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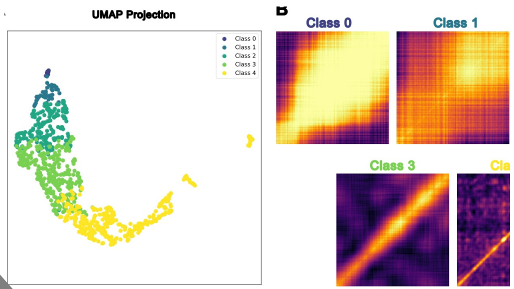
AI4Knowledge



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POSTDOC/INTERN/FELLOWSHIP POSITIONS AVAILABLE

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

MJCherukara

1. Competitive pay & 30 minutes from downtown Chicago
2. Work at the intersection of world's most advanced computing and materials characterization facilities.
3. Lab-wide prioritization of postdoc mentoring, career development and community
4. Hone your ML/data science skills

https://www.anl.gov/hr/postdoctoral-applicants