HPC+AI-ENABLED X-RAY SCIENCE

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Computational X-ray Science

Advanced Photon Source

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YudongYao

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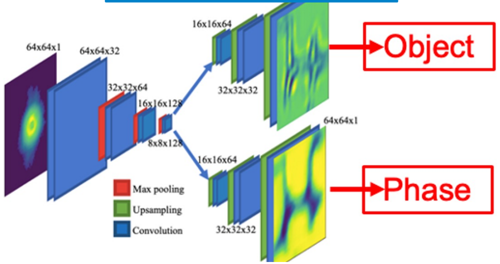
Argonne NATIONAL LABORATORY 75 1946–2021

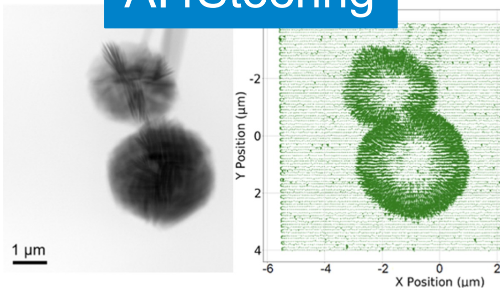
OUTLINE: AI4SCIENCE

AI4Analysis



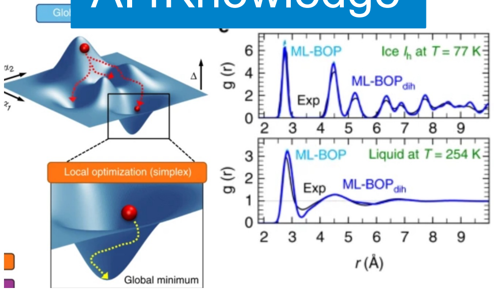
- >100X faster and (sometimes) more accurate analysis
- Enables real-time analysis on Gb/s data streams

AI4Steering



- Self-driving experiments & instruments:
  - – maximize info gain in minimal time

AI4Knowledge

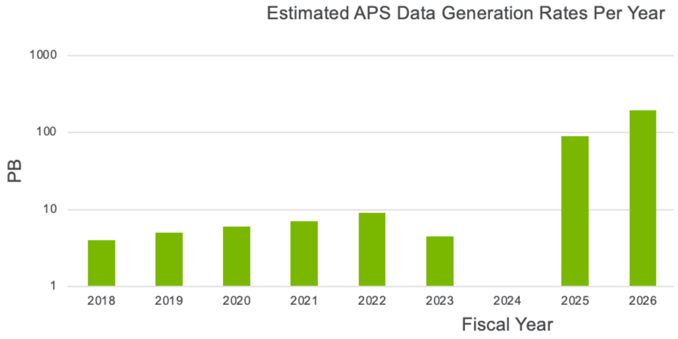


- Get more out of data
- Faster more accurate models, sharper images etc.

MOTIVATION 1: DATA RATES AND COMPUTE NEEDS

AI4Analysis

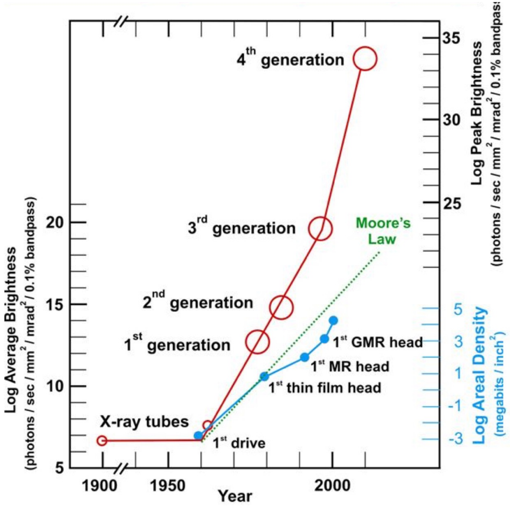
Data & compute



A single instrument (e.g Ptychography) can generate data >GB/s

- Need ~PFLOPs to analyze

APSU: 10-1000X increase in data and compute needs

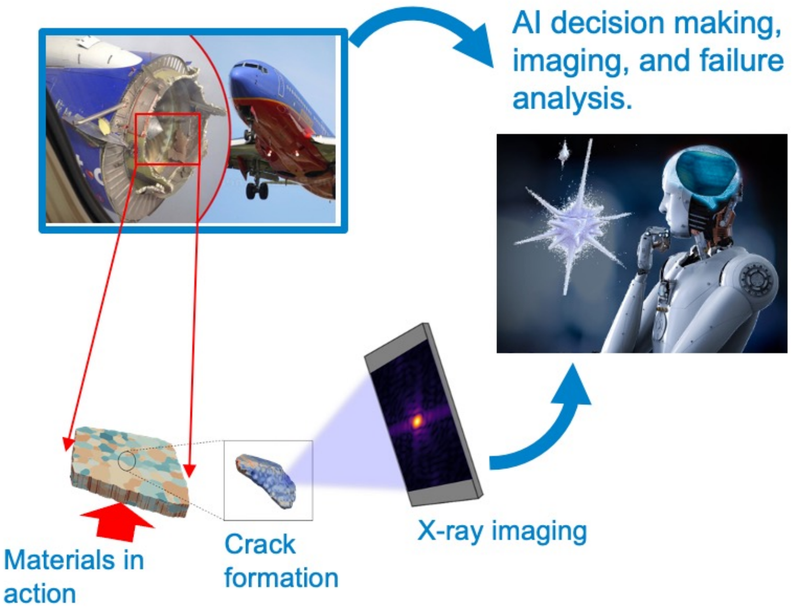


http://archive.synchrotron.org.au/images/AOF2017/Boland---AOF---Future-light-sources-2017-05-29.pdf

Data & compute rates outpace Moore's law

MOTIVATION 2: REAL-TIME FEEDBACK

Experimental steering



Autonomous experiments need real-time data inversion

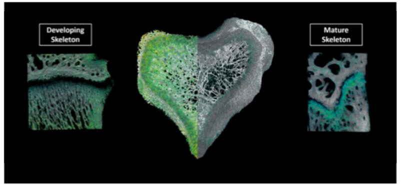
- Need to invert data on order of seconds or less

AI4Analysis

MOTIVATION 3: INVERSE PROBLEMS IN MATERIALS CHARACTERIZATION

1 IMAGING TAKING A SNAPSHOT

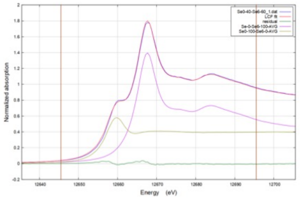
Synchrotron X-rays allow us to take an image of a sample. By studying the interaction of light with an object, we are able to get information about the structure or the function of whatever we are imaging. Our beamlines can take a picture of the tiny airways in a lung or get a three-dimensional image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



E.g.: Projections -> 3D image

2 SPECTROSCOPY ANALYZING THE CHEMISTRY

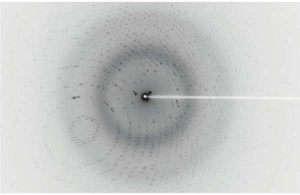
We can see how different wavelengths of light interact with matter, allowing us to analyze what the sample is made of. With spectroscopy we can look at the matter inside of a lentil or model the molecules that exist in space.



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.



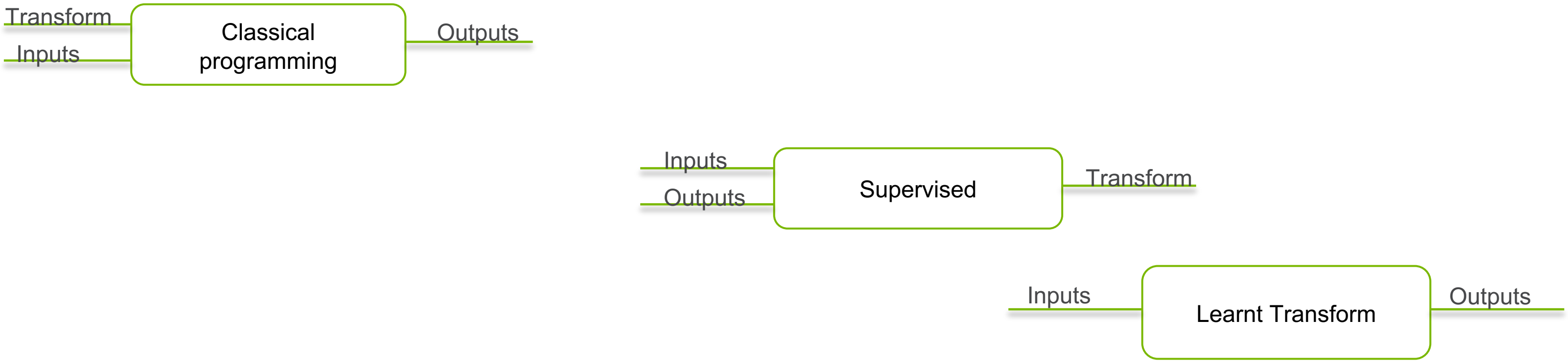
Diffraction -> atomic structure

Inverse problems are computationally expensive!

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

WHY MACHINE LEARNING?

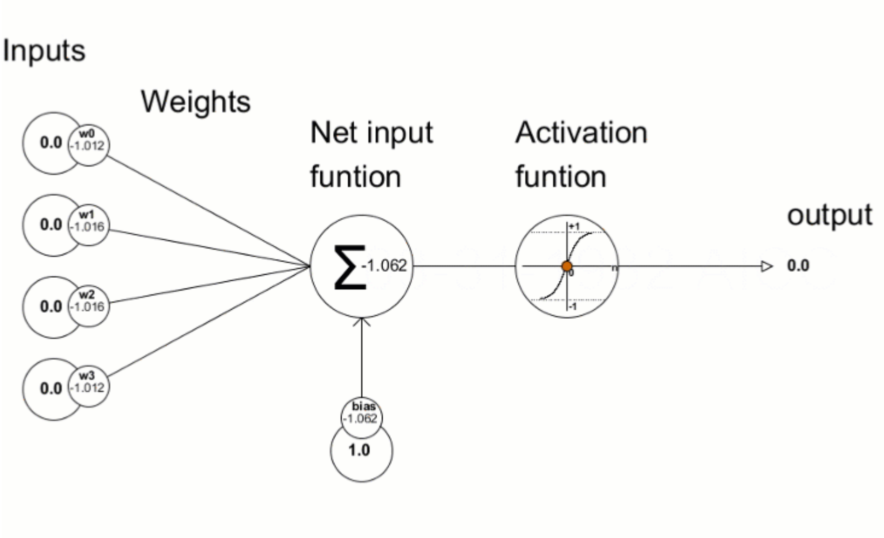
LEARN FROM DATA

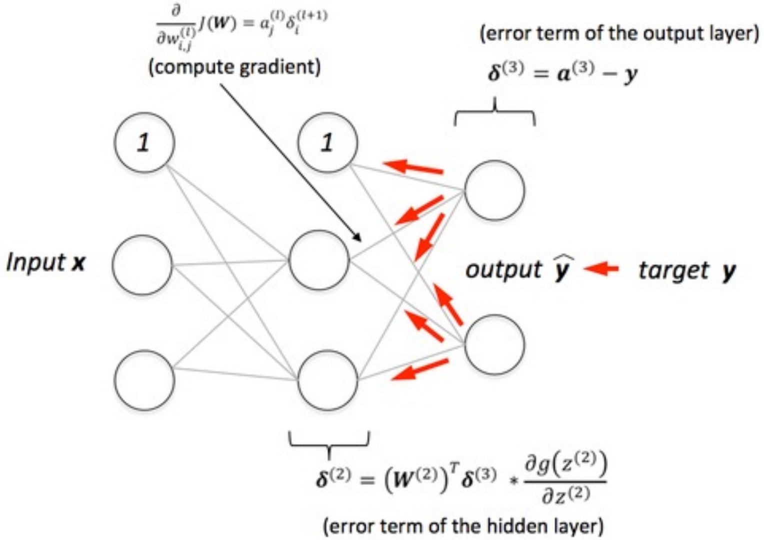


ML lets us solve problems that we cannot with traditional methods

- Just need data
- APSU will have LOTS of data

TRAINING A NEURAL NETWORK: SUPERVISED LEARNING

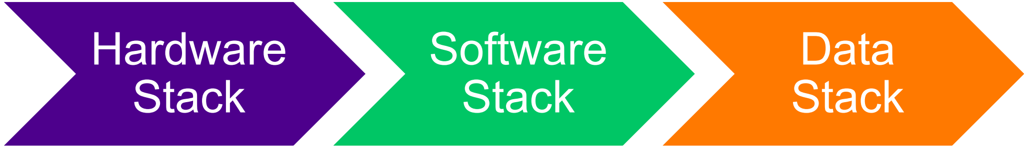




- **Gradient descent 'writes code'**
  - we just provide data

DEEP LEARNING – MORE THAN A NEW TOOL

The advent of 'Software 2.0'



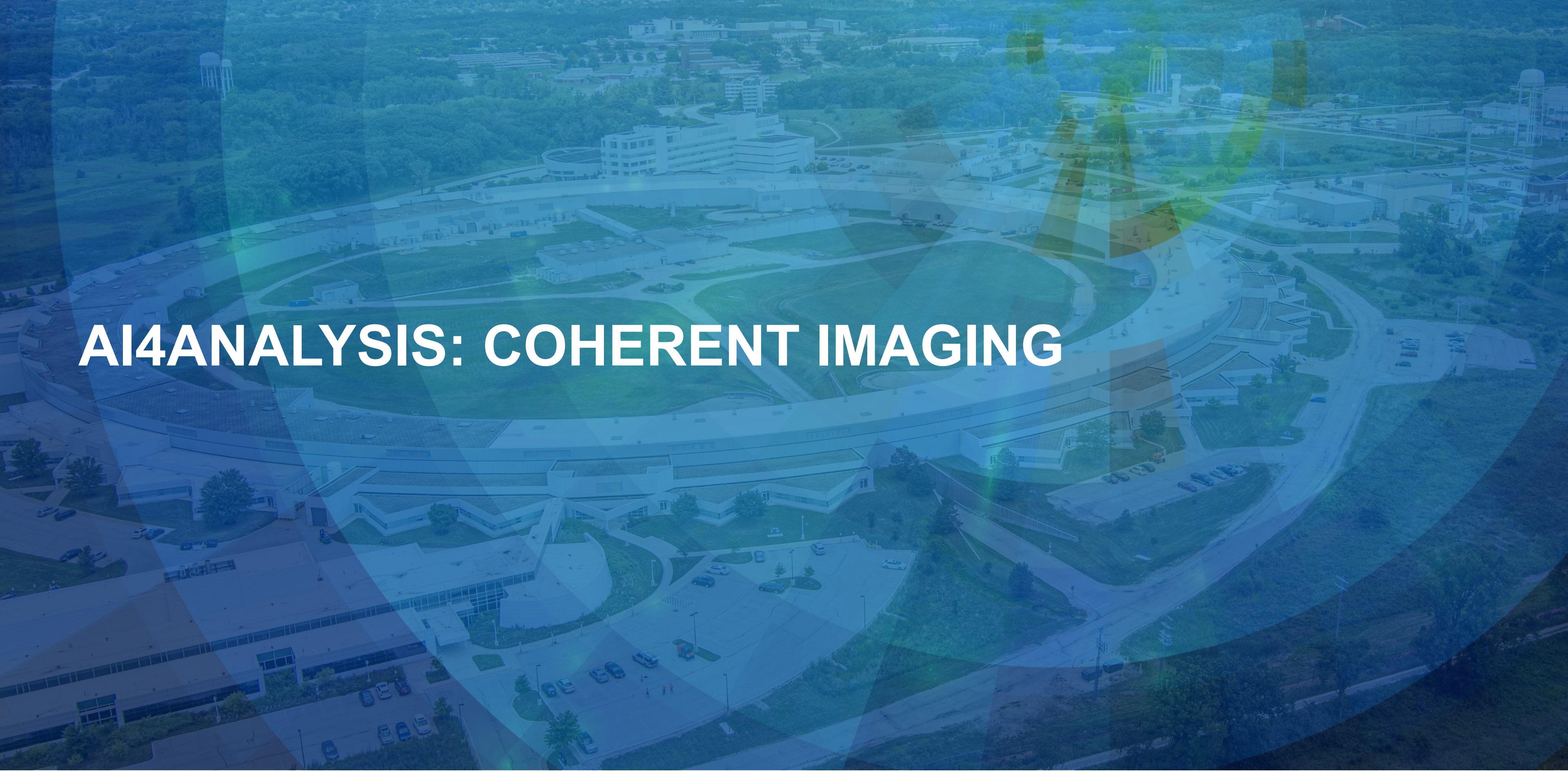
Marc Andreessen
Creator: Mosaic browser
Founder: Netscape & Andreessen-Horowitz (>$10 billion AUM)

Andrej Karpathy
Director of AI, Tesla

Gradient descent can write code better than you. I'm sorry.

2:26 AM · Aug 5, 2017 · Twitter Web Client

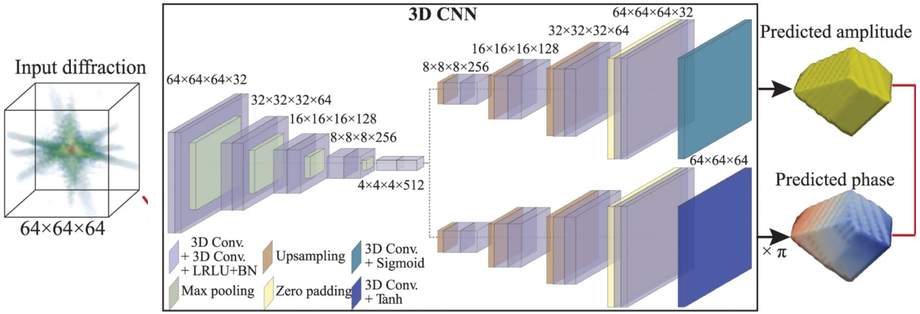
346 Retweets **1.1K** Likes

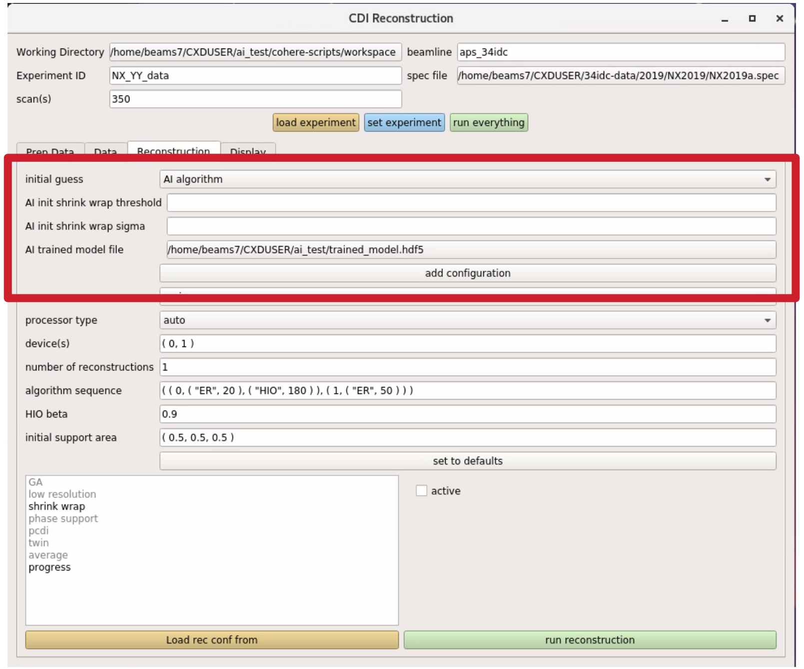


AI4ANALYSIS: COHERENT IMAGING

ML IN PRODUCTION

AI-accelerated User Tools





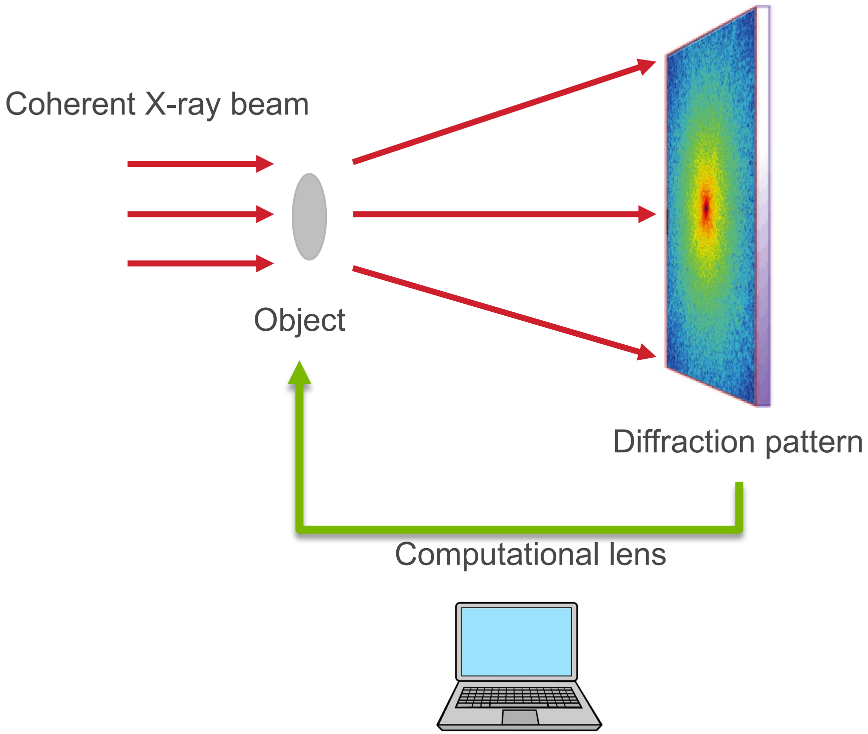
Users do not need to learn ML

Yao, Y., Chan, H., Sankaranarayanan, S., Balaprakash, P., Harder, R. J., & Cherukara, M. J. (2022). AutoPhaseNN: unsupervised physics-aware deep learning of 3D nanoscale Bragg coherent diffraction imaging. npj Computational Materials, 8(1), 1-8.

Frosik, B. and Harder, R. https://github.com/AdvancedPhotonSource/cohere

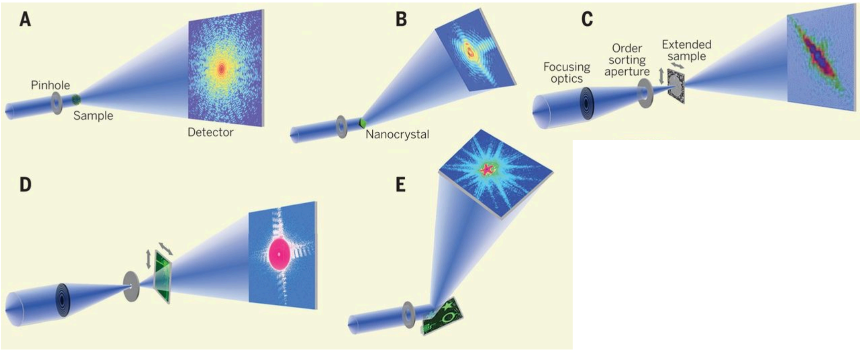
COHERENT DIFFRACTION IMAGING

X-ray Coherent diffraction imaging (CDI)



- Resolution improves with smaller wavelength
- High penetration power
- Coherent-based, lensless imaging
  Resolution not limited by optics

Different CDI geometries and modes



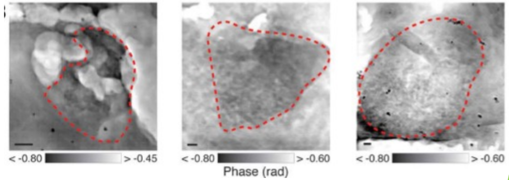
Miao, Jianwei, et al. *Science* 348.6234 (2015): 530-535.

COHERENT DIFFRACTION IMAGING

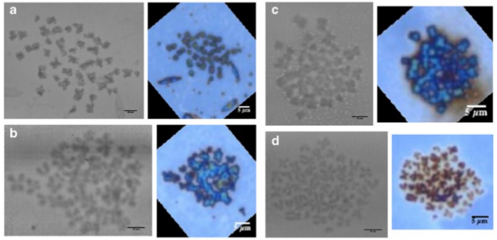
X-ray CDI application

AI4Analysis

Biological imaging

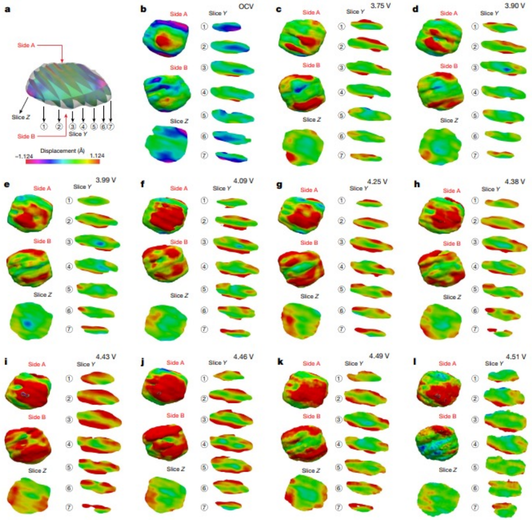


Genoud, S. et al. Chem Sci 11, 8919–8927 (2020).



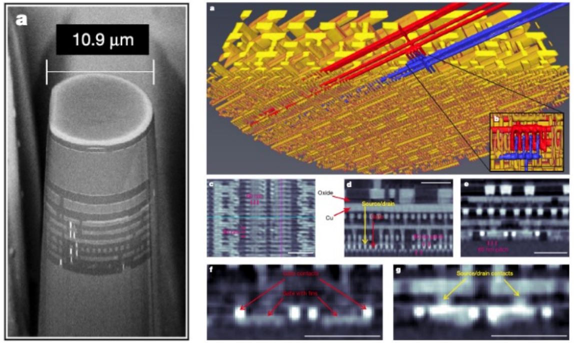
Bhartiya, A. et al. Chromosome Res 29, 107–126 (2021).

Battery materials



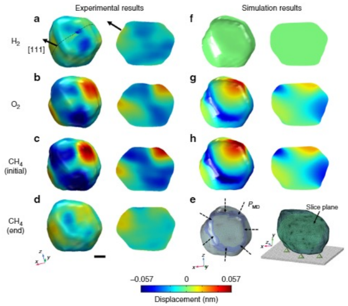
Liu, T. et al. Nature 606, 305–312 (2022).

Semiconductors characterization



Holler, Mirko, et al. Nature 543.7645 (2017): 402-406.

In-situ catalysis



Kim, Dongjin, et al. *Nature communications* 9.1 (2018): 1-7.

COHERENT DIFFRACTION IMAGING

Object

Transmission function

$O = Ae^{j\phi}$

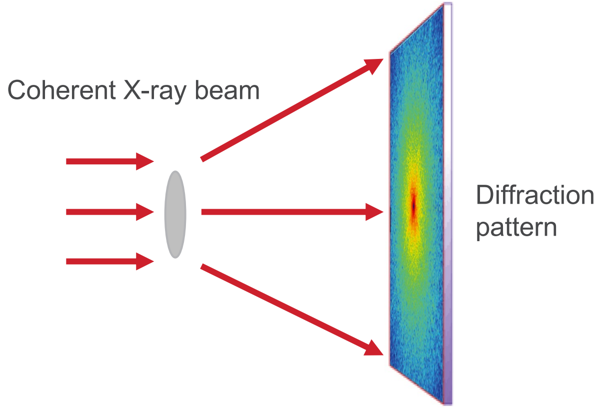
Fourier Transform →

← **Phase retrieval**

Measurement

Diffraction pattern

$I = |\mathcal{F}\{\psi\}|^2$



What's reconstructed?

Refractive index: $n = 1 - \delta + i\beta$

$$\psi = \psi_0 e^{iknt} = \psi_0 e^{ik(1-\delta+i\beta)t} \sim \overbrace{e^{-k\beta t} e^{-ik\delta t}}^{\boldsymbol{O}(\boldsymbol{r})}$$

Absorption contrast: $A = |O(r)| = e^{-k\beta t}$

Phase contrast: $\phi = Arg\big(O(r)\big) = -k\delta t$

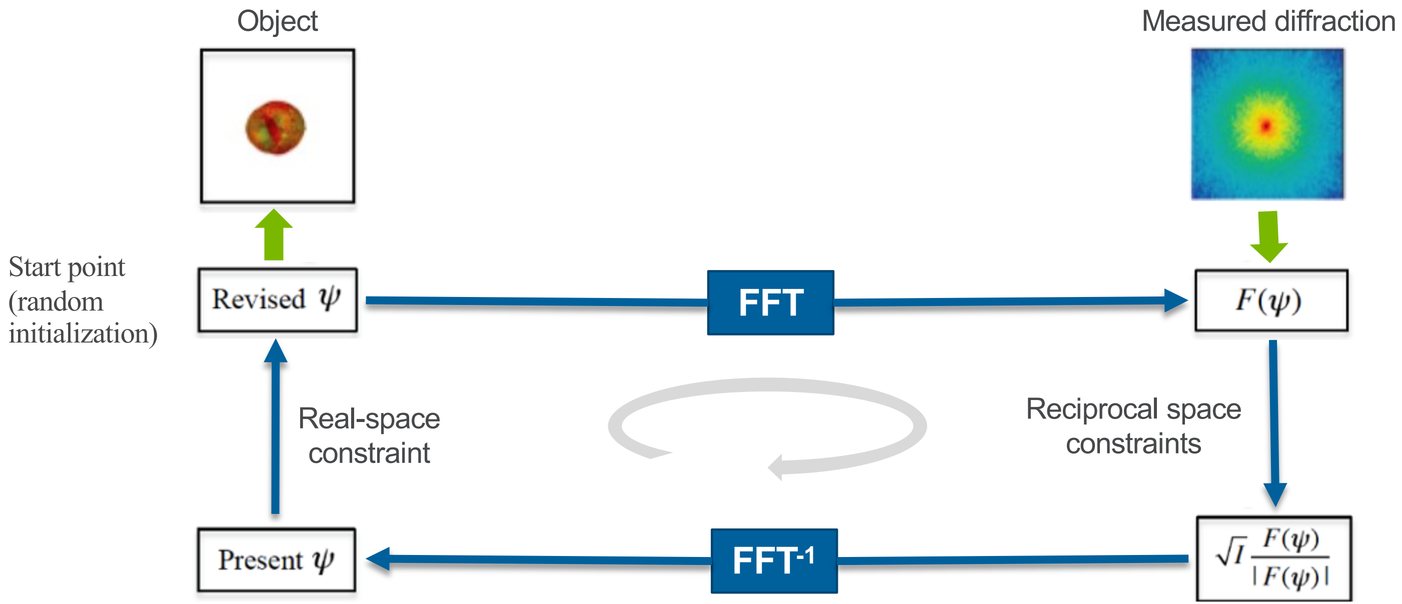
What's measured?

Intensity of the diffraction signal

Phase information lost

PHASE RETRIEVAL-COMPUTATIONAL LENS

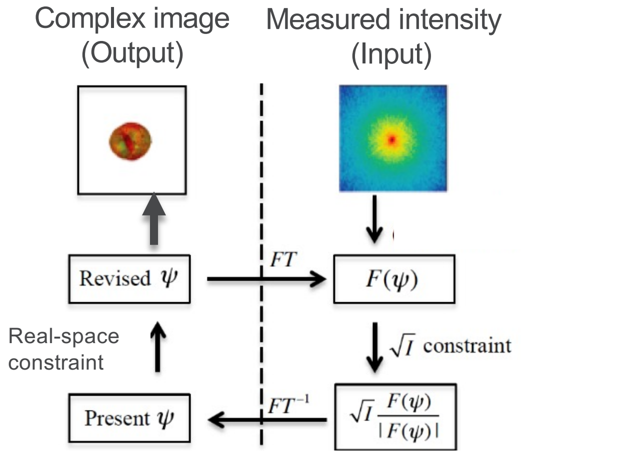
- Fundamental requirement to recover an image of object
- Provide phase imaging
  Better contrast modality in hard x-ray



Error-reduction (ER), Hybrid input-output (HIO), et al

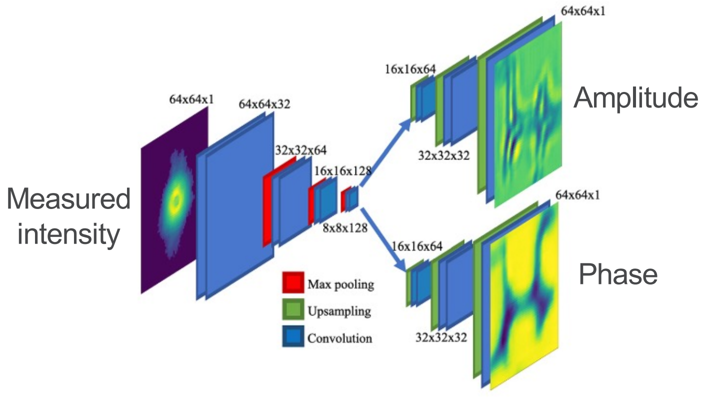
ML FOR PHASE RETRIEVAL

Iterative phase retrieval method



- Computationally expensive
- Sensitive to the initial guess and choice of algorithms

Deep learning



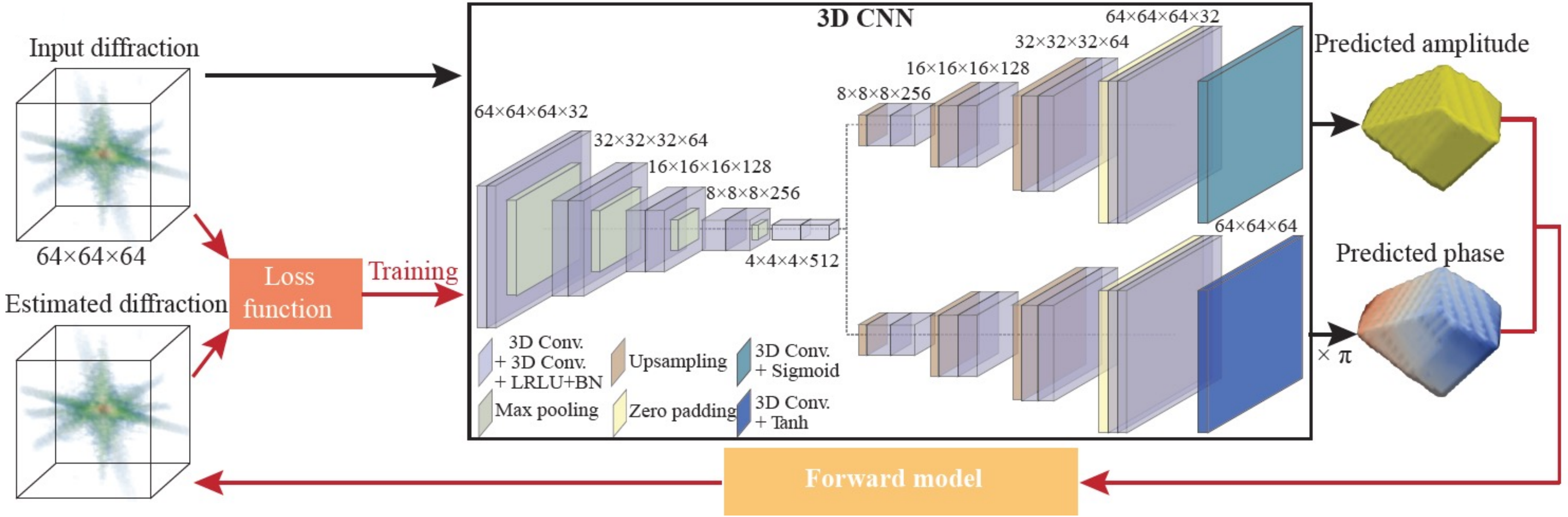
Direct inversion

✓ Faster data inversion speed

- Need for a large volume of labeled training data

AUTOPHASENN

Unsupervised NN for 3D BCDI phase retrieval



3D convolutional neural network:

Learn the inversion from input intensity to images of object

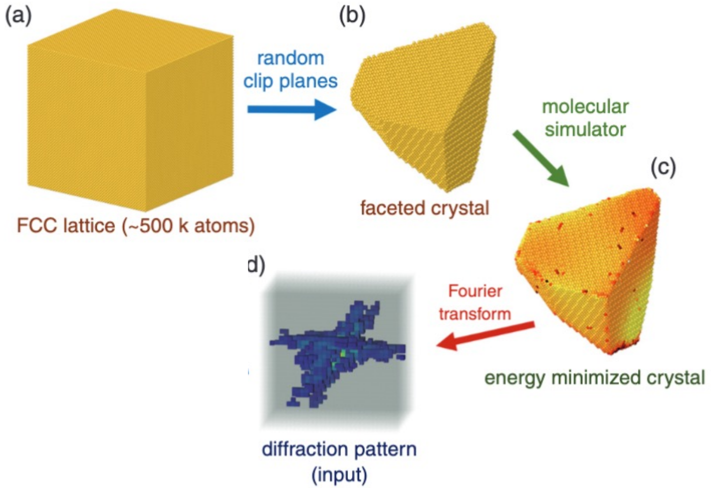
Forward model:

Eliminate the need for ground truth image in training

AUTOPHASENN

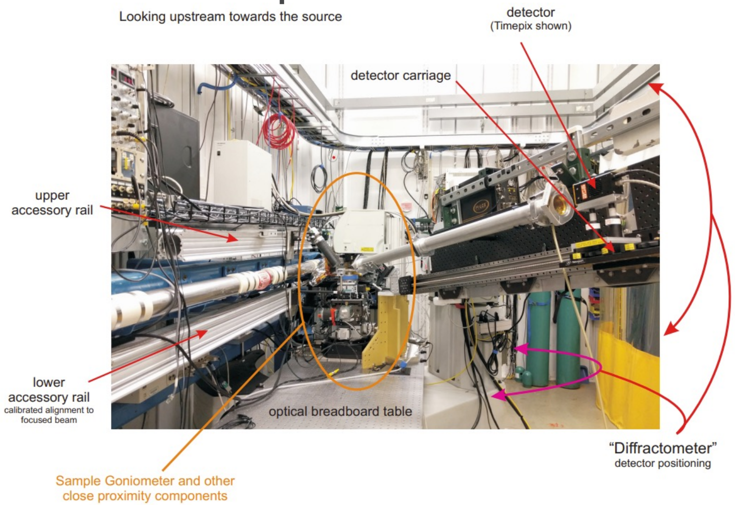
Training data generation

Simulated data



Chan, Henry, et al. *Applied Physics Reviews* 8.2 (2021): 021407.

Experimental data



Acquired at 34-ID-C at APS

104k training data
~12 hours training time on 8 A100 GPUs (40GB)

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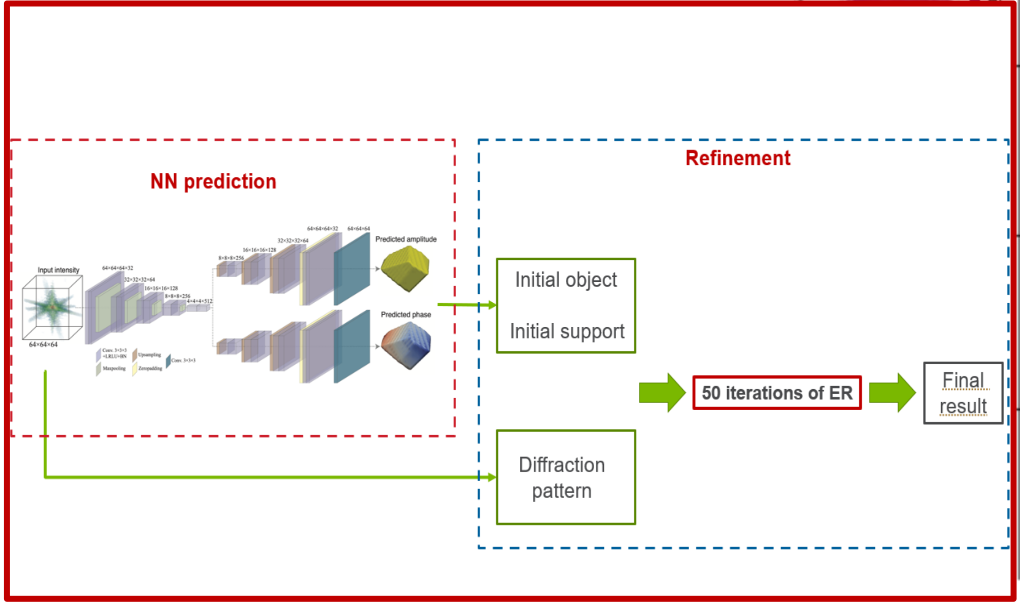
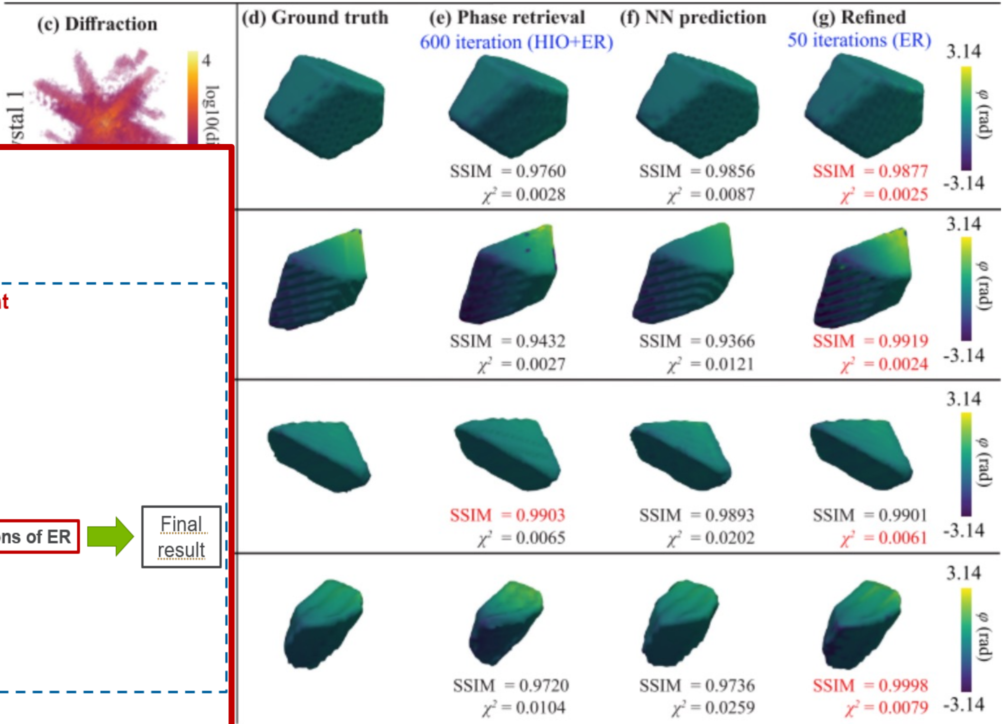
Network performance with simulated data

Tested on ~2k simulated crystals (not seen during the training)





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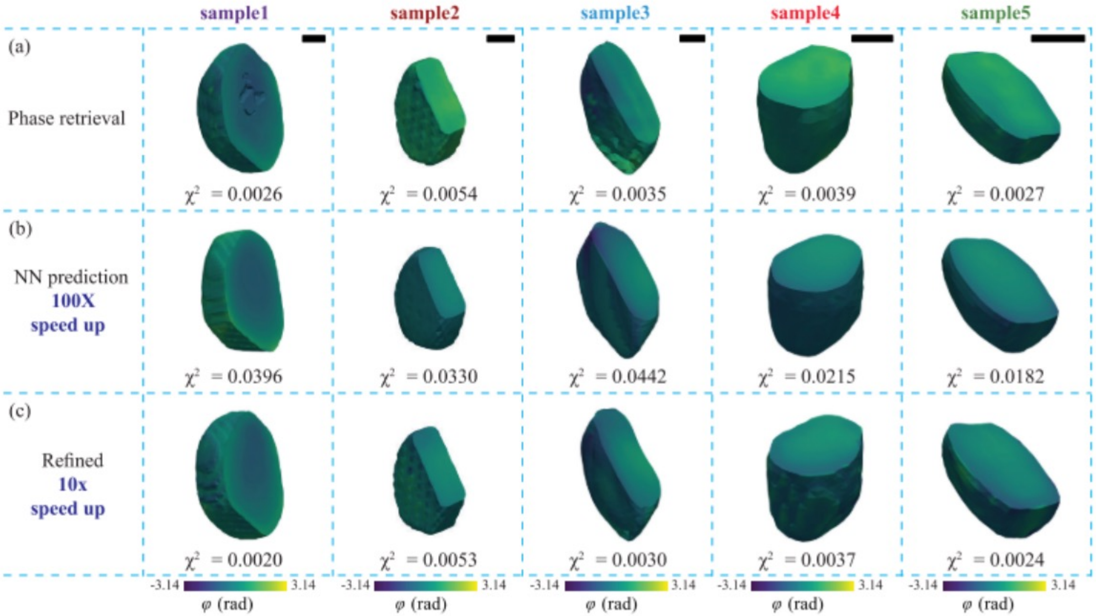
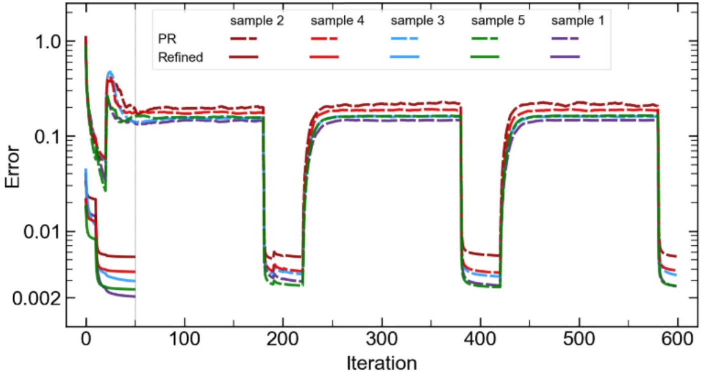
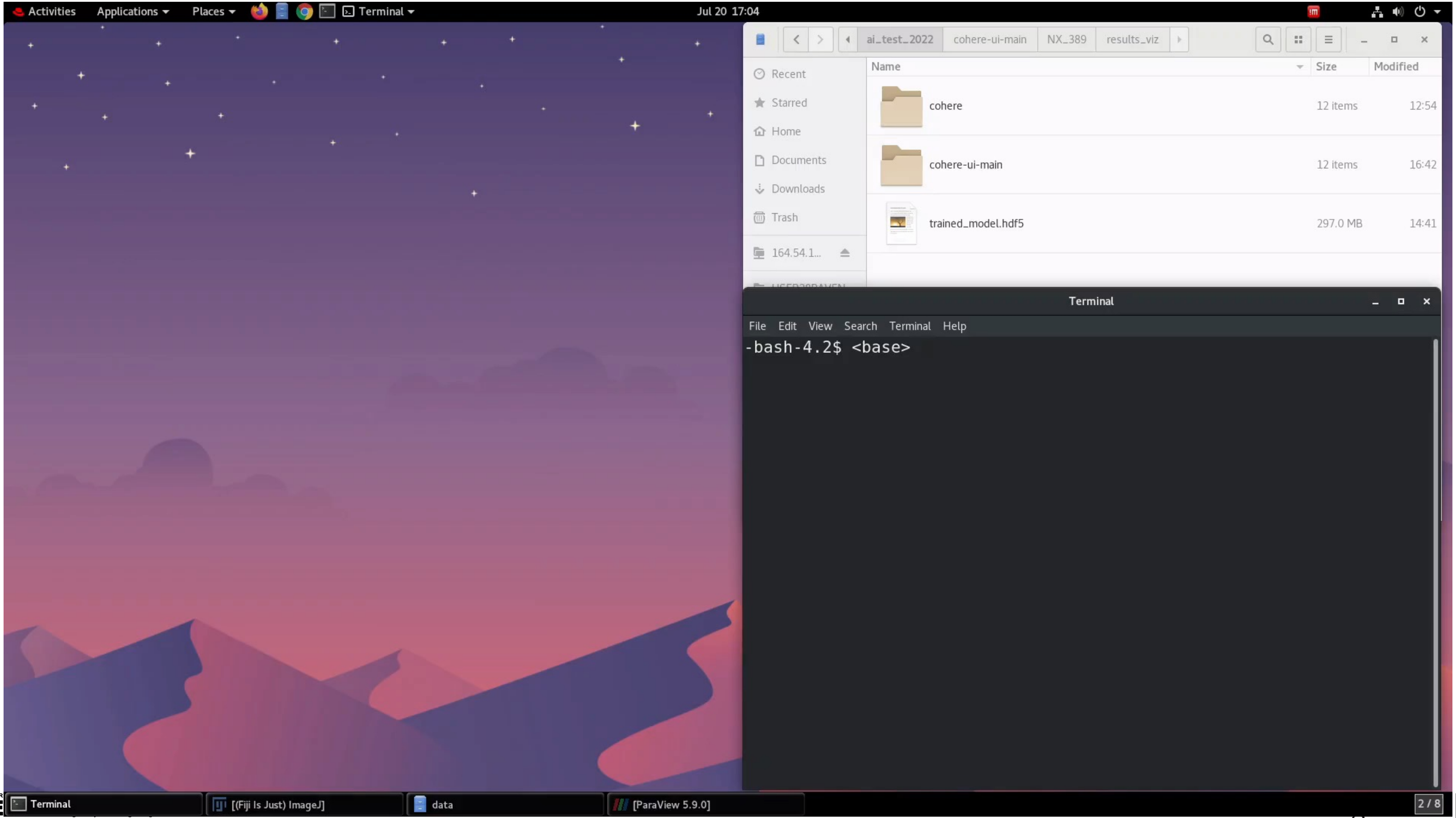
Network performance with experimental data





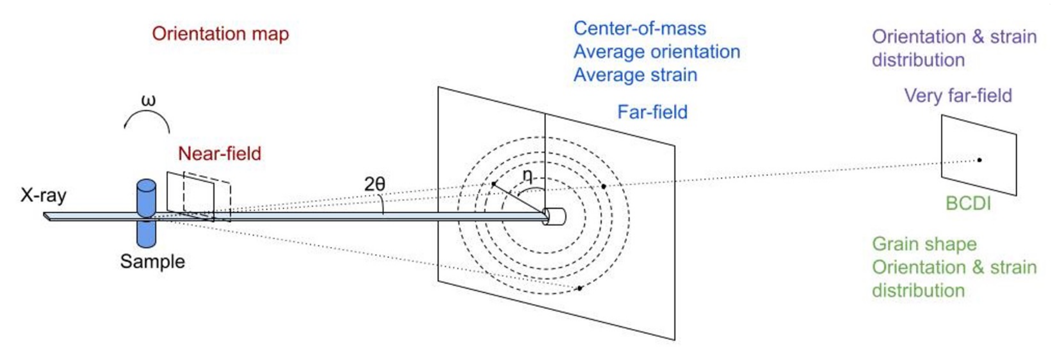
- ❑ 100x speed up compared to conventional iterative phase retrieval
- ❑ Combined with the refinement, the result is comparable/slightly better to the traditional phase retrieval while being ~10 times faster.

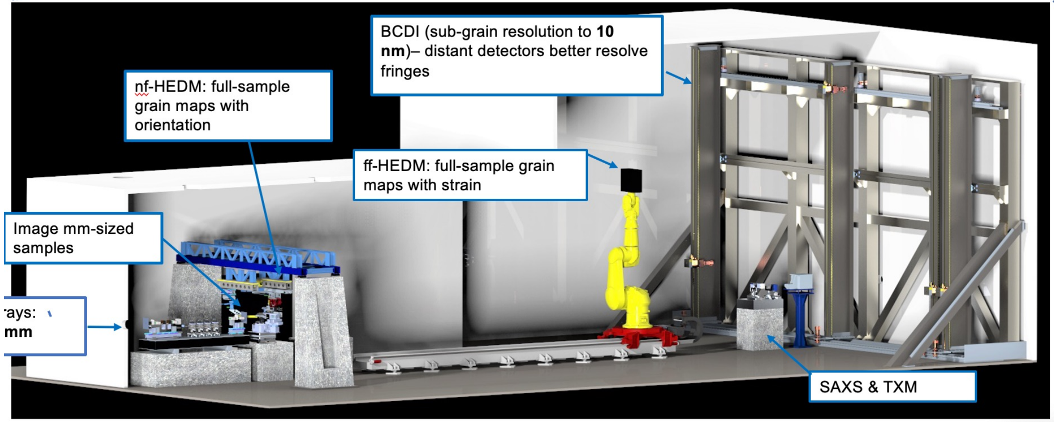
AUTOPHASENN IN COHERE



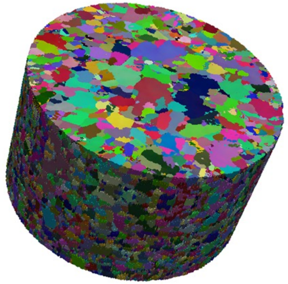
AI4Analysis

BRAGGNN: AI@EDGE FOR HEDM





Today: 1000 cpu-hours per scan (20 mins)
APSU: 10,000 cpu-hours per scan (30 s)

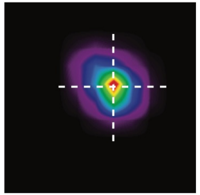


https://www.andrew.cmu.edu/user/suter/HEDMTools.html

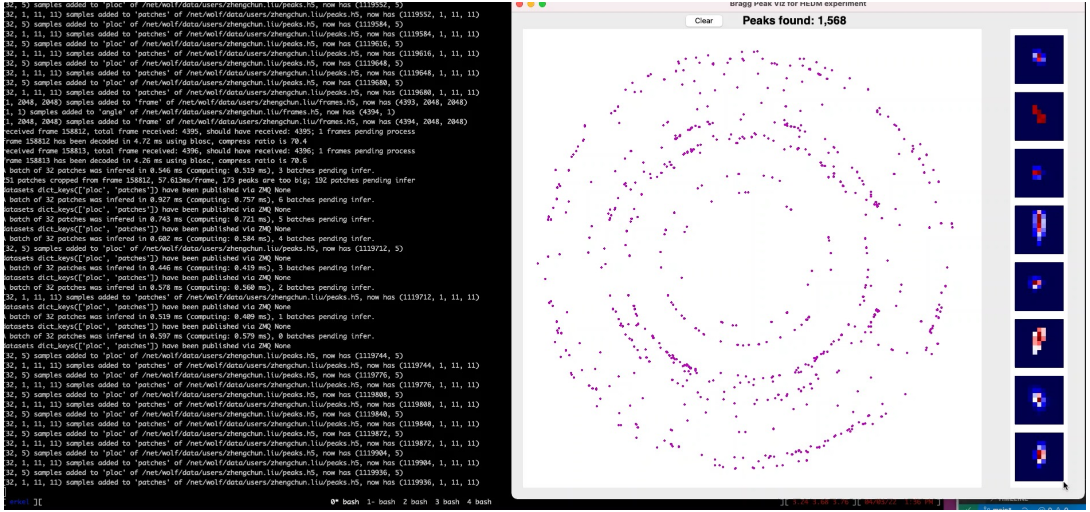
Slide contents from: J. Almer, H. Sharma B. Suter et al.

AI4Analysis

BRAGGNN: AI@EDGE FOR HEDM



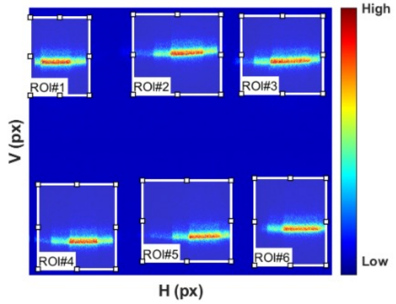
- Deep CNN that outputs peak position
- 200X faster *and* more accurate than pseudo-Voigt fitting
- AI@Edge processes streaming data



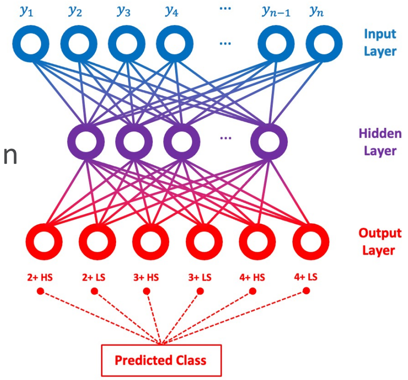
Liu, Z., Sharma, H., Park, J.S., Kenesei, P., Miceli, A., Almer, J., Kettimuthu, R. and Foster, I., 2022. BraggNN: Fast X-ray bragg peak analysis using deep learning. IUCrJ, 9(1).

AXEAP: ARGONNE X-RAY EMISSION ANALYSIS PACKAGE

- Converts emission data into spectra in real-time using Unsupervised ML.



- NN predicts oxidation and spin state from XES spectra



Inhui Hwang, Chengjun Sun et. al., ANL software disclosure SF-21-050

AI4STEERING

AI4Steering

SMART DATA ACQUISITION

Experiment:
- Scanning Bragg diffraction imaging (008 peak) of layered material (WSe_2)

Problem:
- Given an unknown sample, how should we acquire data to maximize information gain in minimal time?

Approach:
- Sample a few (~1%) points randomly
- Use a pre-trained NN to predict the most important points to acquire.
  - Decision is made in ~ 1s

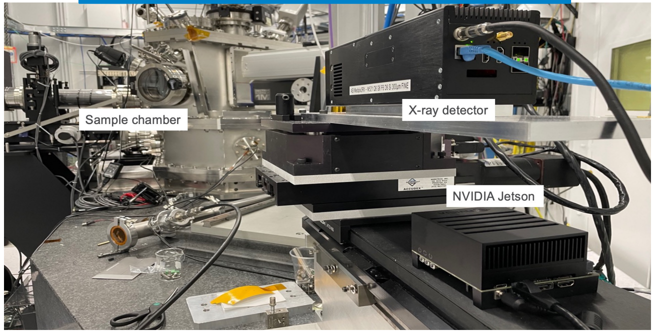
Result:
- AI approach reconstructs image with far fewer points

Saugat Kandel, Tao Zhou et al.

SMART DATA ACQUISITION

AI4Steering

AI@Edge drives instrument

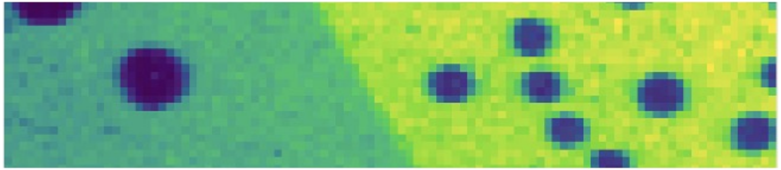


NN inference @ edge

Route optimization

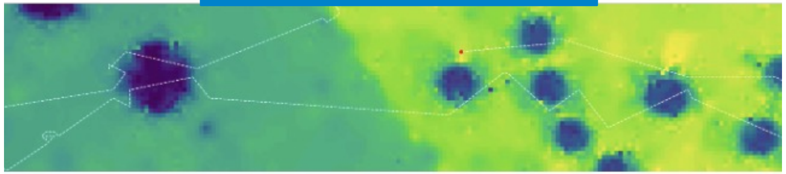
Saugat Kandel, Tao Zhou et al.

Full-res image

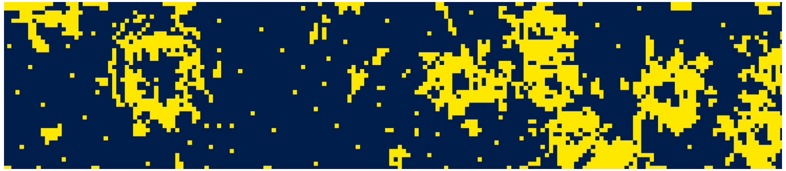


'Ground truth' : 100 nm steps

AI-guided acquisition



4.3X less points



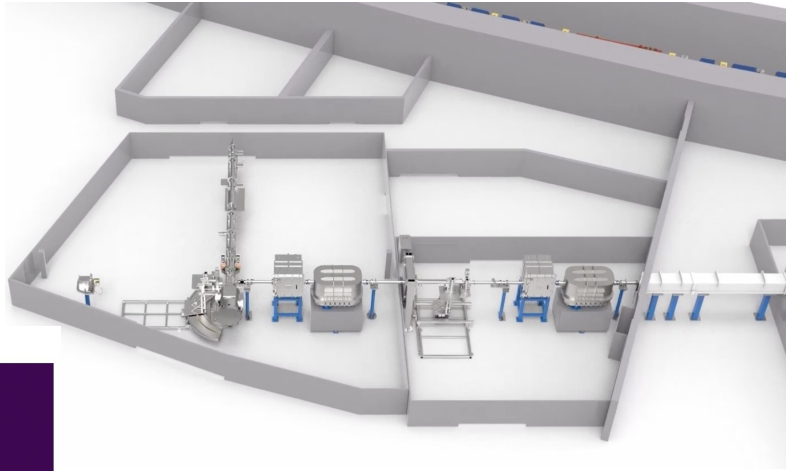
Locations chosen by AI to scan
- Each yellow dot is a scan point

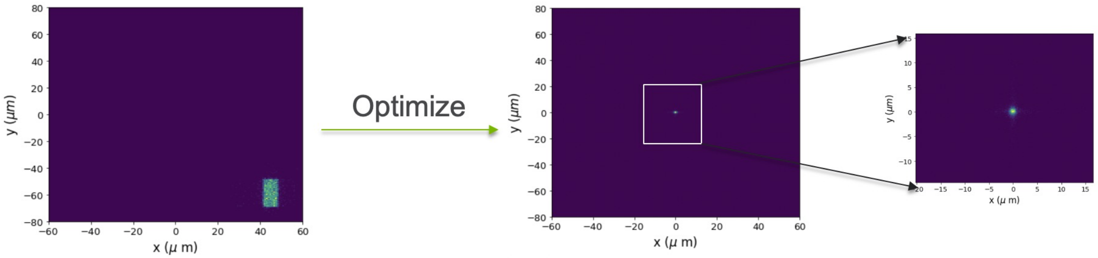
AI4Steering

AI-GUIDED ACQUISITION AT NANOPROBE

Saugat Kandel, Tao Zhou et al.

AUTOFOCUS: AUTOMATED BEAM FOCUS AND ALIGNMENT



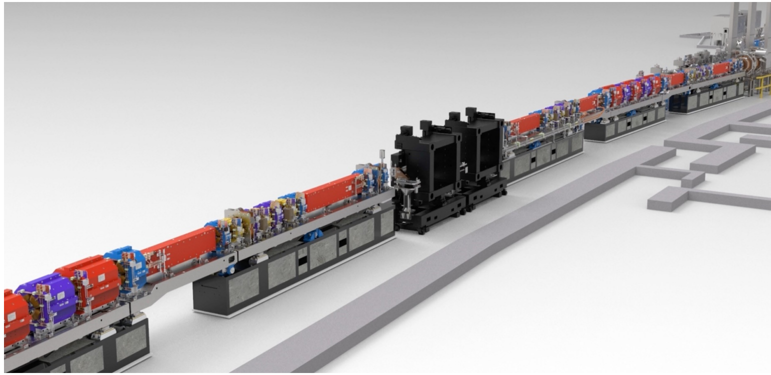


Optimized Mirror focusing
'Digital Twin' of beamline in Oasys

Saugat Kandel, Luca Rebuffi et al.

ACCELERATOR TUNING AND FAULT MITIGATION

- **AI for efficient accelerator operation**
  - Achieve and maintain optimal accelerator performance through reinforcement learning (RL) and Bayesian optimization (BO).
  - Designed a fully integrated 'digital twin' environment for simulation and debugging based on experimentally collected data.
  - Experimental benchmarks have demonstrated new methods to be faster in recovering full performance of the accelerator after a perturbation.



- **AI to predict power supply trips in the storage ring:**
  - Advance warning about an impending PS trip so that preventive action can be taken by the accelerator operator or by the PS maintenance group.
  - Models trained on historical data since 2001.
  - Anomaly detection through autoencoders.

Yine Sun, Nikita Kuklev, Ihar Lobach et al.

AI4KNOWLEDGE

TOMOGAN: DENOISING + ARTIFACT REMOVAL

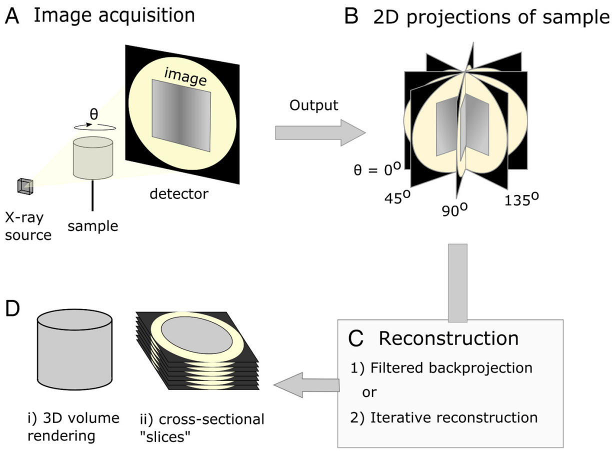
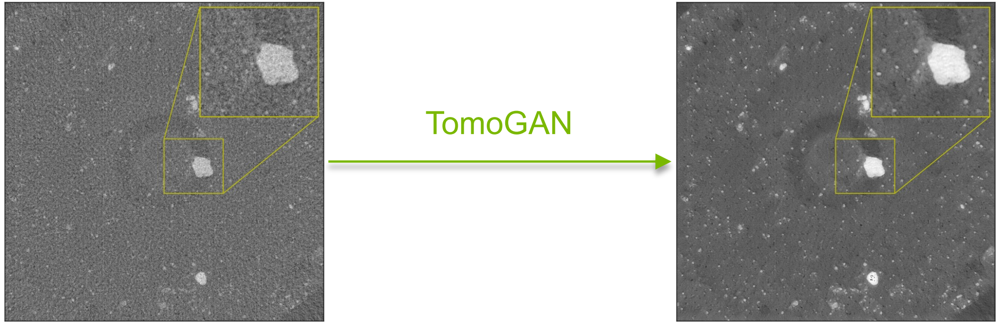


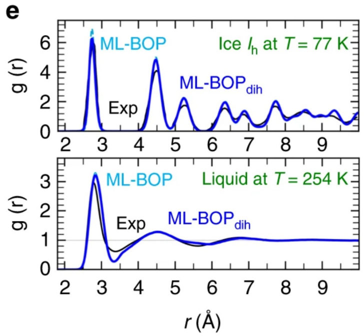
Image from: O'Sullivan, James DB, et al. "X-ray micro-computed tomography (μCT): an emerging opportunity in parasite imaging." Parasitology 145.7 (2018): 848-854.



- Generative adversarial network for denoising and artifact removal
- Up to 1/16th less dose or projections

Liu, Z., Bicer, T., Kettimuthu, R., Gursoy, D., De Carlo, F. and Foster, I., 2020. TomoGAN: low-dose synchrotron x-ray tomography with generative adversarial networks: discussion. JOSA A, 37(3), pp.422-434.

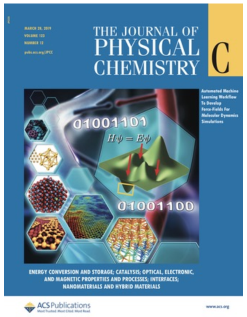
LEARNING MATERIAL MODELS FROM - XRAY DATA



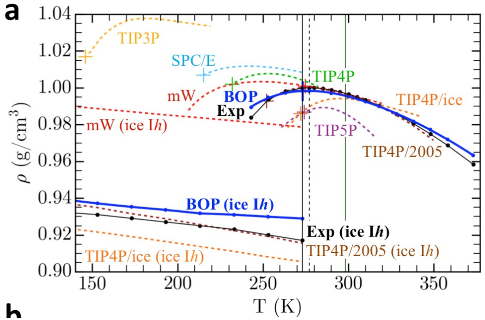
Opportunity

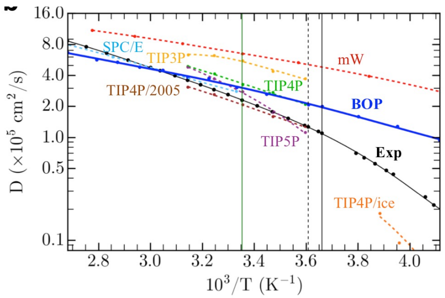
- Build better materials models
  - Machine learnt materials models fit to experimental data
  - Eg Water model: x-ray data (C. Benmore)

Results



- BLAST ML framework for model development
- > 10 widely used models for 2D materials, oxide materials, water etc.



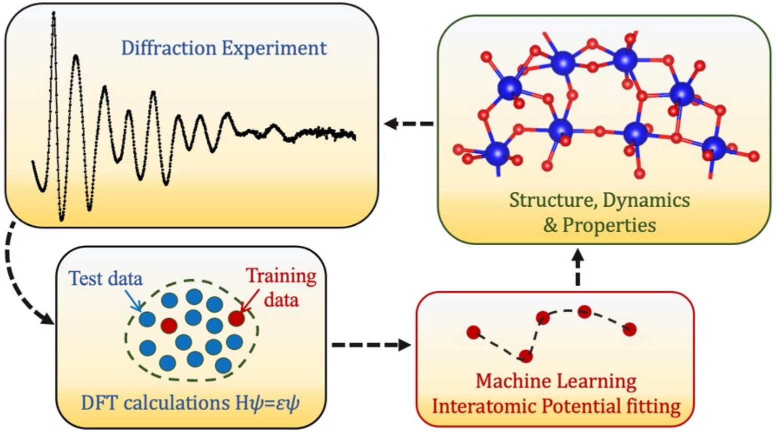


Our water model: ~highest scoring, ~least expensive

Chan, H., Cherukara, M. J., Narayanan, B., Loeffler, T. D., Benmore, C., Gray, S. K., & Sankaranarayanan, S. K. (2019). Machine learning coarse grained models for water. *Nature communications*, 10(1), 1-14.

LEARNING MATERIAL MODELS FROM DIFFRACTION DATA

- **Active learning:**
  - Obtain an atomic models that reproduces the measured x-ray data with quantum mechanical accuracy
  - ML scheme uses an automated closed loop via an active-learner, which is initialized by diffraction measurements, and sequentially improves an unsupervised ML model using a Gaussian Approximation Potential (GAP) approach



Sivaraman, G., Gallington, L., Krishnamoorthy, A. N., Stan, M., Csányi, G., Vázquez-Mayagoitia, Á., & Benmore, C. J. (2021). Experimentally driven automated machine-learned interatomic potential for a refractory oxide. Physical Review Letters, 126(15), 156002.

Sivaraman, G., Guo, J., Ward, L., Hoyt, N., Williamson, M., Foster, I., Benmore, C. and Jackson, N., 2021. Automated development of molten salt machine learning potentials: application to LiCl. The Journal of Physical Chemistry Letters, 12(17), pp.4278-4285.

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FEEDBACK

Lecture – 2:15 – 3:15

AI impacting experiments and analysis – Yudong Yao & Mathew Cherukara

https://forms.office.com/g/GzVHXHCSBg