

# THE ADVANCED PHOTON SOURCE

## PtychoNN for Real-Time Ptychography

Researchers at Argonne National Laboratory have developed and deployed an AI-enabled workflow, PtychoNN, that enables real-time, dose-efficient, coherent imaging of x-ray diffraction data on an x-ray beamline. Their approach to solving the problem is based on a deep convolutional neural network and has been demonstrated to predict real-space structure and phase at each scan point solely from the corresponding far-field diffraction data.

Ptychographic imaging requires scanning a coherent x-ray beam across the sample while measuring the scattered intensities in the far-field. The image is recovered by algorithmically inverting the measured coherent diffraction patterns. Inversion (or image reconstruction) of ptychographic imaging data requires the solution of an inverse problem, e.g., recovering lost phase information from measured intensities alone (or phase retrieval). The phase retrieval problem in ptychography is presently solved using model-based iterative methods that are computationally expensive, precluding real-time imaging. In addition, the convergence of these iterative reconstruction algorithms is often sensitive to factors such as the choice of algorithms and the initial image and probe guess and the choice of these parameters can be subjective. Finally, adjacent measured scan points need to overlap by at least 50%. An overlap in two dimensions can severely limit the area or volume of the sample that can be scanned in a given amount of time.

To demonstrate PtychoNN, the researchers employed the x-ray nanoprobe at beamline 26-ID of the Advanced Photon Source as well as the facilities of the Center for Nanoscale Materials, both of which are Office of Science user facilities at Argonne.

Their results revealed a capability for real-time imaging more than 100 times faster than phase retrieval; they demonstrated live inference at 100 Hz on 512 x 512 images; and lower-dose imaging with 25 times less data than phase retrieval. This speedup is only in the data inversion step; further speedup can be obtained by scanning sparsely, which could potentially lead to 25 times faster scanning from reduced data acquisition. PtychoNN was deployed on a palm-sized edge computing device (NVIDIA Jetson) sitting at the beamline and performed ML-inference on the live data stream from the detector. Finally, in addition to remarkably faster experimental feedback, PtychoNN's ability to recover accurate real-space images from sparse-sampled ptychographic data has the potential to revolutionize ptychography on dose sensitive, dynamic, and extremely large samples.

PtychoNN arrives at a propitious moment given the proliferation of upgraded x-ray sources such as the Advanced Photon Source Upgrade Project, the European Synchrotron Research Facility Extremely Brilliant Source, and PETRA-IV, all of which are designed to increase photon flux and coherence by factors of hundreds or thousands. Traditional iterative phase retrieval methods are simply not able to keep pace with this deluge of experimental data. PtychoNN and other machine learning methods for data inversion will be the key to unlocking the full potential of these upgrades by keeping abreast of the vast data flow generated by coherent imaging experiments.

*This article is adapted from "AI-enabled high-resolution scanning coherent diffraction imaging," Mathew J. Cherukara, Tao Zhou, Youssef Nashed, Pablo Enfedaque, Alex Hexemer, Ross J. Harder,*



Pictured above is the Jetson edge device (circled) running PtychoNN, which makes live predictions from the detector (top) data stream and sends them to the beamline computer. Photo: Mathew Cherukara (Argonne/Advanced Photon Source)

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