The Advanced Photon Source

Better-Educated Neural Networks for Nanoscale 3-D Coherent X-ray Imaging

One of the inescapable realities of imaging techniques is called the "phase problem," which simply refers to the loss of phase information inherent in the nature of imaging methods such as x-ray diffraction. Although inconvenient, it can be dealt with by using mathematical methods to retrieve the phase data from the image with inverse computation. Such methods, however, are not only time-consuming but require a great deal of computer power. A group of researchers working at the APS has demonstrated a new approach to this obstacle by using a deep-learning neural network trained and to perform fast three-dimensional (3-D) nanoscale imaging from coherent x-ray data.

Investigators confronted this problem by using explicitly "physics-aware" training of neural networks that incorporates atomistic simulation data to create diverse training sets based on the physics of the material under study (Fig.1). The neural network predictions are then further refined in the final stage. The research team validated this 3-D convolutional encoder-decoder network (3D-CDI-NN) on 3-D coherent x-ray diffraction data of gold nanoparticles performed at the APS.

To enhance the accuracy of 3D-CDI-NN, the team added a refinement that uses a reverse-mode automatic differentiation (AD) technique on the strain predictions and diffraction data. This proved especially effective in recovering details of structural strain within the examined crystal samples without oversampled data, as when using AD techniques.

The researchers demonstrated the effectiveness of the trained 3D-CDI-NN model with real-world data by imaging gold nanoparticles. Although the initial predictions showed some underestimation of surface details and local strain, these details were recovered after the AD refinement procedure. The 3D-CDI-NN framework was demonstrated to be about 4 times faster compared to typical iterative phase retrieval methods.

When the upgraded APS come online in the near future, with ever brighter and more versatile beams and capable of generating extremely large datasets, faster and more efficient phase retrieval techniques will be essential. The research team notes that machine-learning neural network approaches can be trained to surpass traditional phase retrieval techniques by hundreds of times in speed while placing far lesser demands on scarce computing resources. Such automated methods can also be effectively scaled to different requirements and can even operate on datasets as they are still being collected.

— Mark Wolverton

See: Henry Chan, Youssef S.G. Nashed, Saugat Kandel, Stephan O. Hruszkewycz, Subramanian K.R.S. Sankaranarayanan, Ross J. Harder, and Mathew J. Cherukara, "Rapid 3D Nanoscale Coherent Imaging via Physics-aware Deep Learning," Appl. Phys. Rev. 8, 021407 (2021). DOI: 10.1063/5.0031486

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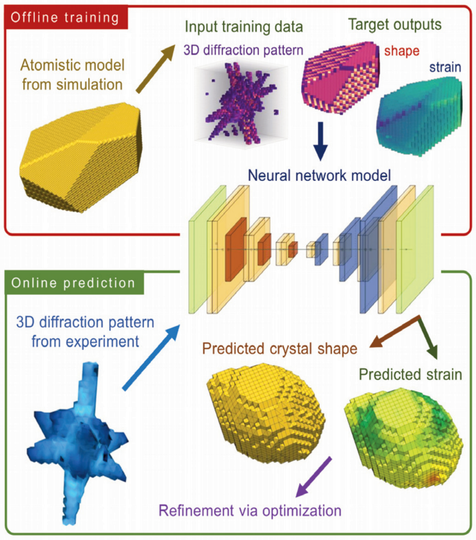

Fig. 1. Schematic of physics-aware framework for phase retrieval in 3-D coherent diffraction imaging. The main component of the framework is a neural network model (3D-CDI-NN) that is trained offline using 3-D data (simulated diffraction pattern, crystal shape, and local strain) derived from atomistic simulations that capture physics of the material. Once trained, the 3D-CDI-NN model can perform real-time prediction of crystal shape and local strain from experimentally measured diffraction pattern. The prediction can then be refined using a gradient-based optimization procedure. From H. Chan et al., Appl. Phys. Rev. **8**, 021407 (2021). ©2021 Author(s). Published under an exclusive license by AIP Publishing.

Call for APS General-User Proposals

The Advanced Photon Source is open to experimenters who can benefit from the facility's high-brightness hard x-ray beams.

General-user proposals for beam time during Run 2022-2 are due by March 4, 2022.

Information on access to beam time at the APS is at http://www.aps.anl.gov/Users/apply_for_beamtime.html or contact Dr. Dennis Mills, DMM@aps.anl.gov, 630/252-5680.

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