APS Scientific Computation Seminar Series

Speakers: Ian Robinson, Brookhaven National Laboratory and University College London
Shinjae Yoo, Brookhaven National Laboratory
Longlong Wu, Brookhaven National Laboratory

Title: Machine Learning Phasing for Bragg Coherent Diffractive Imaging

Date: Monday, April 11, 2022

Time: 1:00 p.m. (Central Time)

Location: **Join ZoomGov Meeting**
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Abstract: David Sayre proposed a solution to the crystallographic "phase problem" immediately after the announcement of Shannon Information Theorem: if diffraction can be sampled more than twice as finely as the Bragg peak spacing, the problem is overdetermined and can be solved [1]. Sayre did not explicitly mention the need for X-ray coherence, which has been happily solved with the development of the latest synchrotron sources, including the APS. X-ray coherence produces speckle in the diffraction patterns which can be oversampled to overdetermine the phase problem. Sayre also did not specifically propose a closed form solution of the phase problem either, however, many methods have been proposed to invert the diffraction to real space images over the 69 years since, all of them iterative algorithms that converge on the solution. But despite "proofs" to the contrary [2], when applied to real data with noise, these methods are usually prone to local minima giving multiple solutions. In this presentation we will introduce the possibility that the speckle inversion "phase problem" may be amenable to Machine Learning approaches in the future. Our first demonstration is published for 2D [3] and 3D data [4].

[1] Some implications of a theorem due to Shannon, D. Sayre, Acta Cryst. 5, 843 (1952)
[2] Uniqueness of solutions to two-dimensional Fourier phase problems for localized and positive images. R. H. T. Bates, Comput. Vis. Graph. Image Process. 25, 205-217 (1984)
[3] Complex Imaging of Phase Domains by Deep Neural Network Longlong Wu, Pavol Juhas, Shinjae Yoo and Ian Robinson, IUCrJ 8 12-21 (2021)
[4] 3D Coherent X-ray Imaging via Deep Convolutional Neural Networks, Longlong Wu, Shinjae Yoo, Ana F. Suzana, Tadesse A. Assefa, Jiecheng Diao, Ross J. Harder, Wonsuk Cha and Ian K. Robinson, npj Computational Materials 7 175 (2021)