

APS Scientific Computation Seminar Series

Speaker: Tao Zhou
Nanoscience & Technology Division, Argonne National Laboratory

Title: Using Automatic Differentiation to Solve the Phase Problem in X-ray and Electron Microscopy

Date: Monday, June 21, 2021

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

Location: <https://bluejeans.com/5625919115?src=calendarLink>

Hosts: Mathew Cherukara and Nicholas Schwarz

Abstract:

In this talk, I will discuss how we applied automatic differentiation (AD) to solve the phase problem in two different fields, namely x-ray Bragg ptychography, and Lorentz transmission electron microscopy (LTEM). We show that with the help of AD, the Takagi-Taupin Equations (TTE) can be used as a general formalism for 3D phase retrieval, applicable to both x-ray Bragg ptychography and Bragg Coherent Diffraction Imaging. Compared to conventional Fourier Transform based methods, our proposed approach accounts for additionally refraction, absorption, interference, dynamical effects, and is applicable to any kind of weakly strained material system. LTEM is a unique characterization technique that enables the simultaneous imaging of both the microstructure and functional properties of materials. Phase retrieval with AD in LTEM allows high spatial resolution and high accuracy to be simultaneously achieved without additional experimental setups. More importantly, this new approach can go beyond recovering just the phase information. We demonstrate this by retrieving the electron-optical parameters of the contrast transfer function.

Biography:

Research

- X-ray Bragg Ptychography for studying structural defects in quantum materials
- Full Field X-ray Diffraction Microscopy under *in situ* and *operando* conditions, e.g., annealing (1000K), cryogenic cooling (50K), electrochemistry cycling, time resolved (150 ps), etc.
- Grazing Incidence X-ray Diffraction and Small Angle X-ray Scattering for studying group IV semiconductor nanowires *in situ* during growth and deformation.

Education

Ph.D., University of Grenoble Alpes, France
M.Sc.Eng., Ecoles des Mines de Saint Etienne, France
B.Eng., Shanghai Jiao Tong University