APS Scientific Computation Seminar Series

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Title: 4D X-Ray Imaging and Modeling of Lattice Dynamics at the Nanoscale

Date: Monday, April 16, 2018

Time: 1:00 p.m.

Location: 401/A1100

Hosts: Nicholas Schwarz and Brian Toby

Abstract:

Observing the dynamic behavior of materials following ultra-fast excitation can reveal insights into the response of materials under non-equilibrium conditions of pressure, temperature, and deformation. Material response under such conditions is challenging to characterize especially at the nano to mesoscopic spatio-temporal scales. Time-resolved coherent diffraction imaging (CDI) is a unique technique that enables three-dimensional imaging of lattice structure and strain on sub-ns timescales. In such a 'pump-probe' technique, stroboscopic x-ray 'probes' are used to image the transient response of a sample following its excitation by a laser 'pump.' Data from these characterization studies also serve as inputs to material models, which are in turn used to make predictions at spatio-temporal scales inaccessible to the experiment. In this talk, I will present some of our recent work on imaging and modeling of phonon transport and lattice dynamics in nanomaterials. I will also describe our work in the development of a machine learning framework that enables rapid and accurate development of material models applicable to a wide variety of materials properties including thermal transport.