

APS Scientific Computation Seminar Series

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Title: Leveraging First Principles Modeling for X-Ray Data Inversion

Date: Monday, February 20, 2017

Time: 1:00 p.m.

Location: 401/A1100

Hosts: Nicholas Schwarz and Brian Toby

Abstract:

The determination of atomistic structures from x-ray diffraction, scattering, and spectroscopic data is challenging due to the complexity of configurational space. In this talk, we will discuss the use of first principles and first principles-based modeling, in conjunction with various optimization approaches, to accelerate the process. Examples include single and multi-objective inversion of PDF data, and resolution of thin film and solid-liquid interface structures from CTR data.