Title: Big data and self-driving labs in small-angle neutron scattering

Abstract:

We are in the midst of a revolution in experimental science. Advances in computing, sources, and data acquisition pipelines have enabled the collection of data at rates orders of magnitude faster that even a decade ago, while machine learning approaches have enabled unprecedented levels of autonomy in experimental execution. In neutron science, this has manifested in event-mode data and the numerous advanced techniques enabled by event mode data acquisition: stopped-flow mixing, stroboscopic measurements, and more. Autonomy is perhaps best exemplified by the Autonomous Formulation Lab at the NCNR, which can use SANS with robotic sample preparation and Gaussian process regression to map a phase diagram of a self-assembling systems with up to 25x fewer samples than a grid search approach. This forthcoming data tsunami is no match for manual fitting approaches using graphical software: new tools are needed. This module will focus on equipping students with foundational skills for working with massive scattering datasets programmatically, explore the self-assembly of a block copolymer micelle system autonomously using the AFL, and introduce some best practices for programmatic fitting of hundreds of individual datasets using the SasView/sasmodels API.