Contribution ID: **59** Type: **Oral**

Rapid, online screening of complex phase spaces using Bayesian Optimization for SAXS measurements

Thursday, 16 March 2023 14:45 (20 minutes)

Small-angle x-ray scattering (SAXS) has been widely used to probe the intricate structure of biomolecules and proteins. Owing to its conceptual simplicity, the technique has also been applied to study the cluster formation in nanoparticles and supercritical fluids (SCF). However, due to the complex thermodynamic state space often encountered in SCF, the effective exploration and identification of the relevant conditions of maximal cluster organization and amalgamation is unknown a priori. This, in turn, necessitates a complete scan of the state space—a laborious and time-consuming process. In this work, we employ Bayesian optimization (BO) as a data-driven method to effectively sample such complex state spaces. We show that the BO algorithm, unaided by human intervention, converges on average 35-50% faster than an expert human user. We also demonstrate the robustness of the implementation by testing on several temperature and pressure ranges while incurring minimal losses in accuracy. This establishes the validity of the method, which has potential to be combined with current and future high acquisition rate experiments conducted at the Linear Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC).

Primary author: YOUNES, Khaled (Stanford University)

Co-authors: POLI, Michael (Stanford University); MUHUNTHAN, Priyanka (Stanford University); ERMON, Stefano (Stanford University); IHME, Matthias (Stanford University)

Presenter: YOUNES, Khaled (Stanford University)

Session Classification: Tracking

Track Classification: Methods