Contribution ID: **36** Type: **Poster**

Simultaneously fitting molecular dynamics simulations to neutron and X-ray diffraction and spectroscopy data with a bayesian approach

Friday 6 December 2024 13:45 (3 hours)

Neutron and X-ray scattering experiments provide valuable insights into the nanoscopic properties of matter, a scale that is also accessible through Molecular Dynamics (MD) simulations. If the simulations reproduce the experiments, they can give greater insight into the material properties on the nanoscopic scale than traditional data analysis methods. However, existing MD forcefields are primarily optimized to reproduce macroscopic quantities.
In our work we establish a connection between published experimental data from neutron and X-ray experiments, specifically focusing on diffuse scattering and quasielastic neutron scattering, and MD simulations.
We integrate tools for MD simulation (LAMMPS) and scattering curve computation (Sassena) in a custom built Bayesian framework that employs a Markov Chain Monte Carlo approach to sample a parameter space. Our approach explores a broad range within the parameter space, enhancing the likelihood of finding the global minimum of forcefield parameters. This approach is highly versatile and can be adapted to different systems. We compare this approach to a simple brute force method of finding an adequate fit. In this work, we utilize liquid water as a proof of concept.

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Session Classification: Poster Session

Track Classification: Neutron Methods