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A Markov Chain Monte Carlo approach to fit Molecular Dynamics simulations to neutron and X-ray diffraction and spectroscopy data on the example of water

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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 on liquid water, 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 parameter space. The fit algrorithm lets us obtain a set of parameters that capture the nanoscopic structure and dynamics as described by neutron and X-ray experiments simultaneously. 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. Here, we utilize liquid water as a proof of concept for the workflow.

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