Contribution ID: **53** Type: **Short talk**

A Bayesian approach to fit Molecular Dynamics (MD) simulations to neutron and X-ray diffraction and spectroscopy data on the example of water

Thursday 22 June 2023 10:00 (15 minutes)

Most of the established MD water models are optimized to reproduce macroscopic water properties, but are then used to study its nanoscopic structure and dynamics.
Neutron and X-ray scattering experiments investigate matter on exactly this nanoscopic level and these experiments can be used to optimize the water models on exactly the same time- and length-scale they will be evaluated on.

In our work, we connect published experimental data of neutron and X-ray experiments on liquid water (diffuse scattering and quasielastic neutron scattering) with MD simulations via a Bayesian fitting algorithm to obtain a set of parameters that can simultaneously fit the real nanoscopic structure and dynamics on an atomic level. To do so, we tie together existing best-of-class tools for MD simulation (LAMMPS) and scattering curve computation (Sassena) using a self-written Bayesian framework that samples the parameter space with a Markov Chain Monte Carlo approach.

Primary author: Mrs REICH, Veronika (GEMS at MLZ, Helmholtz-Zentrum Hereon)

Co-authors: Mr PARDO, Luis Carlos (Departament de Física Escola d'Enginyeria de Barcelona Est, Universitat Politècnica de Catalunya); Prof. MÜLLER, Martin (Helmholtz-Zentrum hereon GmbH); Dr BUSCH, Sebastian (GEMS at MLZ, Helmholtz-Zentrum Hereon, Germany)

Presenter: Mrs REICH, Veronika (GEMS at MLZ, Helmholtz-Zentrum Hereon)

Session Classification: Parallel 5