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Validating Molecular Dynamics Computer Simulations with Neutron Scattering Data

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Neutron scattering data are usually evaluated by analytical models. Computer simulations, for example using the Molecular Dynamics (MD) technique, can give a description of the sample's structure and dynamics on the atomic scale. Using this information, neutron (and x-ray) diffraction and spectroscopy curves can be computed. The scattering data can then be used to validate the simulations and vice versa the simulations can be used to evaluate the scattering data. These evaluations are able to capture complicated structures (e.g., amorphous) and motions (e.g., non-Fickean diffusion).
In this contribution, we focus on the comparison of different exemplary simulations of solids and liquids to scattering data.
For the solids, the influence of different parameters of the simulation such as the size of the simulated box on diffraction patterns is evaluated and the accuracy of the computation results using the program SASSENA is discussed for neutron and x-ray diffraction.
In the case of liquids, the simulated structure and dynamics of water as a prototypical liquid is compared to scattering data and other literature values like the diffusion coefficient. Different force fields are investigated and the influence of their base parameters is studied.

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