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Development of a workflow to calculate the X-ray and neutron diffraction pattern from continuum simulations of macroscopic structures

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It is a common practice in science to approach a problem simultaneously from the theoretical and experimental side. However, it is important to compare theory and experiment as directly as possible in order to validate that the theory describes reality. This contribution focuses on bridging the gap between simulations and scattering experiments with neutrons and X-rays.
Although scattering experiments are a very powerful tool to understand the structure and dynamics of materials on the nanoscale, the analysis of scattering patterns suffers from underdetermination, i. e. different structures can yield the same scattering pattern. One way to help alleviate this phase problem is to run a molecular dynamics (MD) simulation and calculate scattering patterns from it. However, this approach reaches its limits for large systems due to the myriad amount of computation time required.
This work tries to create a workflow in order to generate scattering patterns of large structures with continuum descriptions, i. e. structures that are continuous instead of a summation of atoms. Our final vision is to separate the scattering pattern of inhomogeneities of a macroscopic sample from its environment.

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