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Calculation of neutron and X-Ray scattering data from Molecular Dynamics simulations through optimal use of computation resources

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Optimization of computation time has always been a challenge in the world of computation. In this work, we address the computation of X-Ray and neutron scattering data from molecular dynamics simulations. There are multiple software solutions available for this; we have chosen sassena for our work. Sassena inherits distributed memory parallelization (MPI) from its previous version. This work further augments vectorization and shared memory parallelization (OpenMP) into it and bolsters the computing speed of sassena. Furthermore, the introduction of shared memory parallelization introduces a possibility of doing hybrid parallelization. As a long term goal, we aim to use the benefit of this optimization to validate the simulation of hydrogen storage materials with neutron scattering data.
Keywords:
1) Parallel computing
2) Neutron scattering
3) Molecular Dynamics Simulation
4) sassena

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