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Hybrid high performance computing to covert the molecular Dynamics simulation to neutron and x-ray data

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The world of computing always strives for a faster solution. The current work made an effort to make the program sassena faster, which calculates the neutron and x-ray.scattering data from atomic simulations, such as molecular dynamics (MD). This can be achieved using different parallelization strategies, e.g. vectorization, thread-based parallelism and distributed memory parallelism. Current work, aided by different analysis tools available on the market, tried to find such opportunities of parallelization within sassena and ensured correctness of the code while implementation of any kind of parallelization. The main goal of this work was to build upon advantages of different parallelism strategies and compensate disadvantages of one strategy by the advantages of others. This work expects a gain in the performance by the use of such a hybrid high-performance computing approach. Furthermore, this work plans to benefit from the achieved performance gain and apply this solution to validate simulations of Hydrogen storage materials with scattering data.

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