Possible applications for the Open Molecular Science Cloud: AMBER simulations and development of highly accurate many-body potentials

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The San Diego Supercomputer Center (SDSC) has been recently making efforts to integrate its computational infrastructure with public cloud providers to provide elasticity and an efficient approach for high-throughput computations [1]. In this talk I will be presenting two possible applications related to my research that could take advantage of the Open Molecular Science Cloud (OMSC). The first one is about perming AMBER simulations, and the second one is related to integrating a machine learning software infrastructure with cloud computing for the automated generation of quantum mechanical training sets in a high-throughput fashion.

My work with AMBER consisted of developing new advanced molecular simulation methods. These methods enable the theoretical study at the force field level of electrochemical processes even when pH effects also take place [2], including proton-coupled electron transfer (PCET). This work brings the first implementation of constant redox potential methods in a common software package for molecular simulations. These simulations have high computational performance because they can be done using AMBER's GPU-accelerated code.

My current research project revolves around the development of new highly accurate many-body potentials for molecular simulations. With the advent of elaborate fitting procedures of many-body potential terms to reference "first principles" quantum calculations, the computational cost of fragmentation methods can be significantly decreased. This allowed the construction of very accurate potentials for molecular simulations like the highly successful MB-pol water model [3], which combines a physically motivated representation of long-range interactions with accurate low-order terms of the many-body expansion. My project aims at generating new MB-pol potentials to different systems in order to perform molecular dynamics simulations of gas-phase clusters as well as extended condensed-phase systems. This involves software development, the use of machine learning approaches, and the computation of training data consisting of thousands of highly accurate quantum calculations. These new models will be initially employed to study atmospherically relevant molecules.

References:

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