Statement of Work
Transferring exascale computational chemistry to cloud computing environment and emerging hardware technology (TEC^4)
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I. Background

The primary objective of the US Department of Energy Basic Energy Sciences (DOE BES)-supported TEC4 project is to accelerate the transition process from basic research associated with developing and implementing electronic structure methods to the widespread use of their scalable implementations to complex challenges in industrial chemical sciences. The TEC4 project combines advances in high-performance computing, applied math, and theory to address the factors limiting the wide-scale utilization of computational chemistry tools typically associated with: (1) the inertia in embracing new hardware technologies and algorithms, (2) limited access to HPC resources, (3) insufficient data for accurate data-driven models in chemistry. The role of HIPC is to contribute state-of-the-art parallel implementations of density matrix renormalization group (DMRG) formalisms, which are necessary for describing strongly correlated chemical and material systems.

II. Objective

The main objective is to integrate existing DMRG approaches with the coupled cluster downfolding approaches developed by the PNNL team. This development will fill the gap in existing DMRG approaches associated with the need for more efficient theoretical formulations and algorithms that include dynamic correlation effects in the DMRG theory. The resulting infrastructure will provide novel DMRG formulations capable of delivering unprecedented levels of accuracy in chemistry simulations on HPC cloud computing platforms. This combined algorithmic framework will be also a part of machine learning models developed under the TEC^4 project.

III. Scope of Work

[redacted]

IV. Deliverables

[redacted]