COST REDUCTION OF QUANTUM SIMULATIONS OF CHEMISTRY BY MEANS OF THE DISCONTINUOUS GALERKIN DISCRETIZATION [1]

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Quantum devices potentially enable computational speed up of electronic-structure calculations to the extent that the many-body Schrödinger equation becomes directly solvable and therewith circumvent the multireference problem entirely. However, as an excitingly young technology, quantum computers face several engineering challenges that limit e.g. the number of available quantum bits as well as the number of executable operations. Consequently, when designing novel quantum algorithms one needs to meet these restrictions in the most cost efficient way possible.

Electronic structure methods based on Gaussian and molecular orbital discretizations offer a well established, compact representation that forms much of the foundation of correlated quantum chemistry calculations on both classical and quantum computers. Despite their ability to describe essential physics with relatively few basis functions, these representations can suffer from a quartic growth of the number of integrals. Recent results have shown that, for some quantum and classical algorithms, moving to representations with diagonal two-body operators can result in dramatically lower asymptotic costs, even if the number of functions required increases significantly. We introduce a way to interpolate between the two regimes in a systematic and controllable manner, such that the number of functions is minimized while maintaining a block diagonal structure of the two-body operator and desirable properties of an original, primitive basis. Techniques are analyzed for leveraging the structure of this new representation on quantum computers. Empirical results for hydrogen chains suggest a scaling improvement from $\mathcal{O}(N^{4.5})$ in molecular orbital representations to $\mathcal{O}(N^{2.6})$ in our representation for quantum evolution in a fault-tolerant setting, and exhibit a constant factor crossover at 15 to 20 atoms. Moreover, we test these methods using modern density matrix renormalization group methods classically, and achieve excellent accuracy with respect to the complete basis set limit with a speedup of one to two orders of magnitude with respect to using the primitive or Gaussian basis sets alone. These results suggest our representation provides significant cost reductions while maintaining accuracy relative to molecular orbital or strictly diagonal approaches for modest-sized systems in both classical and quantum computation for correlated systems.

REFERENCES

[1] J. R. MCCLEAN, F. M. FAULSTICH, Q. ZHU, B. O'GORMAN, Y. QIU, S. R. WHITE, R. BABBUSH, AND L. LIN, *Discontinuous galerkin discretization for quantum simulation of chemistry*, arXiv preprint arXiv:1909.00028, (2019).

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