Enabling Scalable VQE Simulation on Leading HPC Systems

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***Abstract*—Large-scale simulations of quantum circuits pose significant challenges, especially in the context of quantum chemistry, due to the number of qubits, circuit depth, and the number of circuits needed per problem. High-performance computing (HPC) systems offer massive computational capabilities that could help overcome these obstacles. We developed a high-performance quantum circuit simulator, called NWQ-Sim, and demonstrate its capability to simulate large quantum chemistry problems on NERSC's Perlmutter supercomputer. Integrating NWQ-Sim with XACC, we have executed QPE and VQE algorithms for downfolded quantum chemistry systems at unprecedented scales. Our work demonstrates the potential of leveraging HPC resources to advance quantum chemistry and other applications of near-term quantum devices.**

I. Introduction

Quantum computing promises the potential to efficiently simulate quantum systems, with applications in areas like quantum chemistry, materials science, and physics. In particular, variational quantum eigensolver (VQE) has emerged as a leading approach for studying the electronic structure problem in quantum chemistry [3].

In the near-term, simulation of VQE on classical computers remains a critical way to verify and benchmark their performance due to the noisy nature of the device. However, scaling the simulation of VQE to tackle larger molecular systems faces several challenges. The memory and computational overhead grow exponentially with system size. Moreover, even for small numbers of qubits (less than 20), the circuit depth and the number of repeated circuit executions required per problem instance remain a major simulation bottleneck.

To address these scaling challenges, we have developed a comprehensive, end-to-end execution workflow for the VQE algorithm. This workflow is optimized for deployment on state-of-the-art High-Performance Computing (HPC) systems. A high-level overview of the execution flow is shown in Figure 1. The execution flow is composed of three core components, which work together seamlessly:

- **Coupled Cluster Downfolding [1]**: Reduces the complexity of the chemical problem for efficient execution.
- **XACC [2]**: XACC is a quantum-classical framework that provides implementations of various quantum algorithms including VQE.
- **NWQ-Sim**: NWQ-Sim is a high-performance quantum circuit simulator built for extensive simulations on advanced HPC systems, such as ORNL Summit and NERSC Perlmutter.

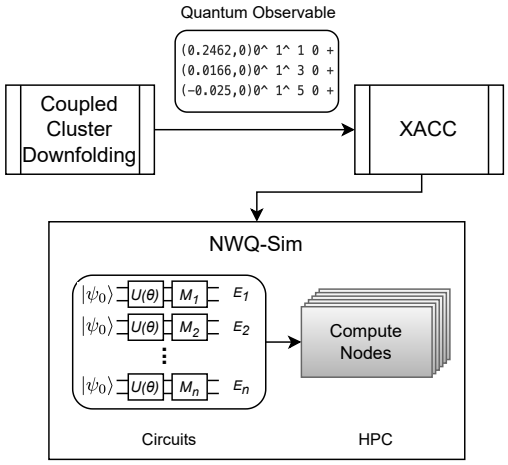

Fig. 1. The schematic illustration of the execution flow for the VQE algorithm. It begins with the Coupled Cluster Downfolding, reducing the complexity of the chemistry problem. The downfolded Hamiltonian then feeds into the XACC, generating quantum circuits for execution. Finally, NWQ-Sim, an optimized quantum circuit simulator, conducts large-scale simulations.

In this study, we showcase the capacity of this VQE execution flow to boost the speed of VQE simulations on leading HPC systems. Through the integration of NWQ-Sim with XACC, we carry out the VQE algorithm on quantum chemistry systems that have been downfolded, reaching scales previously unattained. Our findings underline the transformative potential of optimized simulation capabilities combined with HPC resources, indicating a promising trajectory for advancements in quantum chemistry and other near-term quantum applications.

II. Coupled Cluster Downfolding

Coupled cluster downfolding [1] presents a powerful strategy to substantially reduce the complexity of quantum many-body problems. It does this by breaking the entire system into smaller subsystems and integrating out the external degrees of freedom. This results in an effective Hamiltonian that operates solely within a smaller 'active space' subsystem. The downfolding is achieved using the external cluster amplitudes obtained from the comprehensive coupled cluster calculation. The result is an effective Hamiltonian that incorporates the

effects of the external degrees of freedom through renormalized interactions that operate within the active space. By diagonalizing the downfolded Hamiltonian within a smaller active space, we not only approximate the full system energy but also considerably reduce the complexity of quantum many-body problems, thereby making simulations on quantum computers significantly more manageable while maintaining high accuracy comparable to a full-scale calculation.

III. XACC

XACC is an open-source software framework developed to provide a hardware-agnostic interface for quantum-classical computing. It's designed to lower the barrier to entry for software developers looking to leverage quantum computing. XACC allows the specification of quantum observables directly, typically in the form of Pauli matrices, and makes use of built-in functions to process these observables on the constructed quantum circuits. The results can then be obtained from a quantum circuit simulator, for instance, NWQ-Sim. This simulator will execute the quantum circuit and provide the expectation value of the observable, offering insights into the quantum system under study.

IV. NWQ-Sim for VQE

NWQ-Sim leverages MPI and NVSHMEM to allow for multi-node GPU parallelism and can manage circuits containing over 40 qubits and 1 million gates. Furthermore, it scales effectively to thousands of nodes. NWQ-Sim is specifically designed with a range of optimizations for the VQE algorithm, including the capability to reuse the post-ansatz state for various basis measurements and an enhanced method for calculating expectation values.

A. Ansatz Reuse

The Variational Quantum Eigensolver (VQE) simulations, by their nature, demand repeated execution of the ansatz circuit, causing a significant computational challenge due to the requirement of transforming and measuring states for different bases. Instead of continually running the ansatz for each basis transformation, NWQ-Sim simulates and stores the post-ansatz state once. Then, reuse the post-ansatz state for all subsequent basis calculations. This approach eliminates the need for executing the ansatz circuit thousands of times, saving considerable time during simulations and making VQE simulations more streamlined and efficient.

B. Streamlining Expectation Value Calculation

The traditional approach to calculating the expectation value is to sample measurement outcomes from the quantum state. However, we've taken a more direct, deterministic path that eliminates the need for stochastic sampling. In our approach, the expectation value is calculated by explicitly iterating over all basis states and accumulating their weighted contributions. This efficient strategy takes full advantage of our knowledge of the state's amplitudes.

Together, these features contribute to an efficient process for executing the VQE algorithm on NWQ-Sim.

TABLE I
VQE Energy and Energy error ΔE of Beryllium Molecule

Iteration	Energy (Ha)	ΔE (Ha)
1	-14.6064	0.0164
4	-14.6211	0.0017
7	-14.6211	0.0017
10	-14.6216	0.0012
13	-14.6221	0.0007

V. Preliminary Results

Table I shows the electronic energy of a Beryllium molecule obtained in different iterations of VQE optimization. The exact ground energy is -14.6229262 Hartree. After 13 iterations, the VQE algorithm reaches the chemical accuracy, i.e., energy error to the exact solution $\Delta E < 10^{-3}$ Hartree.

VI. Discussion

Our findings with NWQ-Sim have propelled us a significant step forward in the realm of VQE simulations. However, an exciting frontier remains in the realm of high-performance computing, particularly in leveraging the capacity of GPUs. At present, the execution of VQE simulations involving up to 20+ qubits is predominantly bound by computational power, not memory. Such simulations can comfortably fit within the confines of a single GPU memory. The challenge lies not in the size of these computations but in maximizing the use of available resources to further enhance performance. In view of this, we envisage a potential direction for the future enhancement of NWQ-Sim in the form of a batch mode. This would allow for the simultaneous execution of multiple VQE simulations across numerous GPUs within HPC systems. Efficient synchronization of results across these GPUs could significantly enhance performance and processing times.

VII. Conclusion

In conclusion, we have successfully developed and implemented an optimized workflow for the VQE algorithm on HPC systems. The combination of Coupled Cluster Downfolding, XACC, and NWQ-Sim enables more scalable VQE simulations. Our approach has demonstrated the potential to accelerate VQE simulations to unprecedented scales, providing promising avenues for advancements in quantum chemistry and various quantum applications.

References

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