GCM and VQE Quantum Algorithm Implementation on the NWQSim Accelerator

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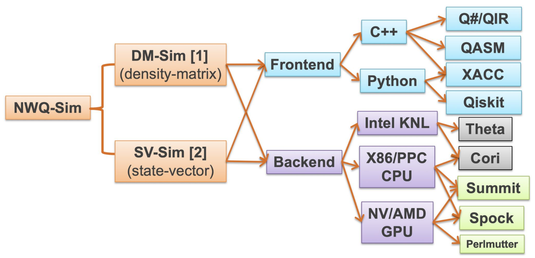
GCM and VQE Near-Term Quantum Algorithms

- The **Generator Coordinate Method (GCM)** is a typically classical algorithm that uses variational parameters in a many-body wave function to model collective atomic motion and, more generally, benchmark molecular systems. As a quantum hybrid algorithm, large subspaces have the potential to be efficiently modeled with relatively low-depth quantum circuits.
- The **Variational Quantum Eigensolver (VQE)** is a well known classical/quantum hybrid algorithm that, given an initial guess or ansatz, calculates an expectation value relative to an observable, then optimizes it to improve the guess, repeating these steps until the ground state (minimum) energy of a system is approximated.
- GCM has interesting potential as an alternative to uses of VQE, where the multi-step classical optimization algorithms necessary in VQE is replaced by a single step to solve the Hill-Wheeler eigenvalue problem.

NWQSim Quantum Simulator

- **NWQSim** is a Quantum System Simulation Environment within the High-Performance Computing group at Pacific Northwest National Lab for classical multi-node, multi-CPU/GPU heterogeneous High-Performance Computing (HPC) systems.
- By creating a streamlined and efficient C++ implementation, these algorithms will expand the quantum chemistry capabilities of NWQSim and provide a foundation for researchers to investigate higher-level quantum chemistry problems.



Methods

The primary goal of this project is to implement GCM and VQE directly in C++ and tie them in to NWQSim. Our implementations of GCM and VQE primarily use matrix representations for all of the operators and calculations, along with more complex natively-created C++ objects for representing strings of operators.

GCM Algorithm

- Based on the system being investigated, a set of fermionic operators and variational coordinates are generated to represent it.

$$\Gamma(\mathbf{Z}) = \sum_{p,q} z_{pq} E_q^p = \sum_{p,q} z_{pq} a_p^\dagger a_q \ , \ z_{qp}^\star = -z_{pq}$$

- These operators are then used in a classical computation and applied to a Hartree-Fock state for evaluation in a quantum device (NWQSim).

$$|\Phi(\mathbf{Z})\rangle = U(\mathbf{Z})|\Phi\rangle = e^{\Gamma(\mathbf{Z})}|\Phi\rangle$$

$$|\Psi_{\mathrm{GCM}}\rangle = \int d\mathbf{Z} |\Phi(\mathbf{Z})\rangle f(\mathbf{Z})$$

- The results are used to solve the generalized Hill-Wheeler eigenvalue problem.

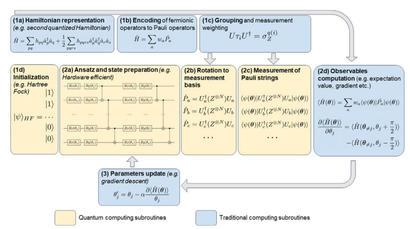
$$\mathbf{H}_{pq} = \langle \Phi(\mathbf{Z}_p)|H|\Phi(\mathbf{Z}_q)\rangle \ ,$$
$$\mathbf{S}_{pq} = \langle \Phi(\mathbf{Z}_p)|\Phi(\mathbf{Z}_q)\rangle \ , \qquad \mathbf{Hf} = E\mathbf{Sf}$$
$$\mathbf{f}_p = f(\mathbf{Z}_p) \ .$$

Algorithm 1 Quantum GCM (QuGCM) for near-term devices

Require: Hamiltonian matrix $H = \sum_j h_j P_j$, HF state $|\Phi\rangle$, and a set $\{\Gamma(\mathbf{Z}_i)\}_{i=1}^M$ where the index i could be a composite up to k terms as in Eq.(23)
1: Transform all $\{\Gamma(\mathbf{Z}_i)\}_{i=1}^M$ using JW transformation
2: Generate unitaries $\{V_i\}_{i=1}^M$ for $V_i := e^{\Gamma(\mathbf{Z}_i)}$ with Eq.(9) and Eq.(20)
3: Trotterize each element in $\{V_i\}_{i=1}^M$ to a linear combination of Pauli strings
4: **for** each V_q in $\{V_i\}_{i=1}^M$ **do**
5: Compute $\sum_j h_j P_j V_q$ classically
6: **for** each V_p in $\{V_i\}_{i=1}^M$ **do**
7: Compute $\sum_j h_j V_p^\dagger (P_j V_q)$ classically
8: Compute $V_p^\dagger V_q$ classically
9: Evaluate $\mathbf{H}_{pq} := \sum_j h_j \langle\Phi| V_p^\dagger P_j V_q |\Phi\rangle$ in a quantum device
10: Evaluate $\mathbf{S}_{pq} := \langle\Phi| V_p^\dagger V_q |\Phi\rangle$ in a quantum device
11: **end for**
12: **end for**
13: Solve the general eigenvalue problem $\mathbf{Hf} = E\mathbf{Sf}$ classically
14: **return** interested eigenvalues and eigenvectors

VQE Algorithm

- Outline of the VQE pipeline[2].



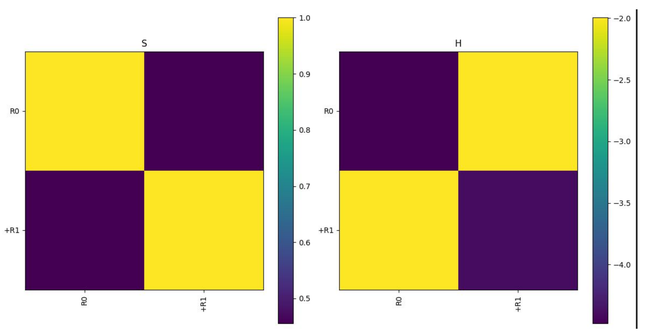
- The unitary coupled-cluster singles and doubles (UCCSD) ansatz is the current VQE ansatz[3].

Algorithm 1 Unitary Selective coupled-cluster

Step 1. Generate single and double excitations for a given molecule.
For all single and double excitations $[i, a]$ and $[i, j, a, b]$ in UCCSD add to ansatz all excitations for which $h_1[i, a]$ and $h_2[i, j, a, b]$ are larger than ϵ_1.
repeat
Step 2. Run VQE with the current ansatz to compute energy, update amplitudes for each excitation present in ansatz.
Step 3. For each single $[i, a]$ or double $[i, j, a, b]$ excitation present in ansatz using t_1 and t_2 values from the previous iteration and additional excitations $[k, c]$ or $[k, l, c, d]$ generate triple and quadruple excitations with the following coefficients:
$t_1[i, a] \cdot h_2[j, k, b, c]$
$h_1[i, a] \cdot t_2[j, k, b, c]$
$t_2[i, j, a, b] \cdot h_1[k, c]$
$h_2[i, j, a, b] \cdot t_1[k, c]$
$t_2[i, j, a, b] \cdot h_2[k, l, c, d]$
Step 4. For each excitation, if the absolute value of the largest coefficient computed in step 3 is larger than ϵ_n on iteration n, add this excitation to ansatz.
until termination condition

Results

The GCM implementation computes the necessary set of unitaries using an inverted Jordan-Wigner transform, and creates a set of qubit operators for quantum computation using a Clifford Transform. The current implementation also has classical and quantum functions along with integration into NWQSim for computing the **S** and **H** matrices at the core of the eigenvalue problem.



The VQE algorithm is currently being implemented using the UCCSD and the Jordan-Wigner transformation.

[2]

Future Work, References, and Acknowledgments

- Solving the final eigenvalue problem with results from GCM calculations
- Make GCM and VQE more user configurable along with configurable Ansatz for ease of use
- Optimization and testing to ensure results are optimal for future work
- Interface the C++ implementations with Qiskit
- Make use of GCM and VQE in real world chemistry problems, and investigate possible use cases of GCM over VQE

[1] Muqing Zheng, Bo Peng, Nathan Wiebe, Ang Li, Xiu Yang and Karol Kowalski, Quantum algorithms for generator coordinate methods. arXiv:2212.09205v1 [quant-ph]
[2] Jules Tilly, et. al, The Variational Quantum Eigensolver: A review of methods and best practices. 2022.
[3] Dmitry A. Federov, Yuri Alexeev, Stephen K. Gray and Matthew J. Otten, Unitary Selective Coupled-Cluster Method. arXiv:2109.12652v5 [physics.chem-ph]

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