QAMP 21: A Protein-Folding Entangler for the Variational Quantum Eigensolver

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Problem Definition / Abstract

The Variational Quantum Eigensolver (VQE) algorithms are one of the most popular solution approaches for quantum optimization problems in the era of Noisy-Intermediate State Quantum (NISQ) devices, but there are certain limitations with the toolset and software libraries used for creating initial circuit states that rarely consider constraints specific to the problem itself. Our objective is to create circuit libraries for an open-source quantum software development tool called Qiskit that will take into consideration the different types of constraints for different problem cases when creating an initial circuit guess for our VQE algorithm, and improve upon existing performance benchmarks. This project will eventually allow users to improve performance for their own optimization problems ranging from simulating complex molecules to solving graph and network problems using VQE. For this research undertaking, we will solve a simple model of the protein folding problem, which is a highly complex computational task and has major applications in biochemical fields such as material discovery and designing targeted molecules. By utilizing these tools, we will be able to accurately calculate important information about a desired protein system such as accurate energy values and reduced computation time.

Details / Background

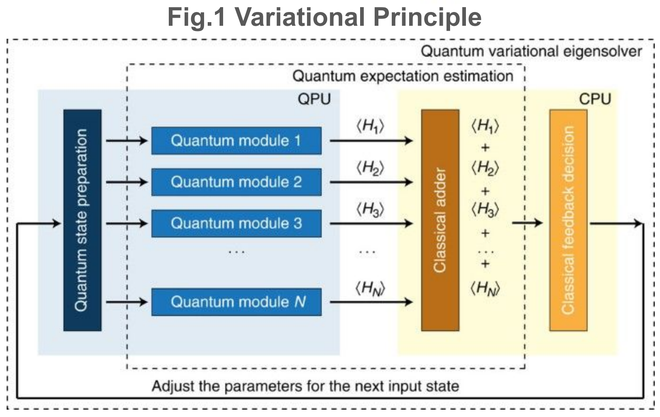
Variational Quantum Eigensolver (VQE):

Variational principle/method states that the expectation value (probability) of any wave function (our initial guess of the solution) will always greater or equal to the minimum eigenvalue (solutions of system) associated with its Hamiltonian, which is a matrix that describes the possible energies of a physical system. To give a brief example of how we use this, we can select a random circuit which represents a state for our selected system, described as an eigenstate “psi”, and we write down a Hamiltonian matrix which describes our selected system, and calculating the probability values of such a system will get us closer and closer to the actual value of the system.

The Variational Quantum Eigensolver algorithm is a quantum computing algorithm based on this principle that helps to estimate the ground state energy of a given quantum mechanical system. This is well suited for solving certain classes of optimization problems.
The basic idea is simply a feedback loop that starts with an initial guess for the eigenstate, measures the differences in the resulting expectation values, and adjusts the initial guess until it reaches a saturation point or minima.

$$\lambda_{min} \leq \langle H \rangle_\psi = \langle \psi | H | \psi \rangle = \sum_{i=1}^{N} \lambda_i |\langle \psi_i | \psi \rangle|^2$$

Fig.1 Variational Principle



[1] Fig.2 VQE Architecture

Entanglers / Variational Forms / Parametrized Quantum Circuits (PQCs):

We optimize our initial state or "ansatz" by using a parametrized circuit with a fixed form, interchangeably called entanglers or variational forms, which is applied to our initial state and generate an output state which on further iteration will give an expectation value close to the minimum eigenvalue.

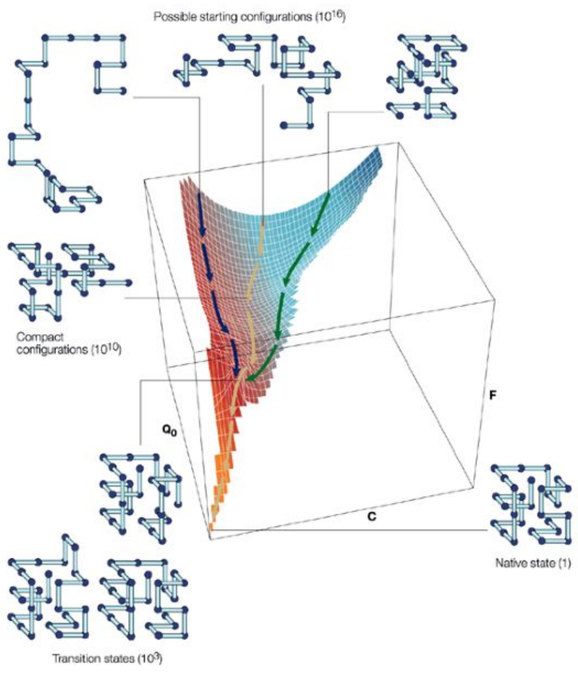
For this project we use Qiskit, which is an open-source quantum development platform designed by IBM Quantum primarily utilizing the Python language and libraries to run code and algorithms on real quantum hardware and simulators. We will be collaborating with IBM Quantum services and the Qiskit toolkit to make additions to the Qiskit Applications modules. [2]

Limitations:

(1) Very few types of entangler circuits are known or available. Even the state-of-the-art library for quantum computers has only four types of entangler circuits such as Ry, RyRz, SwapRz and UCCSD. They are all general entangler circuits with static structures and are used generically for most problems.
(2) Existing entangler circuits do not take into account the feasibility of output answers, and they often output infeasible answers. Results must be feasible answers of corresponding optimization problems when using the VQE algorithm for optimization problems.

Protein-Folding:

Proteins “fold” in nature to their native 3D conformation which enables them to become biologically functional. The structure and functions of many proteins are still not well understood, which means that processes that make use of the knowledge of proteins such as material discovery and designing targeted molecules for applications such as vaccinations, is also heavily underdeveloped.
This is a challenge because unfolded proteins have a very high degree of freedom and thus an enormous number of potential configurations in 3D space which grows exponentially upto the order of 10^{47}, which makes them a computationally intensive task for classical devices alone.
Using quantum computers however, we can can this problem linearly as N^4 in the number of our Hamiltonian terms, where the number of protein molecules is N, thus providing with an exponential speed-up. [3] The number of qubits required to map these conformations scales quadratically.



[4] Fig.3 Energy landscape for protein folding

Key Idea

We initiate by writing an entangler library for problem-specific VQE circuits as described in [5] to improve upon the limitations of current systems defined earlier. The overall vision is to create multiple libraries for different kinds of constraints and for different problems, and combine them into a single circuit library.

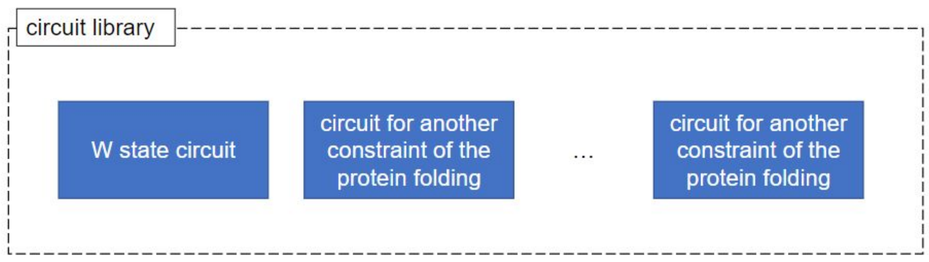
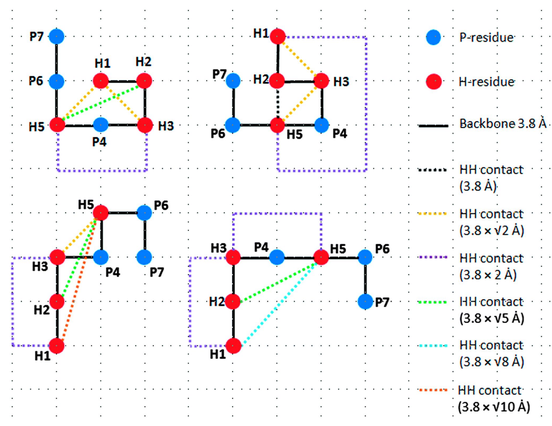


Fig.4 Circuit library schematic for protein folding class

For our project we want to solve the protein folding problem for a very simple protein chain. We start by encoding the different constraints for our sample Hamiltonian. Two of the constraints that we identify are configuration or geometrical constraints, which describe the relative positions of each molecule in the chain and governs its growth, and interaction constraints, which represents energy values that emerge due to electronic interactions between neighbouring molecules in a chain. We will also want to encode penalty terms for representing physical constraints such as local overlap between molecules in a chain, avoiding redundant rotations over an axis, and chirality terms. See Fig. 5 for an example of how these constraints might look like in 2D space.



[6] Fig.5 Scheme representation of 2D hydrophobic models

We then start preparing our PQC class for this protein folding problem by incorporating multi-qubit entanglement schemes to represent our constraints. One such method is to use the W-state circuits which is a superposition of states where exactly one qubit is in state |1> while all others are in state |0>, i.e. hamming weight is 1. Finally we create multiple qubit registers to accommodate for different Hamiltonian constraints and deploying multi-qubit entanglement for each set of identified constraints.
Once the ProblemSpecificVQE class is prepared, we pass a QuadraticProgram instance to this class. It will make an ansatz for our VQE algorithm based on constraints defined above, using circuits in the circuit library and checking for each constraint. If it matches to the specific pattern, it can then call for corresponding circuits in the circuit library.

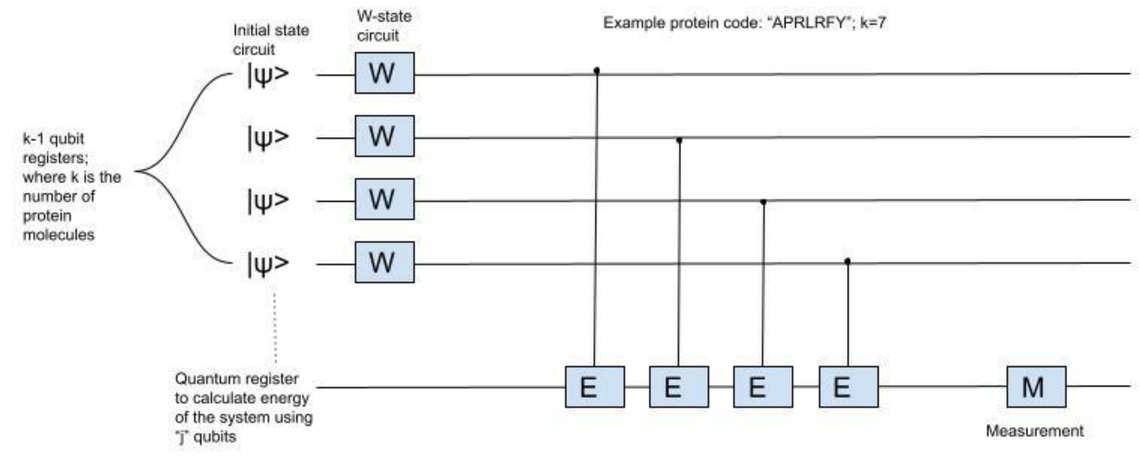


Fig.6 Initial circuit schematic for ProblemSpecificVQE_class using parameterized W states

Expected Results

Once we complete all steps involving designing code, merging libraries with source, and running simulations over different hardware to benchmark our results against existing solutions, we expect to achieve two milestones. One is to have initiated a circuit library that creates dynamic entanglers to reflect the constraints of a simple protein folding model, which in the future can allow additions to the overall library itself to provide other users the flexibility to create improved solutions for their own optimization problems using similar approaches. The other one would be in the simulation results themselves where we expect lower conformational energy values of the system, indicating improved accuracy of the algorithm, and lower optimization time, indicating overall computational speed-up.

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[3] Robert, A., Barkoutsos, P.K., Woerner, S. et al. Resource-efficient quantum algorithm for protein folding. npj Quantum Inf 7, 38 (2021).
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[5] Matsuo, A., Yudai S. and Shigeru Y., Problem-specific parameterized quantum circuits of the VQE algorithm for optimization problems. arXiv preprint arXiv:2006.05643 (2020).
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