2022 Womanium Hackathon

Challenge provided by Quantinuum

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Title: World-class Quantum chemistry with TKET

Hackathon Challenge:

Your company builds hydrogen fuel cell vehicles and is interested in finding new ways for a cost-effective and compact hydrogen storage system. You are working in the research and development (R&D) department and are tasked to evaluate the feasibility to simulate the quantum state of a Lithium Hydride (LiH) molecule using a gate-based quantum device. Based on the known gate sets and the qubit coupling map, you are tasked to find the best quantum device currently available.

Background:

One of the expected applications of noisy, intermediate-scale quantum (NISQ) devices is simulating quantum chemistry. A simple quantum chemistry question is "Given how the electrons and nuclei of a particular molecule are arranged, what is the energy of that configuration?". By examining how the energy of the configuration changes as the nuclei and electrons are moved relative to one another, we can map out an energy surface. The configuration that minimizes the energy is a stable, equilibrium point for the molecule. Knowing this configuration (and its associated energy), we can deduce a variety of molecular properties, such as reaction rates.

To simulate the quantum state of small molecules using a quantum device, we need a quantum circuit that is optimized to run on a quantum computer. Reducing the resources is crucial in the NISQ era, because the noise present in NISQ devices dominates more for larger circuits (with more operations) and reduces the accuracy of the results. Therefore, techniques that reduce circuit requirements can significantly improve the results on real hardware.

Methodology:

Circuit compilation and routing

For this challenge, you will use Quantinuum's TKET compiler via pytket, which integrates with Qiskit. TKET is the leading open-source developer toolkit designed to compile and optimize quantum programs. It is platform agnostic, targeting the world's leading quantum hardware and simulators. It will help you compile and optimize your quantum programs to target a range of hardware and find the most valuable solution for your company.

Pytket is a Python toolkit for quantum programming developed by Cambridge Quantum Computing, an extension of their larger TKET toolchain. TKET encompasses the entire high-performance toolset for quantum programming, primarily written in C++. Hence, pytket is a Python interface to TKET, a platform-agnostic quantum software development kit (QSDK).

Quantum Chemistry:

Most techniques for computing molecular energies on near-term quantum devices rely on the variational quantum eigensolver (VQE) algorithm. This algorithm uses a parameterized ansatz to describe the ground state energy of the Hamiltonian for a given configuration. By examining how the expected energy changes as it varies, one can optimize the parameters to find an estimate for the ground state and its corresponding energy.

Beginner*:* You will first get a feel for how TKET optimizes and compiles sample circuits for a given backend. You can create a sample circuit of your choice, or you can use some circuits, given as QASM code, here. Then optimize and run this sample circuit on different backends. Here is a list of questions to get you started:

1) Which gate-based quantum computers are accessible to you to implement your circuit?
2) Which circuit parameters should be minimized for the most efficient circuit implementation for a given backend?
3) What are the main features of TKET, and how can you apply them here?
4) Which backend is the best for a given sample circuit and why?

Knowledgeable: Instead of using a sample circuit, you will perform the tasks outlined for *Beginner* above for an actual LiH circuit. A given ansatz LiH circuit in the form of a QASM code will be supplied to you for your analysis here. The circuit was obtained by using the simplest qubit mapper/converter called the Jordan-Wigner Mapper. This circuit is quite deep. Before optimization, the circuit will have a total of 12 qubits and more than 16,000 gates.

Advanced: You are comfortable with how TKET can optimally route circuits onto real hardware. You are now asked to use the VQE algorithm to estimate the ground state energy for a LiH molecule. You should create your own ansatz LiH circuit for this challenge. Is it possible to create a 6-qubit ansatz circuit with a different mapper/converter than the Jordan-Wigner Mapper? Do you get different results depending on the quantum computer/simulator used? How do your results compare to known values? Are there any limitations you are confronted with?

Problem expansion for Advanced:
You are also considering how gate fidelity for different operations affects your analysis, i.e. mapping should be noise-aware.

References:

Hackathon tutorial to get you started with pytket

Pytket manual: https://cqcl.github.io/pytket/manual/index.html
Pytket extensions and backends: https://github.com/CQCL/pytket-extensions
Pytket GitHub: https://github.com/CQCL/pytket
Pytket Examples: https://github.com/CQCL/pytket/tree/main/examples

Unitary Coupled Cluster, Single-Double (UCCSD) ansatz:
https://en.wikipedia.org/wiki/Coupled_cluster

Quantum subspace expansion (QSE) technique:
https://journals.aps.org/pra/abstract/10.1103/PhysRevA.95.042308

Qiskit Nature Tutorials: https://qiskit.org/documentation/nature/tutorials/index.html