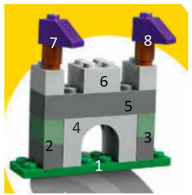
Building Quantum Bridges: Advancing Drug Discovery with QAOA and Explaining Quantum Computing with Building Blocks

Using quantum computers to solve combinatorial optimization problems

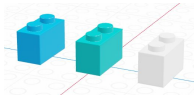
PRESENTER:
B. Maurice Benson

BACKGROUND: Pharmaceutical companies like Novo Nordisk and Johnson & Johnson have begun exploring quantum computers to advance Drug Design and Discovery. Optimization problems are a class of problems which quantum computers are starting to rival their classical counterparts. To demonstrate an example we describe and solve an optimization problem using "interlocking bricks"!

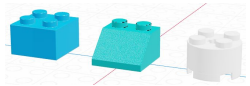
Problem: We have a database of every brick in a box of "interlocking bricks" and want to build a castle. We want to generate multiple castle designs for different conditions. We first divide the castle into regions. Every brick is associated with a region and has the properties:



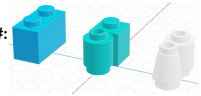
Color:



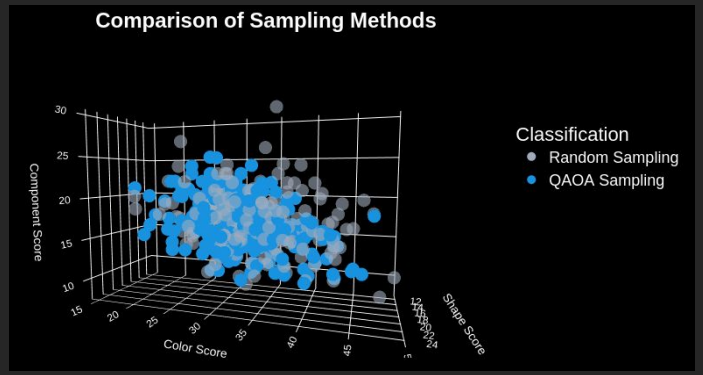
Brick Shape:



Components #:



Quantum Computers are effective at generating a Pareto front of solutions for large combinatorial problems.



Take a picture to **find** the **github repo!**

METHODS:

1. Generate hamiltonians for one brick per region constraint, property constraints, and mixer.
2. Optimize parameters for a 2-layer QAOA circuit.
3. Using the optimal parameters run the QAOA circuit
4. Postprocess results from quantum computer

Results:
Using a database of 48 bricks and a castle with 6 regions quantum sampling with the IBM Eagle was better finding optimal solutions compared to random sampling.

Translating to Chemistry:
Fragment-based drug design involves identifying small chemical fragments that bind to a target protein and optimizing them to develop potent and selective drug candidates. Follow this QR code to learn how PolarisQB achieves quantum utility accelerating the drug design process

B. Maurice Benson, W. J. Shipman, PolarisQB team

QuADD
Quantum-Aided Drug Design from POLARIS qb