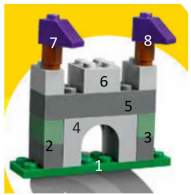
Building Quantum Bridges: Advancing Drug Discovery with QAOA and Explaining Quantum Computing with Building Blocks

Using quantum computers to solve combinatorial optimization problems

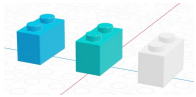
PRESENTER:
B. Maurice Benson

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"!

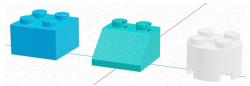
Problem: We have a database of every brick in a box of "interlocking bricks" and want to build a castle. We want to generate multiple castle designs for different conditions. We first divide the castle into regions. Every brick is associated with a region and has the properties:



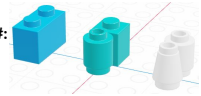
Color:



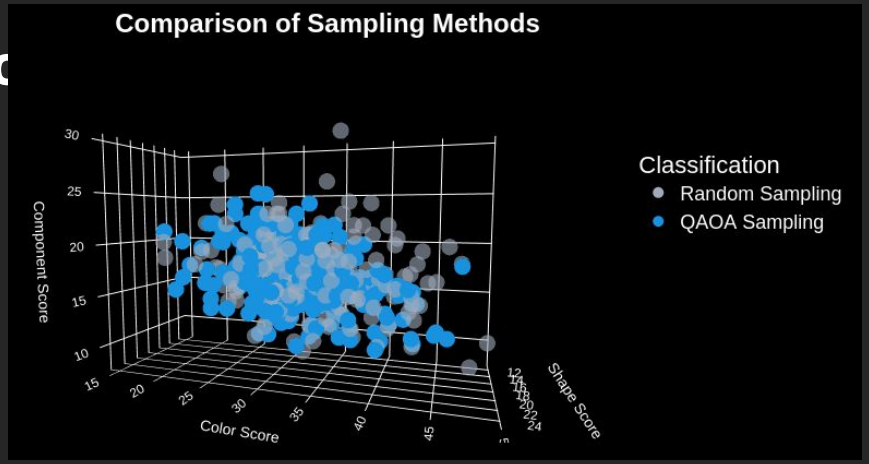
Brick Shape:



Components #:



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



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

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

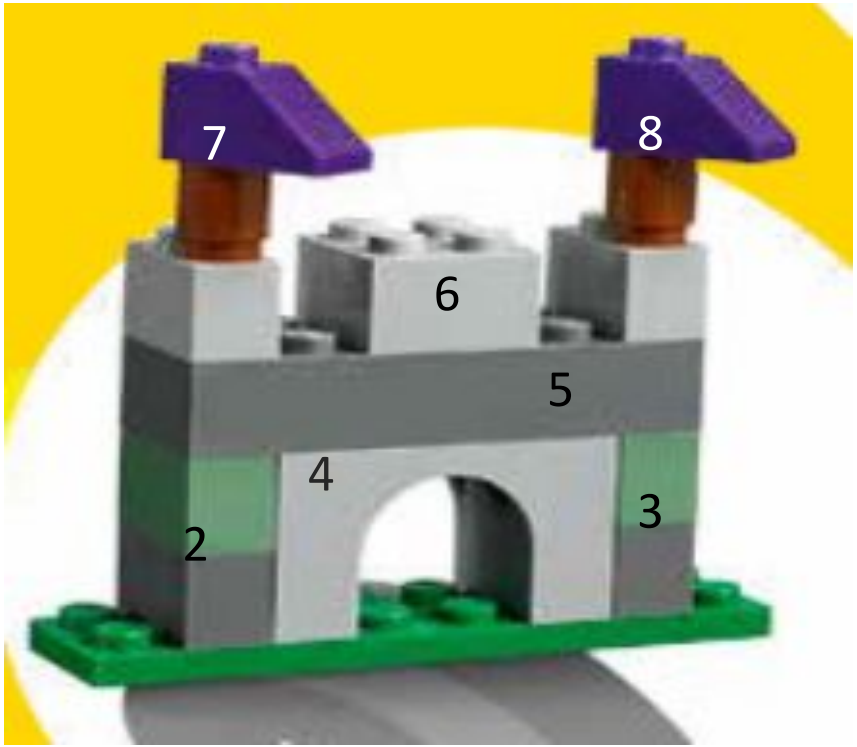
Presented by Maurice Benson
Principal Engineer
PolarisQB

Background

Pharmaceutical companies like Novo Nordisk [1] and Johnson & Johnson [2] 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 [3]. To demonstrate an example we describe and solve an optimization problem using “interlocking bricks”!

Problem

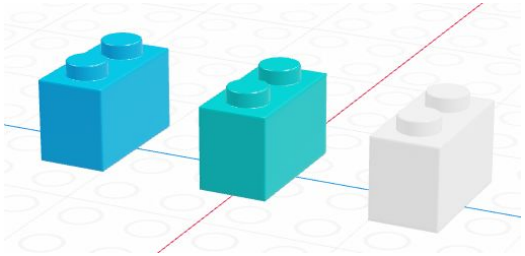
We have a database of every brick in a box of “interlocking bricks” and want to build a castle. We want to generate multiple castle designs for different conditions. We first divide the castle into regions.



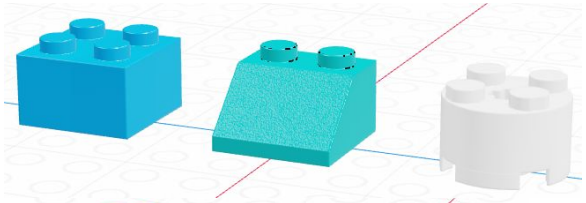
Problem

Every brick is associated with a region and has the properties:

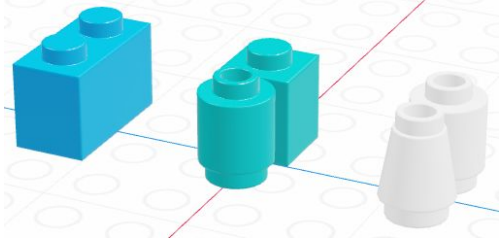
Color:



Brick Shape:



Components #:



Problem

For this problem we will try to optimize for a single color and the least amount of components.

Methods

1. Generate hamiltonians for one brick per region constraint, property constraints, and mixer.
    a. See code for examples and deeper explanation
2. Optimize parameters for a 2-layer QAOA circuit.
    a. Adam optimizer [4]
    b. 150 steps with 18 variables
3. Using the optimal parameters run the QAOA circuit
4. Postprocess results from IBM Eagle QC.
    a. Take 1000 reads from the quantum computer and separated them into sets of 10
    b. The most frequently occurring qubits in these sets were selected for further processing.

Results

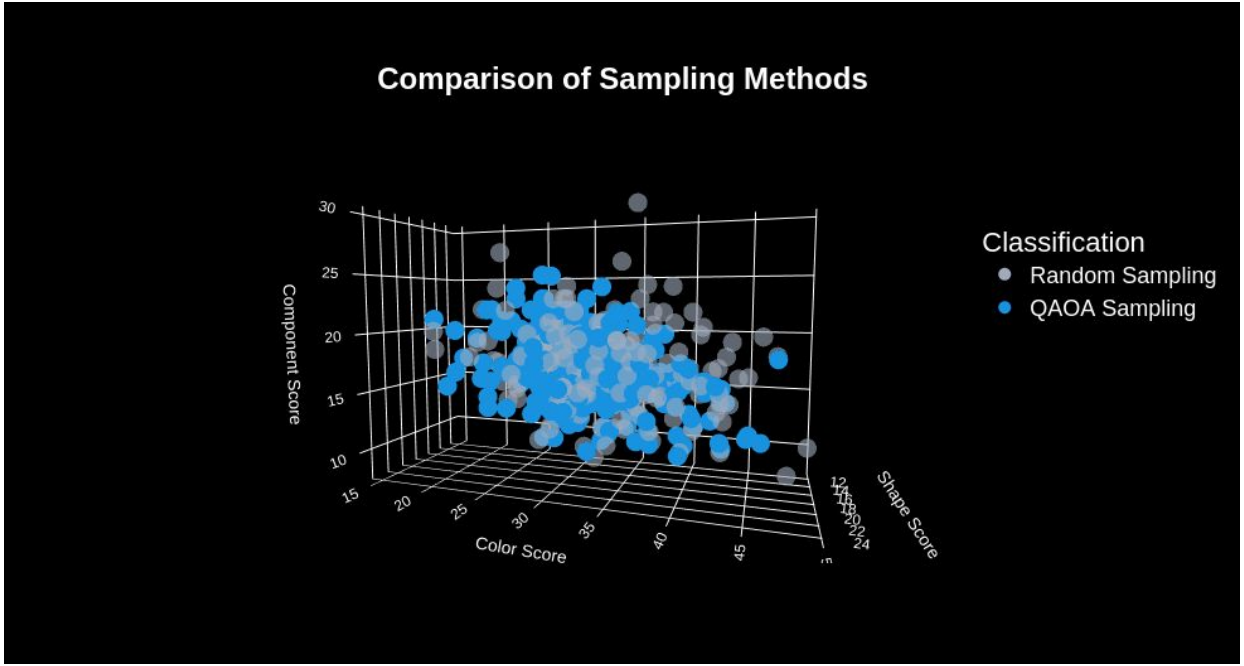
For database of 48 bricks and a castle with 6 regions (262144 possible combinations) quantum sampling with the IBM Eagle was better finding optimal solutions compared to random sampling. We compare the overall scores of solutions obtained from our sampler to those obtained from random sampling using a t-test.

t-statistic: -1.9955901047710478
p-value: 0.04636127256366392

Interpretation:

- **Negative t-statistic:** Mean overall score from the sampler is better (lower).
- **p-value < 0.05:** Statistically significant difference.

Results


Comparison of Sampling Methods
Component Score
30
25
20
15
10
Color Score
15
20
25
30
35
40
45
Shape Score
Classification
Random Sampling
QAOA Sampling

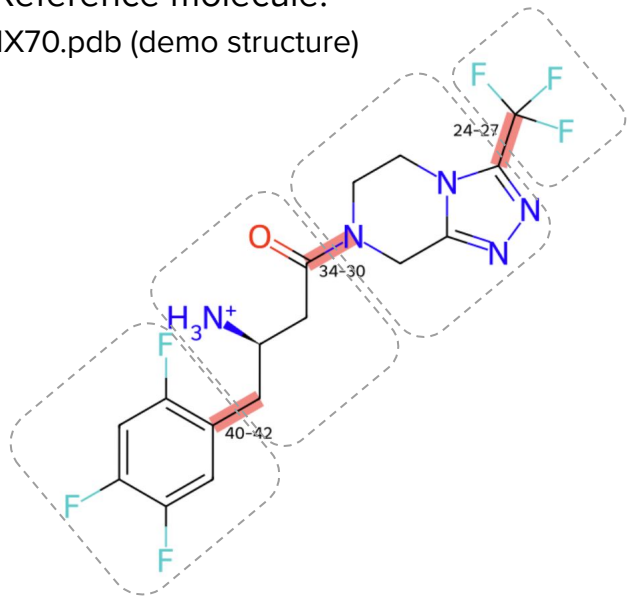
Continuing Conversation

1. Solving multi-objective optimization problems can be used to solve many problems in pharma industry
   a. Drug Trials
   b. Logistics
   c. Sales
2. At PQB we have turned Fragment Based Drug Design into a large combinatorial optimization problem to learn more please take a look at a recent webinar from our “Find your Star Molecule” series.

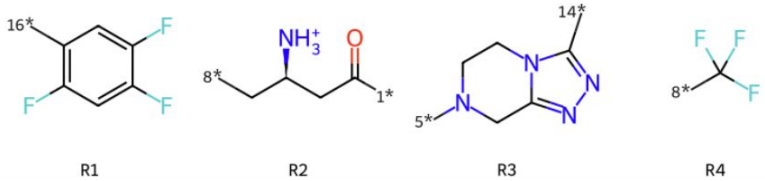
Continuing Conversation Fragment-Based Drug Design

Reference molecule:

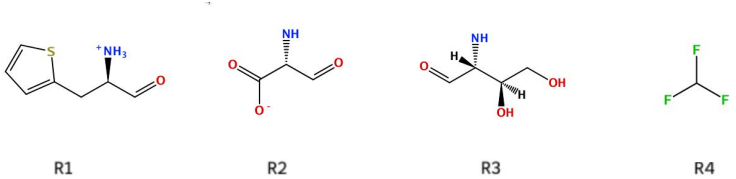
1X70.pdb (demo structure)



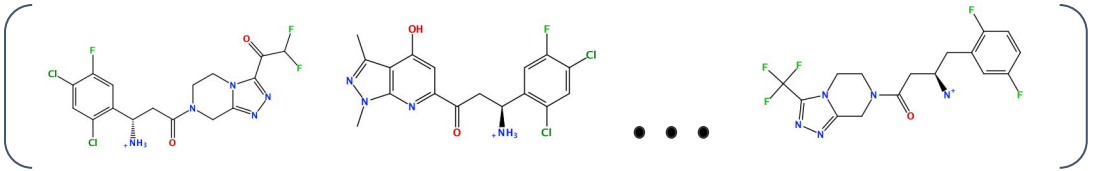
1) Fragment reference molecule



2) Generate numerous fragment options that fit spatial and physiochemical characteristics of the binding pocket



3) Find combinations of fragments that satisfy constraints, assemble into whole molecules



Resources

1. https://thequantuminsider.com/2024/07/04/the-novo-nordisk-foundation-believes-quantum-computing-poised-to-revolutionize-healthcare-drug-discovery/
2. https://thequantuminsider.com/2024/07/01/quantum-computing-for-pharma-with-johnson-johnson/
3. https://arxiv.org/pdf/2312.02279
4. https://arxiv.org/abs/1412.6980
5. https://www.iotworldtoday.com/transportation-logistics/researchers-demonstrate-step-toward-quantum-advantage
6. https://phys.org/news/2024-03-quantum-combinatorial-optimization-problems-easily.html

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