Fouad Ayoub Undergraduate Researcher Department of Aerospace Engineering

Problem-Specific Quantum Linear Solvers and High Entanglement Decompositions: The Poisson Equation Case

Dr. James Baeder Principal Investigator



The Role of the Poisson Equation in Computational Fluid Dynamics

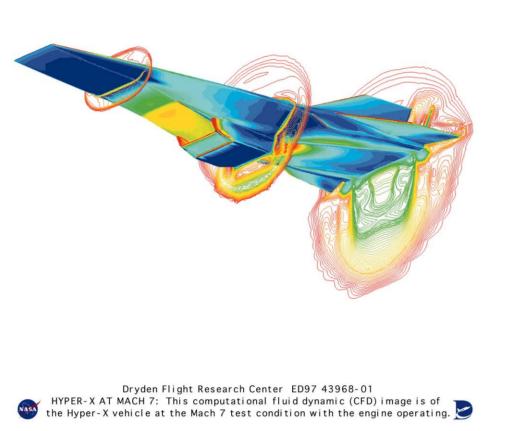
Motivation

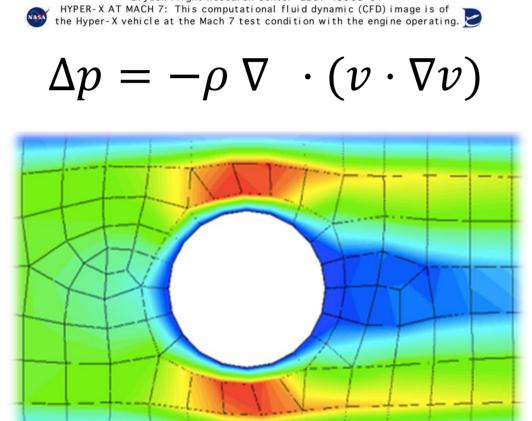
- The Poisson equation relates the pressure and velocity fields of a compressible fluid flow.
- Engineering models and designs require rigorous simulations to get a better understanding of the physical properties of the systems, and often these systems include complicated fluid flow dynamics.

Classical Methods

- Typically, the Poisson equation is solved with Finite Difference Methods. The Poisson is solved at discretized points in space and time as a linear system.
- Classical methods for solving linear systems are generally $O(n^3)$.

Can we do better with Quantum Computing?

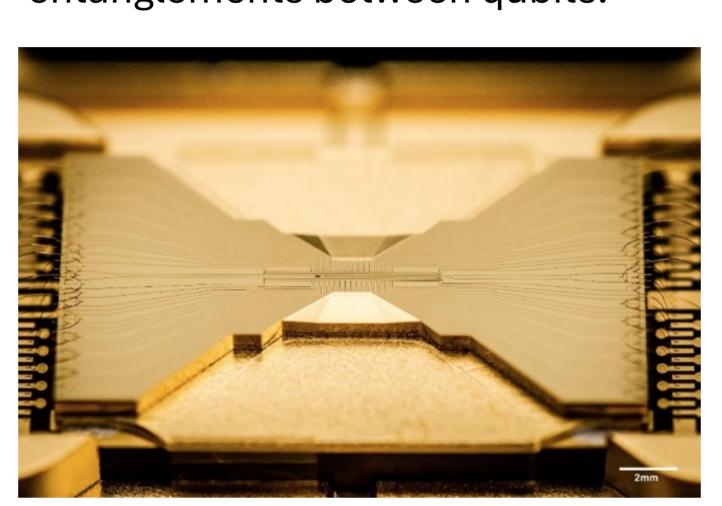




Quantum Computing – Variational Quantum Algorithms

Quantum Computing

- Using Qubits as the method of computation, we can encode large matrices and vectors and perform operations with an exponential space complexity speedup.
- This information is encoded through effective rotations of single qubit states and entanglements between qubits.



Quantum Computer:

Evaluate some cost function by running parameterized quantum circuit

Classical Computer:

Recalculate parameters using gradient descent methods based on most recent cost evaluation.

Variational Quantum Algorithms

- Some quantum gates can be parameterized. We generally call these "rotation gates".
- We can use these gates to make highly expressive, parameterized quantum circuits that can be used in optimization problems.

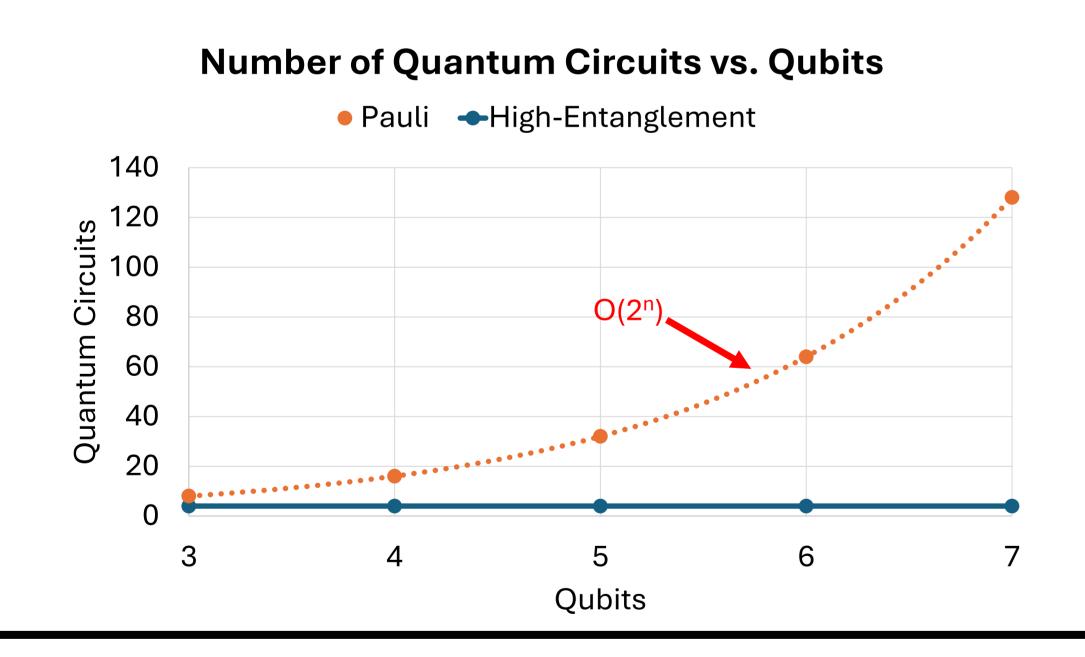
Variational Quantum Linear Solver

- A special case of VQA that solves linear systems of equations
- Develop cost function that quantifies how close Ax is to b.
- Evaluate cost on quantum computer, optimize parameters with a classical computer, and exit when a convergence condition is met.

High-Entanglement Decomposition of Poisson

Pauli Basis Decomposition

- Simple Pauli basis decomposition of the discretized Poisson matrix has an exponential scaling of terms.
- This means doing realistic system sizes will be impractical and diminish any quantum advantage.

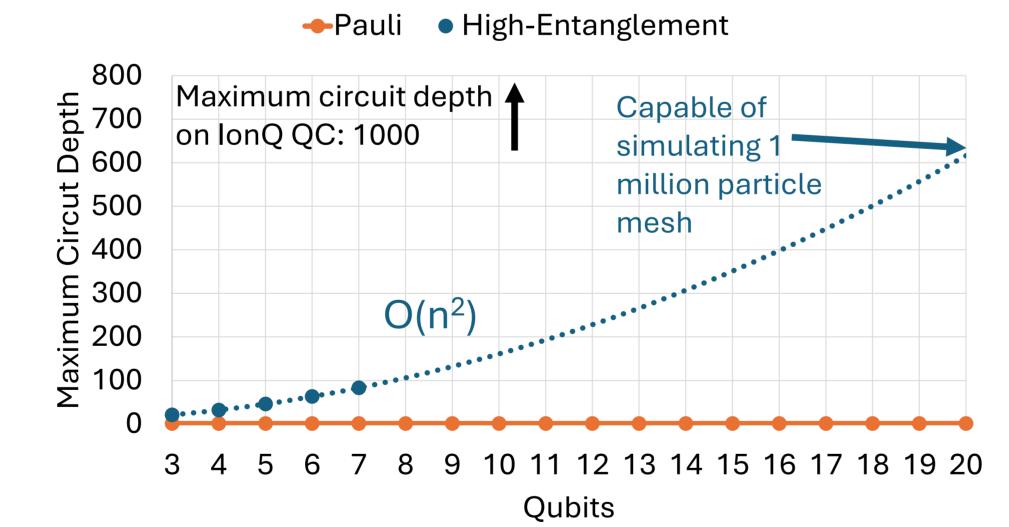


High-Entanglement Decomposition

 Newly proposed high-entanglement decomposition has constant scaling of terms, and only polynomial circuit depth.

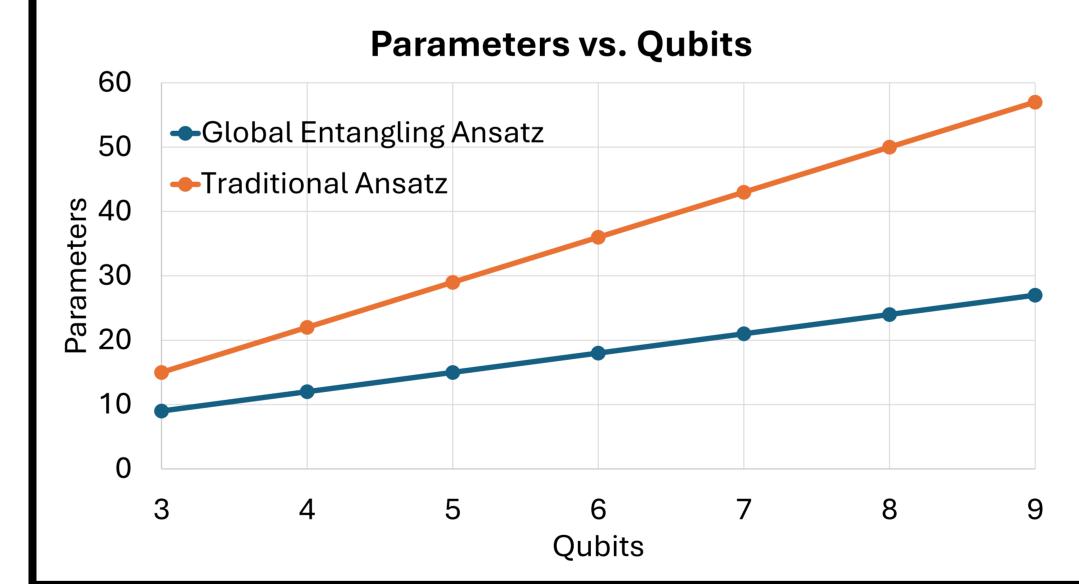
$$A = 2.5I - L_1 - L_2 - 0.5L_3$$





Traditional Ansatz

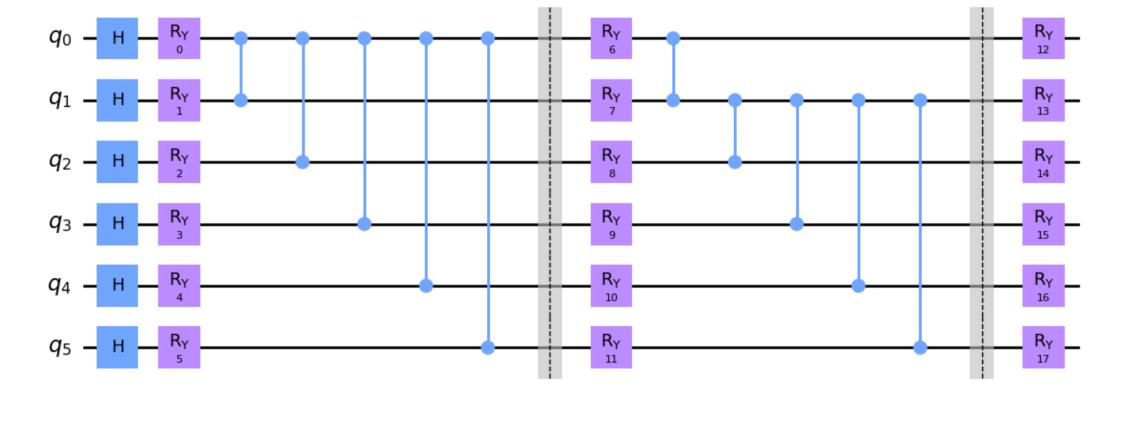
- Typical ansatz used in the literature operate under the limitations that qubits can only entangle with immediate neighbors.
- Results in too many parameters that causes training time to grow unnecessarily.



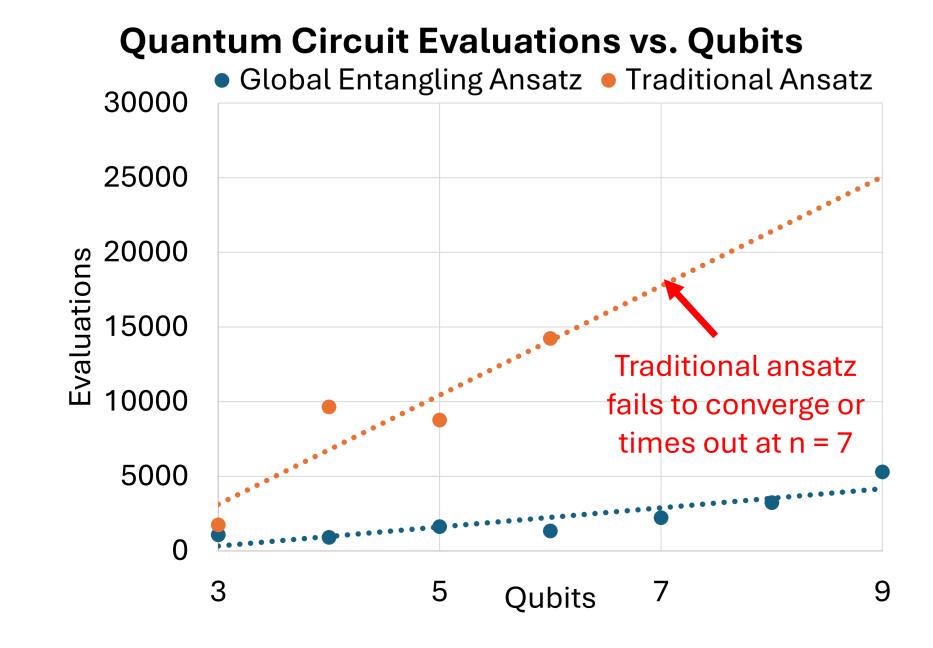
Global Entangling Ansatz

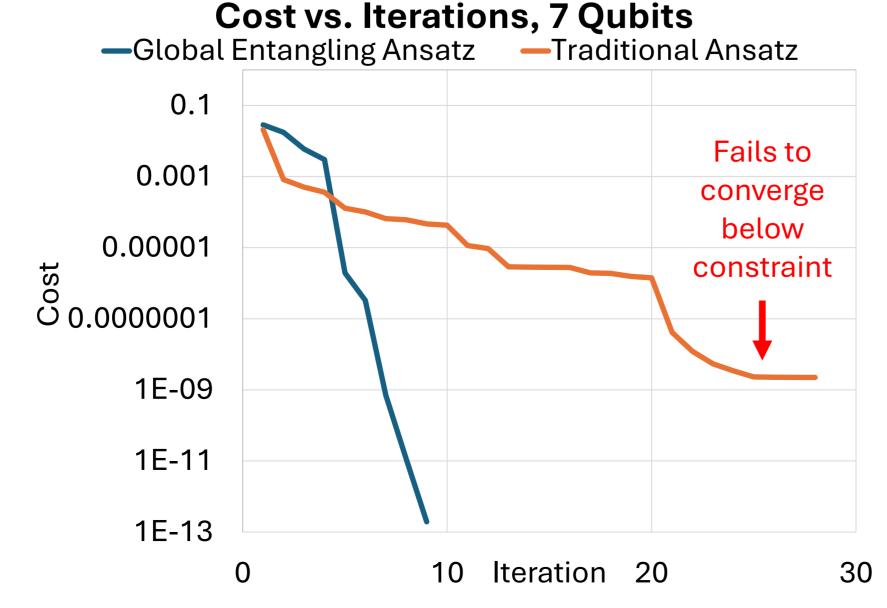
Global Entangling Ansatz

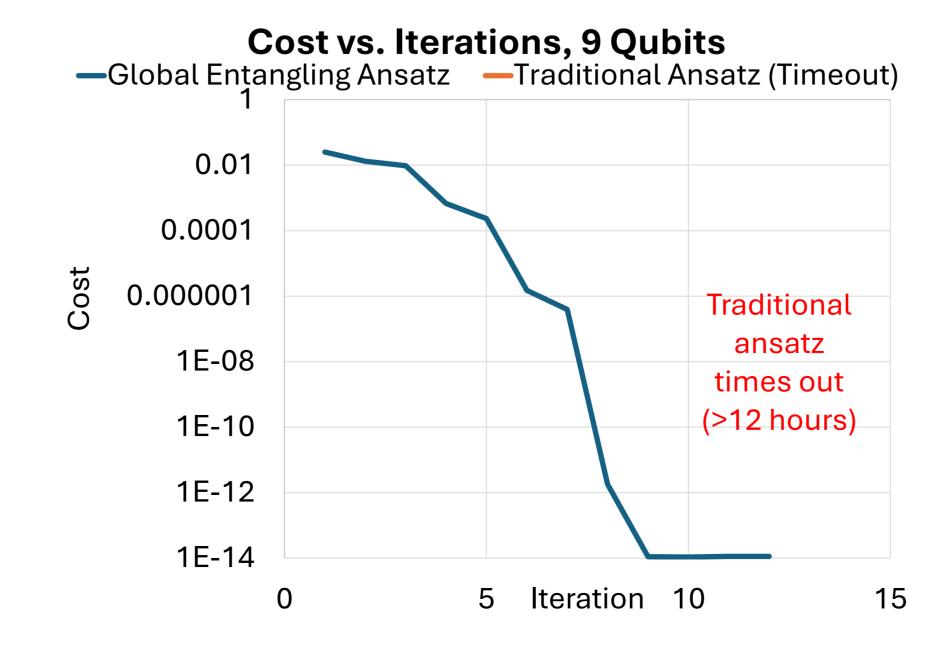
- Using globally entangling layers, each qubit is entangled with each other qubit.
- Without the restriction of locally entanglement, we can create expressible circuits with minimal parameters to optimize across.
- This **shortens the training time** of the circuit, while still maintaining a **high expressibility**.



Numerical Simulations







Results

 High-entanglement ansatz outperforms traditional ansatz, with reasonable scaling of QC evaluations and iterations during optimization. Also, it can converge below required constraint for higher qubit systems.
 Does not time out during optimization.

Future Work

- Attempt to decompose the 2D and 3D discretized Poisson equation matrix in high-entanglement quantum gates.
- Run optimizations on real IonQ Quantum Computers with high-entanglement capabilities.
- Attempt to solve Burgers' equation on quantum computer for time-dependent dissipation solutions.

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