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Optimization, Verification and Engineered Reliability of Quantum Computers

OVER-QC

Sandia National Laboratories
Dartmouth
Los Alamos NATIONAL LABORATORY EST. 1943
THE UNIVERSITY OF NEW MEXICO

https://overqc.sandia.gov

Mohan Sarovar

Integrating ASCR Research to Deliver Scientific Discovery Quantum Computing Workshop

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People

- **SNL**: Jon Aytac, Andrew Baczewski, Matthew Grace, Lucas Kocia, Alicia Magann, Ojas Parekh, Denis Ridzal, Kenneth Rudinger, Antonio Russo, Mohan Sarovar, Greg von Winckel, Wayne Witzel.
- **LANL**: Lukasz Cincio, Patrick Coles, Yigit Subasi.
- **Dartmouth**: James Brown, James Whitfield, Jun Yang.
- **UNM**: Robert Carr, Deepak Kapur.

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Project structure

Thrust 1: Formal verification of quantum algorithm implementations

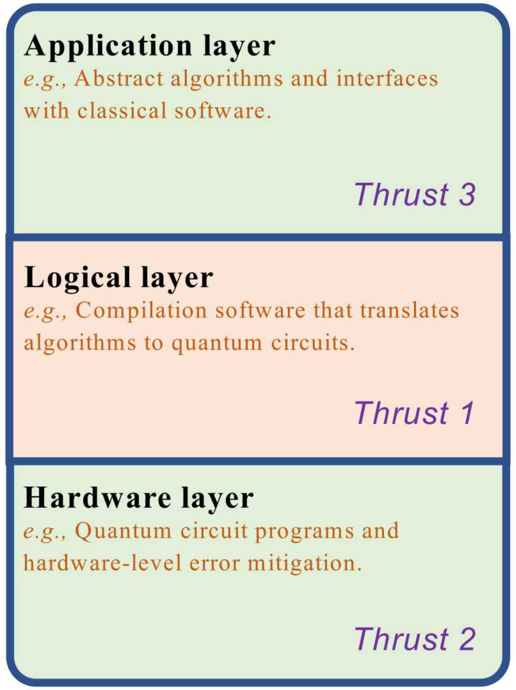
Goal: generate machine-assisted proofs of circuit implementations of quantum algorithms.

Thrust 2: Engineered reliability of NISQ devices

Goal: produce classical software and analysis tools to make near-term devices more reliable.

Thrust 3: Variational devices and classical heuristics

Goal: develop tools to explore synergies between classical heuristics and near-term variational devices (VD).



POP: 2018 - 2022

Highlight 1: Program verification using ProveIt

[Wayne Witzel, Kenny Rudinger, Deepak Kapur, *et al.*]

Algorithm Theory
(What does it do? How efficiently?)

proven algorithm

Algorithm Specification
(from paper or textbook)

proven implementation

Idealized Algorithm Implementation
(set problem size)

proven transformations

proven robustness

Device-Specific Implementation (satisfies hardware constraints, optimized for the hardware)

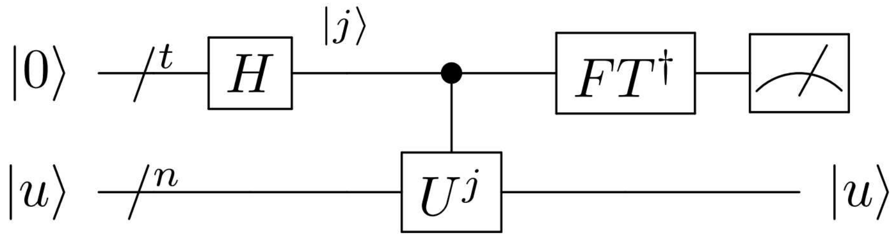
By proving the validity each step along the way, we can be assured that complete validation is feasible.

Highlight 1: Program verification using ProveIt

Prove-It: http://pyproveit.org

- Our open-source Python-based general-purpose theorem-proving assistant.
- Use Jupyter notebooks to render mathematical expressions via LaTeX.

  Example: $\forall_{l \in \mathbb{N}} \left[\forall_{x, \boldsymbol{y}_1, \ldots, \boldsymbol{y}_l} \left(\left(x \in \{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_l\}\right) = \left(\left(x = \boldsymbol{y}_1\right) \vee \ldots \vee \left(x = \boldsymbol{y}_l\right)\right)\right)\right]$
- In a proof-of-concept demonstration,[1] we derived the accuracy of the Quantum Phase Estimation algorithm:



$$\forall_{\varepsilon \in \{1 \ldots (2^{t-1}-2)\}} \left(P_{\text{fail}}(\varepsilon) \leq \left(\frac{1}{2} \cdot \left(\frac{1}{\varepsilon} + \frac{1}{\varepsilon^2}\right)\right)\right)$$

(slightly tighter than textbook[2] bound)

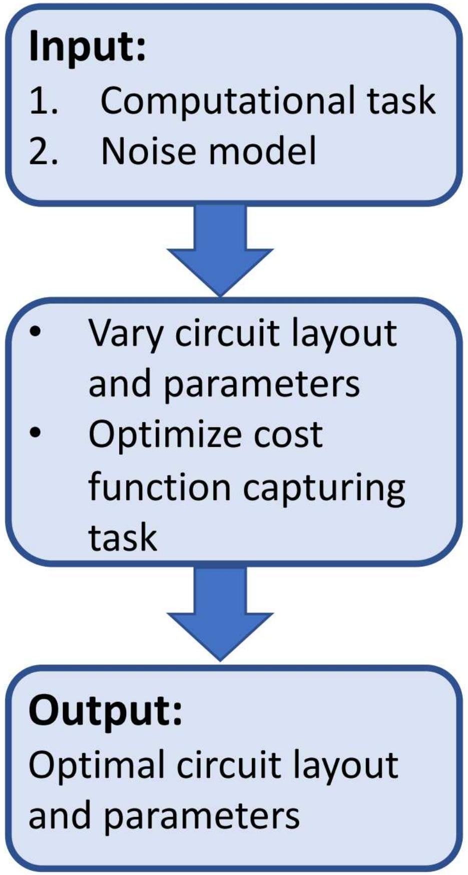
- … and uncovered 3 minor mistakes in the textbook[2] proof and improved the bound of the probability distribution.

1. W. Witzel, M. Sarovar, and K. Rudinger. (2015) Versatile Formal Methods Applied to Quantum Information. [Online]. Available: prod.sandia.gov/techlib/access-control.cgi/2015/159617r.pdf
2. M. A. Nielsen and I. L. Chuang, Quantum computation and quantum information. Cambridge University Press, 2010.

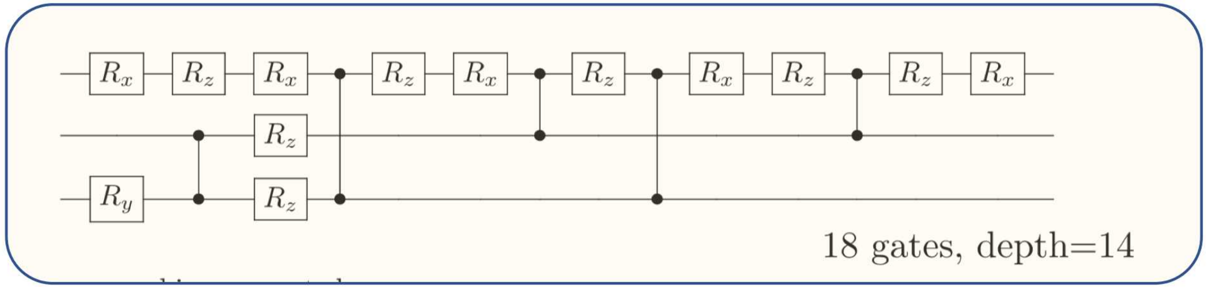
Highlight 2: Machine-learned circuit compilations

[Lukasz Cincio, Patrick Coles, *et al.*]

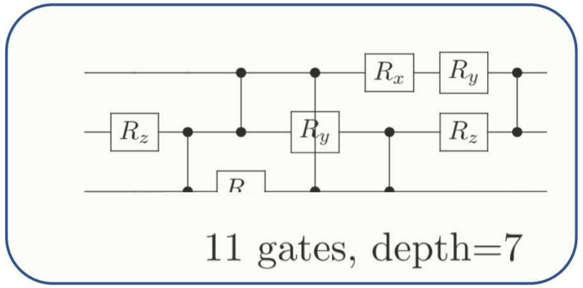
- Compilation of algorithms into circuits typically only consider coarse-grained noise models into account (e.g., limited connectivity, dead qubits)
- Recent characterization tools (e.g., gate-set tomography) yield a wealth of fine-grained error information.
- Can we use this information to improve circuit performance?



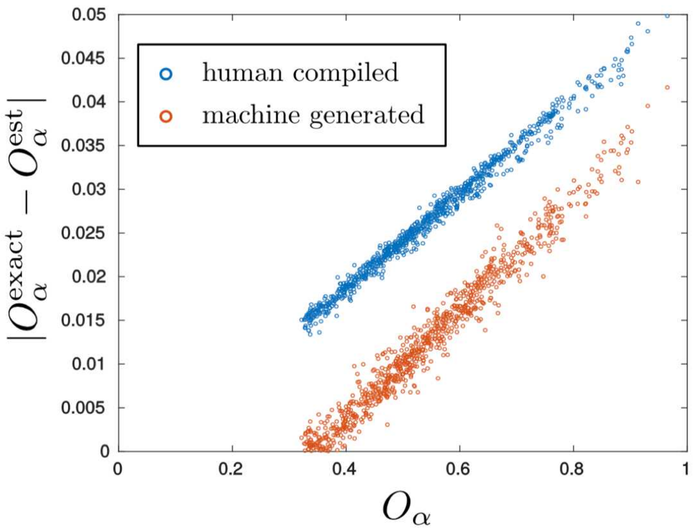
Example: state overlap between two qubits via SWAP test circuit



Human compiled (e.g., Linke et al., PRA 2018)



Machine compiled

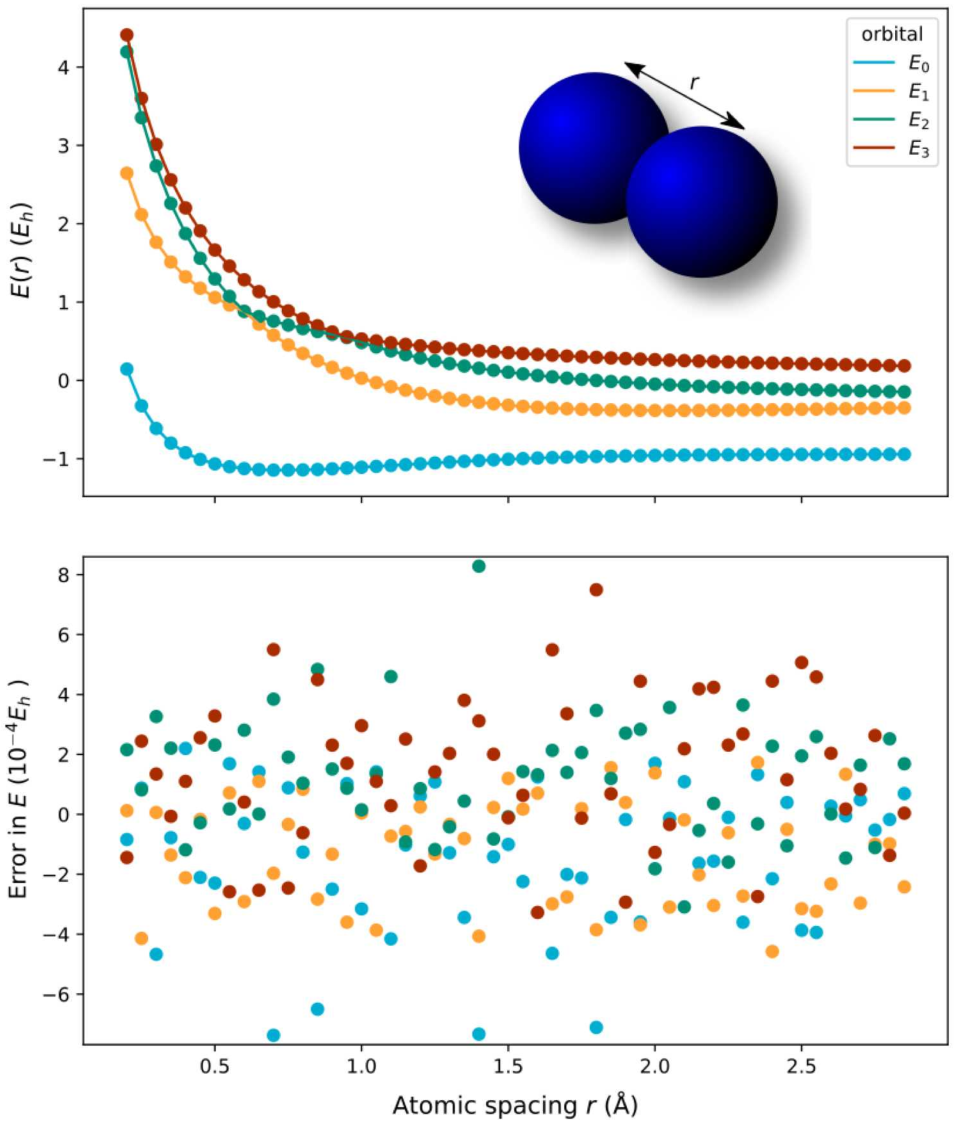


Highlight 3: Improved Q. simulation with RPE

[Antonio Russo, Kenny Rudinger, Andrew Baczewski, *et al.*]

- Robust Phase Estimation (RPE) [Kimmel, Low, Yoder, PRA, 2015] determines the relative phase induced by a unitary between two eigenvectors
- Corresponds to energy differences in the context of Hamiltonian simulation (i.e., molecular spectra)
- **Advantages**:
  - Naturally robust to noise (~31.6%)
  - Does not require controlled unitaries
  - Relies on preparation of superposition of eigenvector pairs
  - Heisenberg scaling

Molecular H_2 energy vs nuclear separation (exact and quantum hardware)



Other work

1. **Large scale QAOA coupled with large-scale classical optimization techniques**
    - QAOA simulations up to 30 qubits
    - Seamless interface with Rapid Optimization Library (https://trilinos.org/packages/rol/)
2. **Development of proxy models for variational QC**
    - Apply probabilistic manifold learning to learn optimization landscape
        - Fewer samples from quantum co-processor
        - Smooths sampling noise and generates smooth landscape for optimizers
3. **New (classical) optimization algorithm tailored to variational QC**
4. **Improved classical solvers for potential inversion when performing TD-DFT with hybrid quantum-classical methods.**
5. **New variational algorithm for quantum linear systems solving**
6. **New analog simulation method for generating, and sampling from, many-body thermal states**

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