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Sandia National Laboratories

Optimization, Verification, and Engineered Reliability of Quantum Computers (OVER-QC)

ASCR Quantum Computing Application Teams Program

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Team

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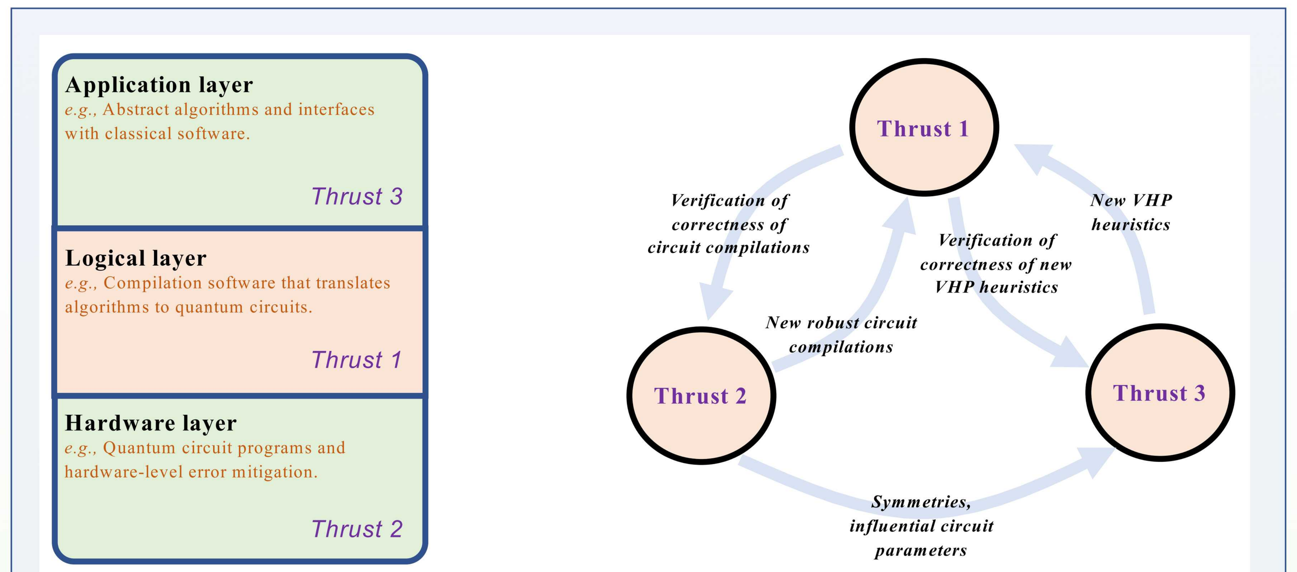
Motivation

Quantum technologies, especially quantum computers, show great promise for revolutionizing high-performance computing and simulation. As prototype quantum computers come online, it is becoming clear that obtaining useful output from such devices will require layers of sophisticated classical software that provide interpretation and analysis of the quantum computer's state and output. We will develop critical components in this ``software stack'' with a particular focus on enabling near-term Noisy Intermediate-Scale Quantum (NISQ) technologies. We have identified three critical needs for near-term quantum computing platforms, and the project is structured around three thrusts that address these needs.

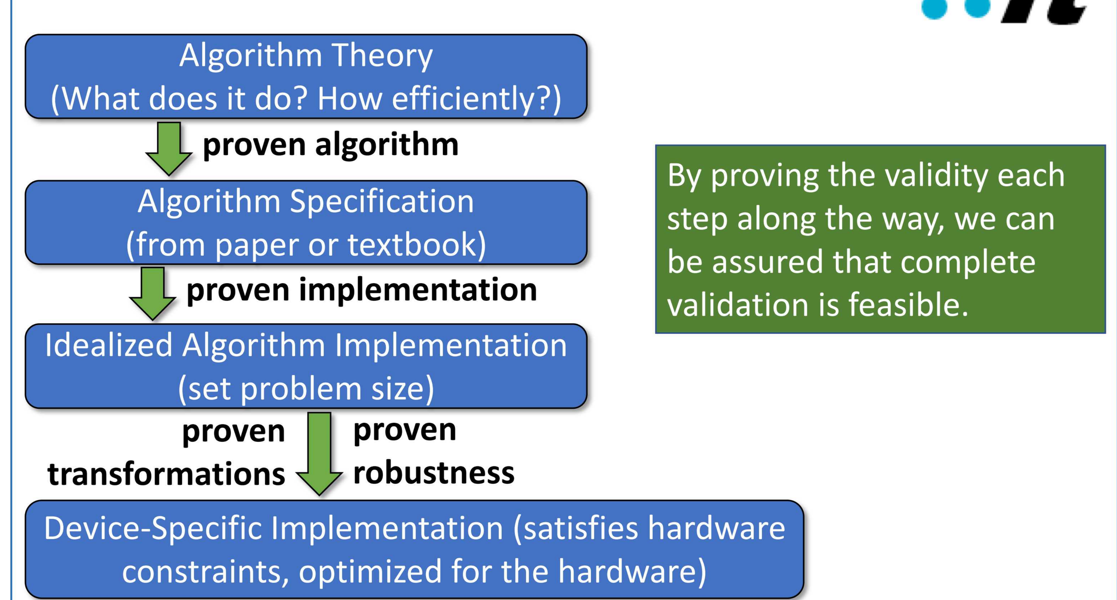


How the project thrusts fit into the conventional picture of a quantum computing software stack, and how the outcomes of each thrust inform the other ones.

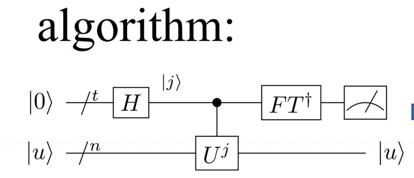
Research Highlights

ProveIt theorem proving assistant

https://github.com/PyProveIt



- Our open-source Python-based general-purpose theorem-proving assistant.
- In a proof-of-concept demonstration,[1] we derived the accuracy of the Quantum Phase Estimation algorithm:



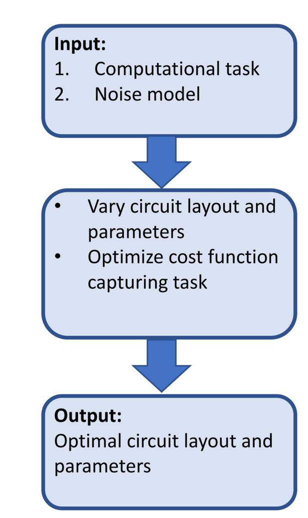
$$\forall_{\varepsilon \in \{1 \ldots (2^{t-1}-2)\}} \left(P_{\text{fail}}(\varepsilon) \leq \left(\frac{1}{2} \cdot \left(\frac{1}{\varepsilon} + \frac{1}{\varepsilon^2}\right)\right)\right)$$

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

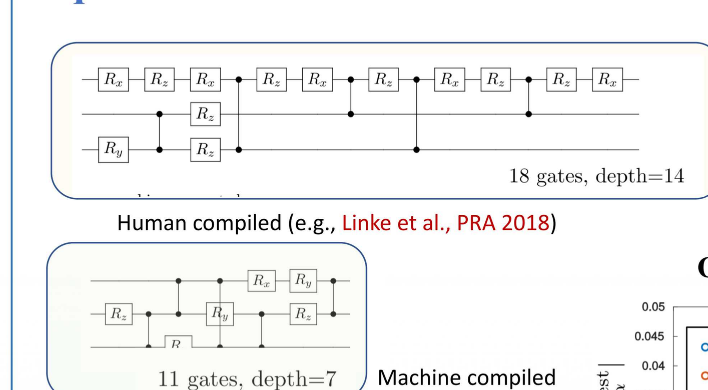
1. W. Witzel, M. Sarovar, and K. Rudinger. (2015) Versatile Formal Methods Applied to Quantum Information. [Online]. Available: prod.sandia.gov/techlib/access-control.cgi/2015/159617r.pdf
2. M. A. Nielsen and I. L. Chuang, Quantum computation and quantum information. Cambridge University Press, 2010.

Noise-aware circuit learning

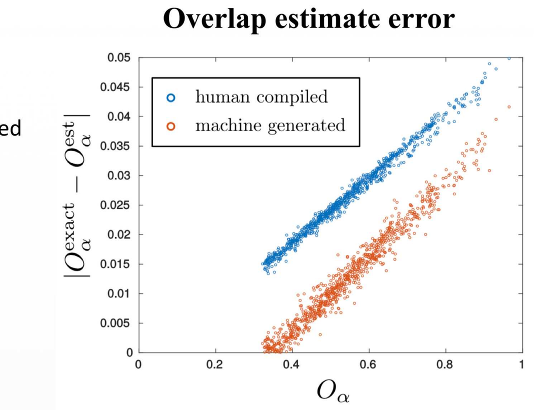
- Compilation of algorithms into circuits typically only consider coarse-grained noise models into account (e.g., limited connectivity, dead qubits)
- Recent characterization tools (e.g., gate-set tomography) yield a wealth of fine-grained error information.
- Can we use this information to improve circuit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



Example: state overlap between two qubits via SWAP test circuit

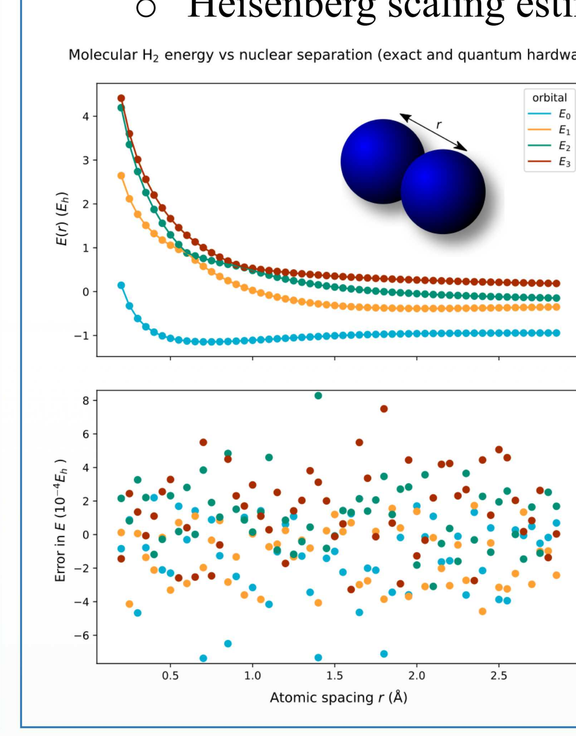


Overlap estimate error

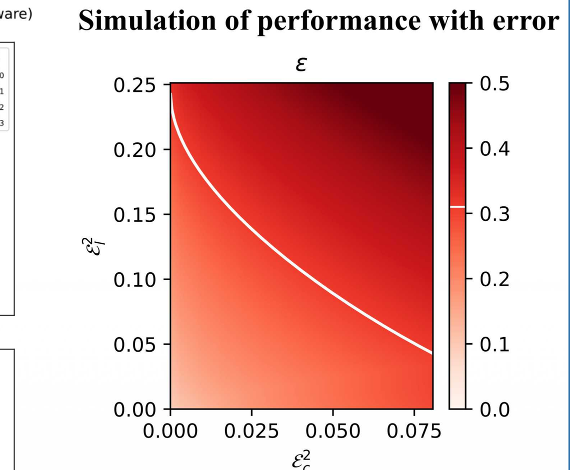


Improved quantum simulation with robust phase estimation

- Robust Phase Estimation (RPE) [Kimmel, Low, Yoder, PRA, 92, 062315 (2015)] determines the relative phase induced by a unitary between two eigenvectors.
- This corresponds to energy differences in the context of Hamiltonian simulation (i.e., molecular spectra).
- We develop a protocol for using RPE to estimate molecular energies that presents an alternative to variational approaches and is possibly suitable for use on NISQ devices.
- Advantages:
  - Naturally robust to noise (~31.6%)
  - Does not require controlled unitaries
  - Heisenberg scaling estimation of energies



Simulation of performance with error



- ε_l is leakage error
- ε_c is state preparation error (portion of state prepared in wrong subspace)
- RPE post-processing can tolerate aggregate errors below the white line

Other work

1. Improved classical solvers for potential inversion when performing TD-DFT with hybrid quantum-classical methods [arXiv:1904.10958]
2. Characterization of noise resilience of variational quantum algorithms [arXiv:1908.04416]
3. New analog simulation method for generating, and sampling from, many-body thermal states [arXiv:1909.02023]
4. Analysis of robustness of measurements and data extraction for TD-DFT on quantum computers [arXiv:1909.03078]
5. New variational algorithm for quantum linear systems solving [arXiv:1909.05820]
6. New (classical) optimization algorithm tailored to variational QC [arXiv:1909.09083]
7. Techniques to reduce quantum simulation resources by exploiting symmetry [arXiv:1910.14644]
8. Characterization of variational optimization landscape and barren plateaus [arXiv:2001.00550]

For more details, visit
https://overqc.sandia.gov

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