SAND2022-7992D

Sandia National Laboratories

Resources estimates for DOE quantum simulation problems

Andrew Baczewski, Quinn Campbell, Lucas Kocia, Ben Morrison, Antonio Russo, Stefan Seritan, UNM AA: Tameem Albash and Conor Smith

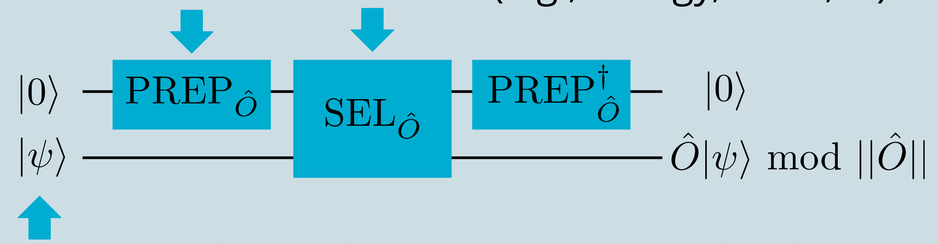
Simulation: DOE's killer quantum computing app

- Identified as the common application of interest across DOE/SC, as well as NNSA/ASC.
- Qubits encode exponentially larger states than classical bits, information extracted at quantum limit.
- Efforts at other institutions typified by time horizons
  - Near-term: noisy hardware, intense SME interest, not scalable.
  - Far-term: error-corrected hardware, mild SME interest, scalable.
- Our approach: improve abstractions for developing new simulation applications on scalable hardware.

Focus on common & scalable abstractions

- Two subroutines shared by scalable applications: block encoding and state preparation.
- Task: calculate a matrix element

Determines the observable (e.g., energy, force, ...)



Determines the application (e.g., materials, plasmas, ...)

Exploring applications answers open questions

- Resource estimates for a variety of DOE problems

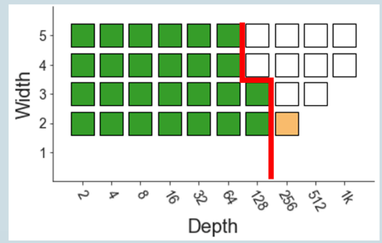
Application	Example	Electrons	Logical qubits	Toffoli count	Physical qubits (est.*)
Bulk solid	Nickel oxide (strong correlation)	64	3,254	2.5×10^{12}	2.0×10^{7}
2D material	Carbon nitride (water splitting)	288	8,592	2.1×10^{12}	5.6×10^{7}
Surface chemistry	Atomic precision doping (nanoelectronics)	726	19,157	1.0×10^{13}	1.4×10^{8}

Based on an algorithm by Su, et al., PRX Quantum (2021)

- These estimates ignore the cost of state preparation, one of the biggest open questions in simulation.
- First estimates including state preparation - *total cost depends on the question that you're asking*.

Broader impacts

- Block encoding circuits are being used as application-inspired benchmarks (collaboration w/SNL Quantum Performance Laboratory)
- Classical benchmarks from collaboration w/Albash group @ UNM.
- Goal: Make Sandia the go-to national laboratory for application-specific quantum computing co-design.



Red line indicates frontier beyond which circuits fail

We are leveraging funding from ASCR (0.4 FTE), ASC (4 FTE), and LDRD (0.8 FTE).

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology &Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.
SAND No. _____