A NASA Perspective on Quantum Computing

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Why Quantum Computing at NASA?

NASA constantly confronting massively challenging computational problems

- Computational capacity limits mission scope and aims

**NASA’s leading supercomputing efforts**

**Low energy and water use supercomputing**

**NASA QuAIL mandate:**

*Determine the potential for quantum computation to enable more ambitious and safer NASA missions in the future*

**Aeronautics:**

Air Traffic Management and Robust Airspace Communication

**Earth Science:**

Data Analysis and image processing

**Space Exploration:**

Resource Allocation and Scheduling
Quantum Computing at NASA

Communication & Networks
- Quantum networking
- Distributed QC

Application Focus Areas
- Planning and scheduling
- Material science
- Fault diagnosis
- Machine Learning
- High-energy physics

Software Tools & Algorithms
- Quantum algorithm design
- Mapping, parameter setting, error mitigation
- Hybrid quantum-classical approaches
- Compiling quantum algorithms to hardware

Solvers & Simulators
- Physics-inspired classical solvers
- HPC quantum circuit simulators

Fundamental Physics Insights
- Co-design quantum hardware


Quantum computing has entered the NISQ Era

Quantum supremacy achieved!

- Perform computations not possible on even the largest supercomputers

Google, NASA, ORNL collaboration

... what about useful quantum supremacy?

- Quantum processors currently too small and non-robust to be useful for solving practical problems

Uses of these still limited, quantum devices?

1. Unprecedented opportunity to explore and evaluate algorithms, both quantum and hybrid quantum-classical heuristic algorithms
2. Investigate quantum mechanisms that may be harnessed for computational purposes

Insights gained feed into next generation

- quantum algorithms
- quantum hardware

Early target: Optimization; Sampling & Machine Learning; simulation of quantum systems

If someone handed you a large, fault tolerant quantum computer, what would you run?
Current status of quantum algorithms

<table>
<thead>
<tr>
<th>Quantum computing can do everything a classical computer can do and</th>
<th>Unknown quantum advantage for everything else</th>
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<tbody>
<tr>
<td>Provable quantum advantage known for a few dozen quantum algorithms</td>
<td>Status of classical algorithms</td>
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<tr>
<td></td>
<td>• Provable bounds hard to obtain</td>
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<tr>
<td></td>
<td>– Analysis is just too difficult</td>
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<tr>
<td></td>
<td>• Best classical algorithm not known for most problems</td>
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<tr>
<td></td>
<td>• Empirical evaluation required</td>
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<tr>
<td></td>
<td>• Ongoing development of classical heuristic approaches</td>
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<tr>
<td></td>
<td>– Analyzed empirically: ran and see what happens</td>
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<tr>
<td></td>
<td>– E.g. SAT, planning, machine learning, etc. competitions</td>
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</table>

A handful of proven limitations on quantum computing

Conjecture: Quantum Heuristics will significantly broaden applications of quantum computing
Fermionic approach to variational quantum sim of Kitaev spin models

Population Transfer algorithms

Quantum-accelerated algorithms for constraint Programming (CP)

M. Sohaib Alam, Stuart Hadfield, Henry Lamm, Andy Li, Quantum Simulation of Dihedral Gauge Theories, arXiv:2108.13305
KEC Booth, B O'Gorman, J Marshall, S Hadfield, E Rieffel, Quantum-accelerated constraint programming, Quantum 5, 550, 2021
The power of pausing: additional control of anneal schedule, increases performance by orders of magnitude

An appropriately placed pause can improve TTS as well as the probability of success - on embedded instances of application interest - consistent region in which pausing helps

Inspired by open systems model of quantum annealing

Heat map of probability of solution, depending on pause location (x-axis) and pause length (y-axis)

Algorithms-hardware codesign II: gate-model processors

Developed the **Quantum Alternating Operator Ansatz**, a generalization of Farhi *et al.* Quantum Approximate Optimization Algorithm framework, inspired by optimization use cases with hard constraints and hardware compilation considerations.

Introduced **more general family of mixing operators**

Inspired Rigetti to pursue native hardware implementation of these gates, with calibration techniques suitable for the family.

Led to joint funding with Rigetti under DARPA ONISQ.

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S. Hadfield *et al.* (2019), From the quantum approximate optimization algorithm to a quantum alternating operator Ansatz, *Algorithms* 12, 34 – *recipient of the Algorithms 2020 Best Paper Award*


M. Streif *et al.* (2021), Quantum algorithms with local particle number conservation: Noise effects and error correction, *PRA*
Avoiding Pitfalls in Algorithm Benchmarking

Mind the Metric!
Even large factor advantages can disappear when moving from one metric to another
Example: Mandrà and Katzgraber showed 100x advantage in TTS on certain problems for D-Wave 2000Q over SoTA classical algorithms, but the advantage disappeared when energy was used as the metric

Mind the Optimizer! Compare like with like.
Don’t claim advantage when a heuristic algorithm numerically beats best classical alg. with a provable guarantee
Example: Don’t compare quantum heuristics for MaxCut with Goemans-Williamson!

Mind the Size!
Challenging to extrapolate to application scale
Small sizes can be misleading when complex behavior only kicks in at large sizes
Polynomial pre-factors may hide true scaling

Mind the Structure!
Algorithms are variously tailored to specific problem classes, taking into account more or less specific problem structure
Tailored algorithms generally perform better, and can remove quantum advantage

General purpose algs have important role

S. Mandra, H. Katzgraber, A deceptive step towards quantum speedup detection, Quantum Sci. Technol. 3, 2018
Tool Development

**Local shadow tomography for error-mitigated expectation values under noise**

![Diagram of local shadow tomography](image1)

**Temporal planning approaches to compiling quantum algorithms**

![Diagram of quantum circuit](image2)

**Extended character randomized benchmarking (RB) derivation to treat non-multiplicity-free groups**

![Diagram of quantum circuit](image3)

**Open quantum system simulations**

![Diagram of quantum circuit](image4)

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D Venturelli, M Do, E. Rieffel, J Frank, Compiling quantum circuits to realistic hardware architectures using temporal planners. Quantum Science and Technology 3 (2), 2018


X Mi, P Roushan, C Quintana, S Mandra, J Marshall, et al. (2021) Information Scrambling in Computationally Complex Quantum Circuits, Science 374, 1479
HybridQ: A Hybrid Quantum Simulator for Large Scale Simulations

Hardware agnostic quantum simulator, designed to simulate large scale quantum circuits.

Can run tensor contraction simulations, direct evolution simulation and Clifford+T simulations using the same syntax

Features:

- Fully compatible with Python (3.8+)
- Low-level optimization achieved by using C++ and Just-In-Time (JIT) compilation with JAX and Numba,
- It can run seamlessly on CPU/GPU and TPU, either on single or multiple nodes (MPI) for large scale simulations, using the exact same syntax
- User-friendly interface with an advanced language to describe circuits and gates, including tools to manipulate/simplify circuits.

Recent Improvements:

- Commutations rules are used to simplify circuits (useful for QAOA)
- Expansion of density matrices as superpositions of Pauli strings accepts arbitrary non-Clifford gates,
- Open-source (soon!) project with continuous-integration, multiple tests and easy installation using either pip or conda

Open source code available at https://github.com/nasa/HybridQ

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A Historical Perspective

Illiac IV - first massively parallel computer
- 64 64-bit FPUs and a single CPU
- 50 MFLOP peak, fastest computer at the time

Finding good problems and algorithms was challenging

Questions at the time:
- How broad will the applications be of massively parallel computing?
- Will computers ever be able to compete with wind tunnels?

NASA Ames director Hans Mark brought Illiac IV to NASA Ames in 1972