National Aeronautics and
Space Administration

Ames

Discovery Innovations Solutions

A NASA Perspective on Quantum Computing

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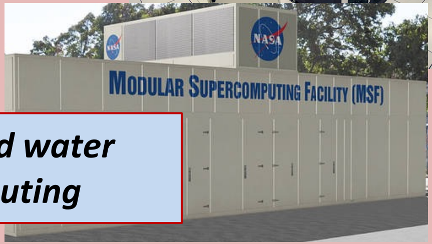
Why Quantum Computing at NASA?

NASA constantly confronting massively challenging computational problems

- Computational capacity limits mission scope and aims

NASA's leading supercomputing efforts

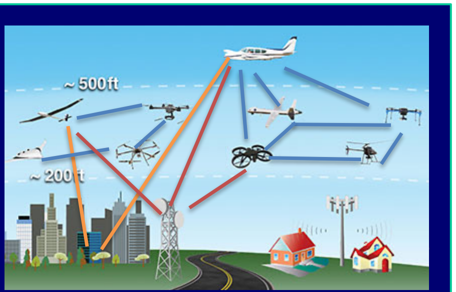


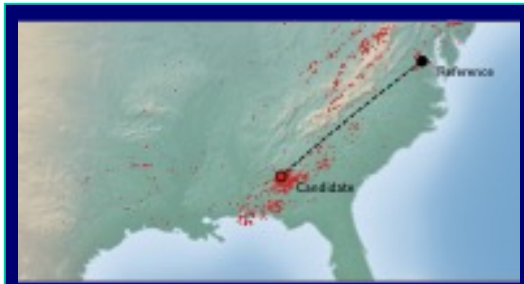
Low energy and water use supercomputing

NASA QuAIL mandate:

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

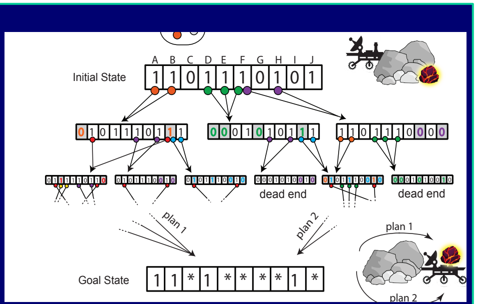
Aeronautics:
Air Traffic Management and Robust Airspace Communication



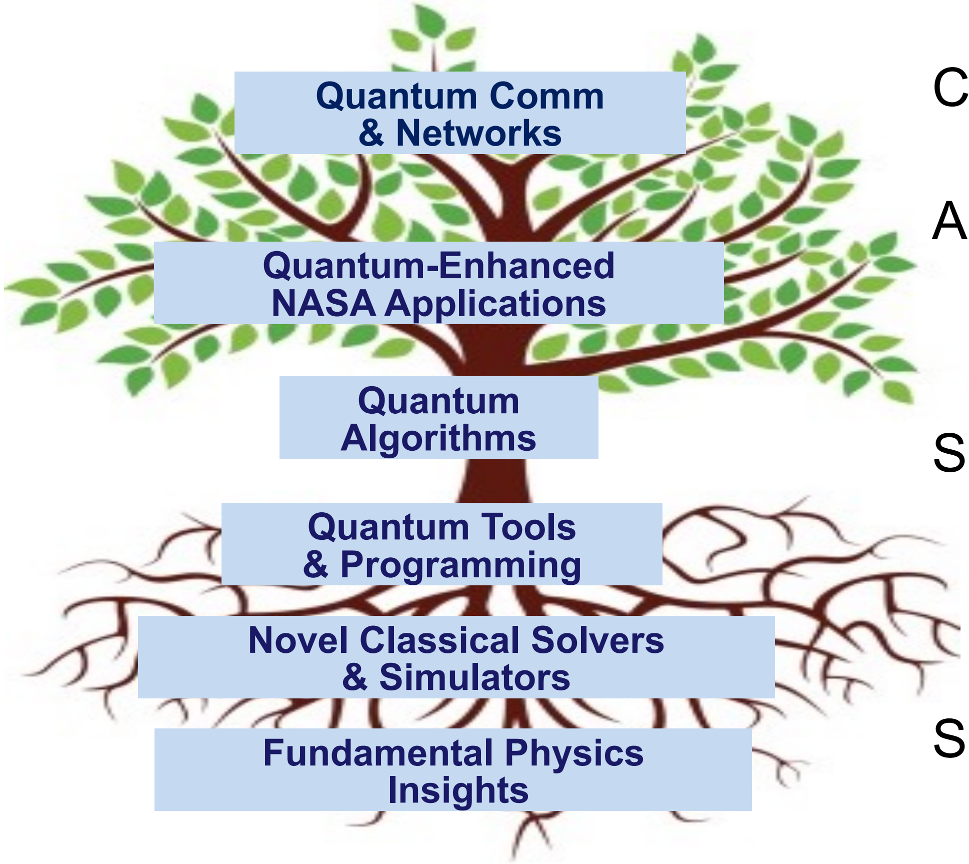


Earth Science:
Data Analysis and image processing

Space Exploration:
Resource Allocation and Scheduling



Quantum Computing at NASA



Quantum Comm & Networks

Quantum-Enhanced NASA Applications

Quantum Algorithms

Quantum Tools & Programming

Novel Classical Solvers & Simulators

Fundamental Physics Insights

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

Physics Insights

Co-design quantum hardware

E.G. Rieffel, et al. (2019) ***From Ansätze to Z-gates: a NASA View of Quantum Computing***, *Advances in Parallel Computing* **34**, 133-160

R. Biswas et al. (2017) ***A NASA Perspective on Quantum Computing: Opportunities and Challenges***, Parallel Computing, Volume 64, p. 81-98

Quantum computing has entered the NISQ Era

Quantum supremacy achieved!

- Perform computations not possible on even the largest supercomputers

Cover article, Nature, 24 Oct 2019

Article

Quantum supremacy using a programmable superconducting processor

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The promise of quantum computers is that certain computational tasks might be executed exponentially faster on a quantum processor than on a classical processor[1]. A fundamental challenge is to build a high-fidelity processor capable of running quantum algorithms in an exponentially large computational space. Here we report the use of a processor with programmable superconducting qubits[2–7] to create quantum states on 53 qubits, corresponding to a computational state-space of dimension 2^{53} (about 10^{16}). Measurements from repeated experiments sample the resulting probability distribution, which we verify using classical simulations. Our Sycamore processor takes about 200 seconds to sample one instance of a quantum circuit a million times—our benchmarks currently indicate that the equivalent task for a state-of-the-art classical supercomputer would take approximately 10,000 years. This dramatic increase in speed compared to all known classical algorithms is an experimental realization of quantum supremacy[8–14] for this specific computational task, heralding a much-anticipated computing paradigm.

In the early 1980s, Richard Feynman proposed that a quantum computer would be an effective tool with which to solve problems in physics and chemistry, given that it is exponentially costly to simulate large quantum systems with classical computers[1]. Realizing Feynman's vision poses substantial experimental and theoretical challenges. First, can a quantum system be engineered to perform a computation in a large enough computational (Hilbert) space and with a low enough error rate to provide a quantum speedup? Second, can we formulate a problem that is hard for a classical computer but easy for a quantum computer? By computing such a benchmark task on our superconducting qubit processor, we tackle both questions. Our experiment achieves quantum supremacy, a milestone on the path to full-scale quantum computing[8–14].

In reaching this milestone, we show that quantum speedup is achievable in a real-world system and is not precluded by any hidden physical laws. Quantum supremacy also heralds the era of noisy intermediate-scale quantum (NISQ) technologies[15]. The benchmark task we demonstrate has an immediate application in generating certifiable random numbers (S. Aaronson, manuscript in preparation); other initial uses for this new computational capability may include optimization[16,17], machine learning[18–21], materials science and chemistry[22–24]. However, realizing the full promise of quantum computing (using Shor's algorithm for factoring, for example) still requires technical leaps to engineer fault-tolerant logical qubits[25–29].

To achieve quantum supremacy, we made a number of technical advances which also pave the way towards error correction. We

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Google, NASA, ORNL collaboration

… what about <u>useful</u> 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

Quantum computing can do everything a classical computer can do

and

Provable quantum advantage known for a few dozen quantum algorithms

Unknown quantum advantage for everything else

Status of classical algorithms

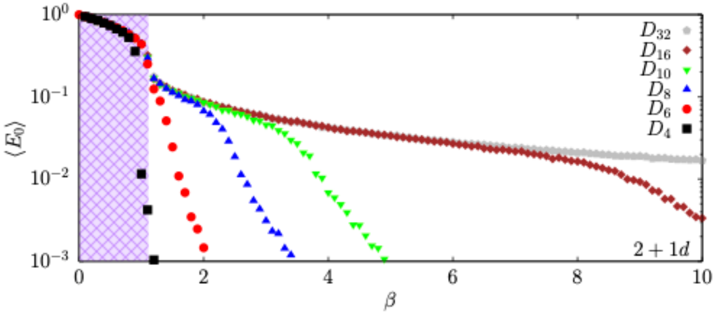
- Provable bounds hard to obtain
  - Analysis is just too difficult
- Best classical algorithm not known for most problems
- Empirical evaluation required
- Ongoing development of classical heuristic approaches
  - Analyzed empirically: ran and see what happens
  - E.g. SAT, planning, machine learning, etc. competitions

A handful of proven limitations on quantum computing

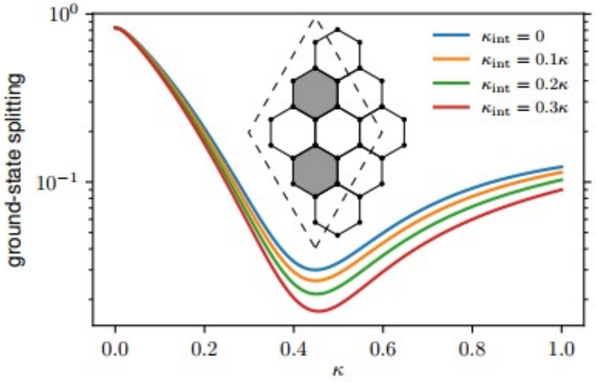
Conjecture: Quantum Heuristics will significantly broaden applications of quantum computing

Algorithms Research

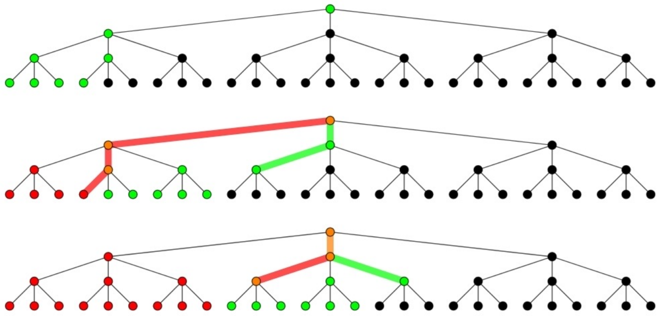
Quantum Sim of Dihedral Gauge Theories



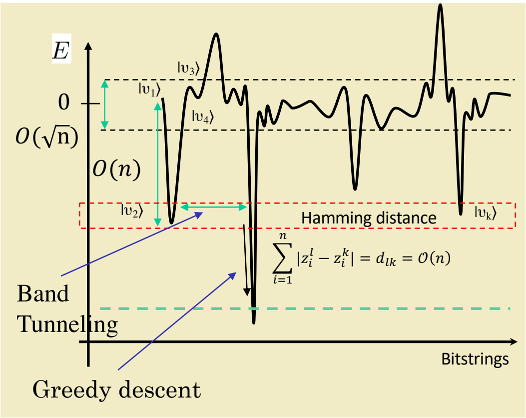
Fermionic approach to variational quantum sim of Kitaev spin models



Quantum-accelerated algorithms for constraint Programming (CP)



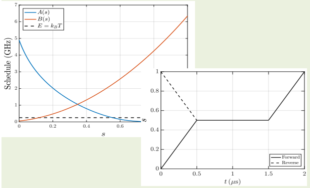
Population Transfer algorithms

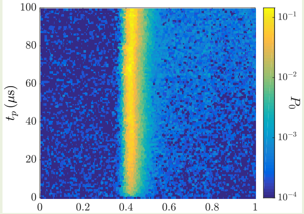


M. Sohaib Alam, Stuart Hadfield, Henry Lamm, Andy Li, Quantum Simulation of Dihedral Gauge Theories, arXiv:2108.13305
Ammar Jahin, Andy C. Y. Li, Thomas Iadecola, Peter P. Orth, Gabriel N. Perdue, Alexandru Macridin, M. Sohaib Alam, Norm M. Tubman Fermionic approach to variational quantum simulation of Kitaev spin models, arXiv:2204.05322
KEC Booth, B O'Gorman, J Marshall, S Hadfield, E Rieffel, Quantum-accelerated constraint programming, Quantum 5, 550, 2021
T Parolini, G Mossi, Multifractal Dynamics of the QREM, arXiv:2007.00315

Algorithms-hardware codesign I: quantum annealing

The power of pausing: additional control of anneal schedule, increases performance by orders of magnitude

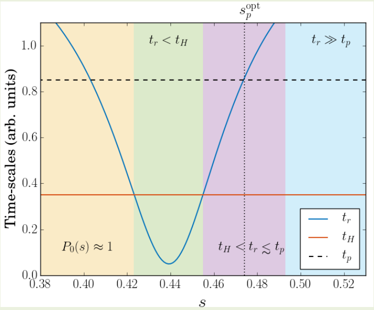




Heat map of probability of solution, depending on pause location (x-axis) and pause length (y-axis)

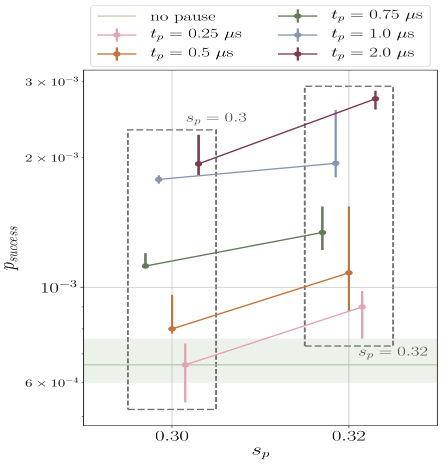
Inspired by open systems model of quantum annealing

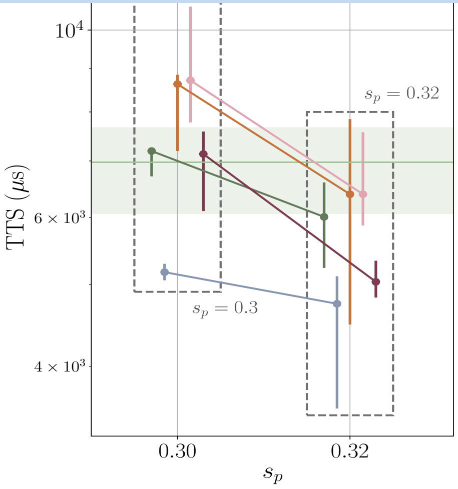
Anneal time regions picture.
Purple region is where pause is expected to be effective.



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

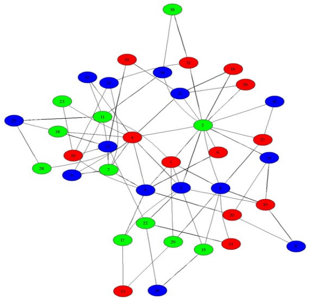




J. Marshall, D. Venturelli, I. Hen, E. Rieffel, **The power of pausing: advancing understanding of thermalization in experimental quantum annealers**, *Phys Rev Applied*, 2019
Z G Izquierdo, S Grabbe, S Hadfield, J Marshall, Z Wang, E G Rieffel, ***Ferromagnetically shifting the power of pausing***, Phys. Rev. Applied 15, 044013
Z G Izquierdo, S Grabbe, Husni Idris, Z Wang, J Marshall,, E G Rieffel**,** The Advantage of pausing: parameter setting for quantum annealers, arXiv:2205.12936

Algorithms-hardware codesign II: gate-model processors

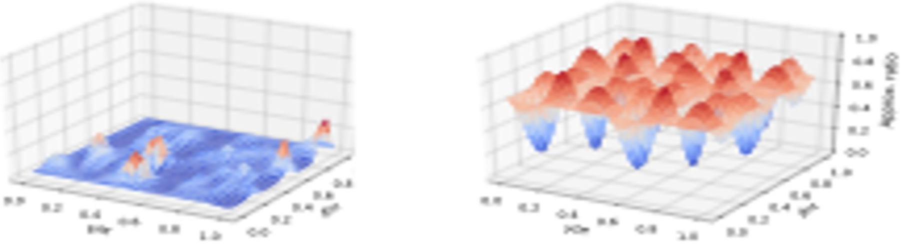
Developed the ***Quantum Alternating Operator Ansatz***, a generalization of Farhi *et al.* Quantum Approximate Optimization Algorithm framework, inspired by optimization use cases with hard constraints and hardware compilation considerations



Problem instance: Max-K-Colorable subgraph

Introduced **more general family of mixing operators**

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



Approximation ratio for 3-coloring a triangle: QAOA with standard X-mixer (left) and with XY-mixer (right)

Led to joint funding with Rigetti under DARPA ONISQ

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*

Z. Wang *et al.* (2020), XY-mixers: analytical and numerical results for QAOA pausing, *Phys. Rev. A* **101**, 012320

M. Streif *el 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

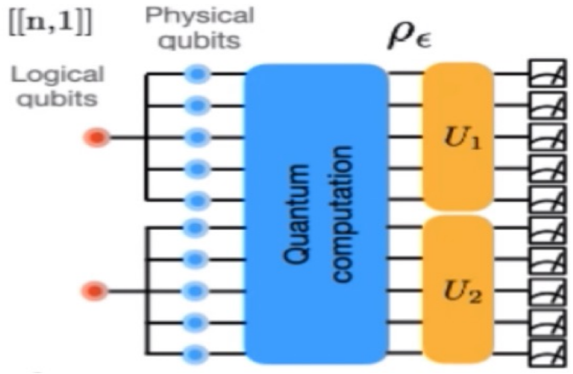
Tailored algorithms generally perform better, and can remove quantum advantage

General purpose algs have important role

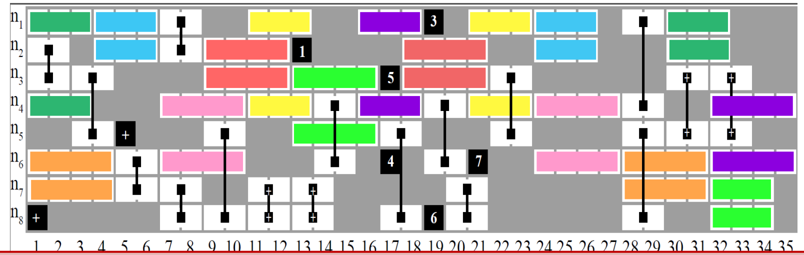
S. Mandra, H. Katzgraber, A deceptive step towards quantum speedup detection, Quantum Sci. Technol. 3, 2018
S. Mandra et al., Strengths and weaknesses of weak-strong cluster problems: A detailed overview of state-of-the-art classical heuristics versus quantum approaches, PRA, 2016

Tool Development

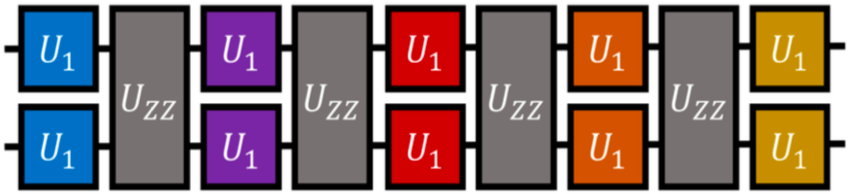
Local shadow tomography for error-mitigated expectation values under noise



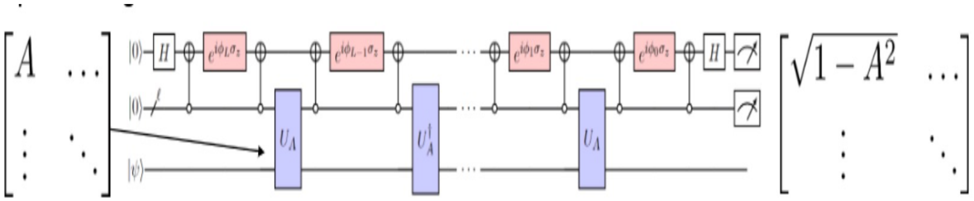
Temporal planning approaches to compiling quantum algorithms



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



Open quantum system simulations



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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
J. Claes, E. Rieffel, Z. Wang (2021), Character randomized benchmarking for non-multiplicity-free groups with applications to subspace, leakage, and matchgate randomized benchmarking, arXiv:2011.00007
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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.

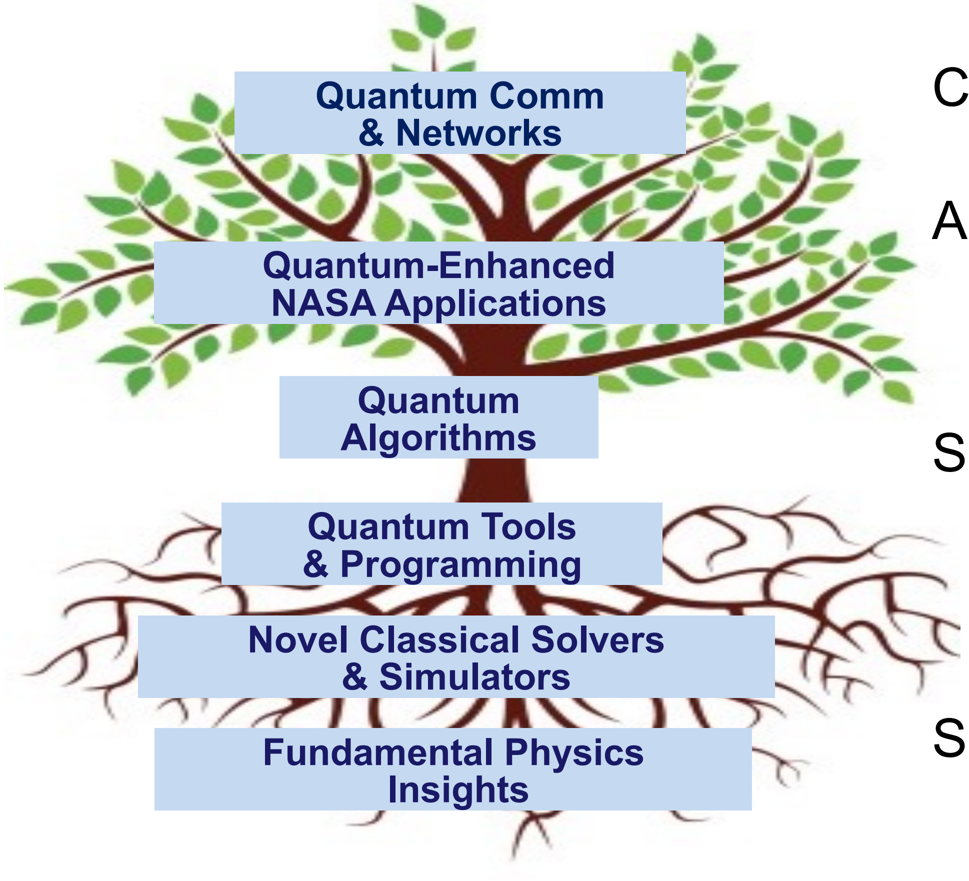
Recent Improvements:

- 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

S. Mandrà, J. Marshall, E. G. Rieffel, R. Biswas, HybridQ: A Hybrid Simulator for Quantum Circuits, arXiv:2111.06868

Quantum Computing at NASA



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HPC quantum circuit simulators

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Co-design quantum hardware

A Historical Perspective

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

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?