A NASA Perspective on
Quantum Computing: Algorithmic opportunities and challenges

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

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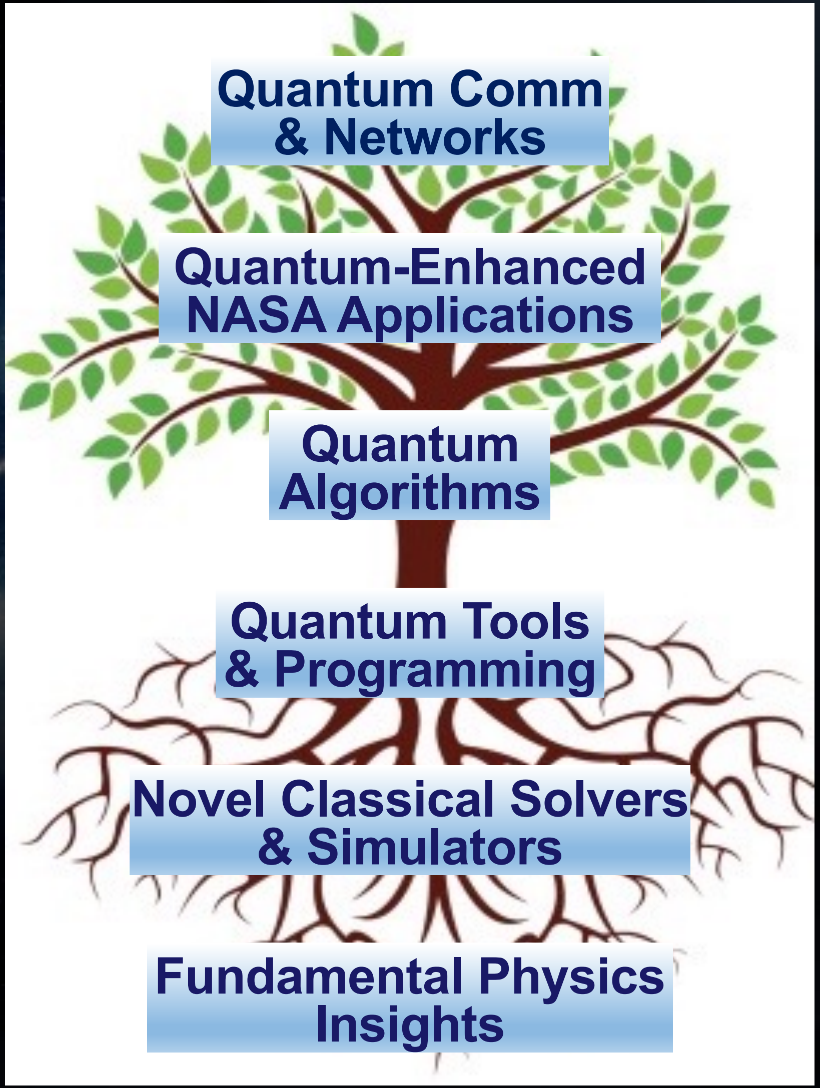
Davide Venturelli
Zhihui Wang

+ active year-round intern program

Quantum Computing R&D at NASA Ames



Communication & Networks

- Quantum networking
- Distributed QC

Application Focus Areas

- Planning and scheduling
- Material science
- Fault diagnosis
- Machine learning
- Recently: Computational fluid dynamics (CFDs)

Software Tools & Algorithms

- Quantum algorithm design
- Compiling to hardware
- Mapping, parameter setting, error mitigation
- Hybrid quantum-classical approaches

Solvers & Simulators

- Physics-inspired classical solvers
- HPC quantum circuit simulators

Physics Insights

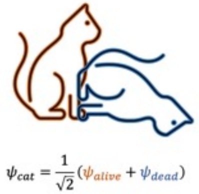
- Co-design quantum hardware

E. Rieffel *et al.* (2019), From Ansätze to Z-gates: A NASA view of quantum computing, *Adv. in Parallel Computing* **34**, 133–160
R. Biswas *et al.* (2017), A NASA perspective on quantum computing: Opportunities and challenges, *Parallel Computing* **64**, 81–98

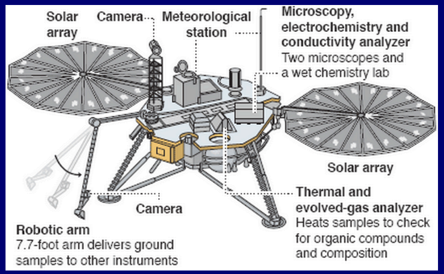
Exploration of Quantum Computing for NASA

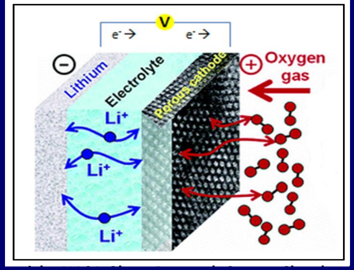
Quantum ML for Earth Science Data Analysis

Superposition



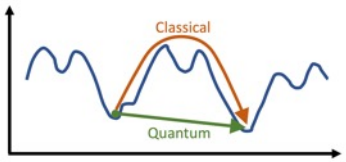
Resource Allocation and Scheduling for Space Exploration



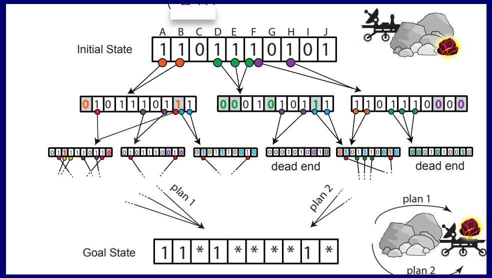


Quantum Simulations for Aerospace Materials

Tunneling



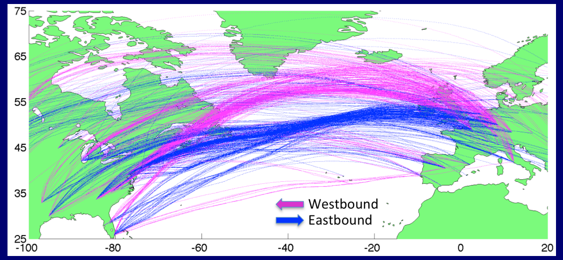
Secure Airspace Communication



Quantum Optimization for Mission Planning & Coordination

Entanglement

Air Traffic Management



<u>Objective</u>: *Find "BETTER" solution*

faster time-to-solution OR more precise solution OR using less energy OR not found by classical methods

What is quantum computing (in one slide)?

The power of quantum computation comes from encoding information in a non-classical way

Quantum computers take advantage of purely quantum effects that are not available classically

- quantum interference; quantum tunneling; quantum entanglement; quantum measurement, quantum many-body delocalization, quantum sampling

These effects can provide more efficient computation and higher levels of security than is available classically

- What Shor's factoring algorithm can compute in days, would take a supercomputer longer than the age of the universe

Emerging quantum hardware enables empirical investigation of quantum optimization for myriad applications

New Era for Quantum Computing

Quantum supremacy achieved

- Perform computations not possible on even largest supercomputers in reasonable time
- Google – NASA – ORNL collaboration

*F. Arute et al. (2019), Quantum supremacy using a programmable superconducting processor, Nature **574**, 505-510*

2023 Update

*A. Morvan, B. Villalonga, X. Mi, **S. Mandrà**, et al., (2023) Phase transition in Random Circuit Sampling, arXiv:2304.11119*

Exp.	1 amp.	1 million noisy samples		
	FLOPs	FLOPs	XEB fid.	Time
SYC-53 [9]	$6.44 \cdot 10^{17}$	$2.60 \cdot 10^{17}$	$2.24 \cdot 10^{-3}$	6.18 s
ZCZ-56 [10]	$6.24 \cdot 10^{19}$	$6.40 \cdot 10^{19}$	$6.62 \cdot 10^{-4}$	25.3 min
ZCZ-60 [11]	$1.32 \cdot 10^{21}$	$1.41 \cdot 10^{23}$	$3.66 \cdot 10^{-4}$	38.7 days
This work	$4.74 \cdot 10^{23}$	$6.27 \cdot 10^{25}$	$1.68 \cdot 10^{-3}$	47.2 yr

… but so far only for a toy problem

- Quantum hardware currently too small for solving practical problems intractable on classical supercomputers
- These devices need to scale up and become more reliable

So what to do in the interim?

- Unprecedented opportunity to invent, explore, and evaluate quantum algorithms *empirically*

NASA QuAIL Focus

- Algorithms and applications to enable safer, more ambitious, and greater time- and energy-efficient missions
- Tools for advancing quantum computing, from quantum circuit simulation, noise characterization, error correction, compilation to realistic hardware

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
- **NISQ era supports unprecedented means for empirical analysis of quantum algorithms**
  - **Quantum heuristics come into their own**

A handful of proven limitations on quantum computing

Conjecture: Quantum Heuristics will significantly broaden applications of quantum computing

Certainty and Randomness in Quantum Computation

Any computation a classical computer can do, a quantum computer can do with roughly the same efficiency

- With the same probability of the outcome
- If the classical computation is non-probabilistic, so is the quantum one
- O(log n) overhead: solely due to making computation reversible

Like classical algorithms, some quantum algorithms are inherently probabilistic and others are not

First quantum algorithm was not probabilistic

- E.g. Deutsch-Jozsa algorithm solves problem with certainty that classical algorithms, of equivalent efficiency, could solve only with high probability

Shor's algorithms are probabilistic

Grover's is not intrinsically probabilistic

- initial search algorithm was probabilistic, but
- slight variants, which preserve the speed up, are non-probabilistic

Some closely related Quantum Optimization Algs: AQO, QA, QAOA

Phase separation operator based on the cost function

Usually $H_P = -\boldsymbol{\Sigma} C(z)|z\rangle\langle z|$ + (optionally) other terms, e.g. "penalty terms" to enforce constraints

Simple Driver/Mixing operator

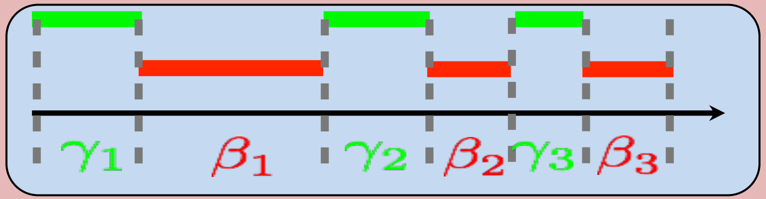
Most frequently $H_M = \sum_j Xj$, though we will shortly see other mixers

Ground state easy to obtain

AQO (special case of AQC)	QA	QAOA
• Evolution under $\boldsymbol{H}(\boldsymbol{t}) = \boldsymbol{a}(\boldsymbol{t})H_P + \boldsymbol{b}(\boldsymbol{t})H_M$ • Slowly enough to stay in the ground subspace	• Evolution under $\boldsymbol{H}(\boldsymbol{t}) = \boldsymbol{a}(\boldsymbol{t})H_P + \boldsymbol{b}(\boldsymbol{t})H_M$ • Many quick runs, thermal effect contribute	• Alternate application of H_P and H_M • For $\boldsymbol{p}$ alterations, the parameters are $\boldsymbol{2p}$ times/angles $\boldsymbol{\gamma_1, \beta_1, \ldots \gamma_P, \beta_p}$

Quantum Approximate Optimization Algorithm

Gate model algorithm due to Farhi et al.



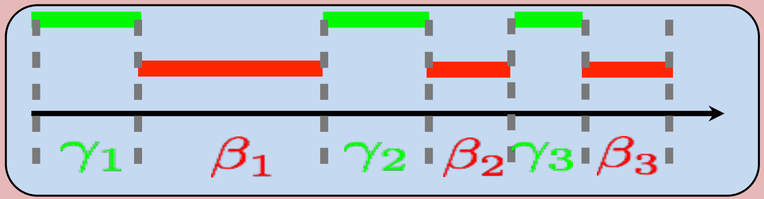
- Alternates between two Hamiltonians, p times
  - Phase separation (cost function dep.)
  - Mixing
  - 2p parameters: amount of time each Hamiltonian is applied
    - Parameter search means often a hybrid quantum-classical algorithm
    - Relation with Variational Quantum Eigensolvers (VQE)
- Aim: Provable approximation ratio

Early results by Farhi and co-authors

- p → ∞: from AQO
  - Converges to optimum for p → ∞
- p = 1: proofs modified from proofs for IQP circuits
  - Provably hard to sample output efficiently classically (up to standard complexity theory conjectures)
  - Briefly beat existing classical approx. ratio on MaxE3Lin2, but inspired better classical algorithm

Quantum Alternating Operator Ansatz

Heuristic based on strutureQuantum Approximate Optimization Algorithm of Farhi et al.



- Alternates between two Hamiltonians, p times
  - Phase separation (cost function dep.)
  - Mixing
  - 2p parameters: amount of time each Hamiltonian is applied
- Aim: ~~Provable approximation ratio~~
- Aim: Good typical performance
- Better support for enforcing constraints, informed by compilation to hardware

Early results

- Alternative algorithm for Grover's unstructured search problem
  - achieves √N query complexity by different means

S. Hadfield et al., **From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz**, Algorithms 12 (2), 34 2019, arXiv:1709.03489

Quantum Alternating Operator Ansatz

Generalization of Quantum Approximation Optimization algorithm

$$Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma}) = U_{\mathrm{M}}(\beta_p)U_{\mathrm{P}}(\gamma_p)\cdots U_{\mathrm{M}}(\beta_1)U_{\mathrm{P}}(\gamma_1)$$

$$e^{-i\gamma H_{\mathrm{P}}}$$

$$\prod_j e^{-i\beta_k H_j}$$

$$|\boldsymbol{\beta}, \boldsymbol{\gamma}\rangle = Q_p(\boldsymbol{\beta}, \boldsymbol{\gamma})\,|s\rangle$$

Phase separator: unitary for which

- The energy spectrum of **H_P encodes the problem's objective function**
- $H_P = -\sum C(z)|z\rangle\langle z|$

Mixer: unitary which:

- Preserves the feasible subspace
- Provides nonzero transitions between all feasible states
- Not necessarily time evolution of a single local Hamiltonian
- β_k depends on the level $1 \leqq k \leqq p$, but independent of H_j

Initial state |s> which:

- is a superposition of one or more solutions in the feasible subspace
- can be prepared efficiently

S. Hadfield et al., **From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz**, Algorithms 12 (2), 34 2019, arXiv:1709.03489

Example: QAOA for Max-κ-Colorable Subgraph

Problem: Given a graph $G = (V, E)$, and k colors $1, \ldots, k$, find a color assignment maximizing the # of properly colored edges

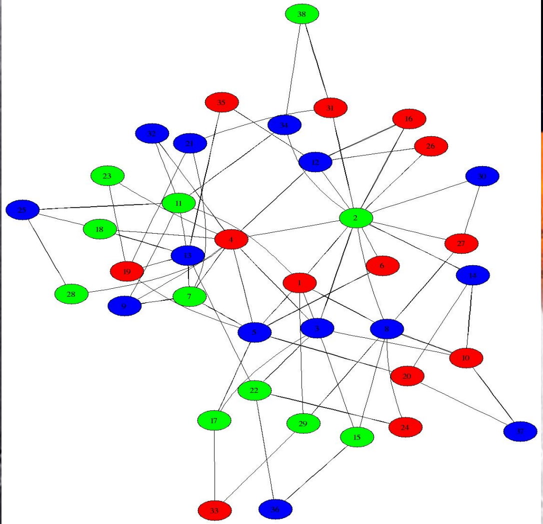
- Properly colored edge means endpoint vertices have been assigned different colors

"One-hot" Encoding: nk variables

$x_{uj} = 1$ iff vertex u is colored color j

Optimization: Write cost function as

$$C(x) = m - \sum_{(uv)\in E}^{m} \sum_{j=1}^{k} x_{uj} x_{vj}$$



Must avoid invalid colorings

e.g. if a vertex is labeled as both red **and** blue, or not colored at all

Requires n constraints: one for each vertex u

$$\sum_{j=1}^{k} x_{uj} = 1$$

Example: QAOA for Max-κ-Colorable Subgraph

Could add constraints to the cost function to enforce penalties

- standard approach in quantum annealing

Better: design mixer to keep evolution in feasible subspace (constant Hamming weight in colors for each vertex)

Feasible subspace is exponentially smaller search space than entire Hilbert space

While still exponentially large

Initial state choice

Any classical feasible state

e.g. all colored red

Any superposition of feasible states

e.g. superposition of all colors (W state)

Use a swap or XY-mixer (XX+YY) on the colors rather than bit flip mixer:

instead of $\sum_j X_j$, use sum of swap operators,

$$|00\rangle\langle 00| + |10\rangle\langle 01| +$$

$$|01\rangle\langle 10| + |11\rangle\langle 11|$$

between colors at a vertex

Ring mixer:

order the colors, and apply swaps to adjacent colors only

Complete mixer:

swap for every pair of colors

Complete mixer mixes more quickly, but has higher circuit depth, especially when compiled to realistic hardware

Example: QAOA for Max-κ-Colorable Subgraph

Partitioned Mixers: Products of $U_{Bv} = e^{-iBv}$. Don't commute, so different orders give different mixers

$$U_{parity}(\beta) = U_{last}(\beta) U_{even}(\beta) U_{odd}(\beta),$$

where

$$U_{odd}(\beta) = \prod_{a \text{ odd},\, a \neq n} e^{-i\beta(X_a X_{a+1} + Y_a Y_{a+1})},$$

$$U_{even}(\beta) = \prod_{a \text{ even}} e^{-i\beta(X_a X_{a+1} + Y_a Y_{a+1})},$$

$$U_{last}(\beta) = \begin{cases} e^{-i\beta(X_d X_1 + Y_d Y_1)}, & \kappa \text{ odd}, \\ I, & \kappa \text{ even}. \end{cases}$$

Many variants of QAOA

- Relation between parameter setting in QAOA and annealing schedule choice in quantum annealing
- Close ties to sampling, e.g. for ML
- Developing General Theory of Iterative Quantum Algorithms

Components of an Iterative Quantum Algorithm

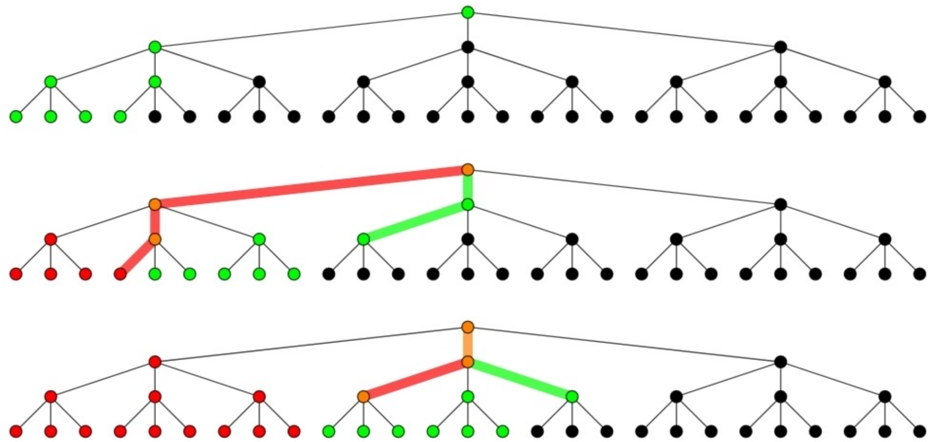
Preparation Rule – Run Quantum (or Classical) Algorithm to get state
Selection Rule – Rank features in the system based on the prepared state
Reduction Rule – Eliminate a feature of the system based on ranking

- Iterative Quantum Algorithms can be designed to guarantee enforcement of constraints
- Classical updates resemble classical greedy algorithms and can pull classical proof techniques
- Special case: IQA for Max Independent Set

L. T. Brady & S. Hadfield, "Iterative Quantum Algorithms for Maximum Independent Set: A Tale of Low-Depth Quantum Algorithms" arXiv:2309.13110
S. Hadfield, L. T. Brady, et al., "Quantum-Enhanced Classical Algorithms" (in preparation)

Brief Glimpse: Quantum-Accelerated Constraint Programming

- In constraint programming (CP), problems are solved with backtracking tree search augmented by logical inference
- Quantum algorithms can accelerate the inference process being performed at each node in the tree
- These quantum inference algorithms can then be integrated within classical, fully-quantum, or partially-quantum backtracking tree search schemes
- Partially quantum backtracking schemes yield speedups for smaller sections of the tree, intended for early, more resource-constrained quantum devices



Other good target state-of-the-art classical algorithms for quantum acceleration?

Booth, Kyle EC, Bryan O'Gorman, Jeffrey Marshall, Stuart Hadfield, and Eleanor Rieffel. **Quantum-accelerated global constraint filtering.** In *International Conference on Principles and Practice of Constraint Programming*, pp. 72-89. 2020
Booth, Kyle EC, Bryan O'Gorman, Jeffrey Marshall, Stuart Hadfield, and Eleanor Rieffel. **Quantum-accelerated constraint programming**. *Quantum* 5 (2021): 550.

Quantum Distributed Algorithms for Approximate Steiner Trees and Directed Minimum Spanning Trees

Joint work with Phillip Kerger, David Bernal Neira, Zoe Gonzales Izquierdo

- We provide quantum distributed algorithms to tackle challenging graph problems
  - Approximate Steiner Tree Problem
  - Directed Minimum Spanning Tree (Arborescence)
- These quantum algorithms provide an asymptotic improvement with respect to the current best known classical algorithm in terms of computational rounds in the CONGEST CLIQUE model
- We provided detailed analysis for the main algorithmic step: finding the all-pairs shortest paths
- We obtained complexity results realizing impractical scales where quantum counterparts become better than classical

Phillip A. Kerger, David E. Bernal Neira, Zoe Gonzalez Izquierdo, Eleanor G. Rieffel, "Mind the Õ: asymptotically better, but still impractical quantum distribute algorithms," Algorithms 16(7), 332, 2023. *arXiv:2304.02825*

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Main results

Quantum distributed algorithms to tackle challenging graph problems

- Approximate Steiner Tree Problem
- Directed Minimum Spanning Tree Problem (Arborescence Problem)

Asymptotic improvement over current best known classical algorithm in terms of computational rounds in CONGEST CLIQUE model

Detailed analysis for the main algorithmic steps

Non-asymptotic complexity results mean both prior classical distributed algorithms and our quantum algorithm only have advantage over simpler schemes at impractically large graph sizes

P Kerger, DE Bernal Neira, Z Gonzalez Izquierdo, EG Rieffel, ***Mind the Õ: Asymptotically better, but still impractical, quantum distributed algorithms****, Algorithms 16 (7), 332, 2023*

New classical distributed algorithm for the broad class of Survivable Network Design Problems (SNDPs) in CONGEST CLIQUE model

New quantum distributed algorithm for SNDPs in QUANTUM CONGEST CLIQUE model

Main ingredients:

- Building on prior distributed all-pair shortest path (APSP) algorithm
- Added routing table computation
- Detailed analysis of constant and log factors

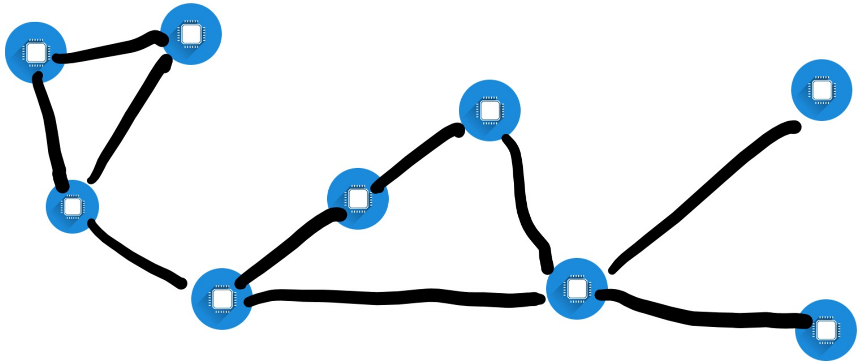
P Kerger, DE Bernal Neira, Z Gonzalez Izquierdo, EG Rieffel, ***Classical and Quantum Distributed Algorithms for the Survivable Network Design Problem****, arXiv:2404.10748*

Background

Introduction: Algorithms on Distributed Data

Algorithms on Distributed Data: Network of Multiple Processors that communicate

- Model as graph where nodes are processors
- Each node its own starting information
  - For graph problems, this is often a list of neighbor nodes



- Example: Network of spacecraft, satellites, or control stations that each have computing power and can communicate
- **Goal**: Answer some question about that distributed information, through communication and computation among the processors

Introduction: Two Classical Models

Graph G = (V,E,W) with n = |V| number of nodes, m = |E| number of edges, and W the weights on the edges

CONGEST Model: Aim is to minimize the number of rounds
Computation happens in rounds (compute, communicate, compute, communicate, …)
Congested: Communication limited by message size: each node can send to each of its neighbors O(log(n)) bits each round
— log(n) is length of a node id

Unlimited local computation at each node
Nodes can communicate only with their neighbors

CONGEST-CLIQUE Model:
1., 2., 3. are the same as for Congest Model
4. All nodes can communicate with each other
Key difference: communication graph distinct from graph G

Initial conditions: Each node knows

- its own ID
- the ID's of its neighbors

  assuming ID's are 1 to n → log(n) bits to encode

Aim: Answer a question about graph in as few rounds as possible

- Ex: Spanning trees, subgraph detection, shortest paths...

What problems can benefit from a distributed *quantum* approach?

Introduction: Models

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Quantum versions: Take CONGEST or CONGEST-CLIQUE, but allow messages to consist of O(log(n)) **qubits**

CONGEST: Negative Results

Main reference: Elkin et al 2012,

“Can Quantum Communication Speed Up Distributed Computation?”

- Proved limitations for quantum CONGEST model
- Quantum communication does NOT provide an improvement for many fundamental problems: **Shortest paths,** Minimum Spanning Tree, **Steiner Tree**, Min Cut, Hamiltonian Cycle…

- **Intuition:** In CONGEST, a significant bottleneck can be communicating between “distant” parts of the network – qubits don’t help with that!

- Elkin, M., Klauck, H., Nanongkai, D., & Pandurangan, G. (2014, July). Can quantum communication speed up distributed computation?. In *Proceedings of the 2014 ACM symposium on Principles of distributed computing* (pp. 166-175).

CONGEST CLIQUE

- Elkin et al.'s results and analysis **do not** carry over to the CONGEST CLIQUE
- So, can quantum communication help in this model?

Surprising **positive results** in in Quantum CONGEST CLIQUE Model (qCCM):

- Faster Triangle Detection, Izumi & Le Gall 2019
- Faster All-Pairs **Shortest-Paths** (APSP), Izumi & Le Gall 2020
  - $\tilde{O}(n^{1/4})$ in quantum versus $\tilde{O}(n^{1/3})$ in classical
  - This was in Elkin's list of problems not admitting speedups!

$$f(n) \in \tilde{O}(g(n))$$
if
$$\exists k: f(n) \in O(g(n) \log^k n)$$

For which other problems can we exhibit improvements in the quantum CONGEST CLIQUE model?

- Elkin, M., Klauck, H., Nanongkai, D., & Pandurangan, G. (2014, July). Can quantum communication speed up distributed computation?. In *Proceedings of the 2014 ACM symposium on Principles of distributed computing* (pp. 166-175).
- Izumi, T., & Le Gall, F. (2017, July). Triangle finding and listing in CONGEST networks. In Proceedings of the ACM Symposium on Principles of Distributed Computing (pp. 381-389).
- Izumi, T., & Le Gall, F. (2019, July). Quantum distributed algorithm for the All-Pairs Shortest Path problem in the CONGEST-CLIQUE model. In Proceedings of the 2019 ACM Symposium on Principles of Distributed Computing (pp. 84-93).

New Algorithms

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Algorithmic Recipe

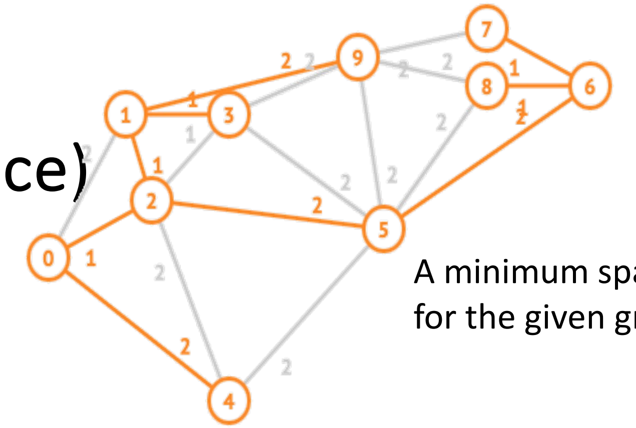
Approach: Make use of previous techniques such as

1. Distributed Grover Search
2. Triangle Finding
3. Distance Products
4. Shortest Paths and Routing Tables

Our Contributions

New algorithms in Quantum CONGEST-CLIQUE Model (qCCM) that succeed with high probability for

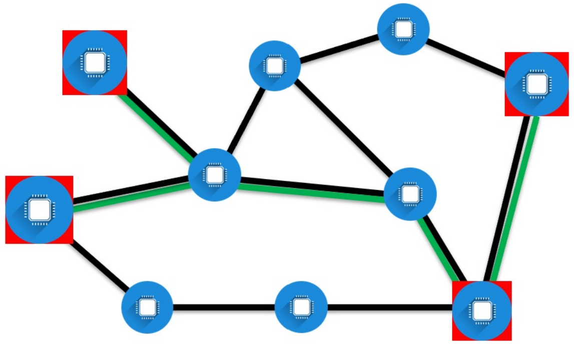
- (approximately optimal) Steiner Trees
- Directed Minimum Spanning Trees (Arborescence)



A minimum spanning tree (orange) for the given graph (grey)

in asymptotically fewer rounds required than for any known classical algorithm

$\rightarrow \tilde{O}(n^{1/4})$ versus $\tilde{O}(n^{1/3})$



Steiner tree (green) for graph with marked terminal nodes (red)

Exact complexity analysis of quantum and classical algorithms reveals improvements needed for both to become practical!

Algorithmic Recipe & Complexity

1. Distributed Grover Search helps with…
2. Triangle Finding helps with…
3. Distance Products helps with…
4. Shortest Paths and Routing Tables helps with…
5. Steiner and Directed Minimum Spanning Trees!

$\boldsymbol{n^{\frac{1}{4}} \log_2(n)^2}$

$\boldsymbol{\log_2(n)^3}$

$\boldsymbol{\log_2(n)}$

$\boldsymbol{c \cdot n^{\frac{1}{4}} \log_2(n)^6}$ rounds

The asymptotic results are exciting! But more work is needed to bring these algorithms into a practical realm

In CONGEST CLIQUE, can solve anything in n rounds:
To be practical, need roughly

$$\boldsymbol{3200 \cdot n^{\frac{1}{4}} \log_2(n)^6 < n}$$

Algorithmic Recipe & Complexity

1. Distributed Grover Search helps with…
2. Triangle Finding helps with…
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4. Shortest Paths and Routing Tables helps with…
5. Steiner and Directed Minimum Spanning Trees!

The asymptotic results are exciting! But more work is needed to bring these algorithms into a practical realm

$n^{\frac{1}{4}} \log(n)^2$

$\log(n)^3$

$\log(n)$

$c \cdot n^{\frac{1}{4}} \log(n)^6$ rounds

In CONGEST CLIQUE, can solve anything in n rounds:
To be practical, need roughly

$$3200 \cdot n^{\frac{1}{4}} \log(n)^6 < n$$

for which

$$n > 10^{18}$$

is required!! 10^{11} for classical $\tilde{O}\left(n^{\frac{1}{3}}\right)$ counterpart.

Distributed quantum algorithms: Future directions

What further improvements be made to bring the asymptotic speedup closer to practical?

Other problems that for which these methods can demonstrate advantages in the quantum setting?

There are other distributed computing models and approaches. What can be shown in quantum versions of these modes?

Pay attention to quantities hidden in $\tilde{O}(N)$ notation!

- Constants and log factors can be important in both the near and long term

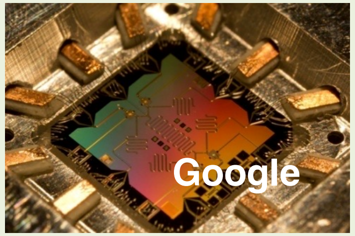
Distributed quantum computing is in its infancy, with few results and many open directions

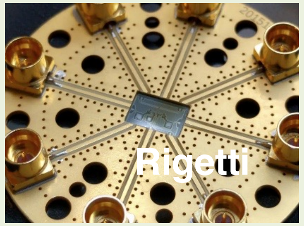
Many opportunities for classical computing to inform quantum computing and to work with or as part of quantum computing

Other Topics

Status of Quantum Hardware

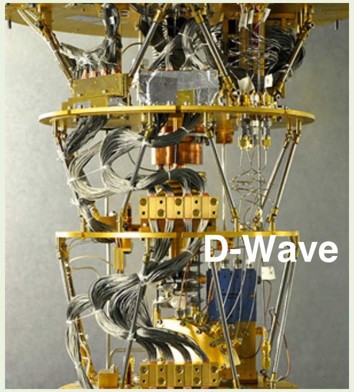
General Purpose:
Universal quantum processors

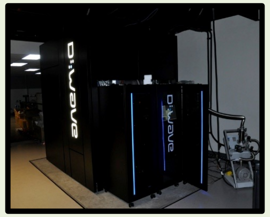




Special Purpose:
E.g. Quantum annealers

Noisy Intermediate-Scale Quantum (NISQ) devices





Many different underlying physical substrates for quantum processors:

- Superconducting
- Trapped ion
- Photonic
- Other
  - -Electron spins in silicon
  - - Neutral atom, cold atom
  - - Topological, anyon based quantum computing

All quantum hardware is small and non-robust

Special purpose vs general purpose processors

- Algorithm/hardware codesign

Number of qubits alone is not a good measure
- Analogy: billions of switches do not a classical computer make

Other key factors
- precision, speed, and generality of the control
  - particularly operations involving multiple qubits
- how long quantum coherence can be maintained
- stability over time
- speed with which processors can be calibrated

Future quantum computers

Application scale quantum computers will resemble supercomputers

Many quantum processing units (QPUs), and classical processing units

Quantum and classical communication

Robustness:

Quantum error correction and fault tolerance are mature areas, with continuous breakthroughs

Tens to thousands of logical qubits per QPUs

Rule of thumb: ~1000 physical qubits per logical qubits

Synergies and differences between quantum computer and supercomputer architectures

2D local structures, higher dimensional comm at larger scales

No cloning severely limits duplication

E.g. Two ways to move quantum info

local quantum physical links

teleportation across arbitrary distances

- requires prior set up of entanglement through local links, and classical comm as part of teleportation

Quantum-inspired classical algorithms and hardware

Quantum Monte Carlo

Improved classical techniques for simulating quantum systems

De-quantized quantum algorithms

e.g. for E3Lin2

e.g. certain sampling and quantum ML algorithms

Quantum proofs for classical for classical theorems (Survey: Drucker & Wolf arXiv:0910.3376)

DARPA's Quantum-Inspired Classical Computing (QuICC) program

PySA: Suite of State-Of-Art classical optimization algs

Features and state-of-the-art implementations:

- Modern C++17 with template metaprogramming for high level of abstraction
- Compile time optimization for improved performance

Algorithms:

- Parallel Tempering
- Ergodic and non-ergodic Isoenergetic cluster moves
- Approximate solution using mean-field theory

Recent augmentations:

- Improved Python interface

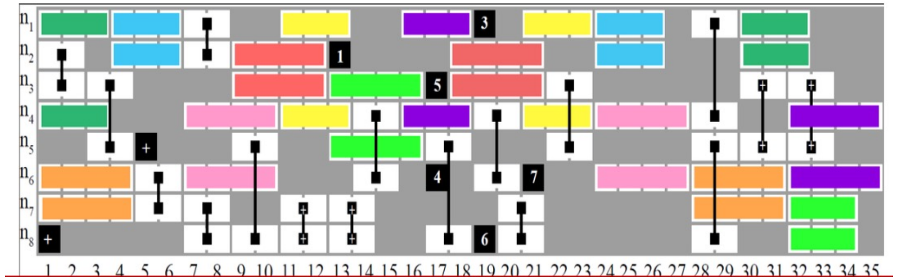
We continuously update PySA with optimized code for state-of-the-art classical optimization, including physics inspired approaches we have developed

Open Source Code: https://github.com/nasa/pysa

Brief Glimpse: Qubit Routing for Quantum Circuits

Quantum algorithms must be compiled before they can be run on quantum hardware

- Gate synthesis: rewrite only in terms of native gates
- Qubit routing: move information around to where two-qubit gates can act, given connectivity constraints



Can be viewed as a temporal planning problem

- Applied state of the art temporal planners
- Minimizes "makespan," the time it takes to carry out the computation
- There is now a quantum circuit compilation domain in the International Planning Competitions temporal planning track
- Combining CP with temporal planning is advantageous

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

Venturelli, Davide, Minh Do, Bryan O'Gorman, Jeremy Frank, Eleanor Rieffel, Kyle EC Booth, Thanh Nguyen, Parvathi Narayan, and Sasha Nanda. "Quantum circuit compilation: An emerging application for automated reasoning." (2019).

Booth, Kyle EC, Minh Do, J. Christopher Beck, Eleanor Rieffel, Davide Venturelli, and Jeremy Frank. "Comparing and integrating constraint programming and temporal planning for quantum circuit compilation." In Twenty-Eighth international conference on automated planning and scheduling. 2018

Quantum Error Correction

- Quantum error correction initially thought impossible!
  - No cloning principle: an unknown quantum state cannot be copied reliably without destroying the original
- Quantum information theory was just too interesting
  - Steane and Shor & Calderbank saw a way to finesse what had seemed insurmountable barriers to quantum error correction
- Now quantum error correction is one of the most developed areas of quantum computing

- Uses properties of quantum measurement and entanglement to its advantage
- Stabilizer code formulation most common
  - Surface code
- Remains active area of research
  - Subsystem codes
  - Dynamical/Floquet codes
  - Quantum Low-Density Parity Check (LDPC) codes
  - Decoders

QuAIL simulation software and theory

Quantum Circuit simulation software

Google – NASA – ORNL collaboration
F. Arute *et al.* (2019), Quantum supremacy using a programmable superconducting processor, *Nature* **574**, 505-510

Recent NASA collaboration with Google AI

A. Morvan, B. Villalonga, X. Mi, **S. Mandrà**, et al., **Phase transition in Random Circuit Sampling**, arXiv:2304.11119, April 24, 2023

Experimental results that are significantly harder to simulate than the 2018 ones

Open Quantum System Simulation

N Suri, J Barreto, S Hadfield, N Wiebe, F Wudarski, J Marshall, Two-Unitary Decomposition Algorithm and Open Quantum System Simulation, Quantum 7, 1002 (2022)

- avoids classically expensive singular value decomposition (SVD)
- requires only a single call to state preparation oracle
- calls to the encoding oracle can also be reduced at the expense of an acceptable error in measurements

Simulation of Photonic Quantum Systems

- Effect of **distinguishability** and **loss** errors in QIP
  - J Marshall, Distillation of Indistinguishable Photons Phys. Rev. Lett. 129 (21), 21360
- Efficient representations
  - J Marshall, N Anand Simulation of quantum optics by coherent state decomposition, arXiv:2305.17099

HybridQ: A Hybrid Quantum Simulator for Large Scale Simulations

Hardware agnostic quantum circuit simulator

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

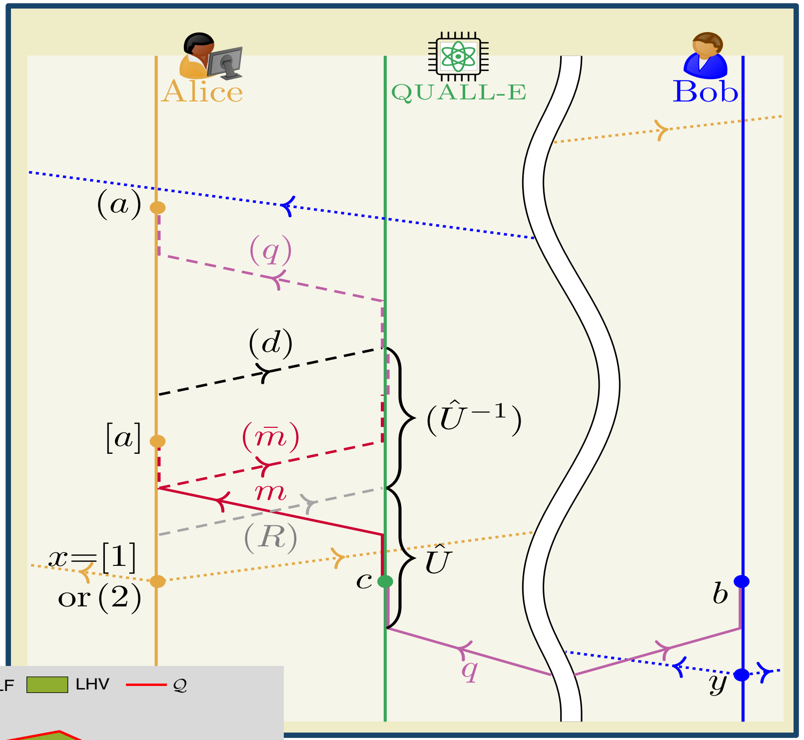
- Fully compatible with Python (3.8+)
- Low-level optimization achieved by using C++ and Just-In-Time (JIT) compilation with JAX and Numba,
- It can run seamlessly on CPU/GPU and TPU, either on single or multiple nodes (MPI) for large scale simulations, using the exact same syntax
- User-friendly interface
- Can run on supercomputers or laptop
- 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 project with continuous-integration, multiple tests and easy installation using either `pip` or `conda`

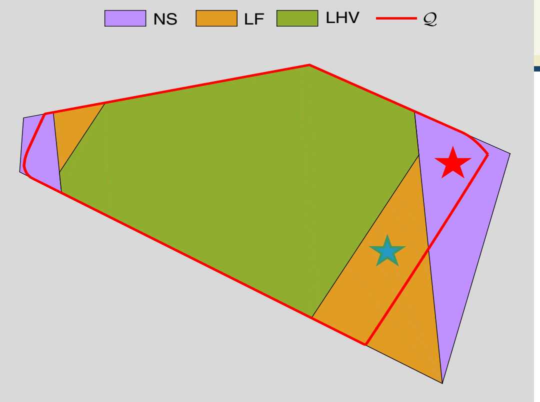
Open source code available at https://github.com/nasa/HybridQ

S. Mandrà, J. Marshall, E. G. Rieffel, R. Biswas, HybridQ: A Hybrid Simulator for Quantum Circuits, QCS 2021, arXiv:2111.06868

Wigner's friend inequalities & Experiments

- Wigner friend scenario recent work
  - new inequalities, with weaker assumptions than Bell's inequalities
  - Proof-of-principle experiments have been done
    - Single photon as friend
- Full experiment would combine Artificial Intelligence and Quantum Computing
  - QUALL-E
- Open research directions for experiments between proof-of-principle and full
  - Space-based experiments





Polytope with 96 extreme points and 932 facets

Bong, Kok-Wei, Aníbal Utreras-Alarcón, Farzad Ghafari, Yeong-Cherng Liang, Nora Tischler, Eric G. Cavalcanti, Geoff J. Pryde, and Howard M. Wiseman. **"A strong no-go theorem on the Wigner's friend paradox." Nature Physics 16, 12 (2020)**
H.M. Wiseman, E.G. Cavalcanti, E.G. Rieffel, **A "thoughtful" Local Friendliness no-go theorem: a prospective experiment with new assumptions to suit,** *arXiv:2209.08491 (Accepted to Quantum)*

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?

For more info

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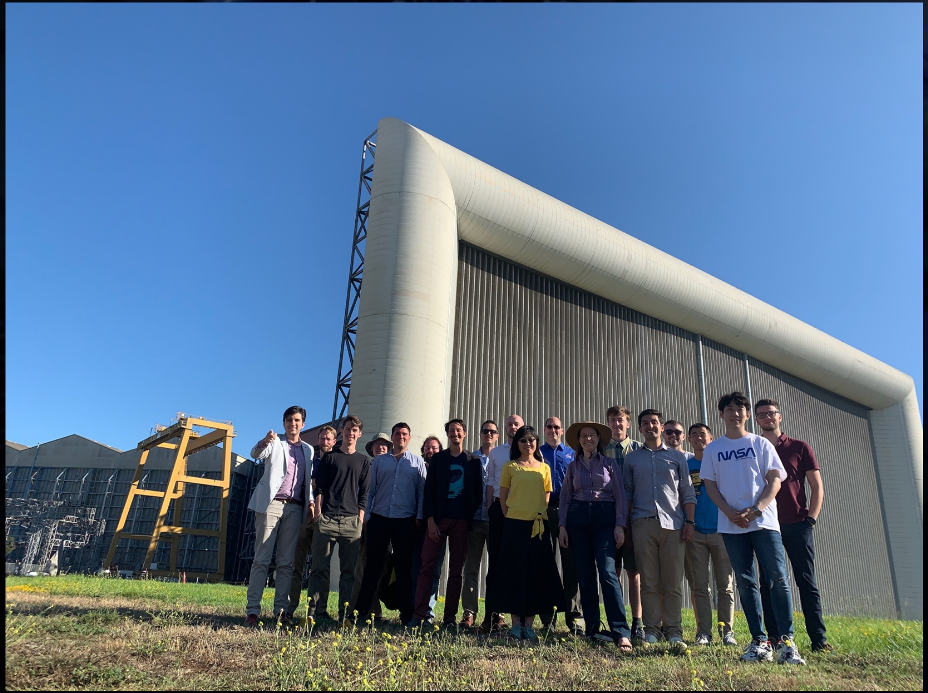

Eleanor G. Rieffel, Stuart Hadfield, Tad Hogg, Salvatore Mandrà, Jeffrey Marshall, Gianni Mossi, Bryan O'Gorman, Eugeniu Plamadeala, Norm M. Tubman, Davide Venturelli, Walter Vinci, Zhihui Wang, Max Wilson, Filip Wudarski, Rupak Biswas, ***From Ansätze to Z-gates: a NASA View of Quantum Computing***, arXiv:1905.02860

Rupak Biswas, Zhang Jiang, Kostya Kechezhi, Sergey Knysh, Salvatore Mandrà, Bryan O'Gorman, Alejandro Perdomo-Ortiz, Andre Petukhov, John Realpe-Gómez, Eleanor Rieffel, Davide Venturelli, Fedir Vasko, Zhihui Wang, ***A NASA Perspective on Quantum Computing: Opportunities and Challenges***, arXiv:1704.04836