

Assessing and Advancing the Potential of Quantum Computing: a NASA Case Study

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Lead

Quantum Artificial Intelligence Lab (QuAIL)

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

QuAIL Team:

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Davide Venturelli

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Past NASA Fellows:

Ryan LaRose (Michigan State)

Sarah Muschinske (MIT)

Bryan O’Gorman (UC Berkeley)

Anthony Polloreno (Univ.
Colorado, Boulder)

+ 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

Software Tools & Algorithms

Quantum algorithm design

Compiling to hardware

Mapping, parameter setting, error mitigation

Hybrid quantum-classical approaches

Solvers & Simulators

Simulation of quantum systems, under noise

HPC quantum circuit simulators

Physics Insights

Co-design quantum hardware

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

Resource Estimation for Solving Utility-Scale Instances



Depends on

Algorithm

Hardware Architecture

Error Correcting Code

Consider all resources

Classical computation

Parameter setting

Energy-to-solve may be a better metric than time-to-solution

DE Bernal Neira, Benchmarking the Operation of Quantum Heuristics and Ising Machines: Scoring Parameter Setting Strategies on Optimization, arXiv: 2402.10255 Applications

DARPA Quantum Benchmarking Program

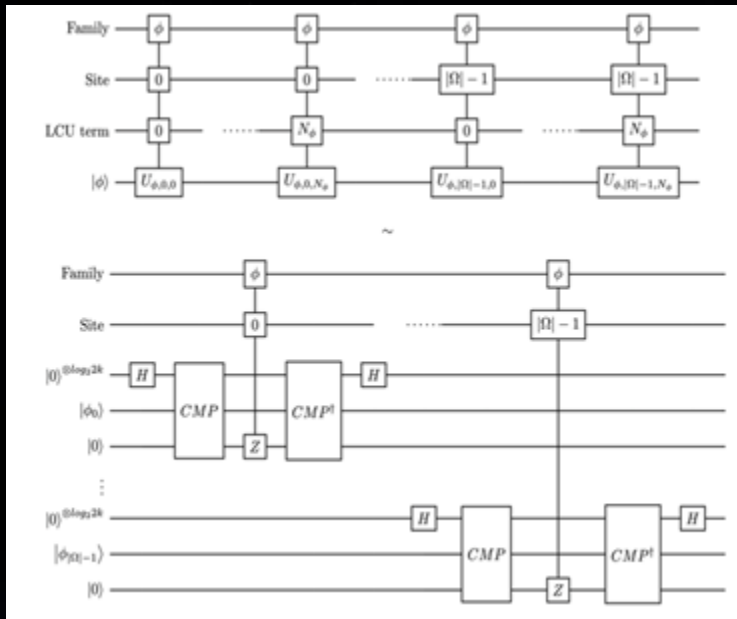
In LISQ (logical intermediate-scale quantum) and early FT (fault tolerant) era, resources will be limited

Even “small” constants and log factors will be critical

Resource estimates support architectural design of quantum computers

Early LISQ and early FT quantum computers may be special purpose, targeted at specific applications

Optimized Quantum Algorithms for Quantum Field Theory Simulation



Example optimization of a circuit used in Φ^4 theory simulation

A. Hardy, P. Mukhopadhyay, **M. S. Alam**, R. Konik, L. Hormozi, **E. Rieffel**, S. Hadfield, J. Barata, R. Venugopalan, D. E. Kharzeev, N. Wiebe, **Optimized Quantum Simulation Algorithms for Scalar Quantum Field Theories**, arXiv:2407.13819 (July 2024)

Quantum computing may provide the only way to simulate the most challenging and intriguing problems in high energy physics

As a step toward realizing that goal, C2QA and SQMS researchers advanced quantum simulation algorithms for Φ^4 theory, a model quantum field theory

This 100+ page paper includes detailed resource estimates for a quantum computer to carry out these algorithms to sufficient accuracy

Provides additional target algorithm that could be run on early fault tolerant quantum computers



One Area of Quantum Computing is Underhyped



These algorithms are the only ones useful today



They are applications of quantum computing but
not of quantum computers

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 theorems (Survey: Drucker & Wolf arXiv:0910.3376)

Quantum Inspired Classical Hardware

Digital Annealers

Coherent Ising Machines

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

Toward establishing useful quantum advantage



Specify utility-scale **instances** (not just problem classes)

Detailed assessment of the utility of solving the problem instance

Size; precision

Speed required

4. How many and how frequently instances need to be solved
5. Best classical algorithms and results

Stepping-stone instance families

Capture key aspect(s) of utility-scale instance(s)

Means to generate instances with

Spectrum of sizes

Tunable hardness

Recent work

S Mandra, G Mossi, E Rieffel, **Generating Hard Ising Instances With Planted Solutions Using Post-Quantum Cryptographic Protocols**, arXiv: 2308.09704

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>

Utility-scale quantum computers



Utility-scale quantum computers will resemble supercomputers

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

Quantum and classical communication

Potentially heterogeneous quantum components

Memory

Magic state factories

Special purpose components targeted
at common quantum subroutines

May have 2D local structures, higher
dimensional comm at larger scales

Surface code is not the end of the story

Many breakthroughs in QEC in the past
few years

New code types

Better decoders

One new type of code:

Dynamical or Floquet codes

Floquet-Bacon-Shor code



To free up space for an additional logical qubit in a Bacon-Shor code

We refrain from fixing one of the gauge degrees of freedom

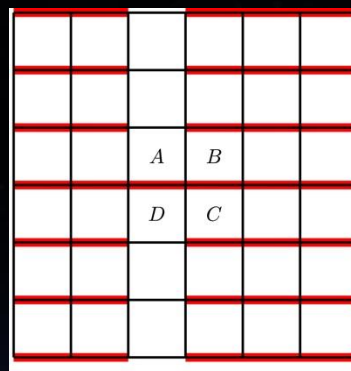
We introduce a “gauge defect”

We need to do so carefully to ensure all Bacon-Shor stabilizers get measured

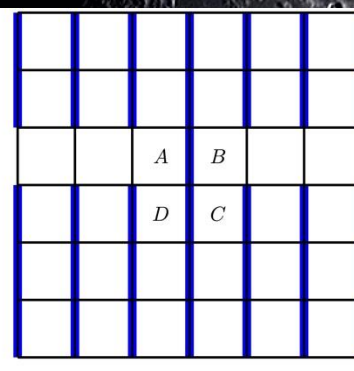
Measurement schedule

Provides insights into design space and design strategies for dynamical codes

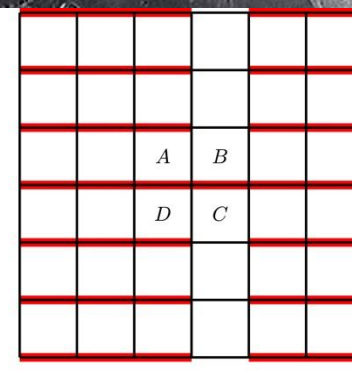
Potential for early experimental realization of a dynamical code



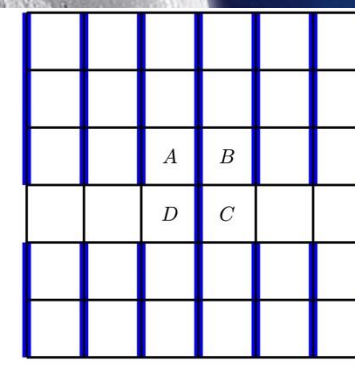
Subset of horizontal XX checks



Subset of vertical ZZ checks



Subset of horizontal XX checks



Subset of vertical ZZ checks

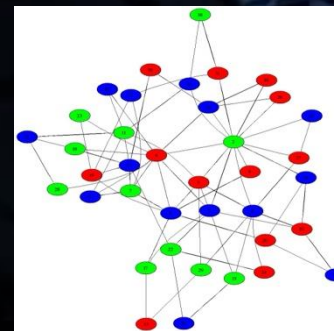
Example: Hardware-Algorithm Co-Design: Gate-Model

Quantum Alternating Operator Ansatz introduced more general “mixing operators”

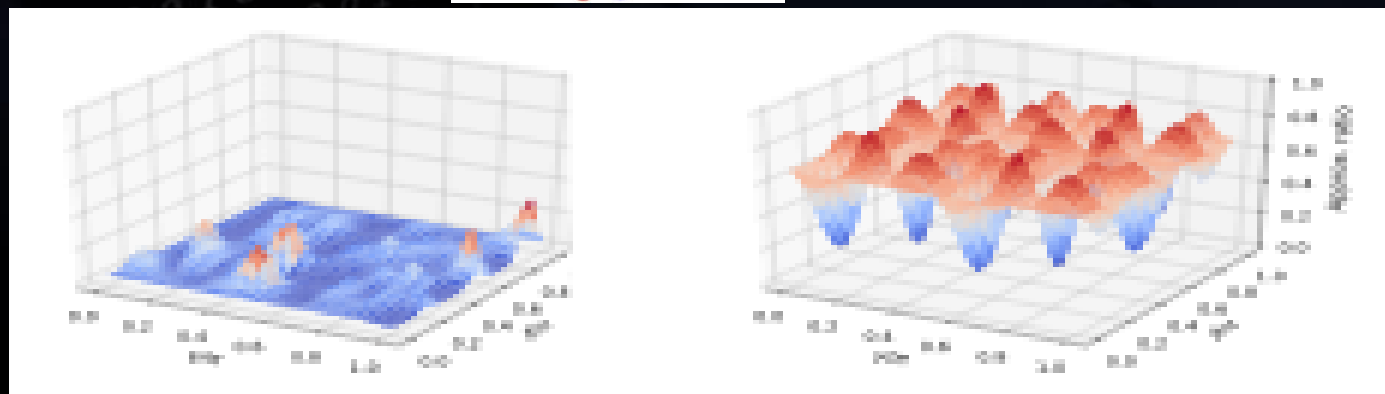
inspired native implementations of these general mixing operators on Rigetti hardware

Rigetti developed novel calibration techniques for this family of gates

Collaboration with Rigetti under DARPA ONISQ project to evaluate QAOA on their gate-model processors



Problem instance: Max-K-Colorable subgraph



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

S. Hadfield *et al.* (2019), From the quantum approximate optimization algorithm to a quantum alternating operator Ansatz, *Algorithms* **12**, 34 Z. Wang *et al.*

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

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

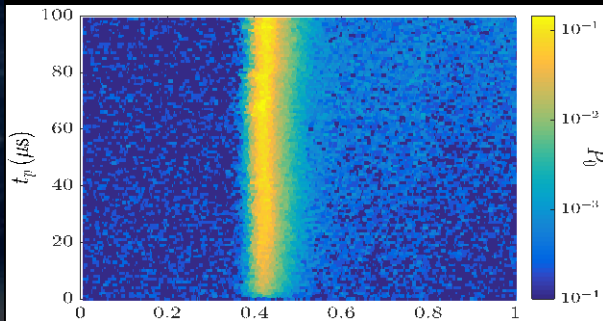
M. Dupont *et al.* (2022), Quantum Enhanced Greedy Solver for Optimization Problems, *arXiv:2303.05509*

FB Maciejewski *et al.* (2023) Design and execution of quantum circuits using tens of superconducting qubits and thousands of gates for dense Ising optimization problems, *arXiv:2308.12423*

Example: Hardware-Alg. Co-Design: Q. Annealing

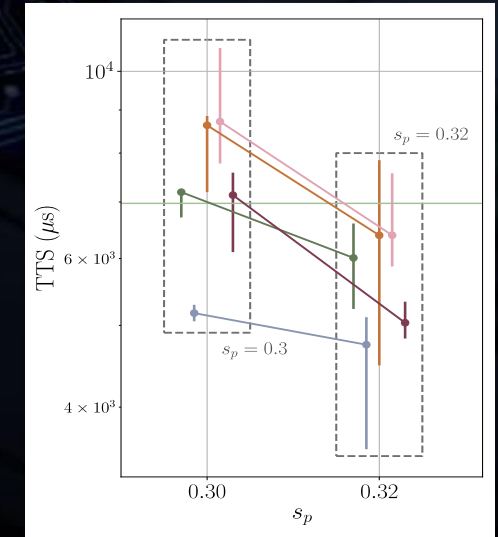
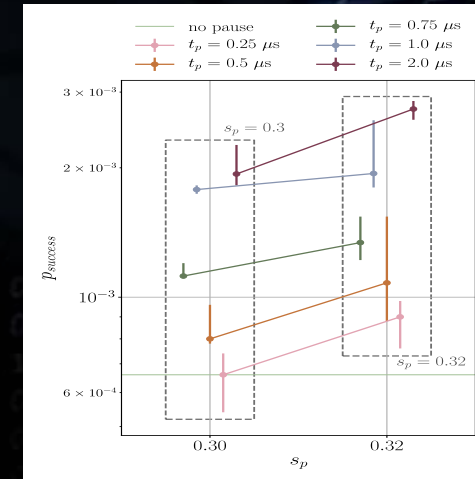
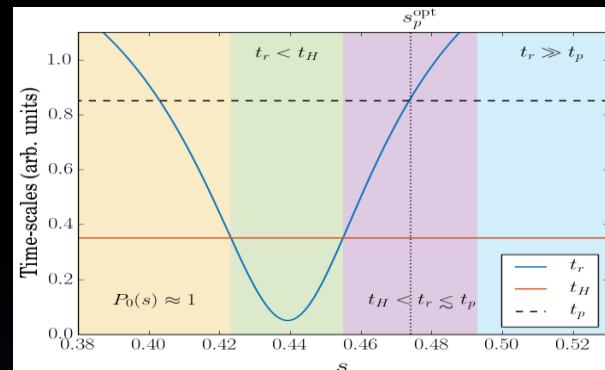


The power of pausing: additional control of anneal schedule, increases performance by **orders of magnitude**



Heat map of probability of solution, depending on pause location and pause length

Anneal time regions. 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 *et al.* (2019), Power of pausing: Advancing understanding of thermalization in experimental quantum annealers, *Phys. Rev. Applied* **11**, 044083
- Z. Izquierdo *et al.* (2021), Ferromagnetically shifting the power of pausing, *Phys. Rev. Applied* **15**, 044013
- Z. Izquierdo *et al.* (2022), Advantage of Pausing: Parameter Setting for Quantum Annealers, *Physical Review Applied* **18** (5), 054056

Quantum Computing for Earth Science



N. Gao *et al.* (2020), High-dimensional similarity search with quantum-assisted variational autoencoder, *KDD '20*, 956-964

Quantum-assisted variational autoencoder

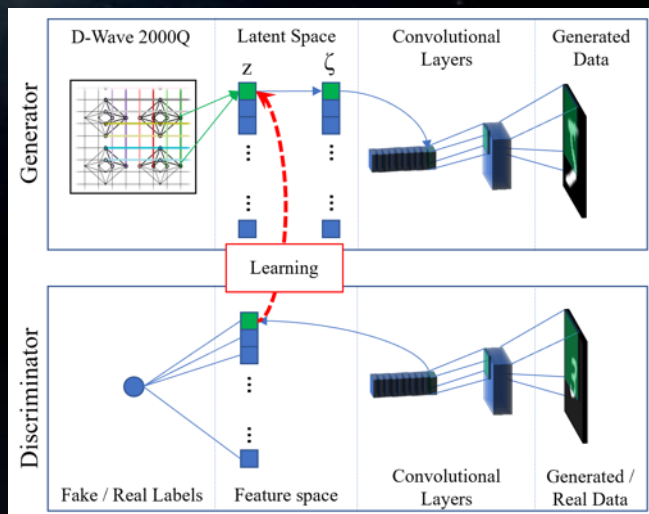
- “Similarity” search applied to NASA’s MODIS dataset
- Multi-variate time series of land cover change
- 17 years of satellite observations over 36 spectral bands
- Extend to segmentation, reconstruction, super-resolution

Quantum inspired
classical algorithms

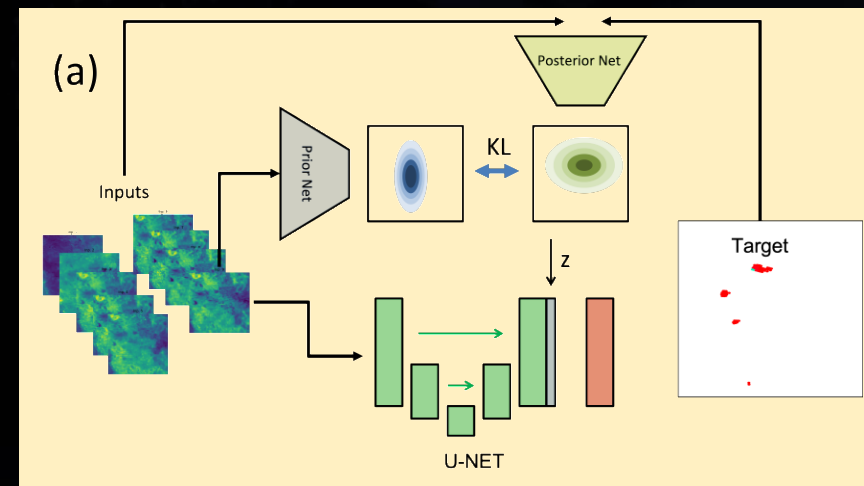
Quantum-ready
classical algorithms

Quantum-assisted associative adversarial network

M. Wilson *et al.* (2021), Quantum-assisted associative adversarial network: Applying quantum annealing in deep learning, *Quantum Machine Intelligence*



Generative Machine Learning for Wildfire Image Processing



A. Asanjan *et al.* (2023), *Probabilistic Wildfire Segmentation Using Supervised Deep Generative Model from Satellite Imagery, Remote Sensing*

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

Mind the constants and log factors!

Quantum Algorithms Intrinsically Distributed problems

Algorithms for problems that are distributed by nature

- each node in the graph has information; no node has all the information
- all nodes need to work together to solve the problem
- minimize number of communication rounds

Novel quantum distributed algorithms for Survivable Network Design Problems

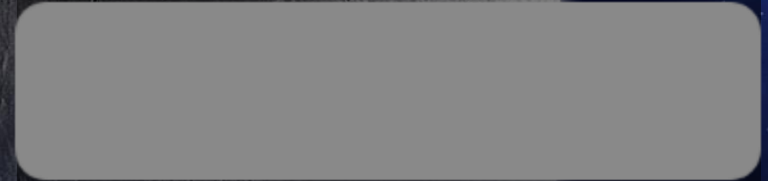
- Broad class that includes Approximate Steiner Tree Problem, K-Connected Network Problem
- Asymptotic improvement with respect to the current best known classical algorithm in terms of computational rounds in the CONGEST CLIQUE model
- Detailed analysis to understand at what scales these algorithms and their classical counterparts out perform a simpler approach

Approximate Steiner Tree in CONGEST CLIQUE can always be solved in n rounds

To be practical, need roughly

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

for which



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



QuAIL simulation software and theory



HybridQ: A Hybrid Quantum Simulator for Large Scale Simulations

- Hardware agnostic circuit simulator
- Tensor contraction simulations, direct evolution, and Clifford+T simulations
- CPU/GPU and/or TPU, either on single or multiple nodes (MPI) for large scale simulations, using same syntax
- Commutations rules are used to simplify circuits (useful for QAOA)

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*

Open Quantum System Simulation

- e.g. 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)

Simulation of Photonic Quantum Systems

- J Marshall, N Anand, Simulation of quantum optics by coherent state decomposition, arXiv:2305.17099
- J Saied, J Marshall, N Anand, S Grabbe, EG Rieffel, Advancing quantum networking: some tools and protocols for ideal and noisy photonic systems, Quantum Computing, Communication, and Simulation IV (2024)

Mitigating distinguishability errors

- J Marshall, Distillation of Indistinguishable Photons Phys. Rev. Lett. (2024)
- J Saied, J Marshall, N Anand, EG Rieffel, General protocols for the efficient distillation of indistinguishable photons, arXiv:2404.14217 (2024)



What can Quantum Computing
tell us about Fundamental Physics?

Wigner's Friend Inequalities and Future Experiments



New inequalities, with weaker assumptions than Bell's inequalities, stemming from Wigner's friend scenario

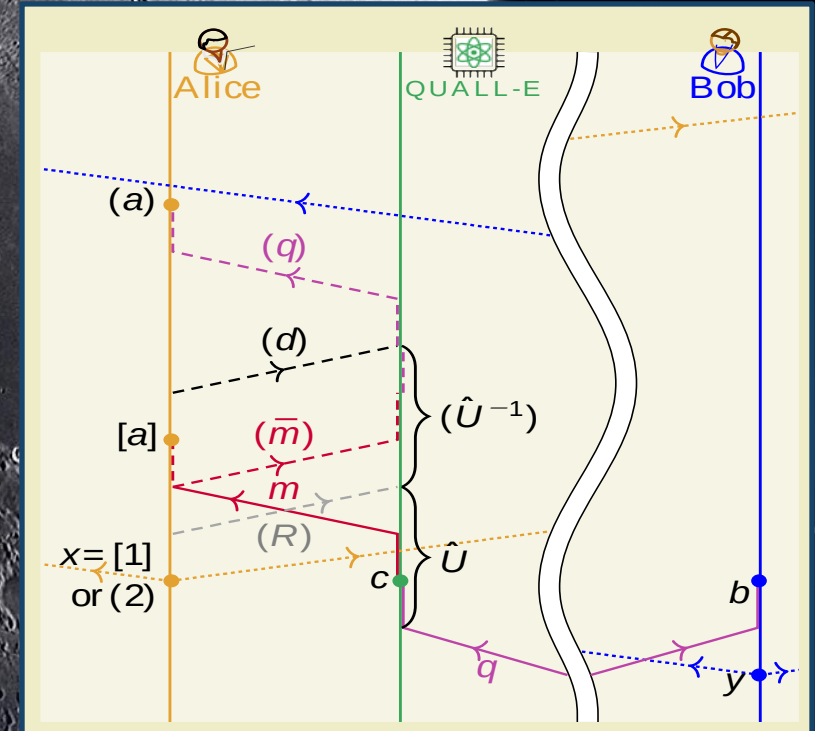
Wigner's friend is less famous than Schrödinger's cat, but equally intriguing

2022 Nobel prize in physics: "for experiments with entangled photons, establishing the violation of Bell inequalities and pioneering quantum information science"

Design of an experiment testing for violations of these inequalities would combine Artificial Intelligence and Quantum Computing

Collaboration between NASA and Australian researchers

Ultimate experiment requires space-based experiments



QUALL-E, an artificial intelligence running on a quantum computer plays a key role WF experiments testing fundamental aspects of quantum physics

H.M. Wiseman, E.G. Cavalcanti, E.G. Rieffel, A "thoughtful" Local Friendliness no-go theorem: a prospective experiment with new assumptions to suit, *Quantum* 7, 1112, 20204

A. Ananthaswamy, Can AI Save Schrödinger's Cat?, *Scientific American*, July/August issue, 2024

A Historical Perspective



Illiacc 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



For more info

Eleanor Rieffel, Ph.D.

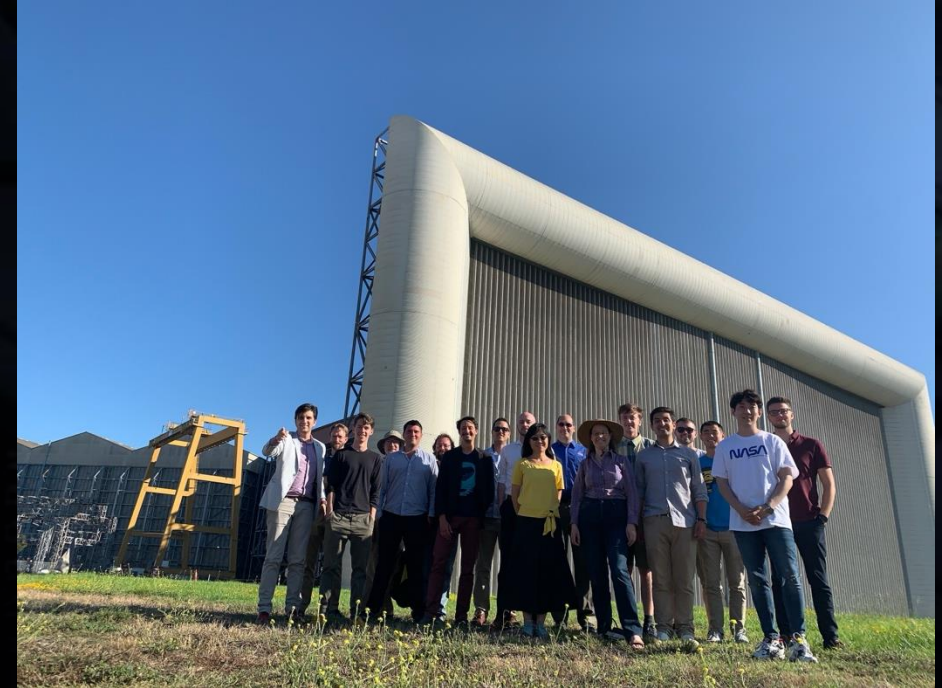
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<https://www.nasa.gov/intelligent-systems-division/discovery-and-systems-health/nasa-quail/>