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Overview of NASA QuAIL Team Research

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Quantum Artificial Intelligence Lab (QuAIL)
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NASA QuAIL Lead: Eleanor Rieffel

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NASA Fellowship: Bryan O’Gorman (UC Berkeley)



Office of the Director of National Intelligence

I A R P A
BE THE FUTURE



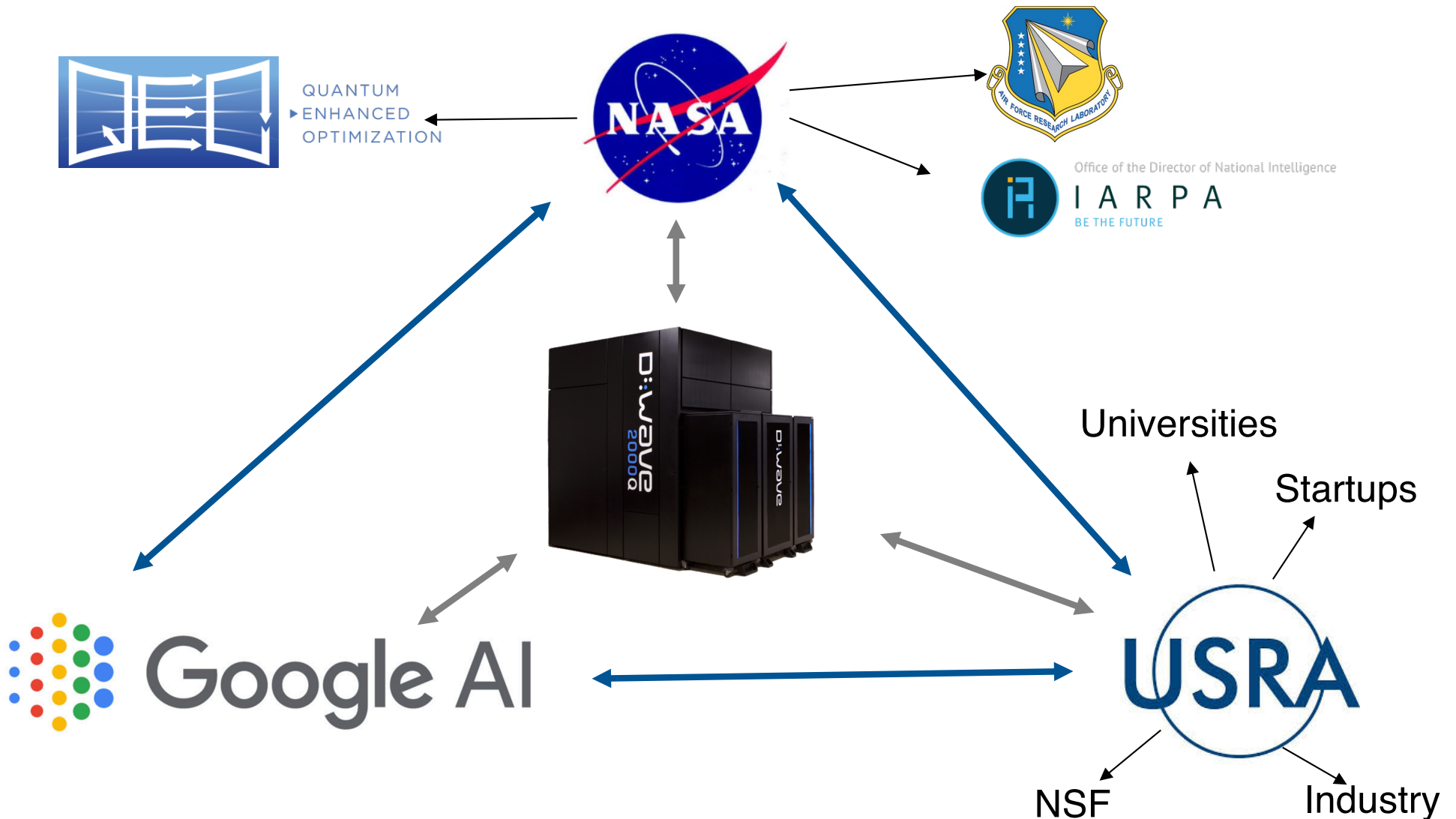
QUANTUM
ENHANCED
OPTIMIZATION



Sept 23, 2019

NASA Ames Research Center

NASA, Google and USRA Collaboration focused on Artificial Intelligence and Quantum Computing (2012-present)





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Users of the D-Wave Machine at NASA

Quantum RFP

<https://tinyurl.com/USRA-RFP2019>

Competitive Selections

Cycle 1 (512 qubit processor): 8 of 14 selected – 57%

Cycle 2 (1152 qubit processor): 10 of 15 selected – 67%

Cycle 3 (2048 qubit processor): 15 of 19 selected – 79%

Diversity of Selected Organizations

Approx 60% Universities + 40% Industrial Research Organizations

Approx 60% U.S. Organizations + 40% International Organizations

Computer Science, Physics, Mathematics, Electrical Engineering, Operations Research, Chemistry, Aerospace Engineering, Finance

Diversity of Research

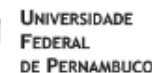
Quantum Physics -> Algorithms -> Applications

Machine Learning for Image Analysis, Communications, Materials Science, Biology, Finance

RFP CYCLE 1 & 2 SELECTIONS



RFP CYCLE 3 (extract)





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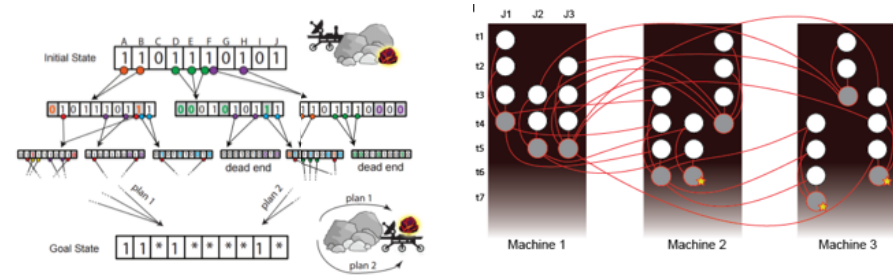
NASA's Interest in Quantum Computing

NASA constantly confronting massively challenging computational problems

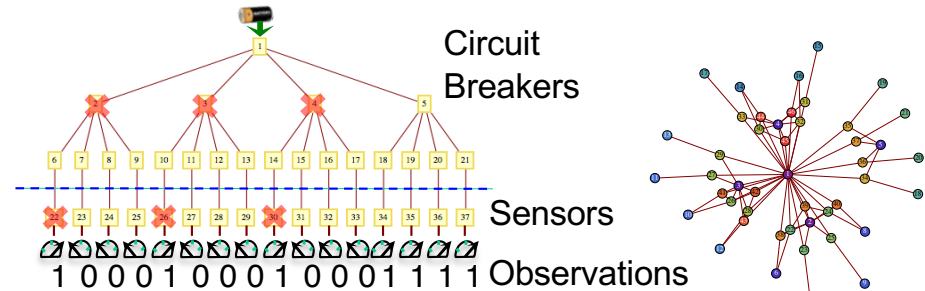
- Computational capacity limits mission scope and aims

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

Complex Planning and Scheduling



Graph-based Fault Detection



Robust network design

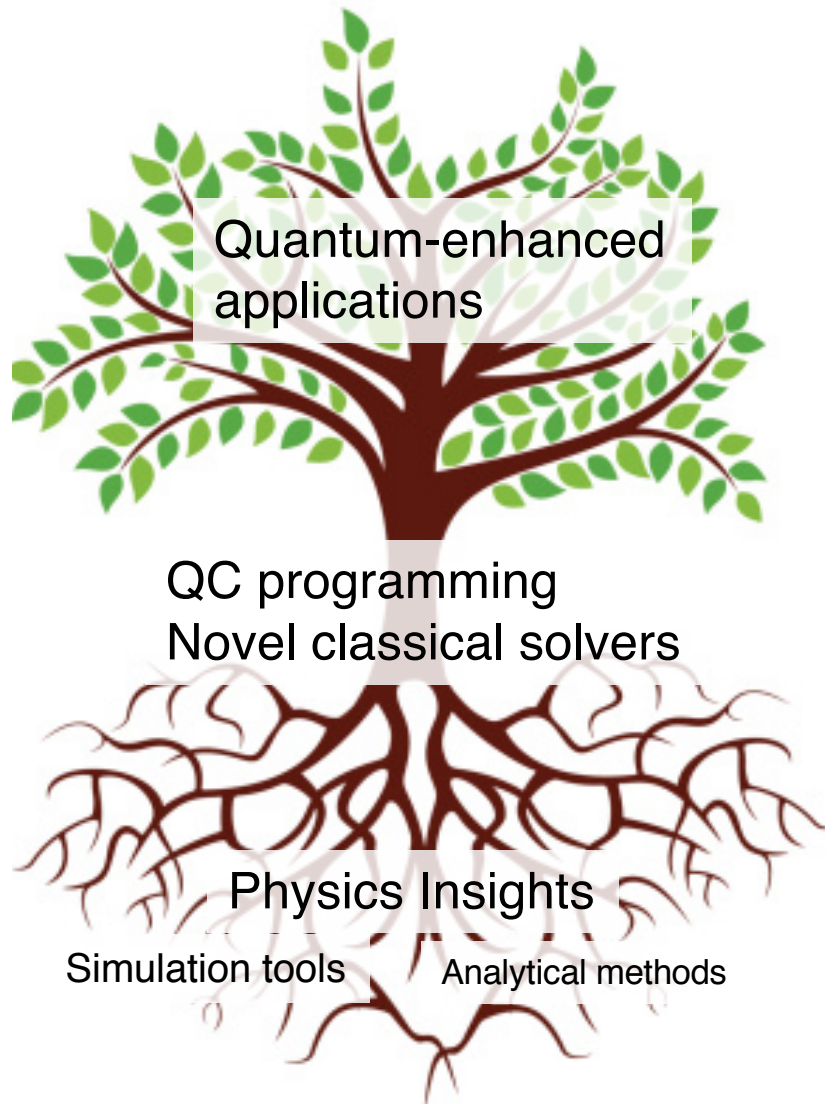




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Approach to Leveraging Quantum Computing to Address NASA's Computational Challenges



Application focus areas

Planning and scheduling Robust networks
Fault Diagnosis Machine Learning
Material science simulations
Wireless Decoding

Programming quantum computers

Quantum algorithm design
Mapping, parameter setting, error mitigation
Hybrid quantum-classical approaches
QC → state-of-the-art classical solvers

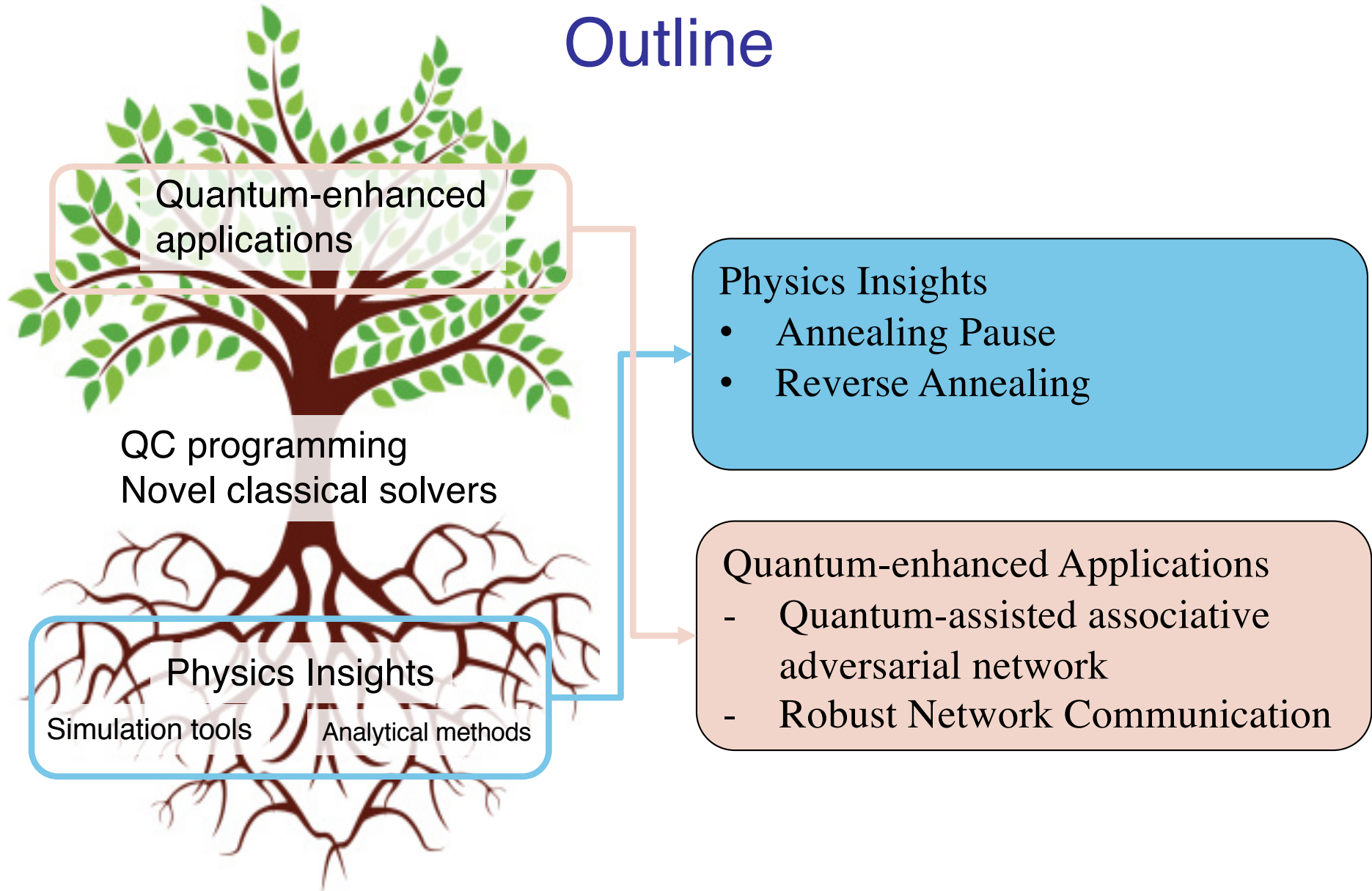
Physics insights into quantum algorithm and quantum hardware design



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Outline





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Pause results for one typical problem

Performance for pause schedules

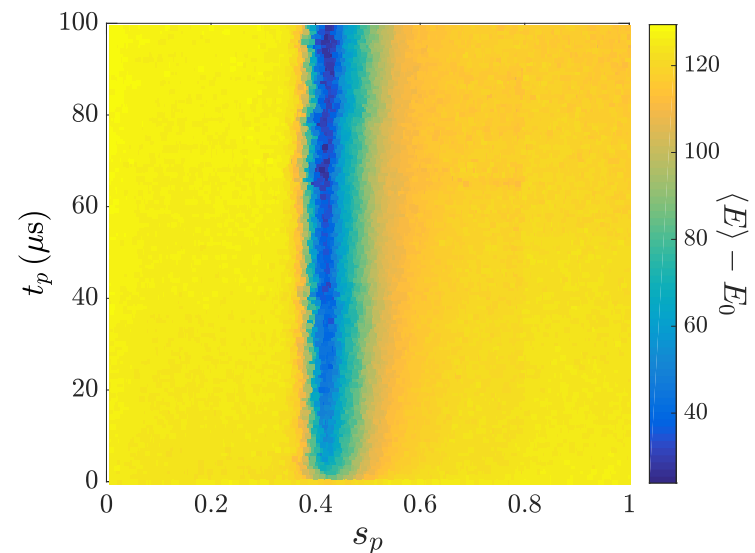
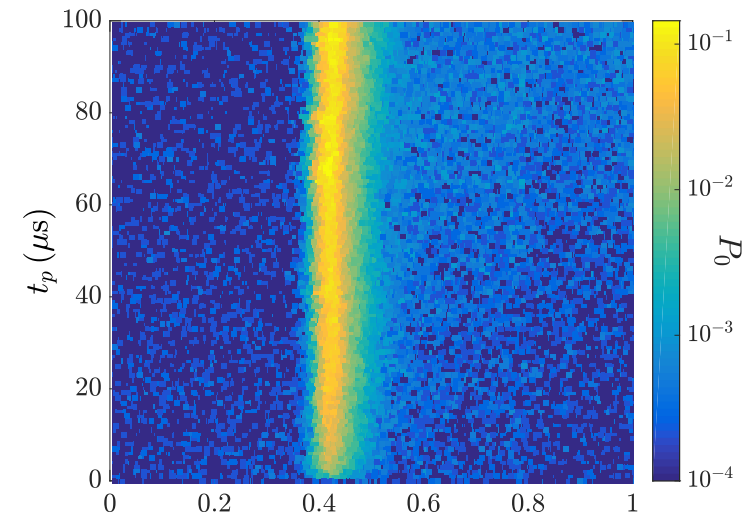
- heat map of probability of solution P_0 as function of pause location s_p and pause length t_p
- heat map of average energy (above ground state) of solution as function of pause location s_p and pause length t_p

Results for single 800-qubit problem

- total anneal time $t_a = 1 \mu s$
- Each point: 10,000 anneals, using 5 gauges
- $P_0 = 10^{-4}$ for anneal without pause

Orders of magnitude improvement for pausing in narrow region of location parameter s_p

J. Marshall, D. Venturelli, I. Hen, E. Rieffel, The power of pausing: advancing understanding of thermalization in experimental quantum annealers, Physical Review Applied 11 (4), 044083, 2019, arXiv:1810.05881





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Theory and relevant time scales

Early times: Ground state is well-separated by rest of spectrum, so $P_0 \sim 1$

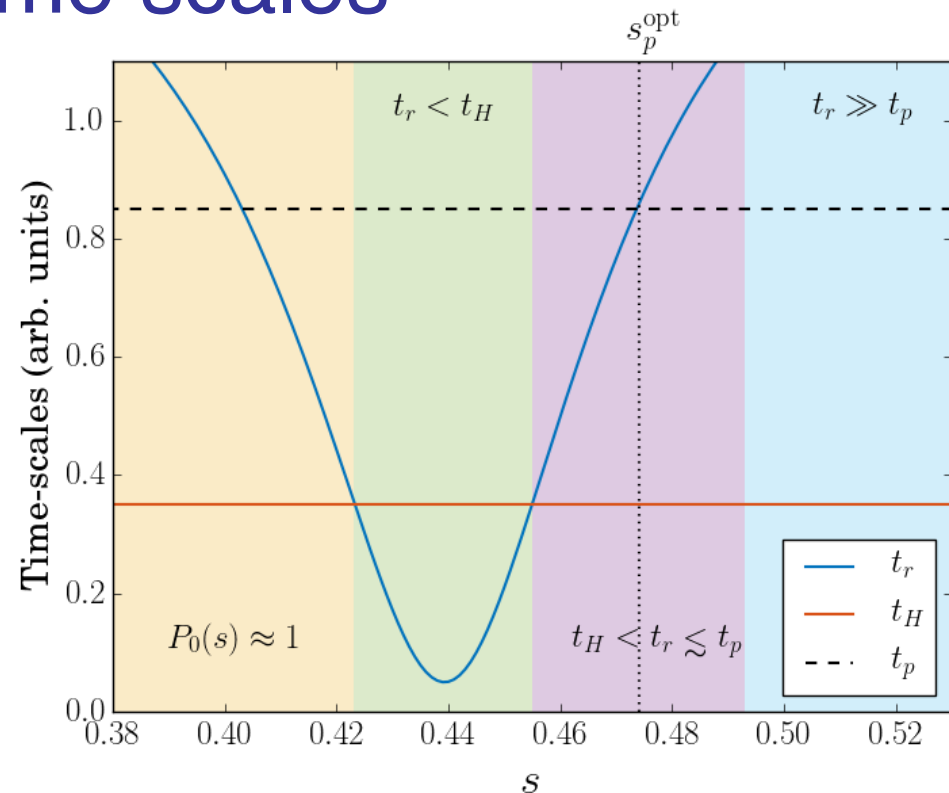
Gap narrows: $t_r < t_H$

Relaxation rate increases, potential for thermal excitation leading to instantaneous thermalization

Gap widens: $t_H < t_r \lesssim t_p$

Instantaneous thermalization no longer occurs, but a pause may enable significant thermalization

Late times: $t_p \ll t_r$ Energy levels well-separated so even with a pause of length t_p , thermalization cannot occur



Cartoon of distinct regions with different behavior focusing on most dynamic part of the anneal

- t_r = relaxation rate
- t_H = Hamiltonian evolution time scale.
For $t_r < t_H$, the system instantaneously thermalizes (we plot t_H as a line only for the purpose of easy visualization of the regions)



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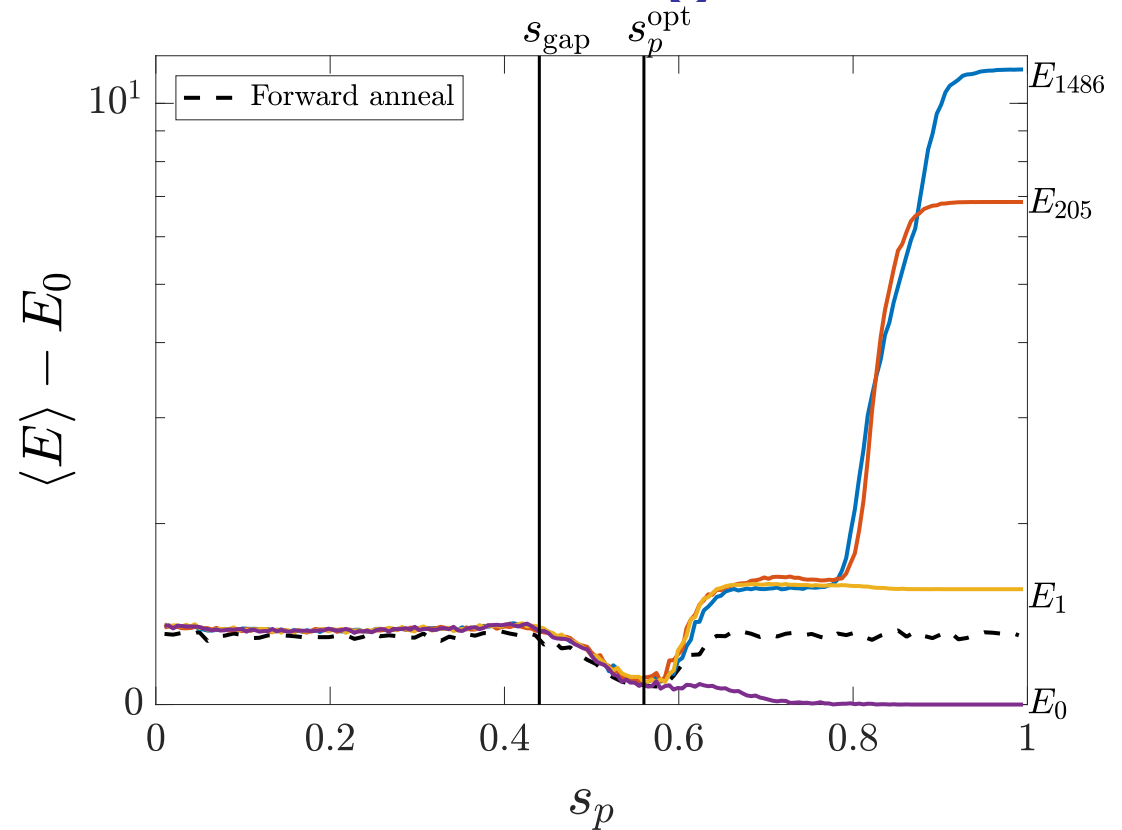
Further insights from reverse annealing

Another feature of the D-Wave 2000Q is reverse annealing

Can start in a classical eigenstate of H_p and evolve backwards from $s = 1$ to a time s_p (where we also pause) and then evolve forward

We see the same optimal pause point after the minimum gap as in the forward anneal case

These reverse annealing results further confirm the key regions and the theory supporting the location of the gap in the $t_a < t_r < t_p$ region



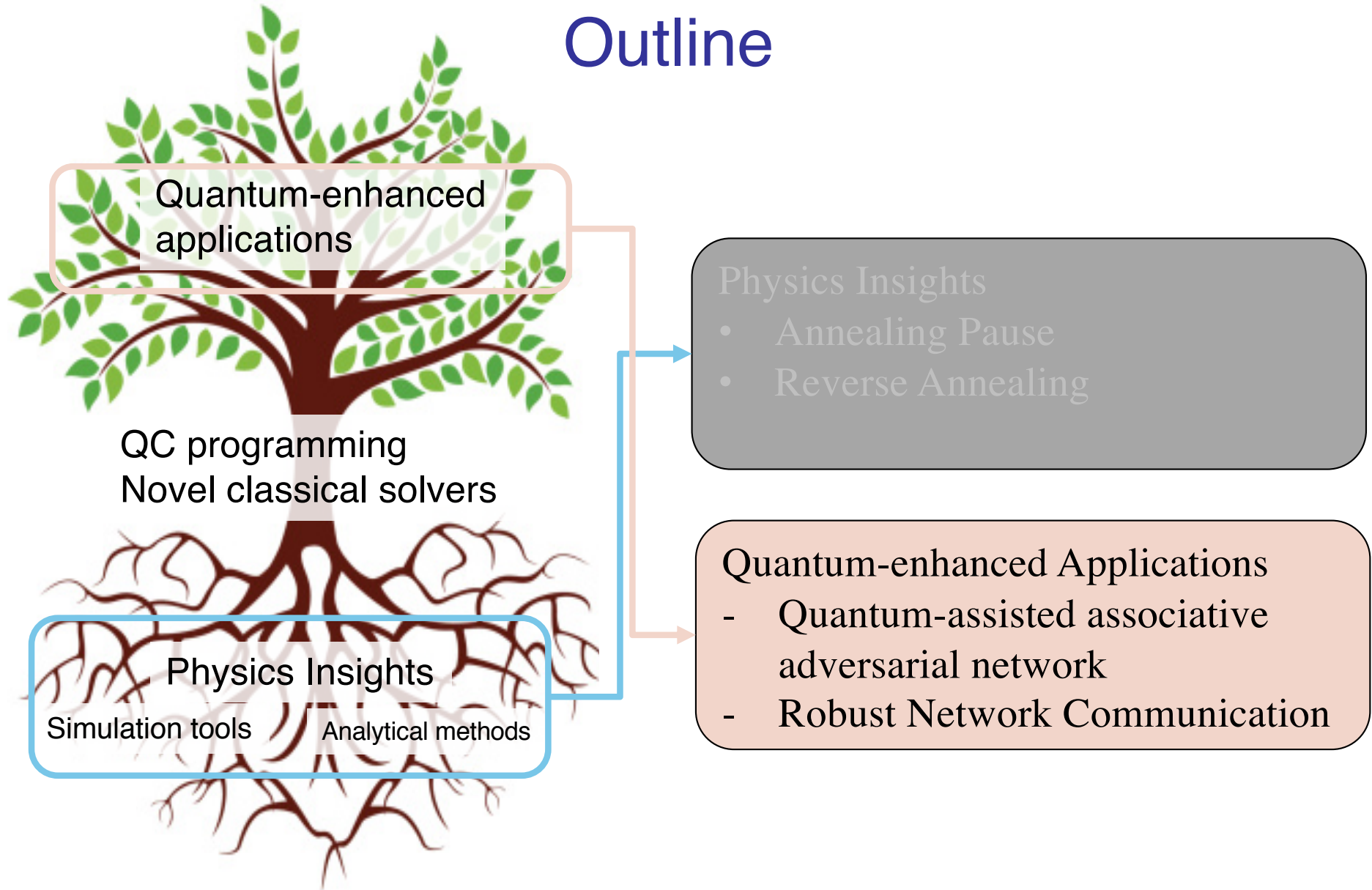
Performance on a single 12-qubit for reverse annealing to point s_p , where a $100 \mu\text{s}$ pause. Dependence of average energy (above ground state) at end of the reverse anneal as a function of the pause location s_p .



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Quantum-assisted associative adversarial network (QAAAN)

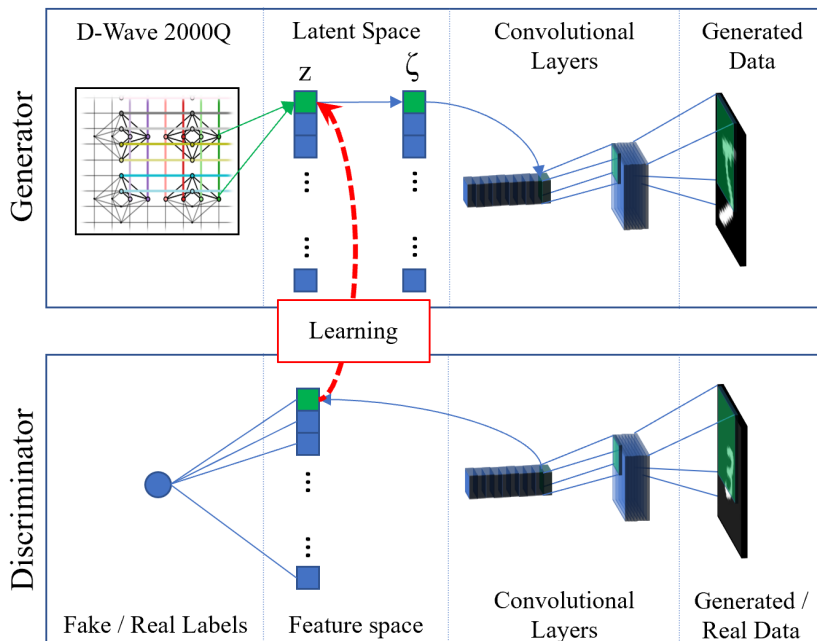
Framework to test potential advantages of quantum-assisted learning in Generative Adversarial Networks (GANs)

Novel algorithm for learning a latent variable generative model via generative adversarial learning

- incorporates Boltzmann sampling from a quantum annealer
- replaced canonical uniform noise input with samples from a graphical model
- graphical model learned by a Boltzmann machine encapsulates low-dimensional feature representation

Compared performance across three topologies (fully connected, symmetric bipartite, Chimera graph)

- QAAAN successfully learns generative model of MNIST dataset for all topologies
- Quantum and classical versions of the algorithm have equivalent performance



M Wilson, T Vandal, T Hogg, E Rieffel, Quantum-assisted associative adversarial network: Applying quantum annealing in deep learning. arXiv:1904.10573



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Robust Communication Network Design

Problem class: *Minimum Weighted Spanning Tree with degree constraints*

Cost function to minimize

$$C_{obj} = \sum_{p,v} w_{p,v} x_{p,v} \quad \text{where } x_{p,v} = 1 \text{ if } p \text{ parent of } v$$

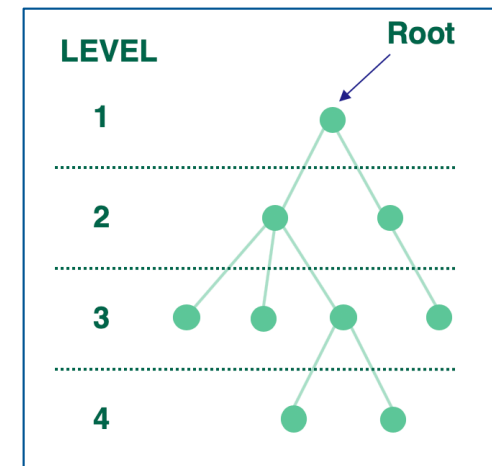
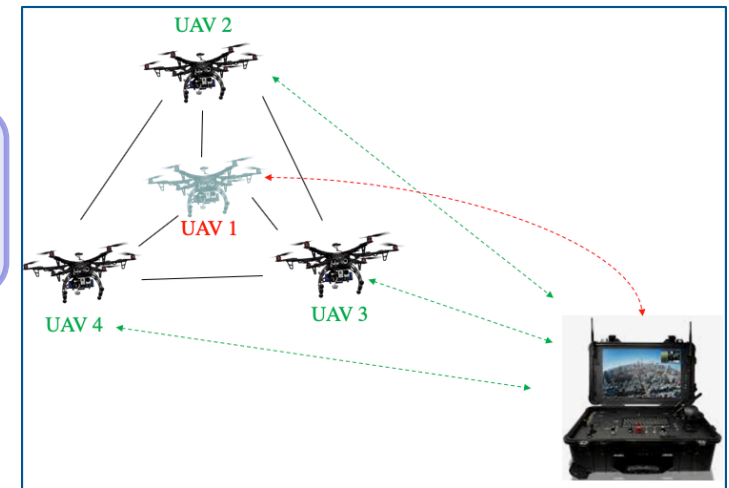
Constraints \longrightarrow Penalties

Every non-root node has one parent

Every node exists at one level

If p parent of v , p 's level is one less than v 's

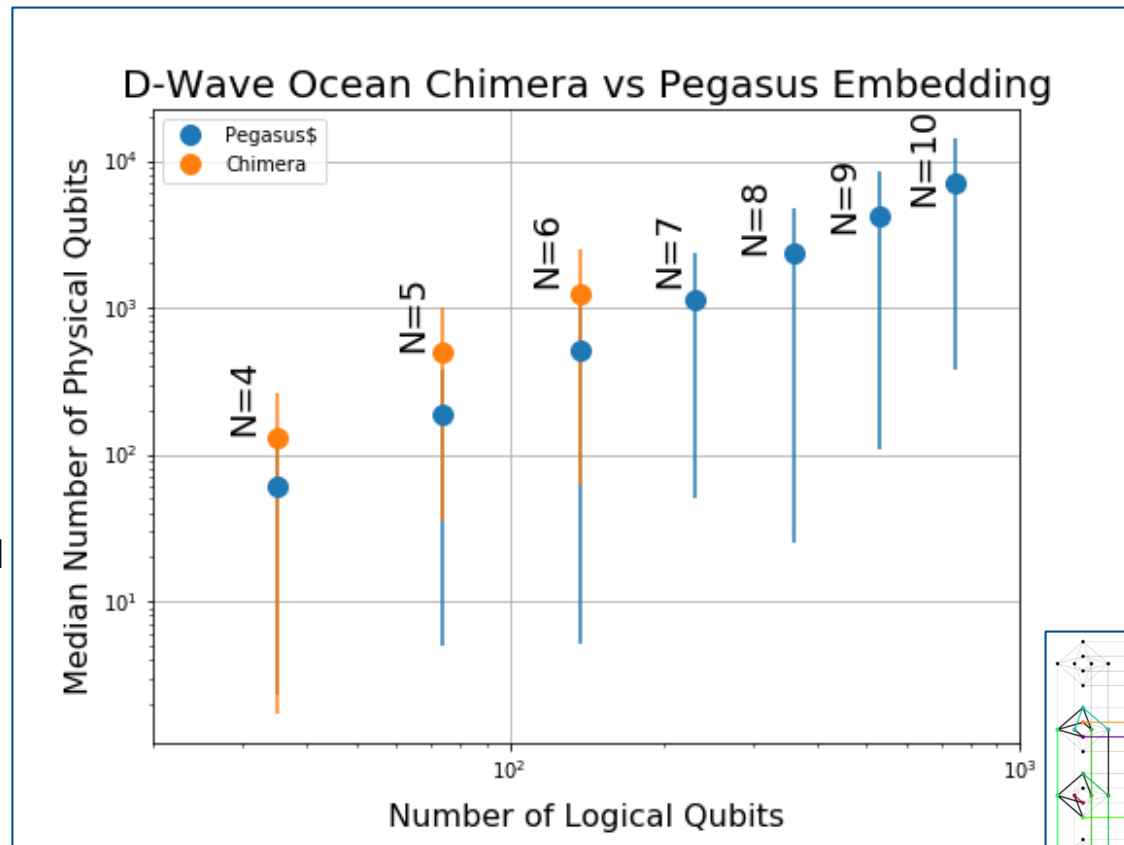
Maximum degree is Δ



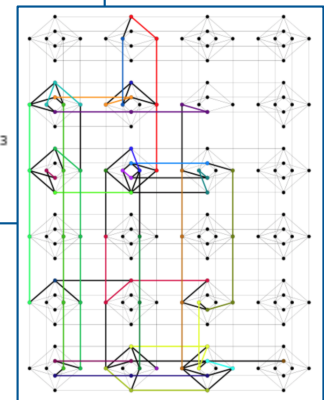


Chimera vs Pegasus Embedding

- Embedding for the fully connected network communication graph with default embedding parameters for N=4 through 10
- Chimera embedding performed with the SAPI2 find_embedding(...) routine with the D-Wave 2000Q hardware adjacency
- Pegasus embedding performed with the Ocean minorminer find_embedding(...) routine
- Pegasus reduces the embedding size by roughly a factor of 2 for this limited comparison



Median Physical Qubits as a function of the number of logical qubits with error bars at 35th and 65th percentiles



Sample Chimera embedding for N=4

Hybrid quantum-classic approaches needed to support real-world network communication applications

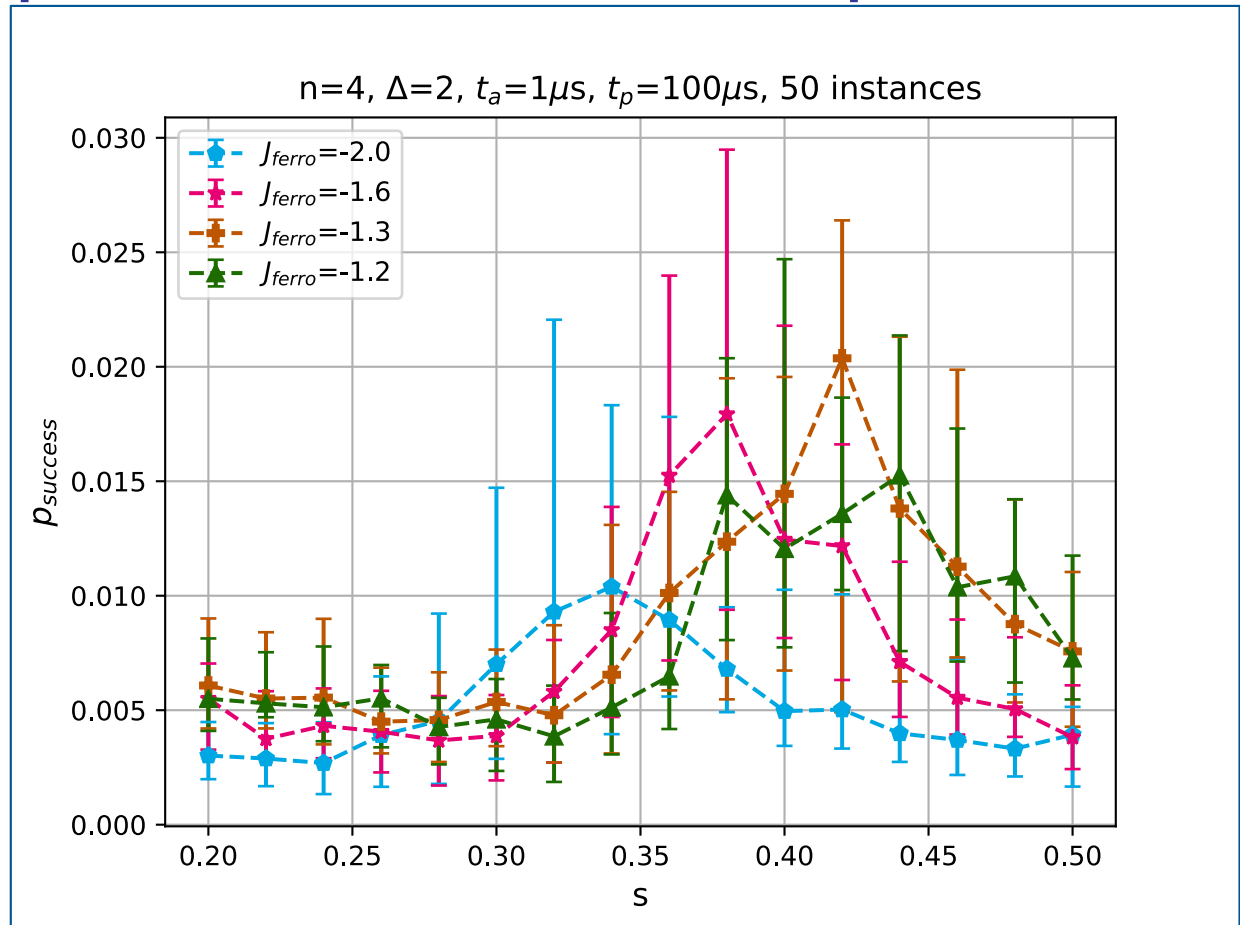


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Effectiveness of pause on embedded problems

- Factor of five improvement in the mean probability of success observed for 50, $N=4$ problem instances (20-35 variables; 50 – 125 qubits when embedded)
- Consistent pause location across instances
- Similar results for $N=5$ problems (not shown)



Median probability of success as a function of the annealing pause for 50 $N=4$ instances, 1 ms anneal, 50K reads. Pause location ranging from 0.2 to 0.5 and J_{ferro} from -1.2 to 2.0 (Error bars are at the 35th and 65th percentiles)

Open question: why is the effect less pronounced for embedded problems?



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Implications:

- Pausing during annealing can increase performance by orders of magnitude
- Improvement only occurs when the pause is within a particular region of the anneal schedule
- Analysis in terms of time-scales suggests the pause should occur in the region where $t_a < t_r < t_p$, well after the min gap

Future work:

- Deeper analysis on more classes of problems, incl. embedded problems
- A faster quench, if available, would enable examination of intermediate dists
- Develop further theory to understand subtler effects, including:
 - trends in optimal pause location with problem size, class, and pause time
 - predicting the effective temperature
- Further improvements with yet more schedule control?
- Any quantum advantage?



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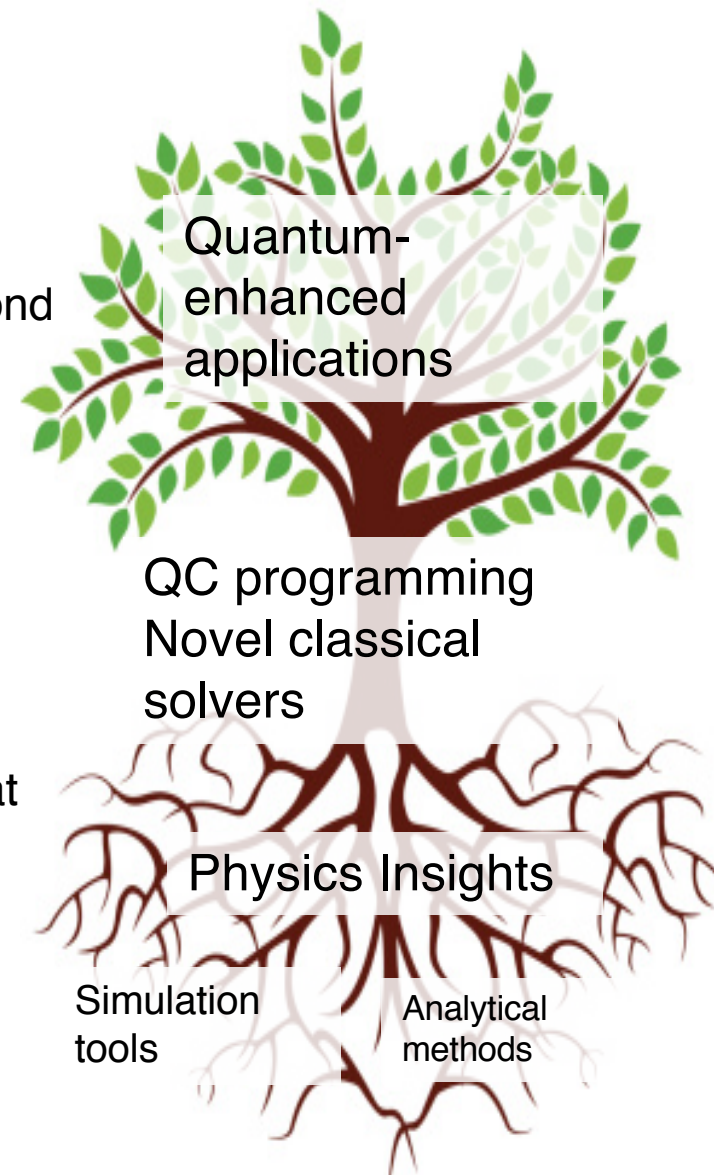
Take away points

Next year will be even more exciting!

- Emerging quantum hardware performing computations beyond the reach of even the largest supercomputers

Many open questions remain:

- When will scalable quantum computers be built, and how?
 - How quickly can special purpose quantum computing devices be built?
- How broad will the impact of quantum computation be? What will the ultimate impact of quantum heuristics be?
- How best to harness quantum effects for computational purposes?



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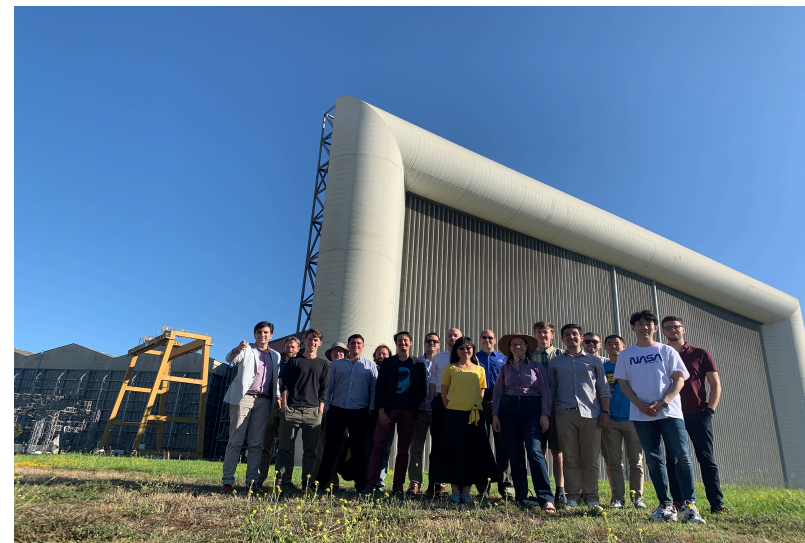


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Rupak Biswas, Zhang Jiang, Kostya Kechezhi, Sergey Knysh, Salvatore Mandrà, Bryan O'Gorman, Alejandro Perdomo-Ortiz, Andre Petukhov, John Realpe-Gómez, Eleanor Rieffel, Davide Venturelli, Fedir Vasko, Zhihui Wang, ***A NASA Perspective on Quantum Computing: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