Overview of NASA QuAIL team Research

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Quantum AI Lab. (QuAIL) at NASA Ames Research Center

NASA QuAIL team: Zhang Jiang, Kostyantyn Kechedzhi, Salvatore Mandrà, Alejandro Perdomo-Ortiz, Andre Petukhov, Davide Venturelli, Zhihui Wang

NASA Fellowship recipient: Bryan O'Gorman

We are hiring!

Funding support:

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QUANTUM
ENHANCED
OPTIMIZATION

Nov 8, 2017 **Langley Quantum Workshop**

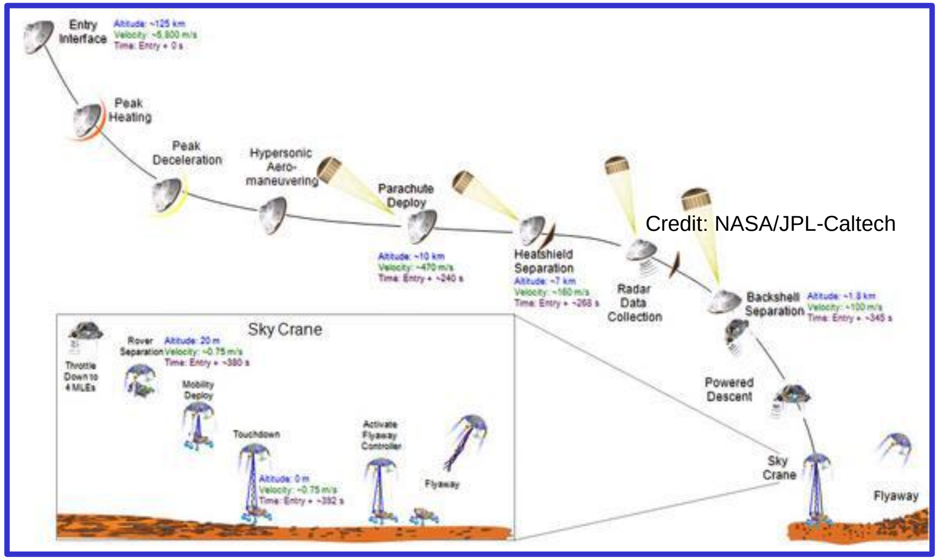
NASA : Centers & Facilities

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

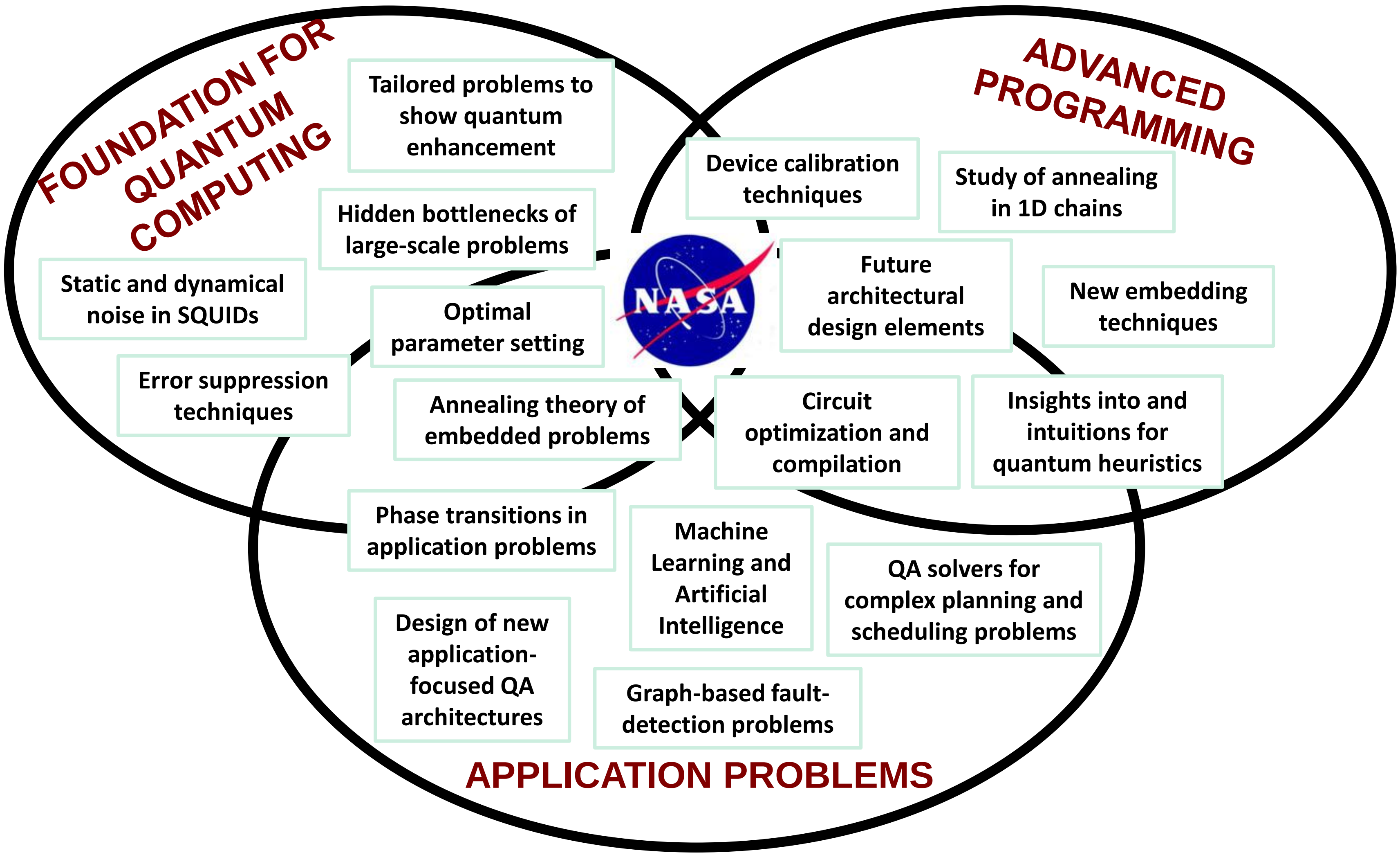


Credit: NASA/JPL-Caltech

Landing sequence for Mars rover Curiosity including "seven minutes of terror."

NASA's Pleiades is one of the top 20 fastest supercomputers in the world

NASA Quantum Research Approach



NASA QuAIL team focus

Long term

- Determine breadth of quantum computing applications
- Evaluate and utilize quantum hardware
  - Develop programming principles, compilation strategies
  - Characterize the hardware capabilities, noise
  - Determine how to harness quantum effects for computational purposes
- Explore potential QC applications of NASA relevance
  - Evaluate most promising near- and middle-term application directions

Ongoing efforts

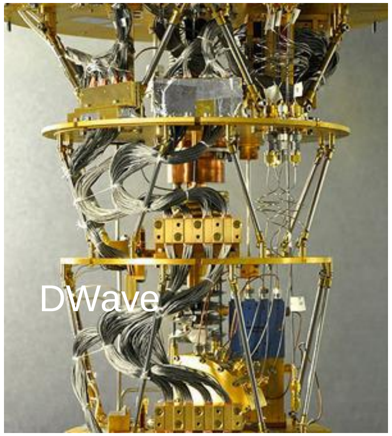
- Initial target: quantum annealing
  - Earliest quantum hardware available: D-Wave quantum annealers
  - Most prominent quantum heuristic
  - Widely applicable to optimization problems
  - Advantages unknown
- Near-term target: emerging quantum computing hardware
  - Small Universal QCs
  - More advanced QAs

Emerging quantum hardware

Special purpose

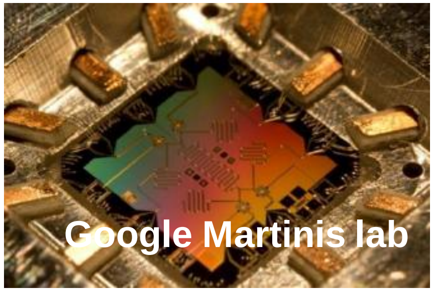
Quantum annealers

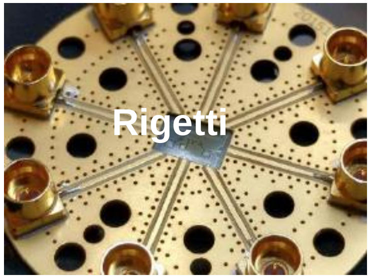
Run one type of quantum heuristic for optimization



General purpose

Universal quantum computers





Uses of emerging, but limited, quantum computational devices?

Currently too small to be useful for solving practical problems

(1) Quantum supremacy

(2) Develop intuitions for quantum heuristic algorithms

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

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

A handful of proven limitations on quantum computing

Conjecture: Quantum Heuristics will significantly broaden applications of quantum computing

Recent NASA Ames Gate-Model QC work

- Extended Framework for QAOA circuits
  - S. Hadfield et al., **From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz**, arXiv:1709.03489
- Analysis for problems with symmetry
  - Z. Jiang et al., **Near-optimal quantum circuit for Grover's unstructured search using a transverse field**, PRA 95 (6), 062317, 2017.
  - Z. Wang et al., **The Quantum Approximation Optimization Algorithm for MaxCut: A Fermionic View**, arXiv:1706.02998
- Compilation to emerging hardware architectures
  - D. Venturelli et al., **Compiling Quantum Circuits to Realistic Hardware Architectures using Temporal Planners**, arXiv:1705.08927
- Quantum supremacy (joint with Google)
  - C. Neill et al., **A blueprint for demonstrating quantum supremacy with superconducting qubits**, arXiv:1709.06678
  - S. Boixo et al., **Characterizing quantum supremacy in near-term devices**, arXiv:1608.00263
- Quantum simulation (joint with Google)
  - J. R. McClean et al., OpenFermion: **The Electronic Structure Package for Quantum Computers**, arXiv:1710.07629

Quantum Alternating Operator Ansatz

Based on the Quantum Approximate Optimization Algorithm

- A gate model heuristic due to Farhi et al.
- Iterates between two Hamiltonians, p times
  - Phase separation (encodes cost function)
  - Mixing

Early results by Farhi and co-authors

- p → ∞: from AQO
  - Converges to optimum for p → ∞
- p = 1: from IQP circuits
  - Provably hard to sample output efficiently classically (up to standard complexity theory conjectures)
  - Beat existing classical approximation ratio on MaxE3Lin2 only to inspire a better classical algorithm

Our Quantum Alternating Operator Ansatz

- Allows more general mixing operators, providing massive improvements in implementability
- Supports broader class of optimization problems having a mix of hard and soft constraings
- Reworked QAOA acronym to support applications to exact optimization and sampling as well as approximate optimization

- Mapped 20+ problems to QAOA formalism

S. Hadfield et al., **From the Quantum Approximate Optimization Algorithm to a Quantum Alternating Operator Ansatz**, arXiv:1709.03489

Parameter setting for QAOA

How hard is it to find good parameters for QAOA?

- Success of QAOA framework will largely depend on this question

For fixed p**, search for optimal parameters poly in** n**, the number of variables**

Exhaustive search quickly becomes inefficient; curse of dimensionality

How complicated is the parameter space?

Explored parameter setting for Maxcut on the ring (arXiv:1706.02998)

QAOA circuit for Grover's problem recovers root N query complexity

- First QAOA result for p>> 1

Strong relation between parameter setting in QAOA and in VQE

Future work

Are there identifiable properties of the evolution that correlate with success

Explore the use of measurement in the course of the algorithm to aid in setting parameters for the next steps

Characterize the parameter space and properties that determine the difficultly of the search for good parameters

Improved classical-quantum loop for parameter setting

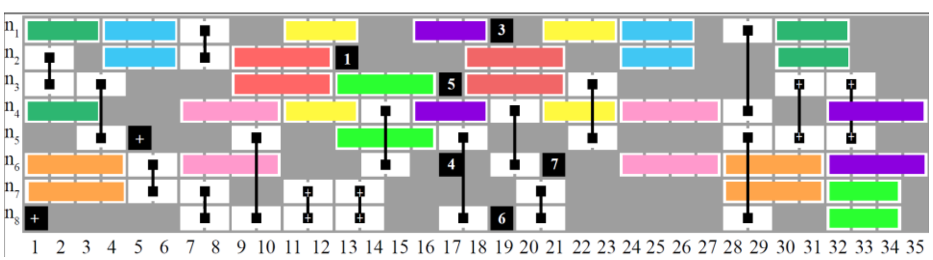
Compilation to realistic hardware

Applied temporal planning to quantum circuit compilation

Initial experiments focused on

- **QAOA circuits for Maxcut because of their high number of commuting gates**
- **A hardware architecture proposed by Rigetti - gates were available between neighboring qubits varied**

Mapped circuit compilation problem to a temporal planning problem, and ran several state-of-the-art temporal planners compile

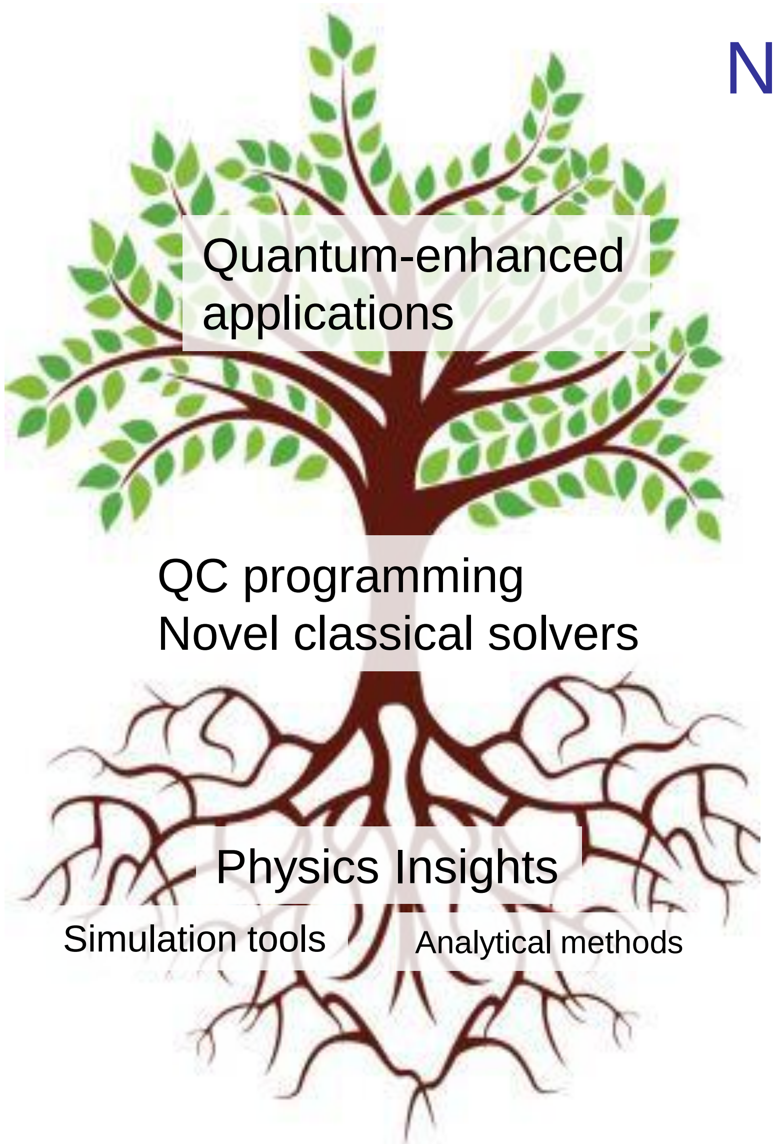


Demonstrated temporal planning is a viable approach to circuit compilation

Future work

- **Map circuit compilation to other formalisms to run state-of-the-art solvers, determining relative advantages of the different approaches**
- **Use insights gained to develop our own compilation approach taking the best properties of existing solvers**
- **Explore different initial starting states, and starting state setting algorithms**
- **Compile more general circuits**
- **Complex hardware requirements, noise tradeoffs and crosstalk**
- **Objectives beyond makespan**

NASA quantum annealing efforts



Biswas, et al. Parallel Computing (2016) – perspective article

Application focus areas

- **Planning and scheduling**
- **Fault Diagnosis**
- **Machine Learning**

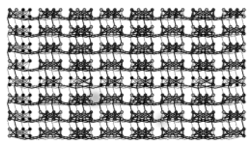
Outcomes from application investigations

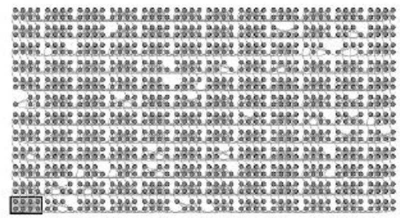
- **Future QA architectural design elements**
- **Programming and parameter setting**
- **Hybrid quantum-classical approaches**

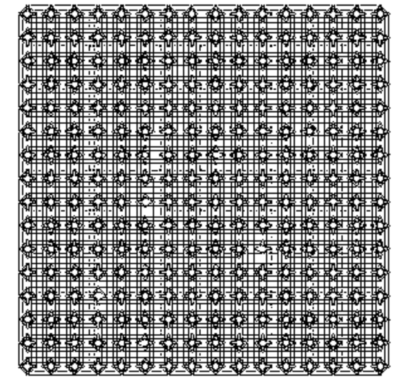
Application-specific and general classical solvers

Physical insights into and intuitions for QA

Upgrade from *Vesuvius* to *Washington* to *Whistler*

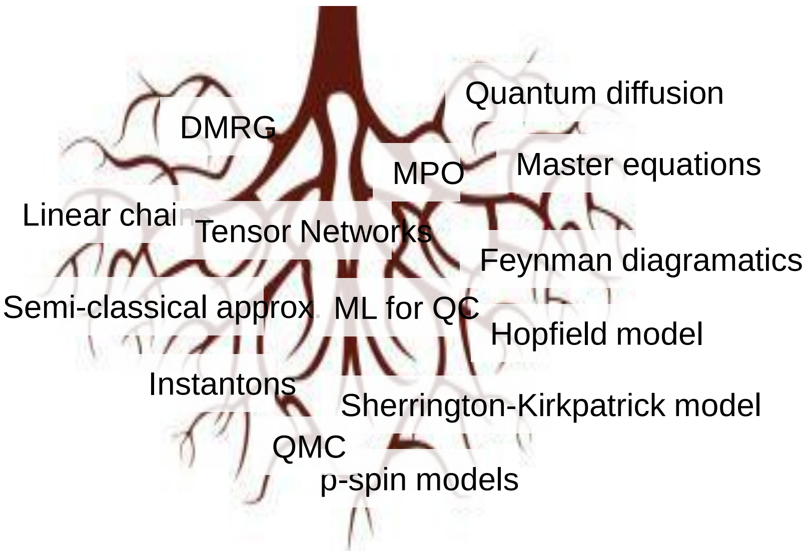




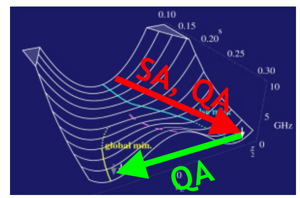


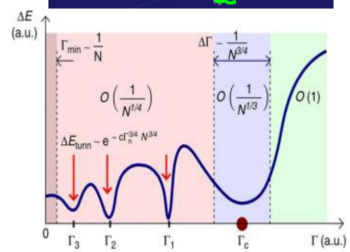
D-Wave Two™	D-Wave 2X™	D-Wave 2000Q™
512 (8x8x8) qubits "Vesuvius"	**1152** (8x12x12) qubit "Washington"	**2048** (8x16x16) qubit "Whistler"
509 qubits working – 95% yield	**1097** qubits working – 95% yield	**2038** qubits working – 97% yield
1472 *J* programmable couplers	**3360** *J* programmable couplers	**6016** *J* programmable couplers
20 mK max operating temperature (**18 mK** nominal)	15 mK Max operating temperature (**13 mK** nominal)	15 mK Max operating temperature (nominal to be measured)
5% and 3.5% precision level for *h* and *J*	3.5% and 2% precision level for *h* and *J*	*To be measured.*
Annealing time **20 μs**	Annealing time improved 4x (**5μs**)	Annealing time improved 5x (**1μs**) Initial programming time improved 20% (**9 ms**). **New anneal offset, pause and quench features.**

Analytical and numerical tools and expertise



Physics insights into QA algorithms





Kechedzhi, et al., PRX 6, 021028 (2016)

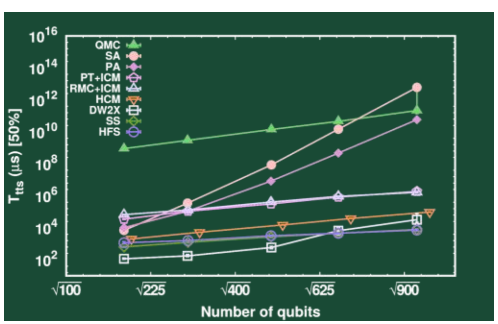
Knysh. Nat. Comm 7,12370 (2016)

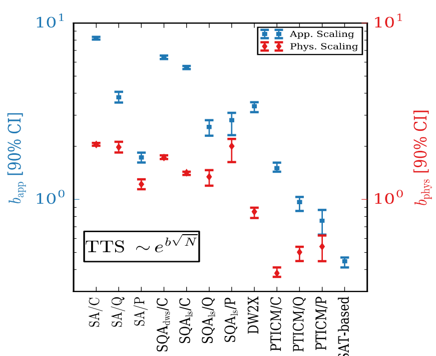
Smelyanskiy, et al. PRL 118, 066802 (2017)

Jiang, et al. PRA 95, 012322 (2017)

Jiang, et al. arXiv:1708.07117 (2017)

Benchmarking QA resources and architectures





Venturelli, et al. PRX 5, 031040 (2015)

Mandrà, et al. PRA 94, 022337 (2016)

Mandrà, et al. Quantum Sci. Tech. 2, 3 (2017)

Mandrà, et al. PRL, 118, 070502 (2017)

Perdomo-Ortiz, et al. arXiv:1708.09780 (2017)

How to **verify** quantum speed-up?

- Any claims of quantum speed-up must be compared to best classical algorithms

- Quantum speed-up can be classified as [1]:
  - Provable quantum speed-up
  - Strong quantum speed-up
  - Potential quantum speed-up
  - Limited quantum speed-up
    - Non-tailored quantum speed-up
    - Tailored quantum speed-up

Theoretical approach

Numerical approach

[1] S. Mandrà, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H.G. Katzgraber, PRE (2016)

State-of-the-art classical algorithms

Open-boundary QMC [1]
Population Annealing [2] (PA)
Isoenergetic Cluster Method [3] (ICM)
Hybrid Cluster Method [4] (HCM)
Hamze-de Freitas-Selby [5] (HFS)
Super-Spin [6] (SS)

Increasingly Tailored

[1] Z. Jiang, V. Smelyanskiy, S. Boixo & H. Neven, In preparation (2017)
[2] J. Machta, PRE (2010) - W. Wang, J. Machta & H.G. Katzgraber, PRE (2015)
[3] Z. Zhu, A.J. Ochoa & H.G. Katzgraber, PRL (2015)
[4] D. Venturelli, S. Mandrà, S. Knysh, B. O’Gorman, R. Biswas & V. Smelyanskiy, PRX (2015)
[5] F. Hamze & N. de Freitas, Proceeding (2004) - A. Selby, arXiv (2014)
[6] S. Mandrà, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H.G. Katzgraber, PRE (2016)

State-of-the-art classical algorithms

Open-boundary QMC [1]

Populati... g [2] (PA)

Is... ethod [3] (ICM...

...ybrid Cluster M...

H... [5] (HFS)

Super-Spin [6] (SS)

Incre... ailored

Many others are coming!

Comparison with application specific algorithms also important

[1] Z. Jiang, V. Smelyanskiy, S. Boixo & H. Neven, In preparation (2017)

[2] J. Machta, PRE (2010) - W. Wang, J. Machta & H.G. Katzgraber, PRE (2015)

[3] Z. Zhu, A.J. Ochoa & H.G. Katzgraber, PRL (2015)

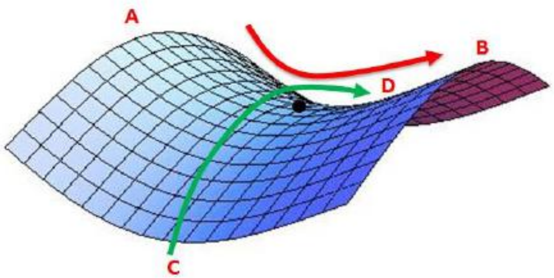
[4] D. Venturelli, S. Mandrà, S. Knysh, B. O'Gorman, R. Biswas & V. Smelyanskiy, PRX (2015)

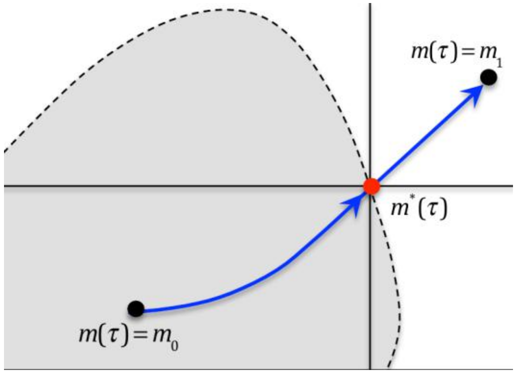
[5] F. Hamze & N. de Freitas, Proceeding (2004) - A. Selby, arXiv (2014)

[6] S. Mandrà, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H.G. Katzgraber, PRE (2016)

Scaling Equivalence of QMC and QA (Stoquastic)

The saddle point of the QMC Hamiltonian is an instanton in the order parameter space





The exponential scaling of the escape rate in QMC at a given temperature is equal to the tunneling rate in QA

S. Isakov, G. Mazzola, V. Smelyanskiy, Z. Jiang, S. Boixo, H. Neven, M. Troyer, "Understanding Quantum Tunneling through Quantum Monte Carlo Simulations", Phys. Rev. Lett. 117, 180402, (2016)

Z. Jiang, V. Smelyanskiy, S. Isakov, S. Boixo, G. Mazzola, M. Troyer, H. Neven, "Scaling Analysis and Instantons for Thermally-assisted Tunneling and Quantum Monte Carlo Simulations", Phys. Rev. A 95, 012322 (2017)

Open-Boundary QMC: A Better Classical Solver?

Open-boundary QMC is **immune** to the kind of topological obstructions that DWave considered in, for example

Andriyash and Amin, "Can quantum Monte Carlo simulate quantum annealing?" arXiv:1703.09277

Numerical results suggested that open-boundary QMC is **quadratically** faster than conventional QMC at an effective zero temperature regime.

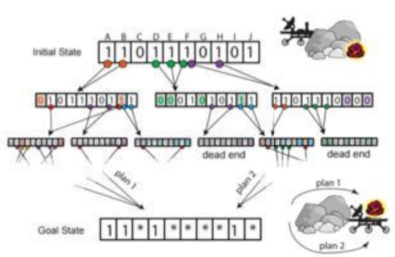
Conjecture: instanton in open-boundary QMC is a half of that in conventional QMC

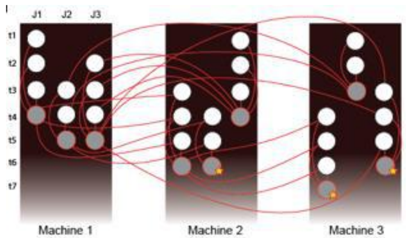
Recent analytical result: Actual situation is more complicated, though the conjecture remains useful in interpreting certain numerical results

Z. Jiang, V.N. Smelyanskiy, S. Boixo, H. Neven, Path-integral quantum Monte Carlo simulation with open-boundary conditions, PRA 96, 042330 (2017)

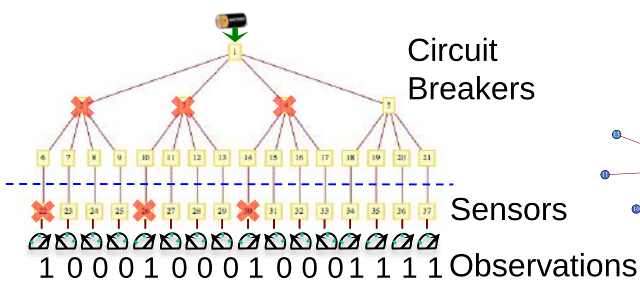
Current NASA Research in Annealing Applications

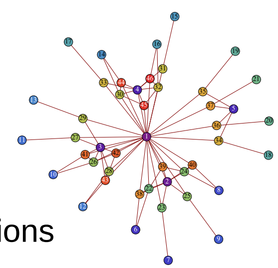
Complex Planning and Scheduling





Graph-based Fault Detection

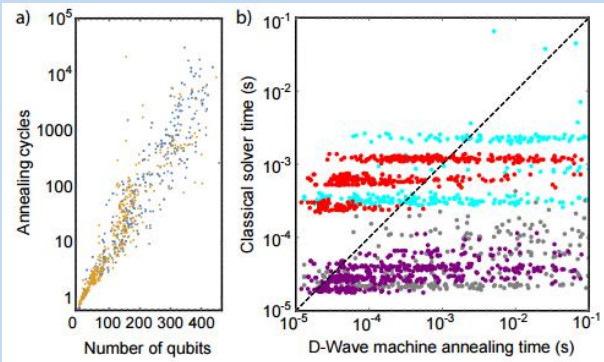


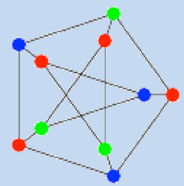


Machine Learning

- General **Planning Problems** (e.g., navigation, scheduling, asset allocation) can be solved on a quantum annealer (such as D-Wave)
- Developed a quantum solver for **Job Shop Scheduling** that pre-characterizes instance ensembles to design optimal embedding and run strategy – tested at small scale (6x6) but potentially could solve intractable problems (15x15) with 10x more qubits
- Analyzed simple graphs of **Electrical Power Networks** to find the most probable cause of multiple faults – easy and scalable QUBO mapping, but good parameter setting (e.g., gauge selection) key to finding optimal solution – now exploring digital circuit **Fault Diagnostics and V&V**
- **Boltzmann sampling** commonly used in **Machine Learning**, particularly Deep Learning. Quantum computing has provable advantage for some sampling problems. Demonstrated learning when using a QA as a Boltzmann sampler.

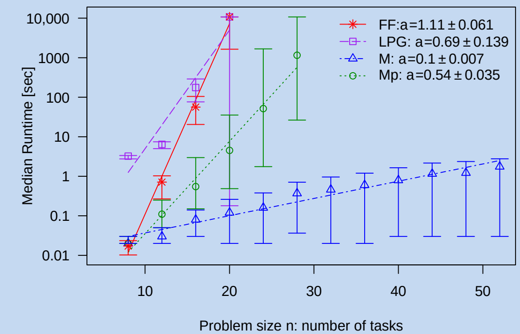
Scheduling Applications





Graph coloring

Comparison with state-of-the-art application-specific algorithms: current best planners



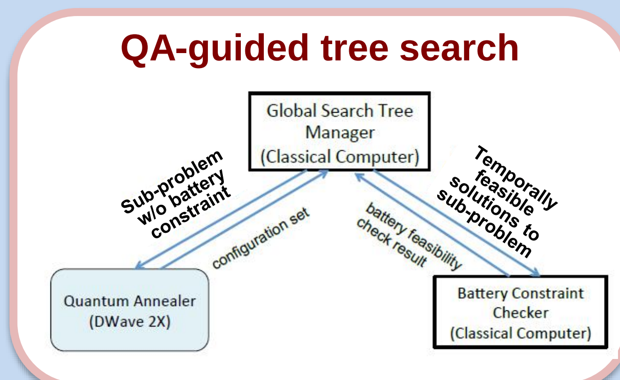
Eleanor G. Rieffel, Davide Venturelli, Minh Do, Itay Hen, Jeremy Frank, **Parametrized Families of Hard Planning Problems from Phase Transitions**, AAAI-14.
E. G. Rieffel, D. Venturelli, B. O'Gorman, M. B. Do, E. Prystay, V.N. Smelyanskiy, **A case study in programming a quantum annealer for hard operational planning problems**, Q. Information Processing, 14, (2014)

D-Wave run results: established baseline performance for QA on these applications

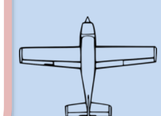
Solved problems with 6 machines and 6 jobs: analyzed scaling of tractability

Job-Shop scheduling: Complete quantum-classical solver framework with pre-processing, compilation/run strategies, decomposition methods

D. Venturelli, D. J.J. Marchand, G. Rojo, **Quantum Annealing Implementation of Job Shop Scheduling,** arXiv:1506.08479



Mars Lander activity scheduling



Airport runway scheduling

Scheduling problems as testbed for resource-bounded tailored embedding methods

- T. Tran, M. Do, E. Rieffel, J. Frank, Z. Wang, B. O'Gorman, D. Venturelli, J. Beck, **A Hybrid *Quantum-Classical Approach to Solving Scheduling Problems***, SOCS'16
- T. Tran, Z. Wang, M. Do, E. Rieffel, J. Frank, B. O'Gorman, D. Venturelli, J. Beck, ***Explorations of Quantum-Classical Approaches to Scheduling a Mars Lander Activity Problem***, Workshops AAAI'16

National Aeronautics and Space Administration

Ames
Discovery Innovations Solutions

Fault Diagnosis

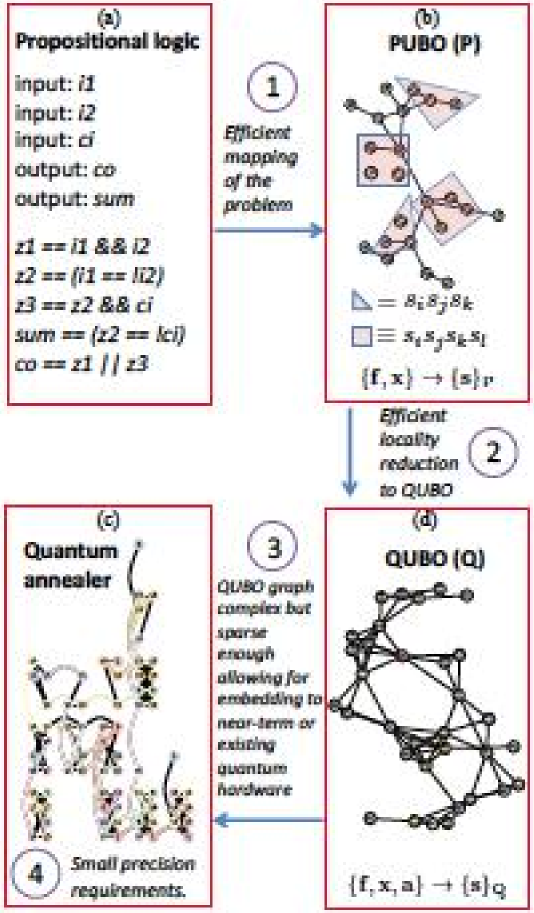
First comprehensive study addressing the readiness of quantum annealing for real-worls applications

Six different algorithms (SA, PT-ICM, QMC, SAFARI, SAT-based, and DWave2X)

In all three problem Hamiltonian representations (PUBO, QUBO, Chimera)

Addressed future quantum annealer design for quantum advantage in applications with practical relevance

- **What is the impact of higher-order terms?**
- **Need for non-stoquastic Hamiltonians?**
- **Impact of connectivity? …**



parc A Xerox Company · QC WARE · Fraunhofer IOSB-INA

A. Perdomo-Ortiz et al., **On the readiness of quantum optimization machines for industrial applications** arXiv:1708.09780

A near-term approach for quantum-enhanced machine learning

Our approach: Hybrid approaches for generative modeling in unsupervised machine learning.

Lesson: **Cope with hardware constraints**

PREDICTIONS

$\mathcal{F}[\,P(\mathbf{s}|\Theta^t)\,]$

LEARNING

Stochastic gradient descent

$\Theta^{t+1} = \Theta^t + \mathcal{G}[\,P(\mathbf{s}|\Theta^t)\,]$

DATA

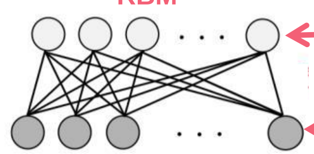
$\mathbf{s} = \{s^1, \ldots, s^D\}$

HARD TO COMPUTE

Estimation assisted by sampling from quantum computer

Ex.: Restricted Boltzmann Machines (RBM)

RBM



Computationally bottleneck

$$\langle v_i u_j \rangle_{p(\mathbf{v},\mathbf{u})}$$

Where,

$$p(\mathbf{v},\mathbf{u}) = \frac{e^{-E(\mathbf{v},\mathbf{u}|\theta)/T_{\mathrm{eff}}}}{Z(\theta)}$$

Widely used in **unsupervised** learning

Challenges solved:

Benedetti, et al. **Estimation of effective temperatures** in quantum annealers for sampling applications: A case study with possible applications in deep learning. **PRA 94, 022308** (2016).

Benedetti, et al. Quantum-assisted learning of **hardware-embedded** probabilistic graphical models. **arXiv:1609.02542** (2016). PRX (accepted).

Benedetti, et al. Quantum-assisted Helmholtz machines: A quantum-classical deep learning framework for **industrial datasets in near-term devices**. **arXiv:1708.09784** (2017).

Perdomo-Ortiz, et al. **Opportunities and Challenges** in Quantum-Assisted Machine Learning in Near-term Quantum Computer. **arXiv:1708.09757**. (2017). Invited article to special QST issue.

Newly funded effort in aeronautics

Assure the **availability** of the UAS Traffic Management (UTM) network against communication disruptions

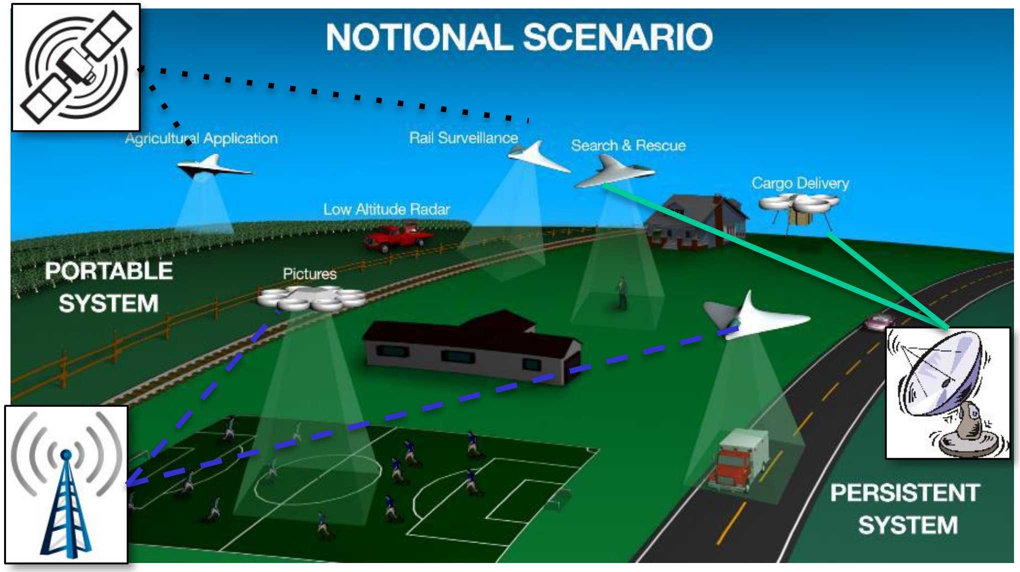
Future

- Higher vehicle density
- Heterogeneous air vehicles
- Mixed equipage
- Greater autonomy
- More vulnerability to communications disruptions

Apply quantum technologies to

- Robust network design
- Track and locate of a moving jammer
- Secure communication of codes supporting anti-jamming protocols

Joint with NASA Glenn, who are working on QKD for spread spectrum codes



Kopardekar, P., Rios, J., et. al., *Unmanned Aircraft System Traffic Management (UTM) Concept of Operations, DASC 2016*

30 month effort: harness the power of quantum computing and communication to address the cybersecurity challenge of availability

THANK YOU FOR YOUR ATTENTION

NASA Ames Research Center

We are hiring!

Opportunities at NASA Quantum AI Lab. (NASA QuAIL)

internships, early career, research scientist

https://usracareers.silkroad.com/
Tracking Code: 629-640

For details, please contact:
Eleanor Rieffel: NASA QuAIL Lead,
eleanor.rieffel@nasa.gov

The End

Selected NASA QuAIL recent pubs and e-prints (1/3)

2017

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