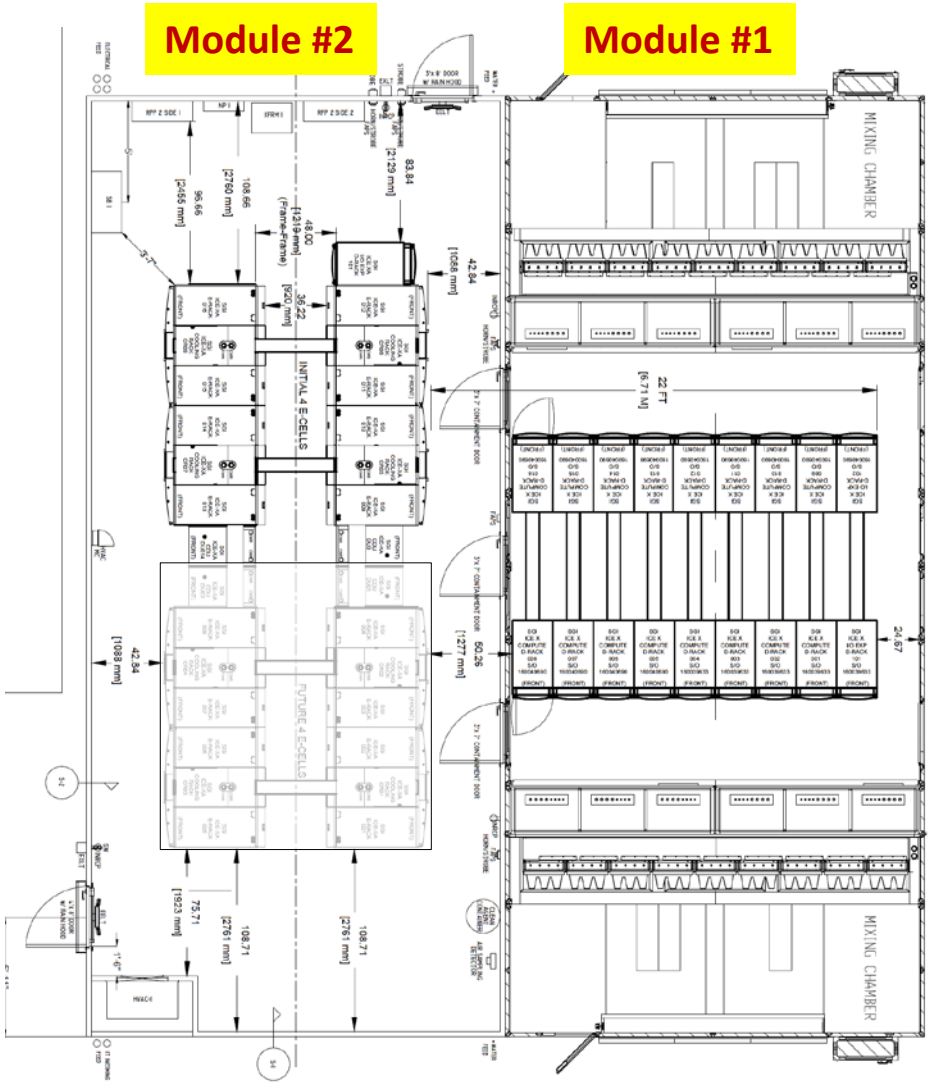
Phase 2: Expand Current MSF



- Facility advances allow more power to 2nd module (from 500 KW to 1.2 MW)
- Doubled compute rack density
  - Electra added 4 E-Cells of ICE-XA with Intel Skylake (total 4.78 PF peak; 369 TB memory)

NASA Earth Exchange (NEX)

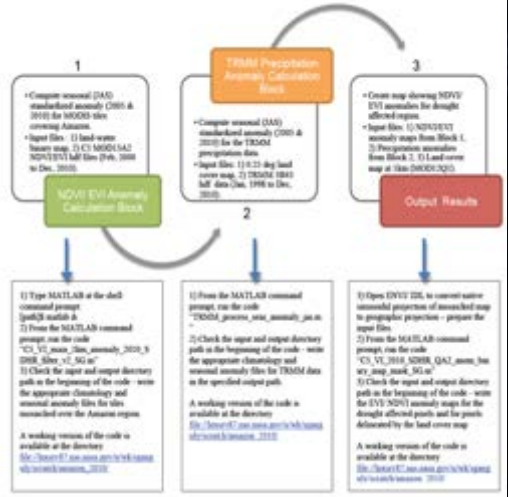
A virtual collaborative environment that brings scientists and researchers together in a knowledge-based social network along with observational data, necessary tools, and computing power to provide transparency and accelerate innovation: **Science-as-a-Service**

VIRTUAL COLLABORATION

Over 650 members

CENTRALIZED DATA REPOSITORY

Over 3.5 PB of observational data



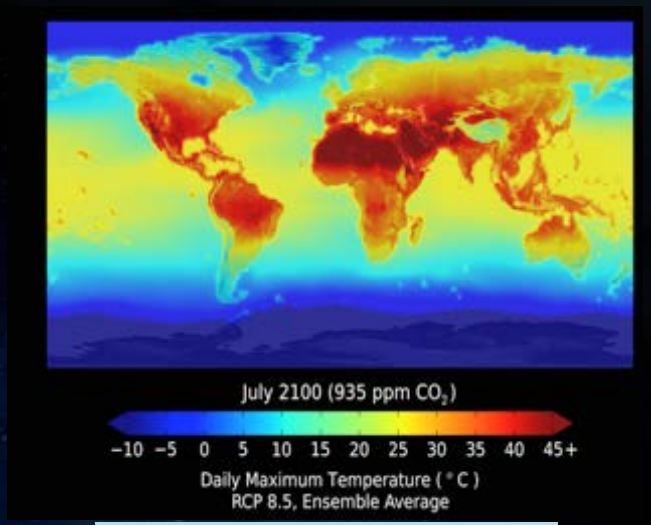
SCALABLE COMPUTING

Heterogeneous and remote, secure access

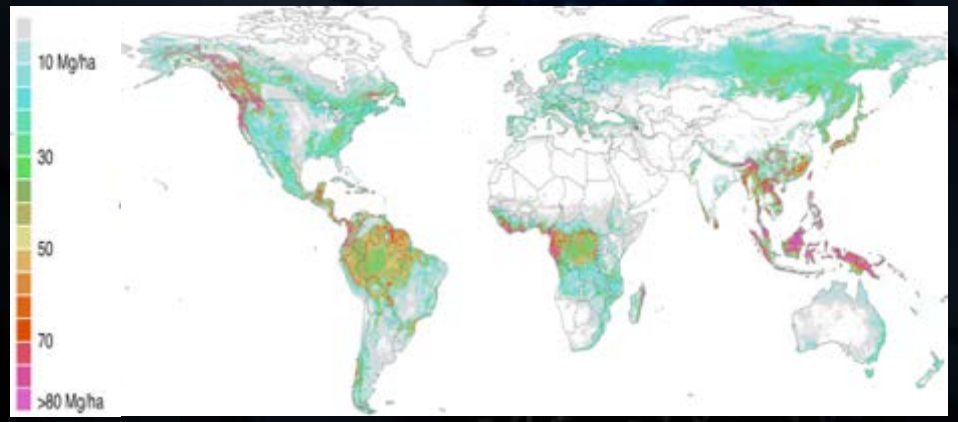
KNOWLEDGE

Workflows, virtual machine images, model codes, and reusable software

Science via NEX



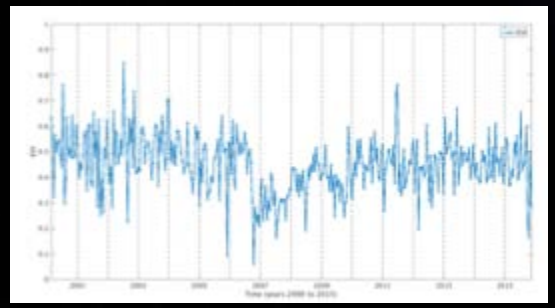
High-resolution projections for climate impact studies

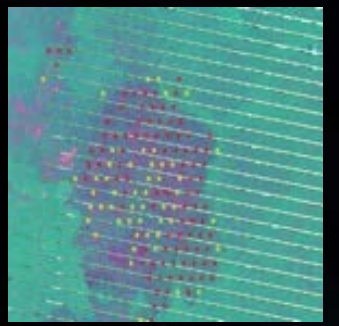


Global vegetation biomass at 100m resolution by blending data from 4 different satellites

High-resolution monthly global data for monitoring crops, forests, and water resources

Sample publication using NEX environment:
Nature 532.7599 (2016): 357

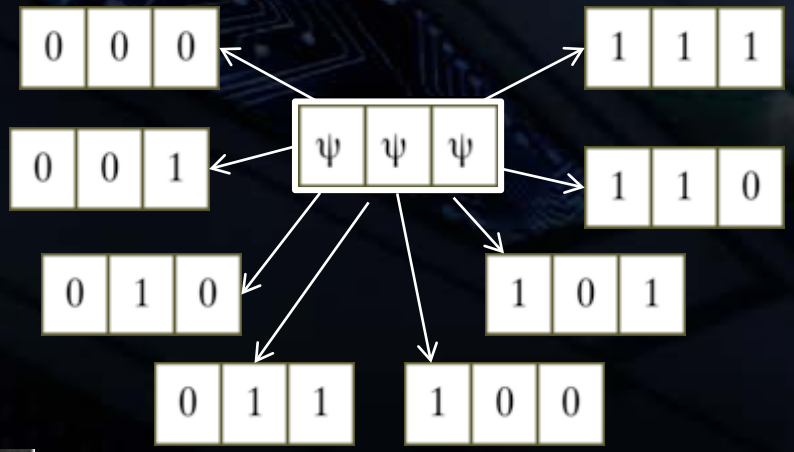




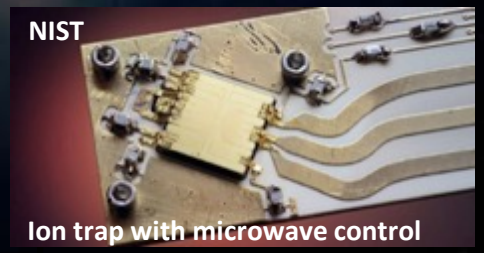
Machine learning and data mining – moving toward data-driven approaches

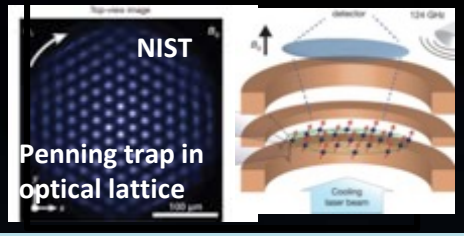
Quantum Computing 101

- Quantum mechanics deals with physical phenomena at very small scales (~100nm) and at very low temperatures (few K) where actions are quantized
- The outcome of a quantum experiment is probabilistically associated both with what was done before the measurement and how the measurement was conducted
- Qubits (quantum bits) can exist in a superposition of states, allowing *n* qubits to represent 2^n states simultaneously
- At the end of a computation, on measurement, the system collapses to a classical state and returns only one bit string as a possible solution

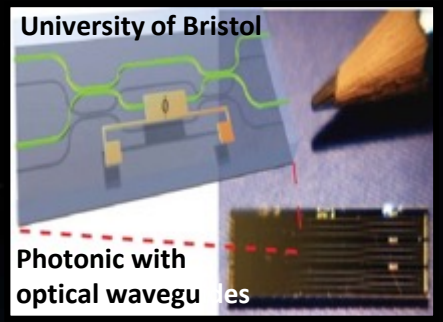


Numerous Implementations

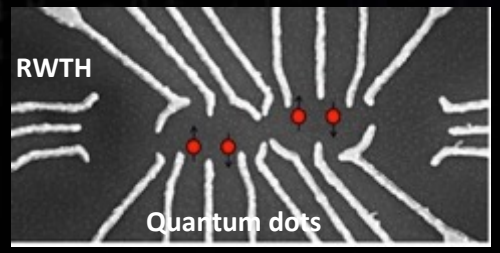


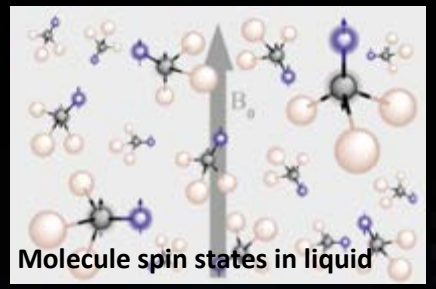


Trapped Ions and Neutral Atoms

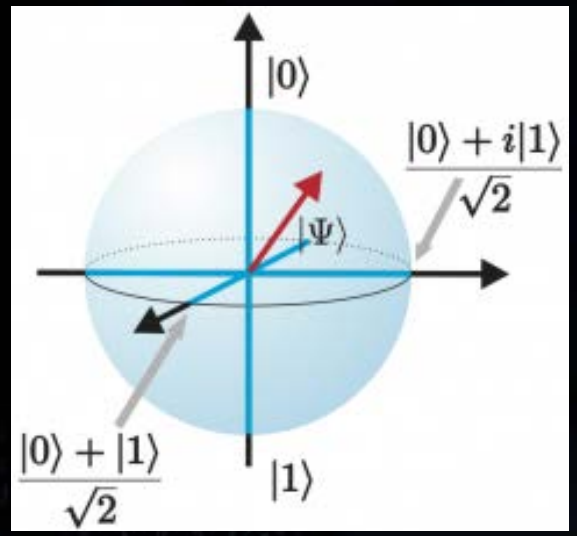


Photonic Quantum Chips



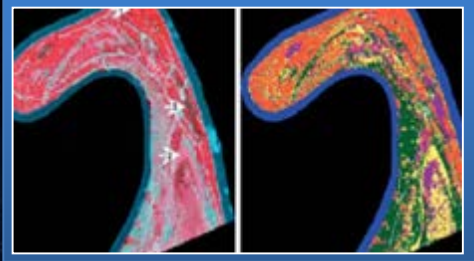


Nanoelectronics, NMR, Diamond Chips, etc.



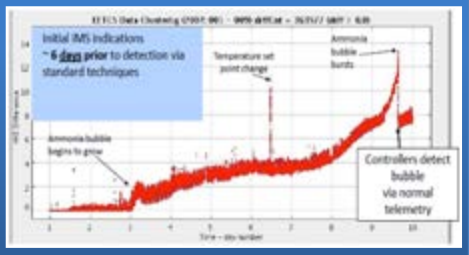
Quantum Computing for NASA Applications

Objective: Find "better" solution
- Faster
- More precise
- Not found by classical algorithm

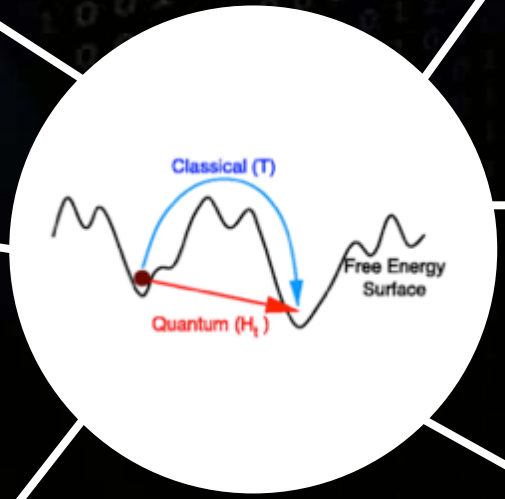


Data Analysis and Data Fusion

Anomaly Detection and Decision Making



Air Traffic Management



V&V and Optimal Sensor Placement

Mission Planning, Scheduling, and Coordination

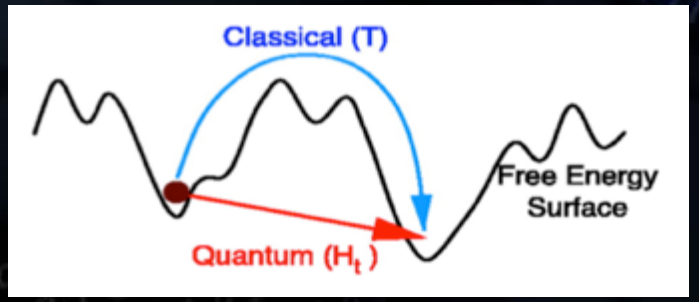
Topologically-aware Parallel Computing

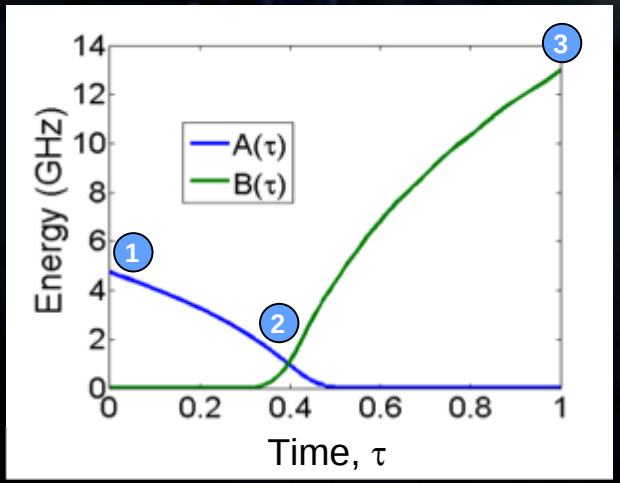
Common Feature: Intractable (NP-hard / NP-complete) problems!

Quantum Annealing

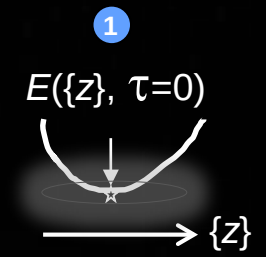
A physical technique to solve combinatorial optimization problems

$$E(z_1, z_2, \ldots z_n) = \underbrace{\left(1 - \frac{t}{T}\right) H_O(\{z\})}_{A(t)} + \underbrace{\frac{t}{T} H_P(\{z\})}_{B(t)}$$

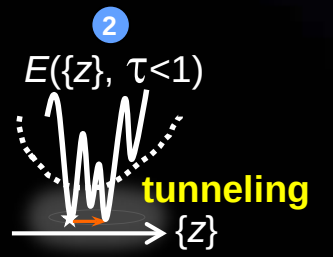




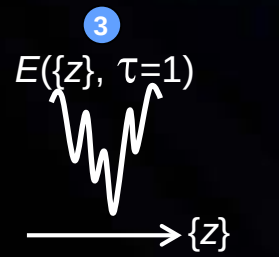
- *N*-bit string of unknown variables {*z*}
- H_0: Hamiltonian with known ground state
- H_P: Hamiltonian whose ground state represents solution to the problem
- Large *A(t)* responsible for quantum fluctuations slowly (adiabatically) lowered to zero while maintaining minimum energy of the system at all times
- In conjunction, cost function of interest *B(t)* gradually turned on
- Transitions between states occur via tunneling through barriers due to quantum fluctuations
- Solution is configuration {*z*} that produces minimum *E* with non-zero probability
- Method similar to simulated annealing where transitions between states occur via jumping over barriers due to thermal fluctuations



Initialize in an easy-to-prepare full quantum superposition



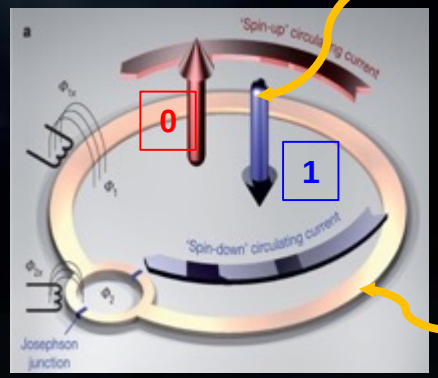
Quantum states explored by quantum tunneling

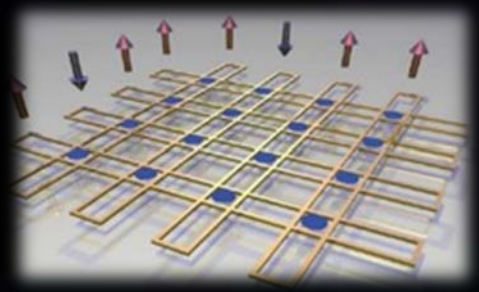


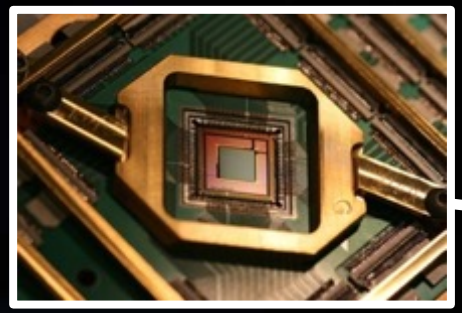
Final state a bit-string encoding solution with probability

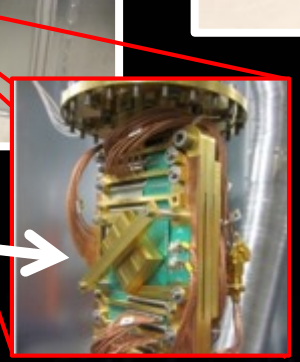
D-Wave System Hardware

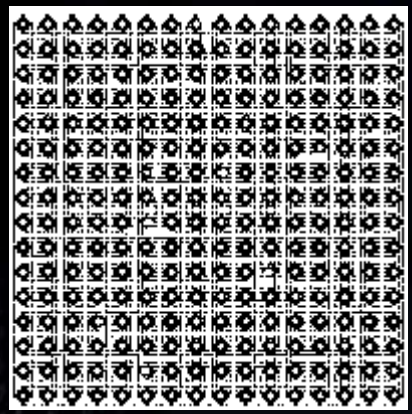
- Collaboration with Google and USRA via Space Act Agreement led to installation of system at NASA Ames in early 2013
- Started with 512-qubit Vesuvius processor – currently 2031-bit Whistler
- 10 kg of metal in vacuum at ~15 mK
- Magnetic shielding to 1 nanoTesla
- Protected from transient vibrations
- Single annealing typically 20 µs
- Typical run of 10K anneals (incl. reset & readout takes ~4 sec)
- Uses 15 kW of electrical power











Focus on solving discrete optimization problems using quantum annealing

Programming the D-Wave System

1 Map the target combinatorial optimization problem into QUBO

No general algorithms but smart mathematical tricks (penalty functions, locality reduction, etc.)

$$\alpha_{ijk} z_i z_j z_k$$

$$\alpha_{ijk}\, y_{ij} z_k + \beta_{ijk}(3y_{ij} - 2z_i y_{ij} - 2z_j y_{ij} + z_i z_j)$$

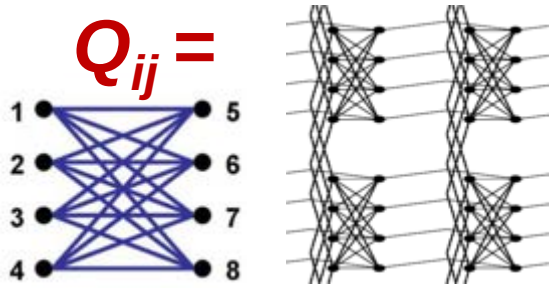
$$\sum_{ij} Q_{ij} z_i z_j \rightarrow \sum_i h_i s_i + \sum_{i,j} J_{ij} s_i s_j$$

Mapping not needed for random spin-glass models

2 Embed the QUBO coupling matrix in the hardware graph of interacting qubits

D-Wave qubit hardware connectivity is a Chimera graph, so embedding methods mostly based on heuristics

$Q_{ij} =$

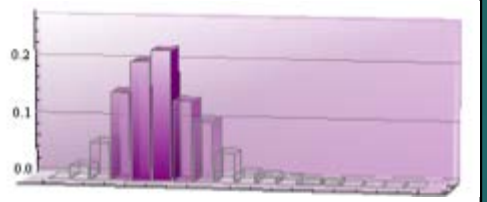


Embedding not needed for native Chimera problems

3 Run the problem several times and collect statistics

Use symmetries, permutations, and error correction to eliminate the systemic hardware errors and check the solutions

Probability

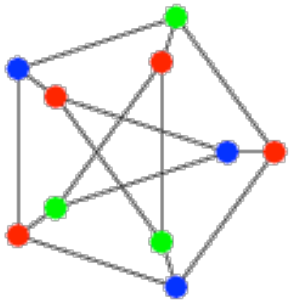


Solution's energy/cost

Performance can be improved dramatically with smart pre-/post-processing

Mapping to QUBO: Graph Coloring Example

Graph Coloring Problem:
Assign one of *k* colors to each vertex so that no two vertices sharing an edge have the same color



Binary variable:

$$x_{v,c} = \begin{cases} 1 & \text{vertex } v \text{ with color } c \\ 0 & \text{vertex } v \text{ not with color } c \end{cases}$$

Violation of requirements encoded as cost:

- (1) unique assignment: Each vertex v must be assigned exactly one color:

$$H_v^{(unique)} = (\sum_{c \in C} x_{v,c} - 1)^2 \Leftarrow \sum_{c \in C} x_{v,c} = 1$$

Costing cases

(1) No color or Multi-colored

- (2) Connected vertices cannot use the same color

(2) Same color for connected vertices

$$H_{v,v',c}^{(exclude)} = x_{v,c}x_{v',c} \text{ if } vv' \in E$$

Final QUBO form:

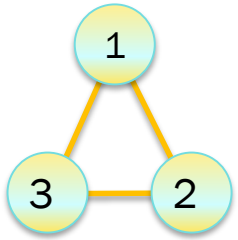
$$H = \sum_v H_v^{(unique)} + \sum_{v,v' \in E} \sum_c H_{v,v',c}^{(exclude)}$$

H = 0 corresponds to a valid coloring

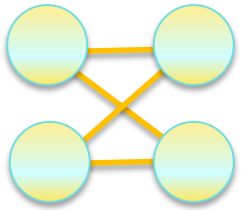
Embedding the QUBO

Embed a triangle onto a bipartite graph

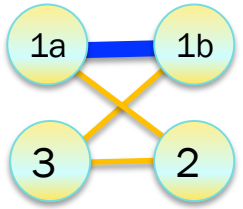
original QUBO



hardware connectivity



QUBO embedded



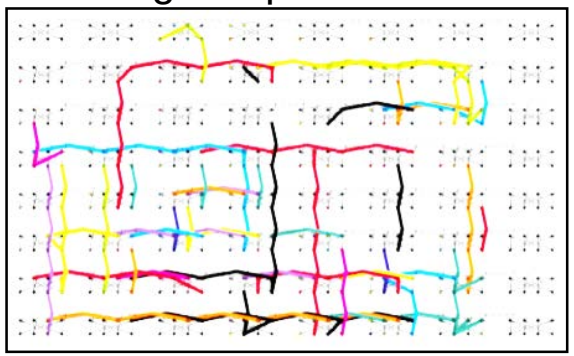
$$H_0 = J_{12}x_1x_2 + J_{23}x_2x_3 + J_{13}x_1x_3$$

$$H_1 = J_{12}x_{1a}x_2 + J_{23}x_2x_3 + J_{13}x_{1b}x_3 + J_{\text{Ferro}}x_{1a}x_{1b}$$

Strong, but not too strong, ferromagnetic coupling between physical qubits x_{1a} and x_{1b} encourages them to take the same value, thus acting as a single logical qubit x_1

Embedding a realistic problem instance:

Physical qubits on each colored path represent one logical qubit

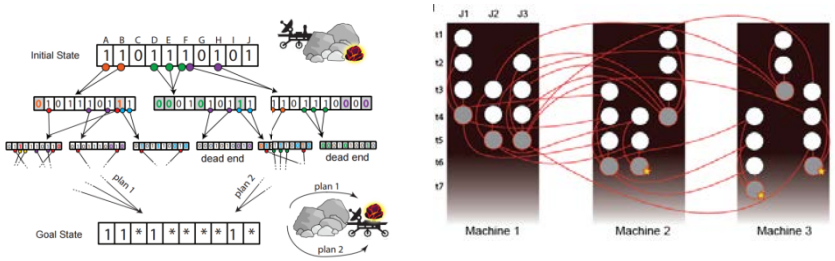


H_0 and H_1 have the same ground state but the energy landscape of the search space differs

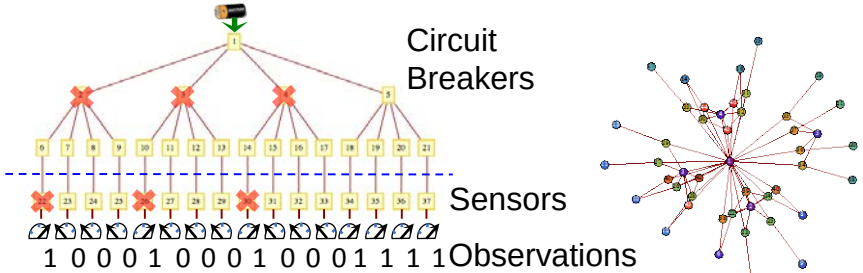
Current research investigation: How best to set the magnitude of these “strong” couplings to maximize probability of success

Other NASA Research in Applications

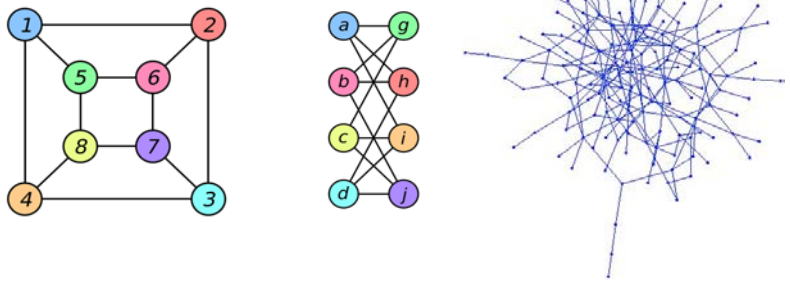
Complex Planning and Scheduling



Graph-based Fault Detection



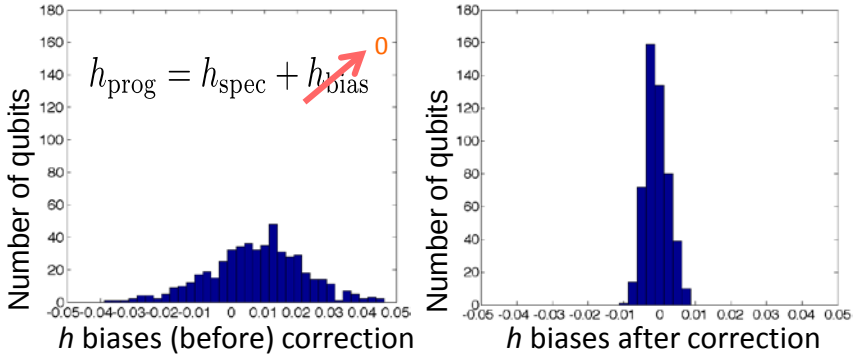
Graph Isomorphism



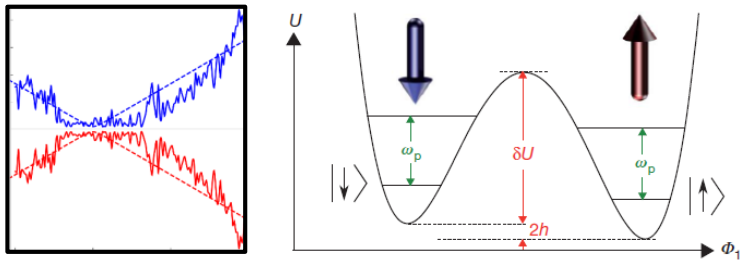
- General **Planning Problems** (e.g., navigation, scheduling, asset allocation) can be solved on a quantum annealer
- Developed a quantum solver for **Job Shop Scheduling** that pre-characterizes instance ensembles to design optimal embedding and run strategy – tested at small scale (6x6) but potentially 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**
- **Subgraph Matching Problems** are common in applications of interest to the intelligence community – similarly, finding **Longest Matching Sequences** important in genomics and bioinformatics

Current NASA Research in Quantum Physics

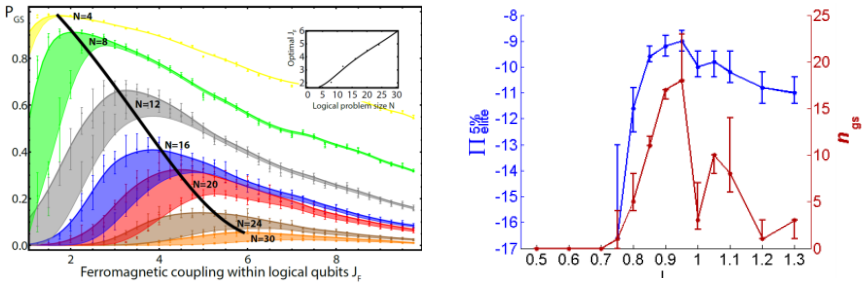
Calibration of Quantum Annealers



Effect of Noise on Quantum Annealing

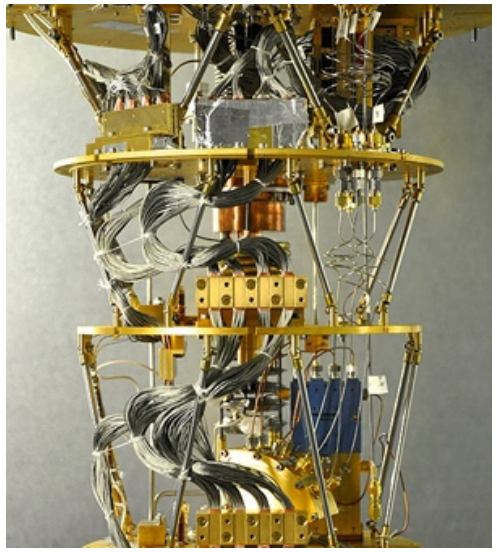


Optimal Embedding & Parameter Setting



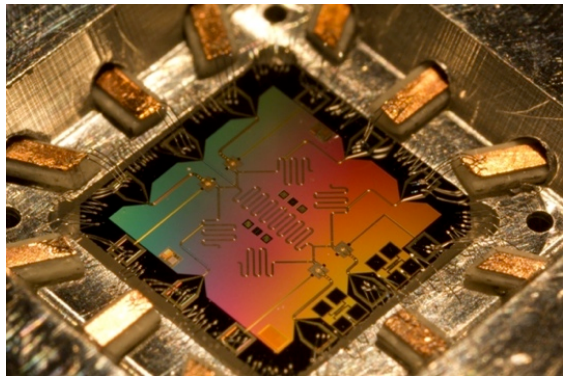
- Developed technique to determine and correct **residual persistent biases** in the programmable parameters of quantum annealers (*h* and *J*) – correction significantly improves performance and reliability (reduction in variability)
- First **realistic noise analyses** show how low-frequency noise dramatically affects the performance of quantum annealers – results being used to design hardware improvements
- Limited hardware connectivity makes embedding challenging – good runtime parameters determined by considering the **nature and dynamics of chains** – quick scans can be used to predict performance of extensive scans
- Small instances of **hard problems at phase transitions** in combinatorial optimization are intractable – they can be designed by looking at solvability phase transitions
- Predict **tractability of application problems** by studying the scaling of energy gaps and density of bottlenecks in spin glass phase

Emerging Quantum Hardware

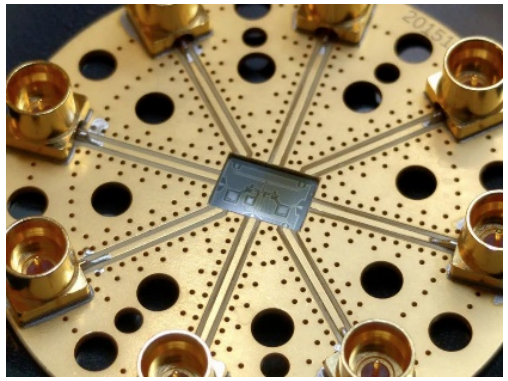


D-Wave Systems

- What should we do with the emerging and very exciting, but quite limited, quantum computational devices?
  - Still too small for solving practical problems
- Couple of possibilities:
  - Quantum supremacy
  - ***Develop intuitions for quantum heuristics***



Google

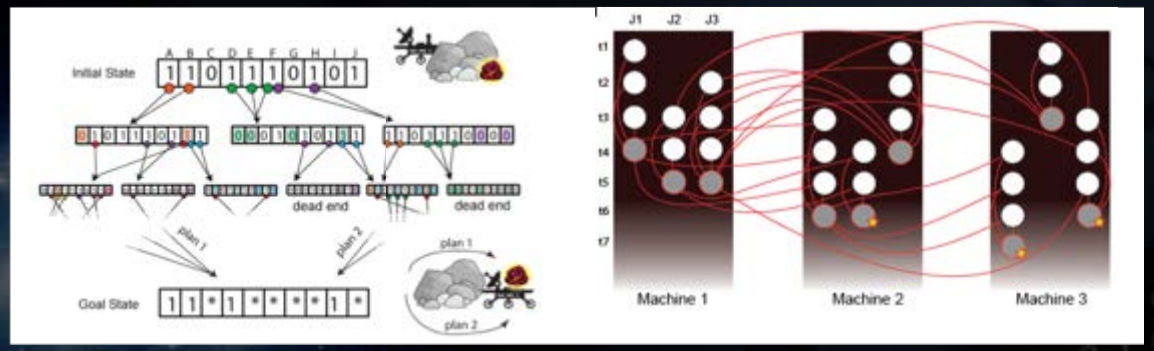


Rigetti

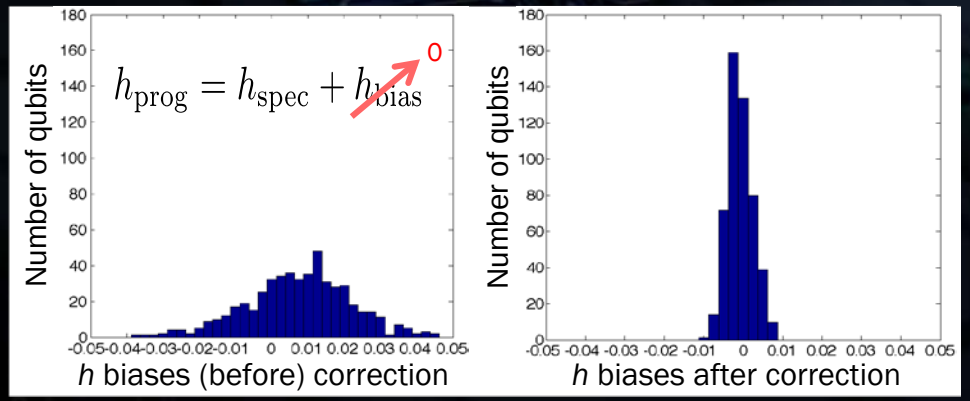
IARPA

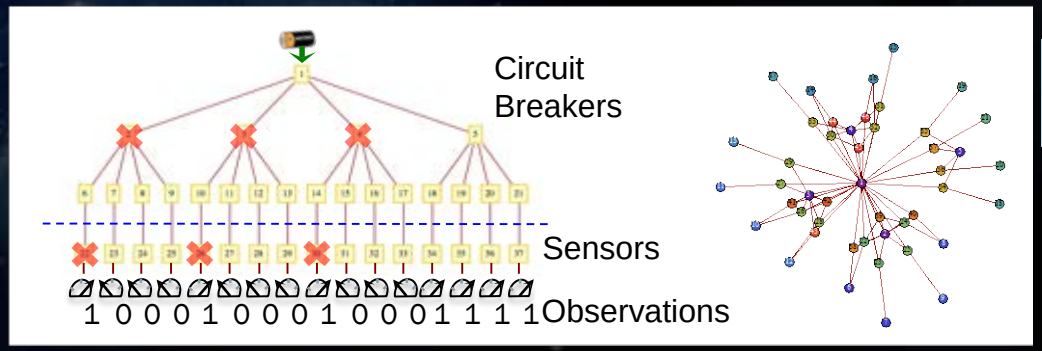
Current NASA Research in Quantum

Complex Planning and Scheduling



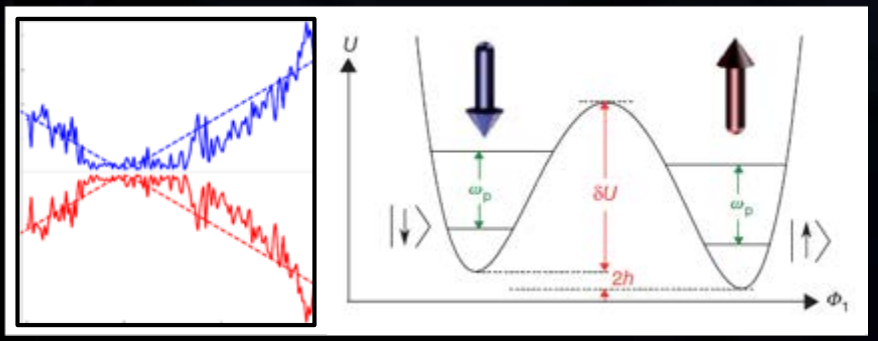
Calibration of Quantum Annealers

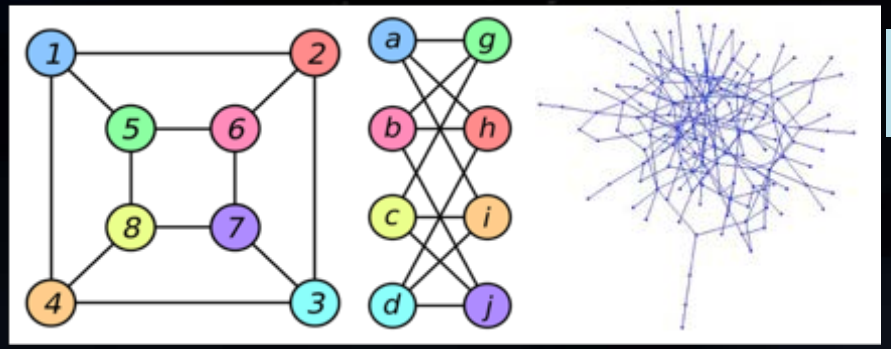




Graph-based Fault Detection

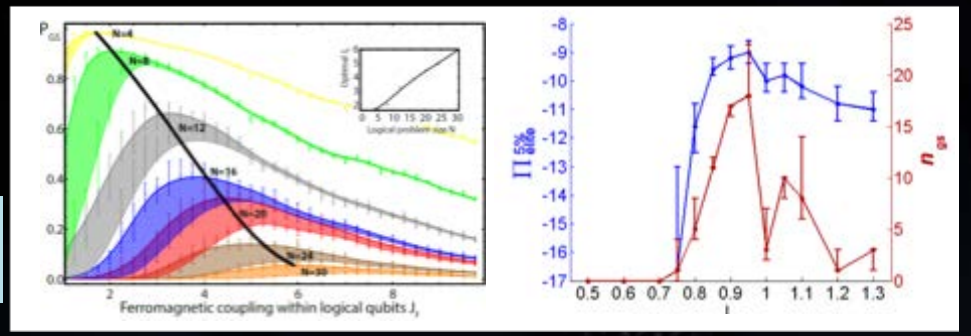
Effect of Noise on Quantum Annealing





Graph Isomorphism

Optimal Embedding and Parameter Setting



Assured Availability of UTM Network

UTM: UAS Traffic Management

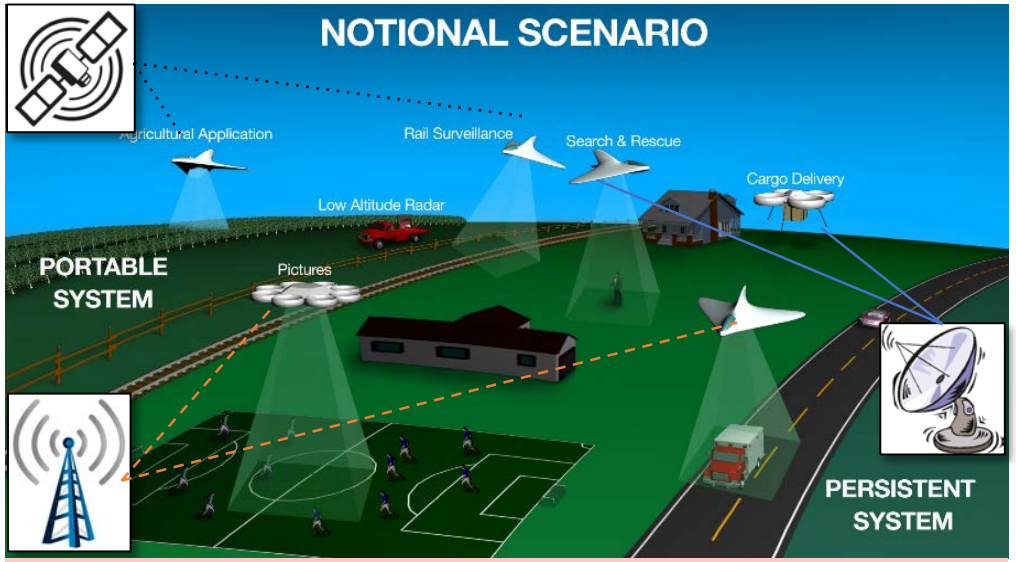
UAS: Unmanned Aerial System (includes UAV, ground control, and comm.)

Future

- Higher vehicle density
- Heterogeneous air vehicles
- Mixed equipage
- Increased autonomy
- Greater vulnerability to communication disruptions

Explore quantum approaches for:

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



- Harness power of quantum technologies to address cybersecurity challenge of assured availability
- Leverage work on QKD for spread spectrum codes

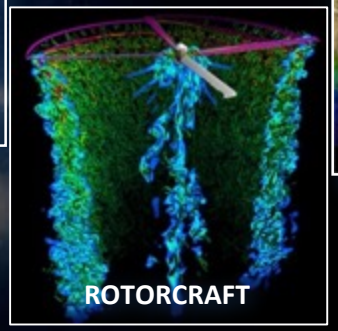
P. Kopardekar, et al., ***Unmanned Aircraft System Traffic Management (UTM) concept of operations***, AIAA 2016-3292

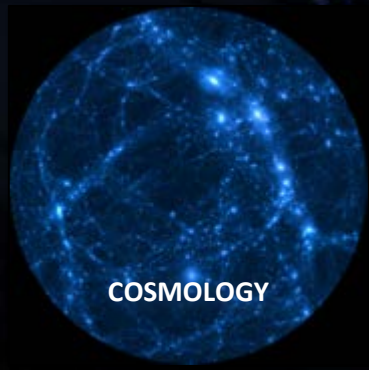
Quantum Communication

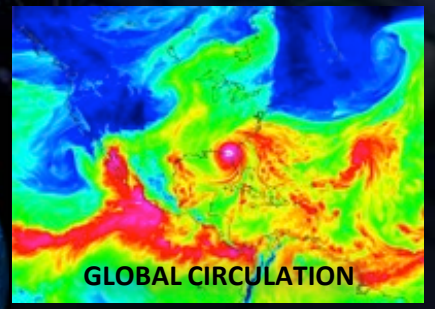
- Quantum Cryptography
  - Uses single or entangled photons to distribute a secure random key → QKD
- Teleportation
  - Uses entangled photons to send quantum information → necessary for quantum repeaters and networks
  - However, requires pre-shared entanglement, 3 photons, and hard (impossible?) to implement 2-photon gate
- Superdense Teleportation (SDT)
  - Uses entangled photons and restricted space to send quantum information
  - Remotely prepare quantum information with reduced resources
  - Requires only 2 photons of which only one has to be sent
- NASA funding development of SDT demo from ISS for last 5 years
  - Lab work performed at UIUC under auspices of Paul Kwiat
  - Independent assessment and flight system engineering conducted by MIT-LL
    - 2023: SDT from ISS to ground
    - ~2026: Demo on multi-spacecraft (i.e., swarm of small sats)
    - Late 2020's: QKD from Mars orbiter

Advanced Computing Mission

Enable the science & engineering required to meet NASA's missions and goals







Effective, stable, production-level HPC environment

Advanced technologies to meet future goals