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Title: Rapid Response: D-Wave Effort Debrief Welcome, Logistics

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Information Science & Technology Institute

Rapid Response: D-Wave Effort Debrief
Welcome, Logistics

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Information Science & Technology Institute (ISTI)

October 6, 2016

Los Alamos NATIONAL LABORATORY EST.1943

ISTI INFORMATION SCIENCE & TECHNOLOGY INSTITUTE

*Thanks to ***Denny Dahl*** and ***Scott Pakin*** for letting me reuse some of their slides

Purpose

- **ISTI Rapid Response Call for "getting feet wet" on the D-Wave Quantum computer issued in June 2016 for FY16 work (about 3 months of time)**
- ***Main Objectives***
  - Develop a diverse and sizable workforce, community, interest within LANL for D-Wave and Quantum Computing
  - Identify promising application areas/problems for future projects
  - Complement other D-Wave work at LANL (LDRD DR, ASC)
- **Funded 11 proposals**
  - PIs from CCS, T, XCP, A, EES divisions
- **Debrief Presentations today by PIs, followed by discussion led by J. Sarrao and M. Anderson**
- **Brief Welcome Presentation**
  - Information Science & Technology Institute (ISTI)
  - The D-Wave Machine at Los Alamos
  - How to program a D-Wave machine

Overview Information Science & Technology Institute (ISTI)

Mission

The Information Science & Technology Institute (ISTI) enables the execution of LANL's institutional IS&T pillar through revitalization of technical IS&T areas, recruiting and retention of IS&T staff.

ISTI manages, organizes sponsors and/or co-sponsors (1) Summer School programs, (2) University Collaborations, (3) Workshops, (4) the IS&T Seminar Series, (5) Program Development, and (6) the Visualization Co-Laboratory at LARP.

Main Activities

Summer Schools

- 2nd Parallel Computing School
- 11th Computer Systems, Clusters, and Networking Summer Institute
- 7th Computational Co-Design School *(co-sponsor)*
- 5th Data Science at Scale School *(co-sponsor)*
- New Schools in FY17: *Machine Learning, Cyber Security*

University Collaborations

- CMU: Failure at Scale, Data Intensive Computing
- UCD: Data Visualization
- Missouri S&T: Cyber security

Workshops

- CoDA: Data Science across DOE
- Physics Informed Machine Learning
- Data Science and Optimal Learning for Materials Discovery and Design

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- Discuss ideas for novel IS&T activities
- Volunteer on ISTI Science Advisory Committee
- Schedule IS&T Seminar speakers
- Reserve LARP Visualization Co-Lab

Why LANL Procured a D-Wave 2X System

- **Paid for by NNSA's ASC program**
  - Supports most supercomputer work at LANL, LLNL, and SNL
- **Concern about the end of Moore's Law**
  - How will we get more performance?
  - Considering alternative computing paradigms (primarily quantum and neuromorphic) as possibilities

National Nuclear Security Administration

Advanced Simulation & Computing™

- **Forward-thinking approach**
  - Invest in new technologies now, *before* the situation becomes dire
  - Perhaps even influence the development of these new technologies
  - For the D-Wave, even if 1K qubits isn't enough to be useful, we want to be ready for future generations that *do* have enough qubits

LANL's D-Wave Timeline

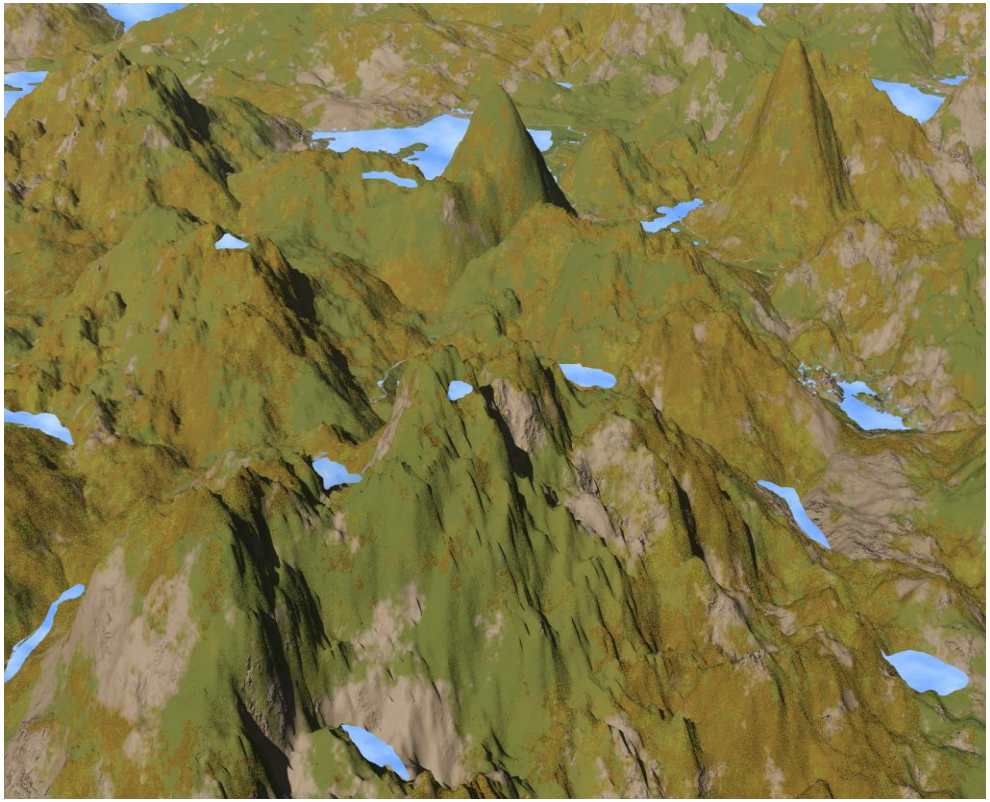
- **September 2015**
  - Order placed with D-Wave
- **October 2015**
  - Factory acceptance
- **November 2015**
  - Announcement and press releases
- **December 2015**
  - First QED 101 class at LANL
- **January 2016**
  - Denny Dahl from D-Wave relocates to Los Alamos (rapid turnaround for technical questions and programming advice)
- **March 2016**
  - Second QED 101 class at LANL
  - Included physics deep dive from Trevor Lanting—very well received

LANL's D-Wave Timeline (cont.)

- **May 2016**
  - System shipped to LANL
- **June 2016**
  - Third QED 101 class
  - Dropped hands-on pieces
  - One day
  - Held in a large auditorium
  - Videoconferencing for remote attendees
  - Huge success—173 attendees (about 50:50 remote/local) from across DOE
- **August 2016**
  - QED 201 tools class
  - System released to LANL (August 31)

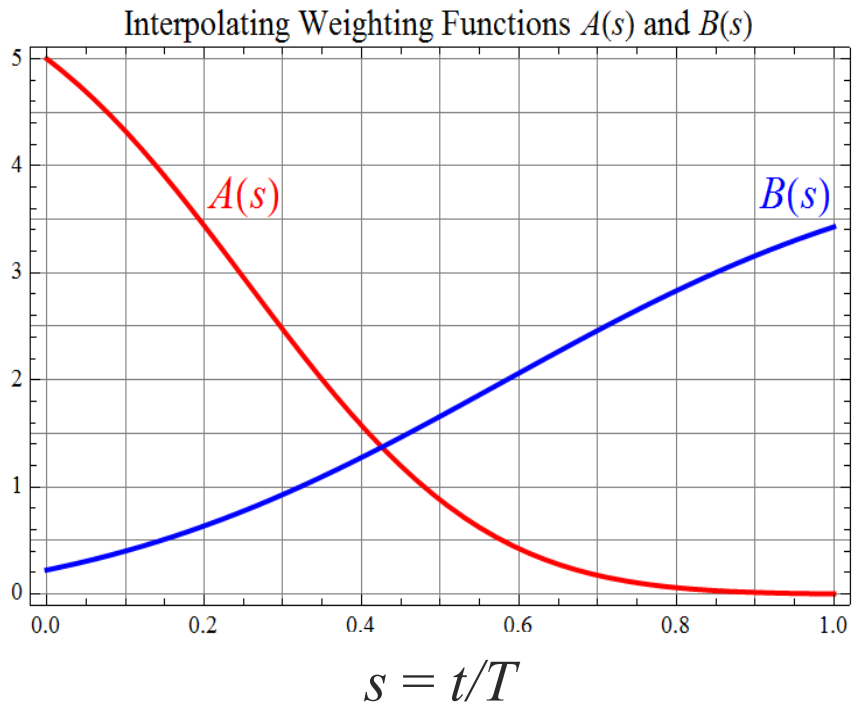
Quantum Annealing: The Landscape Metaphor
See http://dwave.lanl.gov/ for Detailed Material

- The solution space of an optimization problem can be viewed as an energy landscape with best solution in lowest valley
- Classical algorithms can only walk over this landscape
- Quantum annealing uses quantum effects to go through the hills



Adiabatic Perspective on Quantum Annealing

- A system will remain in the ground state of all the instantaneous Hamiltonians passed through – as we change the "landscape" – provided the change is made sufficiently slowly ("adiabatically")
- $H(s) = A(s)\, H_{\text{initial}} + B(s)\, H_{\text{final}}$
  where $s = t/T$
  - H_{initial} is a simple landscape with an obvious minimum,
  - H_{final} is the landscape that models our problem instance
  - $A(s)$ and $B(s)$ are weight functions that change with time up to annealing time T



Quantum Enhanced (Combinatorial) Optimization

Quantum Hamiltonian is an operator on Hilbert space:

$$\mathcal{H}(s) = A(s)\sum_i {\sigma_i}^x + B(s)\left[\sum_i a_i\,{\sigma_i}^z + \sum_{i<j} b_{ij}\,{\sigma_i}^z{\sigma_j}^z\right]$$

Corresponding classical optimization problem:

Quadratic Unconstrained Binary Optimization (QUBO)

$$\mathrm{Obj}(a_i, b_{ij}; q_i) = \sum_i a_i q_i + \sum_{i<j} b_{ij} q_i q_j$$

q_i: binary variables of qubits
a_i: qubit weights (“h”)
b_{ij}: coupler weights (“J”)

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However: Not all possible couplers exist (only linear number). Embedding required on underlying qubit graph (Chimera), and actual physical implementation

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Also: Computation is not deterministic, not guaranteed to find global minimum. Repeated runs required to gain confidence in result and also find interesting alternate solutions

Meta Algorithm

1. Express problem as an optimization problem in QUBO form
2. Compute an embedding for concrete problem instance
3. Run sufficient number of iterations of D-Wave annealing steps
4. Analyze results

Unique Aspects of LANL's D-Wave 2X Installation

- **LANL is at high altitude**
  - 7355′ (2242m)
  - Affects system calibration
- **Installation in a secure facility → lots of extra paperwork**
  - Approvals for structural modifications (concrete slab to reduce vibration)
  - Approvals for uncleared foreign nationals to have access
- **Huge UPS unit**
  - 4 hours of backup power (100 kWh)
  - Covers time to bring in and attach a diesel generator

Parameter	Value
# of qubits	1,095 (95.1%)
# of couplers	3,061 (91.1%)
Temperature	10.45 mK
Annealing time	5–2000 μs
h range	[-2, +2]
J range	[-1, +1]

Today's Presentations in Diverse Application Domains

- Combinatorial Optimization
- Machine Learning
- "Reverse-engineering" the physics, testing quantum nature
- Quantum software stack development