18-819F: Introduction to Quantum Computing 47-779/47-785: Quantum Integer Programming & Quantum Machine Learning

Quantum Annealing, Quantum-Inspired Heuristics, Benchmarking, and Parameter setting Lecture 9

10.03.2022







Benchmarking: our tool to observe optimization speedups

- When addressing problems using quantum algorithms there is usually a main question...
 - Is it better than classical?
 - The definition of Quantum Speedup depends on how the question is asked
 - Provable Quantum Speedup (e.g., Grover algorithm)
 - Strong Quantum Speedup (e.g., Shor's algorithm)
 - Observed Quantum Speedup (potential and limited)
- Optimization problems pose a challenge to speedup analysis
 - Problems can be in NP: Exponential speedups are believed as unreachable
 - This does not discourage us from developing methods given applications
 - Speedup should be observed at application scale for the problem of interest, and heuristically observed \rightarrow We need **Benchmarks** of our solution methods

In the real world what you care about is «speedup at application scale» for your problem of interest.





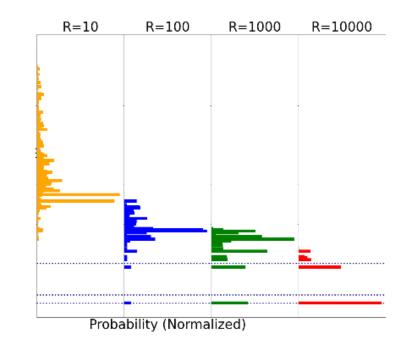


 $S(N) = rac{C(N)}{O(N)}$ Speedup as a function of problem size

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Parameterized Stochastic Solvers for Optimization Problems

- Solver
 - End-to-end solution method: hardware and software running algorithm
- Our definition of Stochastic
 - Solvers are understood as samplers of random variables X of distributions characterized by a CFD and a threshold $F_X(X \le x)$
 - Solvers are modifiers of these distributions with resource such that distribution shifts towards optimal solution as resource increases
- Definition of parameterized
 - Several parameters in the algorithms with strong effects in performance
 - In some cases, unknown dependance of performance w.r.t parameters







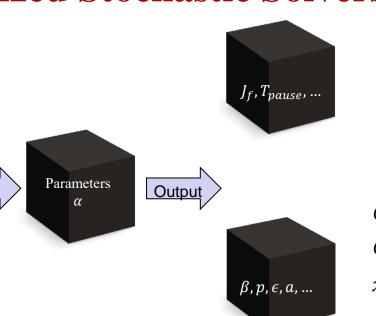


Carnegie Mellon University

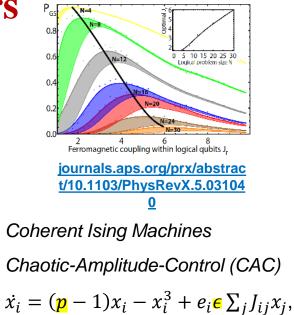
Optimization Parameterized Stochastic Solvers

Input

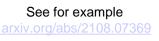
- Classical algorithms
 - Simulated Annealing
 - Parallel Tempering
 - Genetic Algorithms
- Quantum Annealing (QA)
- Coherent Ising Machines
- Quantum Alternating Optimization Ansatz (QAOA)
- Unconventional processors for Ising models

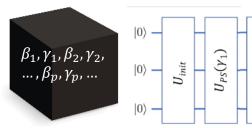


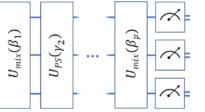
EPPER



 $\dot{e_i} = -\frac{\beta}{\beta} (x_i^2 - \mathbf{a}) e_i,$











Quantum and Quantum-Inspired Ising Solvers Examples

 Quantum Annealing: D-Wave Systems
 Coherent Ising Machines and Bifurcation Machines







The Quantum Adiabatic Algorithm for Ising Machines



(1) Map objective function into energy of a quantum Ising system

 $H_p = \sum_{ij} J_{ij} Z_i \otimes Z_j + \sum_i h_i Z_i$

(2) Start from easy problem to solve with known solution

$$H_D = \Gamma \sum_i X_i$$
 (transverse field)
 $|\Psi\rangle_{Nqubits} = \frac{1}{\sqrt{2^N}} \sum_{n=1}^{2^N} |solution(n)\rangle$

(3) Do any Schrödinger evolution (no measurement! No noise!) that changes the energy states «sufficiently slow».

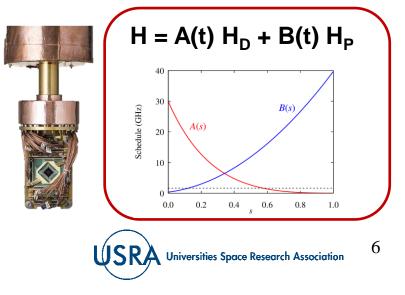
How slow? It depends on the problem, on H_D and on the <u>Annealing Schedule</u> No way to predict efficiently. Try!



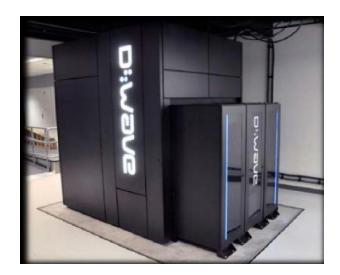


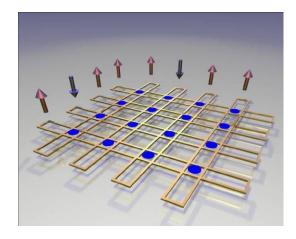
 $H|s_{1}s_{2}...s_{N}\rangle = EN|s_{1}s_{2}...s_{N}\rangle$ $\exp(iH)|s_{1}s_{2}...s_{N}\rangle = e^{iE_{N}}|s_{1}s_{2}...s_{N}\rangle$ $X = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad Y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ $R_{x}(\pi/2)|0\rangle = |1\rangle$ $R_{x}(\pi/2)|1\rangle = |0\rangle$

If this field is always on and constant the minimum energy state is the **all-superposed state**

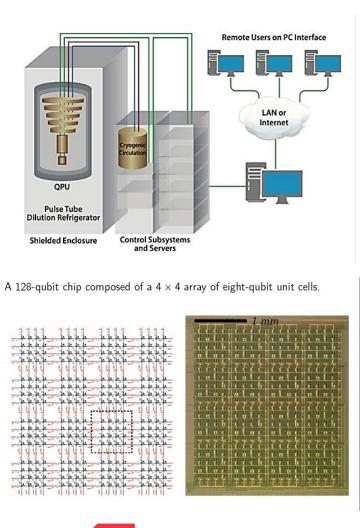


Quantum annealing à la D-Wave



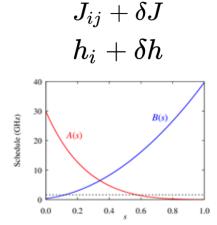


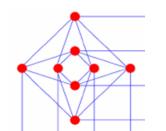


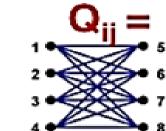


TEPPER

 J_{ij} and h_i have maximum value and fluctuating intrinsic control errors:

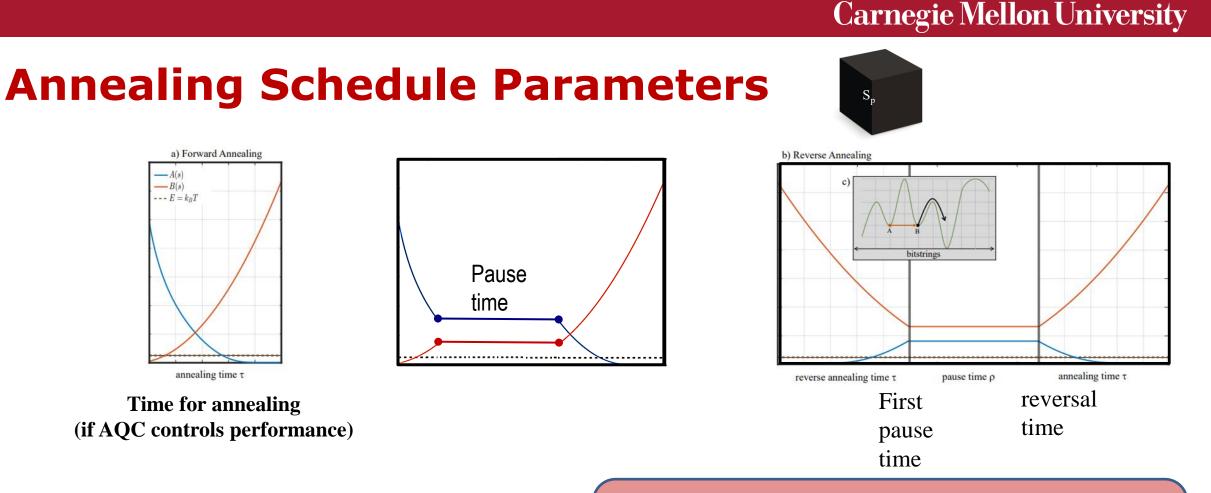








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These are all parameters that influence performance.

Only for elegant problems they can be derived ab-initio. In the real world you have some physics guidance for best guess then you use a heuristics to find them





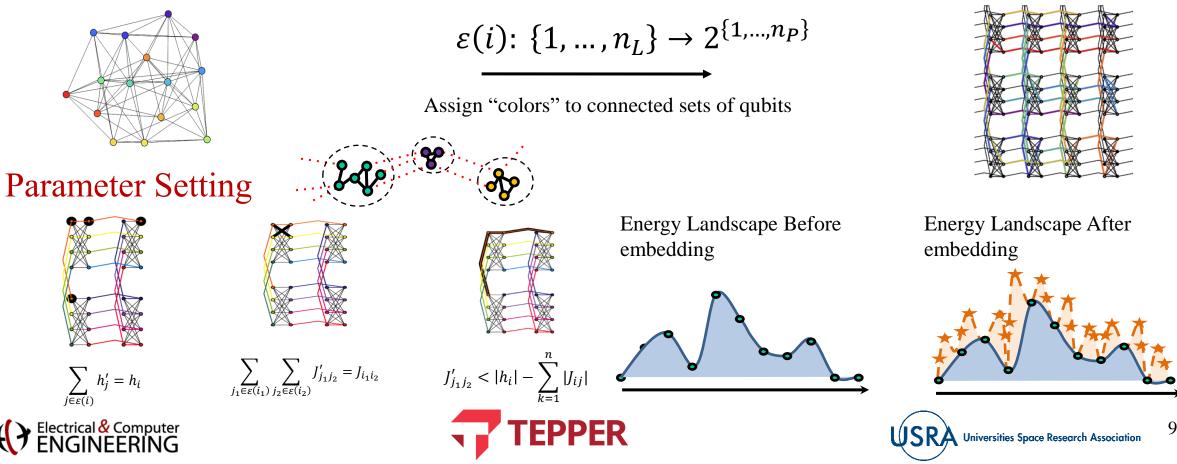


 $(n_{\rm P} \text{ logical bits})$

Minor Embedding

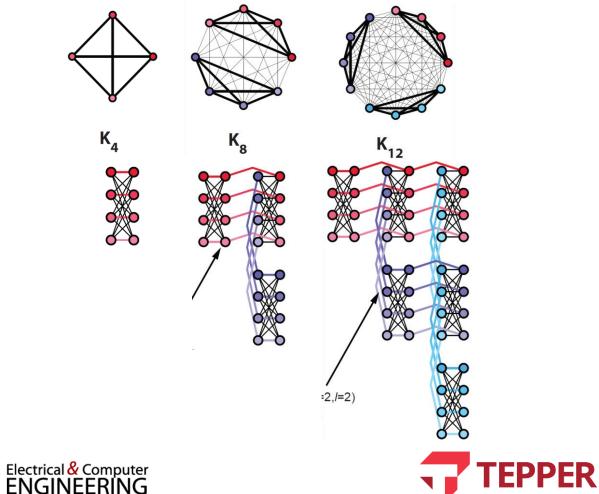
Topological Embedding

(n_H hardware qubits)

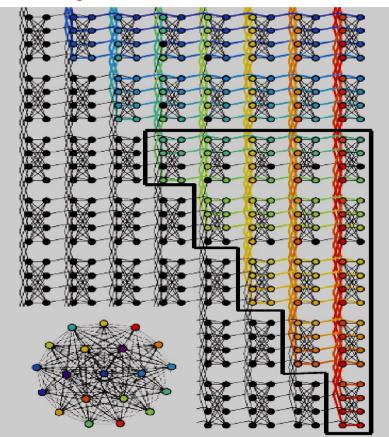


Minor Embedding of a fully connected graph

Systematic Rule for Embedding



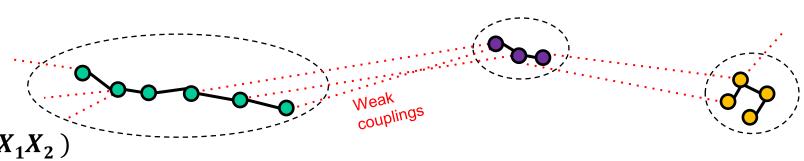
Quadratic overhead

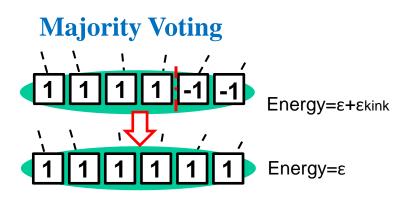




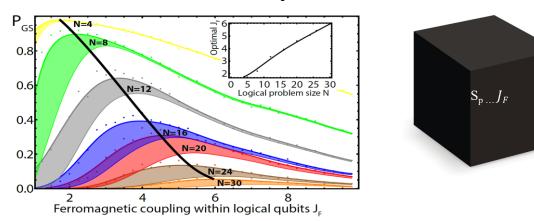
Unembedding

Ferromagnetic Coupling $f(S_1, S_2) = -JF s_1 s_2$ $f(X_1, X_2) = -4JF(-X_1 - X_2 + X_1X_2)$





What is the correct J_F ?



Not too large, not too small. Trial and error. (See Venturelli et al.

https://journals.aps.org/prx/abstract/10.1103/PhysRevX.5.031040)



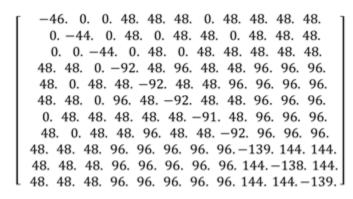




Minor Embedding - Example

https://colab.research.google.com/github/bernalde/QuIPML22/blob/main/notebooks/Notebook%204%20-%20DWave.ipynb

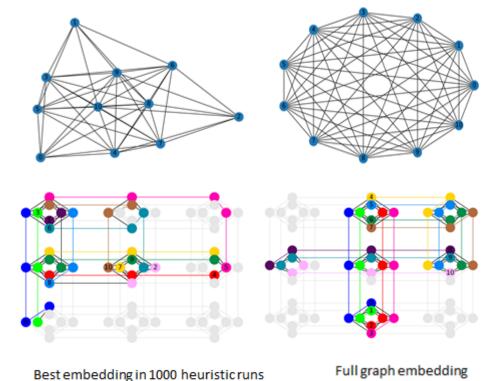
From our main example



And embed it into a Chimera graph (subgraph of the Chip) Notice that we need to "duplicate" certain variables into several qubits

This step is non-trivial:

Either use heuristic methods or solve highly constrained problem

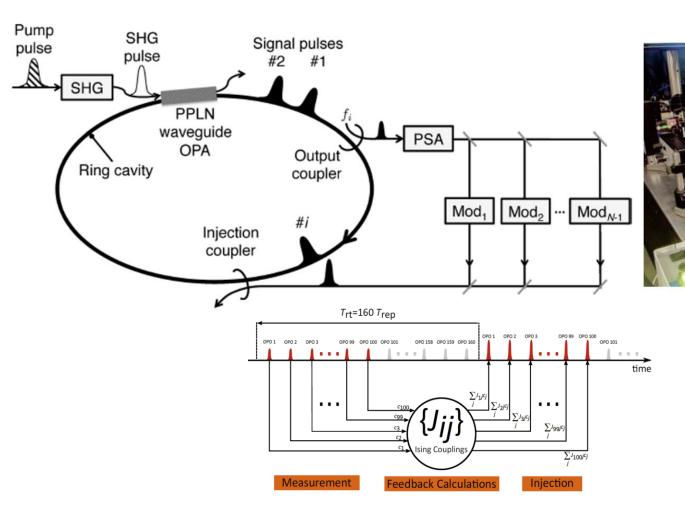


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Coherent Ising Machines



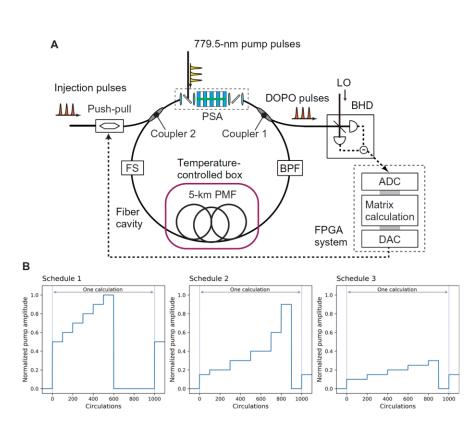








NEWS: 100,000 Spins



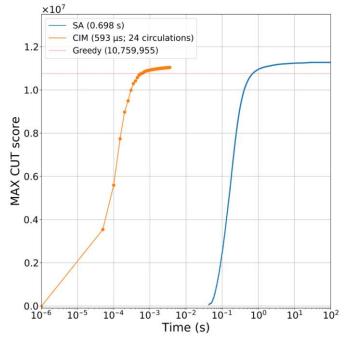


Fig. 3. MAX CUT score as a function of computation time obtained with the CIM (orange line) and SA (blue line). The data points exhibit the scores evaluated at the intermediate steps in the CIM and SA computation. The dotted line denotes the score obtained with SG (10,759,955).

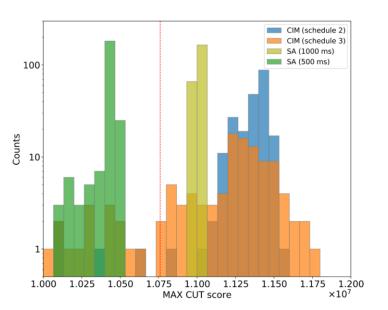


Fig. 6. Histograms of MAX CUT score with CIM and SA. The vertical dashed line shows the SG score (10,759,955).

SCIENCE ADVANCES | RESEARCH ARTICLE

COMPUTER SCIENCE

100,000-spin coherent Ising machine

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Coherent Ising Machines: Stochastic Differential Equations

Describing the system with zero quantum noise, and neglecting the out-of-phase component of the signal

$$\dot{x_i} = (p-1)x_i - x_i^3 + \epsilon \sum_j J_{ij} x_j$$

$$(\dot{x}_{i} = \frac{\partial V}{\partial x_{j}})$$

$$V \coloneqq \sum_{i} \left(\frac{(p-1)x_{i}^{2}}{2} + \frac{x_{i}^{4}}{4}\right) - \epsilon \sum_{ij} J_{ij} x_{i} x_{j}$$

$$S_{i} = sign(x_{i}) \text{ is the bit variable}$$





Chaotic-Amplitude-Control (CAC) or Amplitude Heterogeinity Correction or Error-variable Feedback

$$\dot{x}_{i} = (p-1)x_{i} - x_{i}^{3} + e_{i}\epsilon \sum_{j} J_{ij}x_{j},$$

$$\dot{e}_{i} = -\beta (x_{i}^{2} - a)e_{i},$$

Various architectures

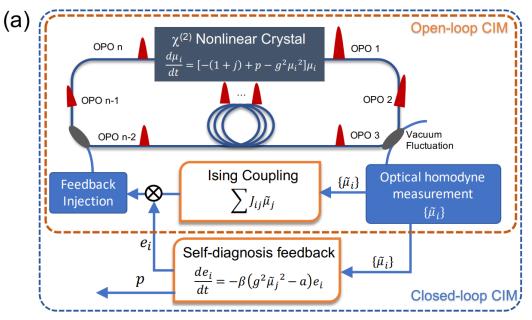
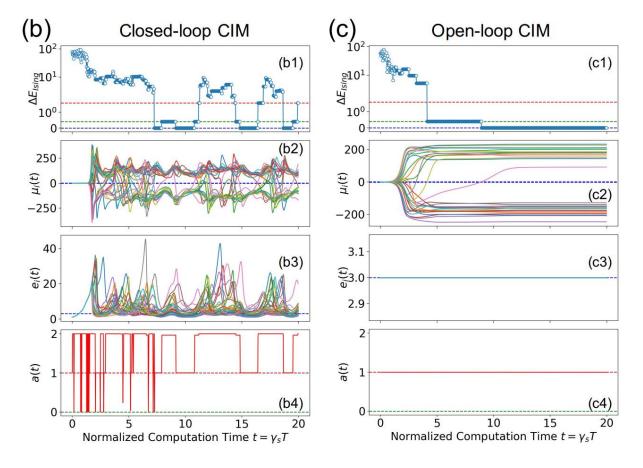


FIG. 1: (a) Schematic diagram of the measurement-feedback coupling CIMs with and without the self-diagnosis and dynamic feedback control (closed-loop and open-loop CIMs) indicated using dashed blue and orange lines, respectively. (b) and (c) Dynamical behaviour of the closed-loop and open-loop CIMs, respectively. (b1) and (c1) Inferred Ising energy (the dashed horizontal lines are the lowest three Ising eigen-energies). (b2) and (c2) Mean-field amplitude $\mu_i(t)$. (b3) and (c3) Feedback-field amplitude $e_i(t)$. (b4) Target squared amplitude a(t). (c4) Pump rate p(t).



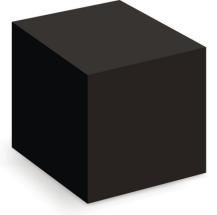
https://arxiv.org/abs/2105.03528







Coherent Ising Machines: Stochastic Differential Equations



In our simulation, the x_i variables are restricted to the range $\left[-\frac{3}{2}\sqrt{\alpha}, \frac{3}{2}\sqrt{\alpha}\right]$ at each time step. The parameters p and α are modulated linearly from their starting to ending values during the T_r time steps and are kept at the final value for an additional T_p time steps. The initial value x_i is set to a random value chosen from a zero-mean Gaussian distribution with a standard deviation of 10^{-4} and $e_i = 1$. Furthermore, 3200 trajectories are computed per instance to evaluate TTS. The actual parameters used for simulation are listed below:

N step	3200
ΔT	0.125
T_r	2880
T_p	320
p	$-1.0 \rightarrow 1.0$
α	$1.0 \rightarrow 2.5$
β	0.8

Chaotic-Amplitude-Control (CAC) or Amplitude Heterogeinity Correction or Error-variable Feedback

$$\begin{aligned} \dot{x}_i &= (p-1)x_i - x_i^3 + e_i \epsilon \sum_j J_{ij} x_j, \\ \dot{e}_i &= -\beta (x_i^2 - a) e_i, \end{aligned}$$

See for instance:

https://arxiv.org/pdf/2108.07369.pdf

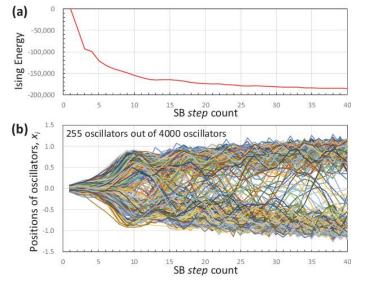






Oscillation Based Machines, Bifurcation Machines, MemComputers etc.

The Kuramoto Model describes synchronization of oscillators The Toshiba Simulated Bifurcation Machine, Memcomputing



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The Fujitsu Digital Annealer



https://ieeexplore.ieee.org/document/8892209







Time-to-Solution and variants

- Fix parameters, run many times (num_{trials}) estimate cost of being above certain quality measure PDF $f(X \le x) = f(x)$
- Define a success test: ok if X = cost < target = x
- Estimation of success probability

•
$$F_X(x) = CDF(x_{OK}) = P_{success} = \frac{num_{OK}}{num_{trials}} = \int_{x < x_{OK}} dx f(x)$$

- Probability of succeeding at least once in *R* attempts is given by new random variable $Y_R = \min\{x_{[i]}\}$ with CDF
- $f(Y_R \le x) = F_{Y_R}(x) = P(R) = 1 (1 P_{success})^R$
- Invert to find *R* required to achieve success with at least probability *s* (*usually* 0.99) scaled by a resource factor (e.g., time per shot/read)

•
$$TTS = t \frac{\log(1-s)}{\log(1-Psuccess)}$$

Academic Benchmarking Standard: median $\langle TTS \rangle(N)$

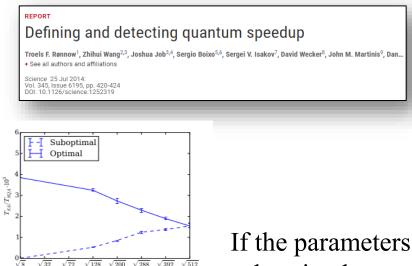


FIG. 2. Pitfalls when detecting speedup. Shown is the speedup of SQA over SA, defined as the ratio of median time to find a solution with 99% probability between SA and SQA. Two cases are presented: a) both SA and SQA run optimally (i.e., the ratio of the true scaling curves shown in Figure 1), and there is no asymptotic speedup (solid line). b) SQA is run suboptimally at small sizes by choosing a fixed large annealing time $t_a = 10000$ MCS (dashed line). The apparent speedup is, however, due to suboptimal performance on small sizes and not indicative of the true asymptotic behavior given by the solid line, which displays a slowdown of SQA compared to SA.

Linear problem size \sqrt{N}

If the parameters are suboptimal you can be fooled into thinking the complexity decreases with problem size!

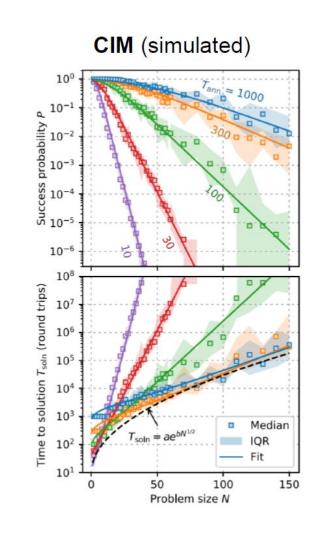


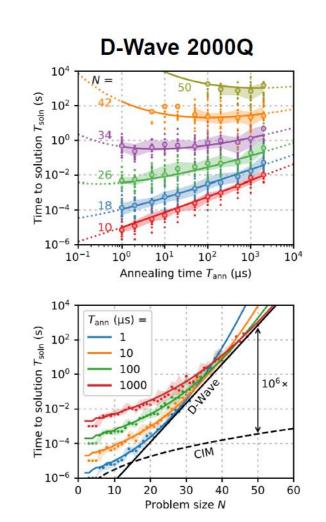




Example 1: CIM vs D-Wave (2020)

https://www.science.org/doi/ 10.1126/sciadv.aau0823











Example 2: Sim-CIM vs Adiabatic QAOA

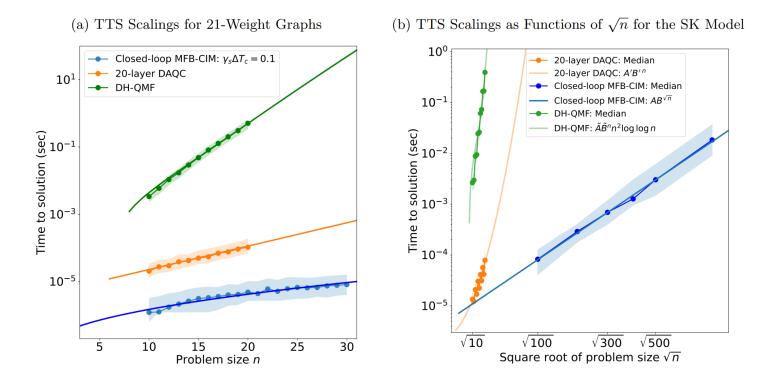


FIG. 14: Comparison of the time-to-solution (TTS) scalings for the MFB-CIM, DAQC, and DH-QMF in solving MAXCUT. (a) Wall-clock time of a closed-loop CIM with a low-finesse cavity ($\gamma_s \Delta T_c = 0.1$), DAQC with an optimum number of layers (p = 20), and DH-QMF with an a priori known number of optimum iterations versus problem size n. (b) TTS of the closed-loop CIM on the fully connected SK model for problem sizes from n = 100 to n = 800, in steps of 100. For each problem size, the minimum TTS with respect to the optimization over t_{\max} is plotted. In comparison, the SK model TTSs are shown for 20-layer DAQC and DH-QMF for problem sizes ranging from n = 10 to n = 20. The straight, lighter-blue line (a linear regression) for the CIM demonstrates a scaling according to $AB^{\sqrt{n}}$. The lighter-orange and lighter-green best-fit curves for DAQC and DH-QMF are extrapolated to larger problem instances, illustrating a scaling that is exponential in n rather than in \sqrt{n} . In both figures, the shaded regions show the IQRs.

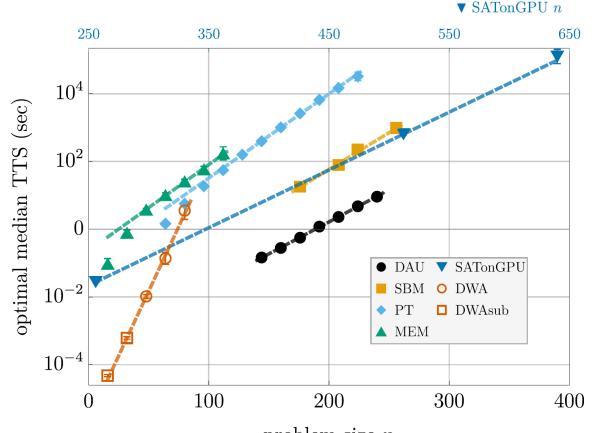




https://arxiv.org/abs/2105.03528



Example 3: D-Wave vs Digital Annealer and Parallel Tempering



problem size n

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https://arxiv.org/abs/2103.08464

FIG. 2. Median optTTS for different solvers for the quadratic 3R3X instances at different problem sizes n. The error bars correspond to 2σ confidence intervals calculated using a Bayesian-bootstrap. Each solver is represented with a different marker and color, as denoted by the legend. DAU is Fujitsu's Digital Annealer Unit, run in parallel mode on 25 April 2020. SBM is Toshiba's Simulated Bifurcation Machine, accessed via Amazon Web Services on 20 August 2020. PT is our implementation of parallel tempering. MEM is the Virtual MemComputing Machine. SATonGPU is the data from Fig. 5 of Bernaschi *et al.* [37], after converting their native three-body 3R3X results in n/2 variables to n two-body variables by simplying doubling their reported n values. Note that the SATonGPU results are plotted on a separate, shifted horizontal axis (top, blue), as this solver reached significantly larger problem sizes than the other solvers; its optTTS is smaller by at least two orders of magnitude than the rest. DWA is the D-Wave Advantage1.1 device accessed via LEAP on 31 October 2020. DWAsub are suboptimal points in which the optimal runtime is below 1 μ s, the lowest runtime possible on the Advantage1.1 device. The lines correspond to the exponential fits [Eq. (3)] of the data, with the coefficients given in Table II. The DWAsub points were not used in computing the DWA scaling exponent reported in Table II.

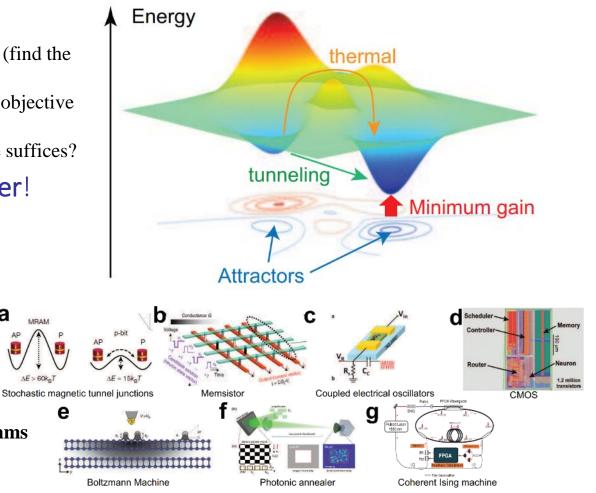


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Example 3: Ising Solvers Review

"Solving the Model"

- **Physicists:** identifying the value of thermodynamics expectation values (find the ٠ thermal distribution of energies)
- **Optimizers:** find the actual bitstring/variable values that minimizes the objective function (find the ground state)
 - **BIG CAVEAT!** Do we return the optimal solution, or a good one suffices?
- How to solve the Ising model? With an **Ising solver**!
- What is an Ising solver? An end-to-end solution method including ٠ software/algorithms and hardware/machines
 - **Classical Thermal Annealing**
 - Other classical algorithms
 - Quantum-inspired classical algorithms
 - Dynamic System solvers
 - Oscilator-based computing, Coherent Ising Machines
 - **Quantum Approaches**
 - **Quantum Annealing, Hybrid Quantum-Classical Algorithms**



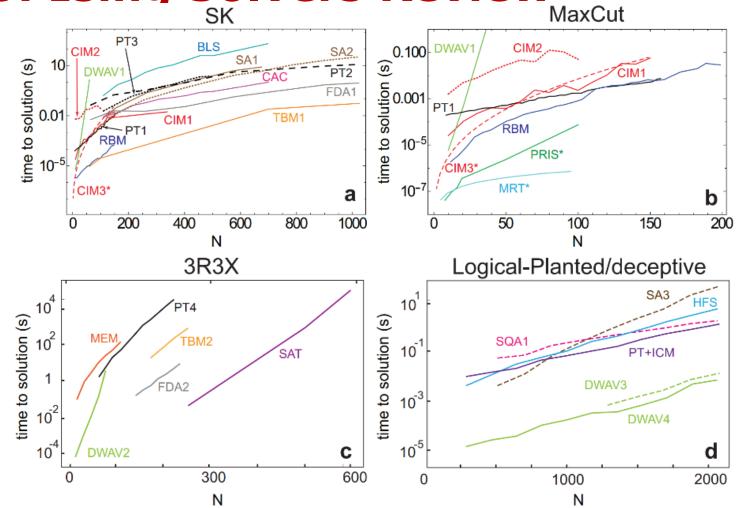
Mohseni, Naeimeh, Peter L. McMahon, and Tim Byrnes. "Ising machines as hardware solvers of combinatorial optimization problems." Nature Reviews Physics 4.6 (2022): 363-379.





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Example 3: Ising Solvers Review



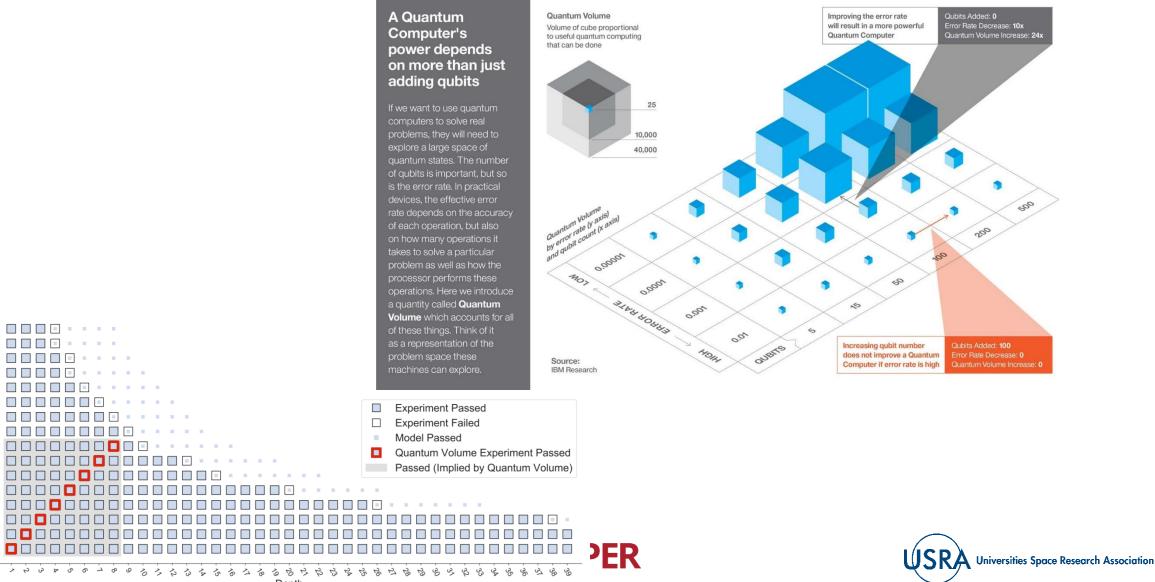
Mohseni, Naeimeh, Peter L. McMahon, and Tim Byrnes. "Ising machines as hardware solvers of combinatorial optimization problems." Nature Reviews Physics 4.6 (2022): 363-379.







Quantum Volume and variants



15 -

14 -

13 -

12 -

11

10

Width 8

Quantum Volume and variants

How large and how long are the programs that a quantum processor can run reliably today?

https://quantum-journal.org/papers/q-2020-11-15-362/ https://arxiv.org/abs/2110.03137

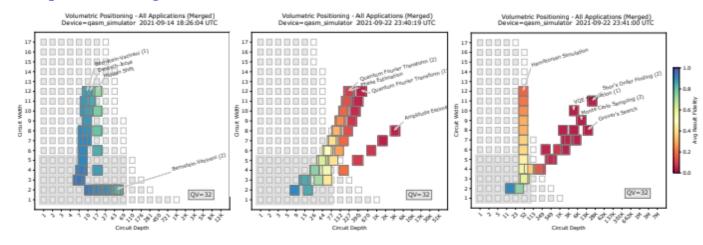
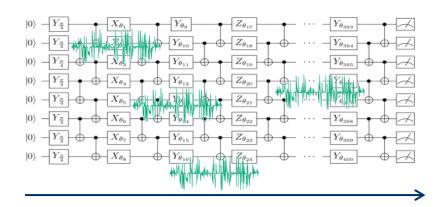


FIG. 1. Quantum Application-Oriented Performance Benchmarks. The results of executing our quantum application-oriented performance benchmarking suite on a simulator of a noisy quantum computer, with results split into benchmarks based on three loose categories of algorithm: tutorial, subroutine, and functional. For each benchmark, circuits are run with a variety of widths, corresponding to the problem size, here ranging from 2 to 12 qubits. The result fidelity, a measure of the result quality, is computed for each circuit execution, and is shown as a colored square positioned at the corresponding circuit's width and normalized depth. Results for circuits of equal width and similar depth are averaged together. The results of the application-oriented benchmarks are shown on top of a 'volumetric background' (grey-scale squares) which extrapolates from a device's quantum volume (here, 32) to predict the region in which a circuit's result fidelity will be above 1/2 (the grey squares).







Fidelity of two pure quantum states is a distance metric that could be defined as the overlap/transition probability: $F(\psi, \phi) = |\langle \psi | \phi \rangle|^2$ Can be generalized for noisy quantum states.



Performance Ratio as a function of resource

Inspired in approximation ratios, considers that we are only interested in "best" samples/reads

- The probability that R random variables are all less than x is $RF_E(x)$
- The PDF for the maximum of R iid runs is

$$PDF = \frac{dF}{dE} = R F_E(x)^{R-1} P_E(x)E(x)$$

• For a discrete distribution:

$$\mathbb{E}(Y_N) = \sum_{k=1}^{L} \left[\left(\sum_{r=k}^{L} p(x_r) \right)^N - \left(\sum_{r=k+1}^{L} p(x_r) \right)^N \right] x_k$$

N total number of runs, r rank index of solution within L different solutions, $p(x_r)$ probability of obtaining r^{th} solution and x_k being the resource cost of each sample/read

- Can be obtained by bootstrapping!
- Generate *N*>>1 runs. Select randomly *R*<<*N*. Compute the max of *R*. Repeat and average.
- Using our "rigorous notation"

$$f_{Y_R}(X_k) = F_{Y_R}(X_k) - F_{Y_R}(X_{k-1}) = \left[\left(1 - F_X(X_{k-1}) \right)^R - \left(1 - F_X(X_k) \right)^R \right]$$







How to evaluate the parameter setting Windows Sticker

- We propose using experimental data to respond to questions regarding new instances
- Addressing main question of "speedup at application scale" for your problem of interest.
 - Expectation of metric quality at a fixed resource and confidence
 - With X% confidence, will we find solution with Y quality after using R resource?
- Bonus:
 - Explainable, Simple, Automatic!
- In our notation

•
$$X_E(R,c) = F_X^{-1} \left(1 - (1-c)^{\frac{1}{R}} \right)$$

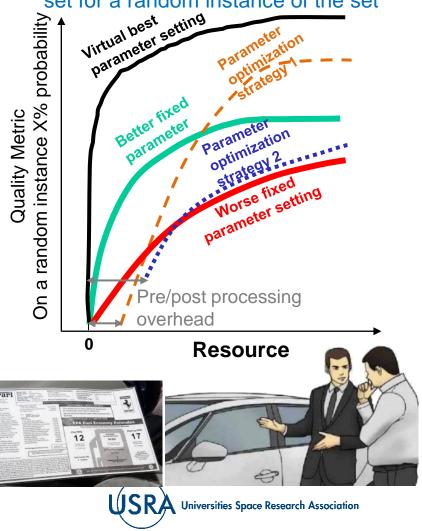
"Classic car Windows Sticker" licensed under CC0 1.0

"Slaps Roof of Car" licensed under CC0 1.0





Obtain the profile across the benchmark set for a random instance of the set



Let's go to Colab <u>https://colab.research.google.com/github/bernalde/QuIPML22/blob/</u> <u>main/notebooks/Notebook%205%20-%20Benchmarking.ipynb</u>







Check the AWS Exercises

Let's go to the AWS Braket

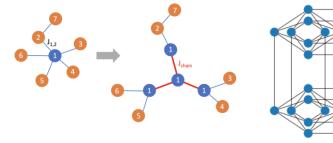
https://console.aws.amazon.com/braket Quantum Annealing tutorials from Quiz III

quantum_annealing/Dwave_Anatomy.ipynb

(also found in <u>GitHub</u>) but if you want to execute it open it in AWS.

- Great background information on
 - Quantum Annealing
 - Embedding
 - Ising Model / MAXCUT / QUBO

Electrical & Computer





Anatomy of quantum annealing with D-Wave on Amazon Braket

This tutorial notebook dives deep into the anatomy of quantum annealing with D-Wave on Amazon Braket.

First, the concept of quantum annealing as used by D-Wave is introduced to show how it probabilistically finds the (approximate) optimum to some optimization problem.

The next section introduces the structures of the D-Wave QPUs and the concept of **embedding**. Amazon Braket provides two D-Wave devices, 2000Q and Advantage. The 2000Q device has the **Chimera** topology, while the Advantage device has the **Pegasus** topology. Running a problem on a particular D-Wave device requires to map the original source graph onto the targe graph. This mapping is called embedding.

Finally, an example QUBO problem is solved using both the classical annealers and QPU to demonstrate the sampling process and a breakdown of the QPU access time.

Background: quantum annealing

Introduction: On a high level, quantum annealing (QA) is a specific approach to quantum computing, as opposed to the common gate-based model. Quantum annealers are specific-purpose machines designed to solve certain problems belonging to the class of Quantu functuration (QUBO) problems. The QUBO model unifies a rich variety of NP-hard combination problems, such as Quadratic Assignment Problems, Capital Budgeting Problems, Task Ilocation Problems and Maximum-Cut Problems, just to name a few [1]. Since quantum annealers do not have to meet the strict engineering requirements that universal gate-based machines have to meet, already today this technology features ~ 5000 superconducting qubits, compared to less than 100 qubits on gate-model quantum computers. Amazon Braket offers access to the superconducting quantum annealers provided by D-Wave Systems that can be programmed using the high-level, open source tool suite called Occan.

Adiabatic quantum computing: The paradigm of QA is closely related to adiabatic quantum computing (with only subtle differences discussed later) [2]. In essence, adiabatic quantum computing makes use of an adiabatic process where parameters are changed sufficiently slow for the system to adapt to the new parameter configuration quasi-instantaneously. For example, in a quantum mechanical system, some Hamiltonian starts from H_0 and slowly changes to some other Hamiltonian H_1 , with (for example) a linear ramp (also called schedule):

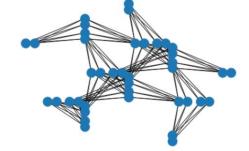
 $H(t) = (1 \text{Unknown character Unknown character Unknown character})H_0 + tH_1$

where $t \in [0, 1]$ on some time scale. Accordingly, the system's final dynamics at t = 1 is governed by H_1 while initially it is determined by H_0 . If the change in the timedependent Hamiltonian H(t) is sufficiently slow, the resulting dynamics are very simple (according to the adiabatic theorem): if the system starts out in an eigenstate of H_0 . It he system remains in an instantaneous eigenstate throughout the evolution. Specifically, if the system started in the ground state (the eigenstate with minimal energy), the system stays in the ground state, if the condition of adiabaticity (that is related to energy difference between the ground state and the first excited state called the gap) is satisfied. This means, to solve a (unknown) ground state of a Hamiltonian for a (hard-to-solve) problem, one can start from an easy-to-solve Hamiltonian with a known ground state.

Quantum Annealing: In practice, it is very difficult to fulfill the adiabaticity conditions, because of undesired noise. Therefore, quantum annealers forego the stringent, theoretical adiabaticity conditions and heuristically repeat the annealing procedure many times, thereby collecting a number of samples from which the configuration with the lowest energy can be selected as the optimal solution. However, there is no strict guarantee to find the true ground state.

Typically the Hamiltonian H_0 has the form: $H_0 = \sum_i \sigma_i^+$; with well-known ground state (the equal superposition of all bitstrings). And H_1 is described by the canonical Ising model

 $H_{\text{Ising}} = \sum_{i, j} J_{i, j} \sigma_i^z \sigma_j^z.$





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Other exercises on DWave

In AWS Braket <u>https://console.aws.amazon.com/braket</u> there are other interesting Quantum Annealing tutorials

quantum_annealing/*

(also found in <u>GitHub</u>) but if you want to execute it open it in AWS.

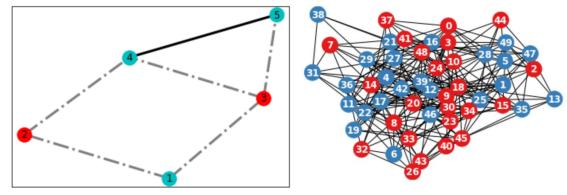
- Classical combinatorial problems: MAXCUT, Graph partitioning, Min vertex cover, Traveling Salesman Person
- Other cases: Factoring, Structural Imbalance

Check (and run) them all



Your plot is saved to maxcut_plot.png

EPPER



Result to MVC problem: [1, 3, 4, 6, 8, 9] Size of the vertex cover: 6

