Université Paris-Saclay,
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Benchmarking DWave Quantum Computers within the BACQ initiative

Aspect of programming and optimizing for Quantum Annealers

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TQCI seminar Dec. 4th 2025

Section 1

Context

Context: French QC applicative benchmarking “BACQ”

A polyvalent suite of benchmark for applications of QC addressing several fields

Simulation of Quantum Physics
(Quantum phase transition: Ising model in transverse field, 2D Hubbard model)

Optimization
(including Q-Score/MAXCUT)

Linear Systems Solving

Prime factorization

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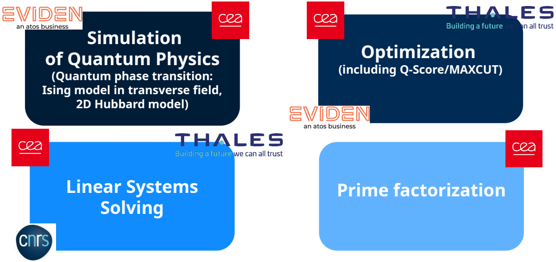

We aim to address all possible kind of QC harware, including:

- gate-based quantum computers
- analog quantum computers and quantum annealers

Application to quantum annealers (D-Wave)

D-Wave quantum annealers are a series of quantum computers:

- The oldest commercial series of quantum computers
- Not universal QCs (not gate-based)
- Primarily aimed at optimization problems (all generations) or quantum simulations (Advantage-2 only)

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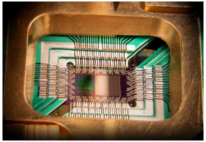
- Optimization:
  - ATOS/Eviden Q-Score (MaxCut), SotA TNO:
    - DW-2000Q **QScore= 70**
    - DW-Advantage **QScore= 180**
  - **MCM Gn series (to be presented)**
- Prime factorization:
  - SotA: DW-Advantage current best: factorization of $8,219,999 = 32,749 \times 251$
- **Linear System Solving (to be presented)**

D-Wave Quantum Annealers: main points



Canadian Enterprise funded in 1999. Provider of quantum computing solutions since 2009

- Superconducting flux qubits (nobium)
- 5 generations of QPU: 128, 1152, 2048, 5000+
- next generation: Advantage 2, 7440 qubits (end of 2024?)
- Principle: Quantum Annealing (QA)

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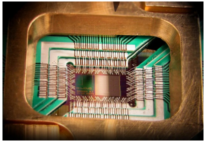

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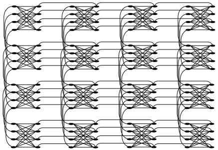

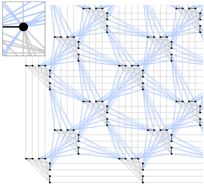

- Chimera= 6 connections/qubit
- Pegasus= 15 connections/qubit
- Zephyr= 20 connections/qubit

Really sparce compared to the number of qubits

Image credits: D-Wave™

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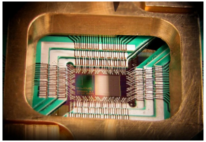

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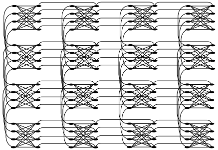

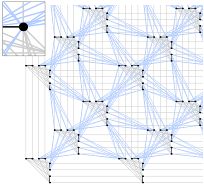

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Ising Hamiltonian

$$\mathcal{H}_{Is} = \sum_{i=0}^{n-1} h_i \sigma_i + \sum_i \sum_{j \neq i} J_{ij} \sigma_i \sigma_j \qquad \text{equiv. to QUBO problem} \qquad (1)$$

Section 2

Computing on DWave Annealers, what it means

QUBO problem, Ising Hamiltonian and Adiabatic evolution

- Generalized Ising problem (2D): $\mathcal{H}(\mathbf{h}, \mathbf{J}, \mathbf{s}) = \sum_i h_i s_i + \sum_{i<j} J_{ij} s_i s_j$ with s_k spins and $J_{i,j}$ coupling constants
- QUBO problems e.g. $f = x^T Qx = \sum_{i \leq j} q_{i,j} x_i x_j$ with $x_i \in \{0, 1\}, \forall i$

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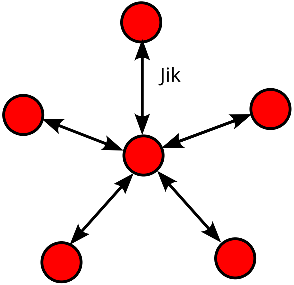
Quantum Annealing (QA) is inspired by the **Adiabatic theorem** of QM

$$\mathcal{H}(t) = f(1 - \frac{t}{\tau})\mathcal{H}_d + f(\frac{t}{\tau})\mathcal{H}_t \textbf{ with}$$
$$\begin{cases} \mathcal{H}_d = & \sum_i \sigma_i^x \\ \mathcal{H}_t = & \sum_i h_i \sigma_i^z + \sum_{(i,j) \in G} J_{i,j} \sigma_i^z \sigma_j^z \end{cases} \tag{2}$$

- $\mathcal{H}_d$ driver Hamiltonian
- $\mathcal{H}_t$ target Hamiltonian
- τ annealing time

Principles and caveats of minor-embedding on D-Wave

Illustration: case of an architecture with 4 couplings/qubit and a problem with 5 couplings



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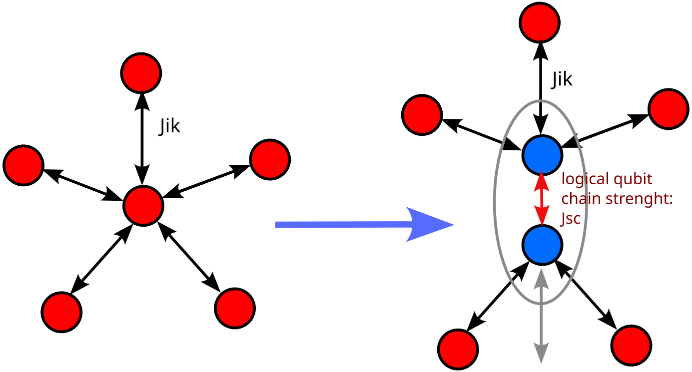

- Decide variable allocation and mapping (minor-embedding, NP-hard)
- Decide the chain-strenght: usually as a ratio (Relative Chain Strength, RCS)

Solving a problem on a D-Wave QPU: modus operandi

- Transform the problem into a QUBO problem or an Ising Hamiltonian
- Embed the Ising problem on the graph topology of the target QPU
  - It is utterly rare to match the topology of the DWave QPU
  - Method 1: use the hybrid solver from D-Wave
    - con: black-box, no guarantee that the QPU will be usefully taken into the work
  - Method 2: use the embedding tools of the D-Wave Ocean toolbox
    - con: quickly augments the number of qubits utilized. May fail, and rarely achieve a near optimal embedding, expect results up to $\simeq 150$ variables
- Use SRT to lower the impact of spin biases in the QPU
- Tweak the large amount of internal parameters of the QPU, notably:
  - Annealing time
  - Pause in annealing (from DW2000Q+) or reverse annealing (from Advantage+)
  - Try to obtain better embeddings and optimize the relative chain strength (RCS)
- Postprocess the results: statistical analysis, resolve logical-qubit discrepencies

Reducing biases: Spin Reversal Transform (SRT)

- The idea of SRT is to inverse a spin or negate a given variable, so:
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For auxiliary variables/qubits a simple way (e.g. to circumvent the topological limitations)

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- for r^* a good choice is generally between 0.5 and 3
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- **in case of logical qubits: possible to use open or closed chains, and use majority vote when the values of L-qubits don't agree at the Ph-qubit level**
- **auxiliary qubits are also necessary for quadratization methods (going from HOBO to QUBO where HOBO cost function is a generic polynomial of x_i)**

Quadratization

Quadratization is a tool to transform higher order polynomial cost functions into QUBO.
Several method exist e.g.:

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- NTR-KZFD (Negative Term Reduction by Kolmogorov, Zabih, Freedman and Drineas)
  - con: produces more terms, necessitate some rewriting
  - pro: the coefficients are (much) smaller

Section 3

Benchmarking Optimization problems on DWave

The choice of the Gn series as a benchmarking tool

Quantum Annealing being a heuristic we should treat it as such

- Finding a combinatorial problem with a simple to evaluate optimum
- ATOS defined the Q-Score [1] based on the Max-Cut problem (NP-hard, unconstrained)

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- A matching is a single bound between 2 populations (= constrained problem)
- A maximum matching is the configuration of matchings that maximize their number
- The G_n series = instances of MCM, easy to solve
  - demonstrated the slow convergence of the **Simulated Annealing** in some cases
  - $(n+1)^3$ possible matchings but only $(n+1)^2$ in the solution
  - Selecting randomly a given matching is increasingly counterproductive as n grows

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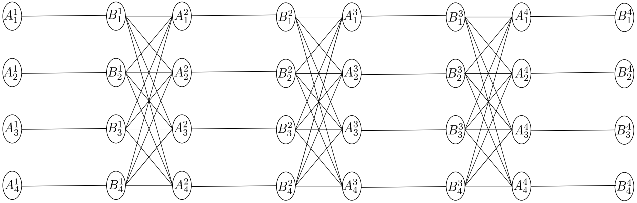
The G_n series = good candidate to complement the Q-Score on optimization

G_n series illustration

Exemple: G_3



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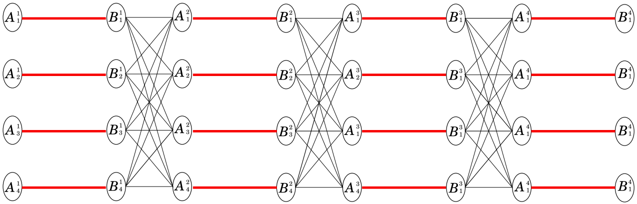

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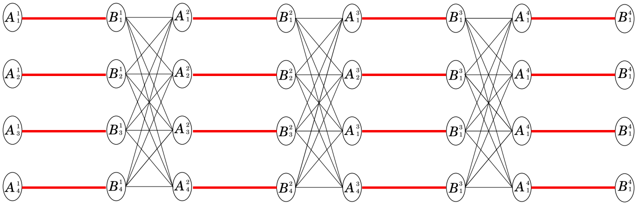

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We must adapt it to an Ising Hamiltonian/QUBO formulation

- The maximum matching problem is constrained $\neq$ QUBO/ISing
- Change the economic function (the Hamiltonian) to take the constraints into account
- Doing so transform the problem from hard constrained to soft constrained (good enough)

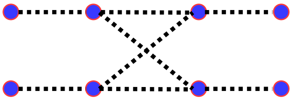
QUBO formulation

QUBO (for minimazation):

$$q_{ee} = -1 - 2\lambda \text{ et } q_{ee'} = \begin{cases} 2\lambda & \text{si } \exists v \in N / e \in \Gamma(v) \text{ and } e' \in \Gamma(v) \\ 0 & \textit{otherwise} \end{cases}$$

As $\sum_{e \in E} x_e \leq card\{E\}$ we can decide for $\lambda = card\{E\}$ as an upper value [3]

- Example: G1



$$Q_{G_1} = \begin{bmatrix} -17 & 0 & 16 & 16 & 0 & 0 & 0 & 0 \\ 0 & -17 & 0 & 0 & 16 & 16 & 0 & 0 \\ 0 & 0 & -17 & 16 & 16 & 0 & 16 & 0 \\ 0 & 0 & 0 & -17 & 0 & 16 & 0 & 16 \\ 0 & 0 & 0 & 0 & -17 & 16 & 16 & 0 \\ 0 & 0 & 0 & 0 & 0 & -17 & 0 & 16 \\ 0 & 0 & 0 & 0 & 0 & 0 & -17 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -17 \end{bmatrix}$$

QUBO formulation

QUBO (for minimazation):

$$q_{ee} = -1 - 2\lambda \text{ et } q_{ee'} = \begin{cases} 2\lambda & \text{si } \exists v \in N/e \in \Gamma(v) \text{ and } e' \in \Gamma(v) \\ 0 & \textit{otherwise} \end{cases}$$

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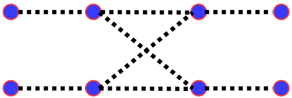

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- When n grows, the number of edge per vertex increases linearly
- $\Rightarrow$ the minor-embedding is rapidly an issue

Relevant parameters for improving the outcome

- In [3] the oldest architecture (Chimera), embedding constraints limited the achievable problems to G_4 in the best case (with at most 2000 qubits)
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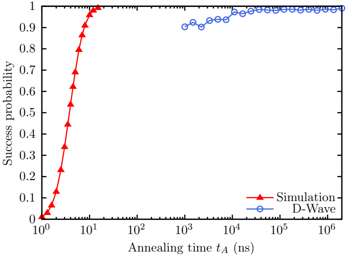


Comparing resolution of Schrodinger eq. on supercomputer vs D-Wave experiments (Advantage-2)

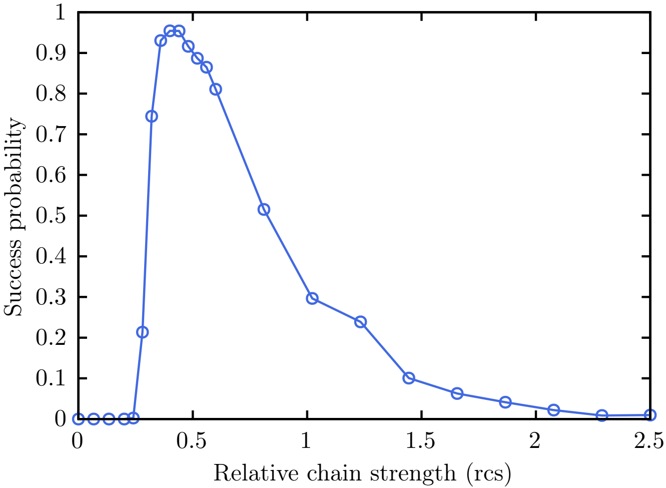
- Different from theoretical but not relevant

Section 4

Experiments on DWave familly of QPUs

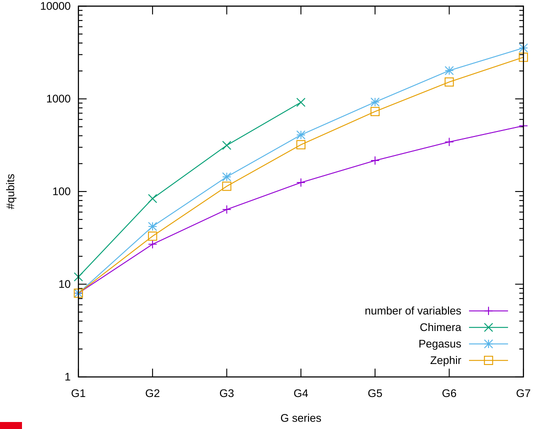
Impact of chain strength and minor-embedding

Relative Chain Strength must be well chosen to optimize the outcomes



Impact of minor-embedding

The number of qubits in the minor embedding should be reduced as much as possible to improve results



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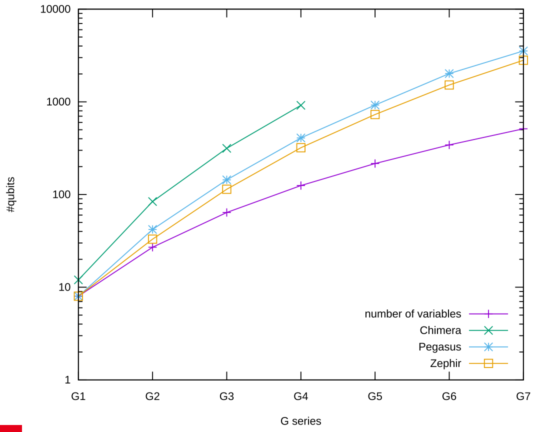

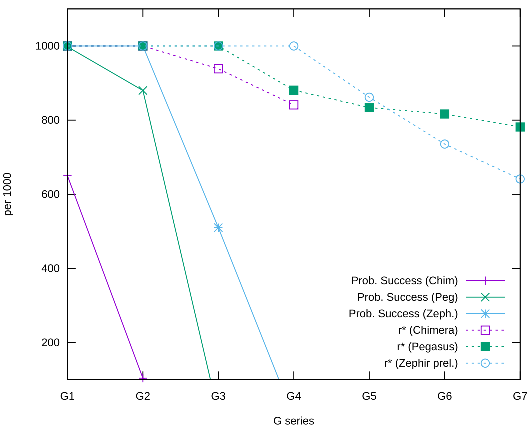

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- Cases where an exact solution is mandatory (e.g. LSS)
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- Cases where approximate solutions can be acceptable (e.g. Optimization problems)
  - Distance to optimum:
    - Hamming distance to optimum,
    - optimality score pondered by constraints violations

In the case of MCM (optimization problem we decided to mix both)

Definition of G-score

- The relative Hamming distance to the optimal solution

$$r_H = \frac{d_H}{(n+1)^3} \tag{3}$$

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- We define a ratio of optimality for the first “failed” G_n

$$r_o = \frac{1}{2}(1 - r_H + r_d) \tag{5}$$

G-score results

We define a weighted-score based on the probability of finding the optimal on the last "non-failed" G_n

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QPU architecture	n_s	r_o	p_o	S_G
DWave-2000Q (Chimera)	2	0.9375	84.9%	54.7
DWave Advantage (Pegasus)	3	0.904	1.8%	64.8
DWave Advantage-2 (Zephir)	3	0.936	11.0%	69.1
SA	5	0.92	4%	220
VA2	7	0.93	0.7%	513
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There is still a significant gap between QA and classical optimization heuristic. We can see improvements, nonetheless

Section 5

Linear System Solving

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Quantum Annealing / D-Wave quantum computers

- Are not easily comparable to gate-based QC
- Are specialized computer for Ising Hamiltonian simulations or QUBO solving
- Are not expected to reach exponential speedup (only polynomial)

State of the art: solving linear systems on D-Wave's QCs

Solving problem on D-Wave quantum annealers

To convey calculation on a D-Wave computer means finding a QUBO or Ising formulation whose minimum solves the initial problem

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N.B.: it is possible to solve non integer systems, but for benchmark, integers are fine

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Allows to express any integer in $\{-2^{r-1}, \cdots, 2^{r-1} - 1\}$ (same as 2's complement)

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$$c_i(\mathbf{x}) = \left[\sum_{j=0}^{N-1} a_{ij} \left(\sum_{k=0}^{r-1} x_{jk} 2^k - x_{jr} 2^r \right) - b_i \right]^2 \quad \text{and} \quad \mathcal{C}(\mathbf{x}) = \sum_{i=0}^{n-1} c_i(\mathbf{x}) \tag{9}$$

$\mathcal{C}(\mathbf{x})$ is quadratic, binary, its minimum is what we want$=$ a QUBO problem

First results and caveat of this method

The higher order coefficients of the QUBO cost function: $\mathcal{M}(\boldsymbol{x}) \propto 2^{2r} \sum_{i=0}^{n-1} x_{i,r}$

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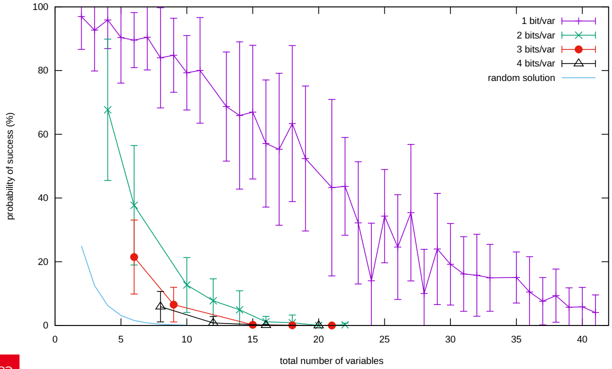

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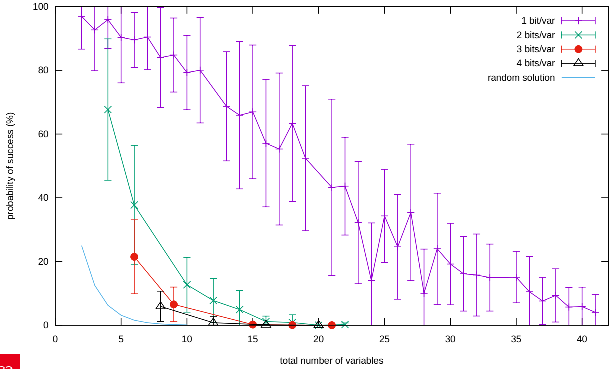

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The method is not scalable

First simple benchmark: 1 bit resolution, LSS

Limiting to binary solutions (1 bit resolution) avoids the exponential problem

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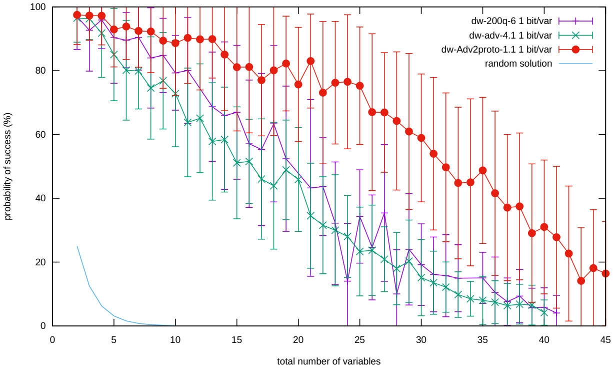

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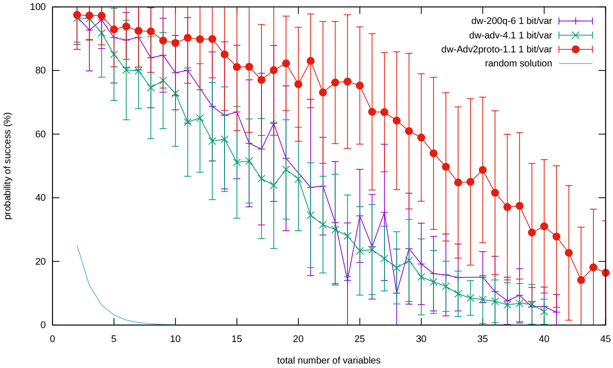

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QPU generation	x_o
Chimera (dw-2000q)	20.1 ± 1.8
Pegasus (dw-advantage)	17.8 ± 0.8
Zephyr (advantage2-proto)	31.8 ± 0.8

Improving the results: tweaking the minor-embedding

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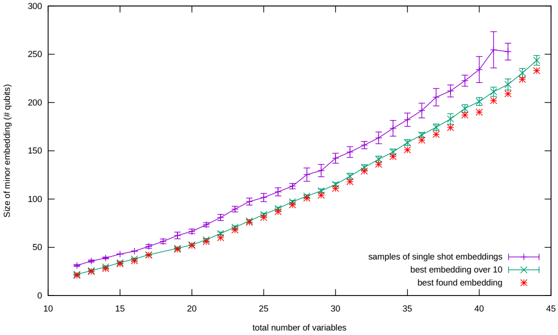

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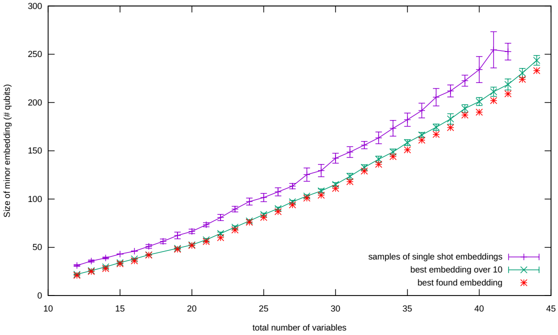

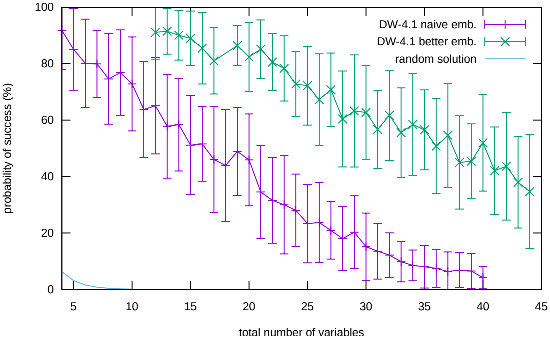

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inflection point: $17.8 \pm 0.8 \longrightarrow 37.0 \pm 1.2$

Much better benchmark result

Avoiding the exponential problem, a novel algorithm

Introduction on a simple example:

$$\begin{cases} X + Y + 1 = 0 \\ -X + Y + 3 = 0 \end{cases}$$

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$$\left\{ \begin{array}{llllllll}
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& & x_2 & & & +y_2 & & +c_1 - 2c_2 = 0 \\
\hline
x_0 & & & +y_0 & & & +1 & -2c'_0 = 0 \\
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And the cost function (QUBO problem):

$$\mathcal{C}(X, Y) = (x_0 + y_0 + 1 - 2c_0)^2 + \cdots + (x_0 + x_1 + x_2 + y_2 + c'_1 - 2c'_3 - 4c'_4)^2$$

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Nonetheless, this provide the base of an utility measure of solving linear systems with QA. We choose a large probability of finding the solution e.g. 20%

Experimental results

	2 vars, 3bits/v		2 vars, 4bits/v		3 vars, 3bits/v		3 vars, 4bits/v	
	std	2's	std	2's	std	2's	std	2's
Adv-4.1	22.1±6.3%	21.2±25%	4.5±3.4%	2.7±3.3%	2.0%	2.9%	0.12%	≈ 0.01%
Adv2-proto 40μs annealing	na	na	na	na	2.0%	2.7%	0.12%	0.19%
Adv2-proto 1ms annealing	25.3±21%	29.5±18%	9.4±7.9%	17.1±17%	1.9%	5.8%	0.25%	0.65%

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	2 vars, 3bits/v		2 vars, 4bits/v		3 vars, 3bits/v		3 vars, 4bits/v	
	std	2's	std	2's	std	2's	std	2's
Adv-4.1	**22.1$\pm$6.3%**	21.2$\pm$25%	**4.5$\pm$3.4%**	2.7$\pm$3.3%	2.0%	**2.9%**	**0.12%**	$\approx$ 0.01%
Adv2-proto 40μs annealing	na	na	na	na	2.0%	**2.7%**	0.12%	**0.19%**
Adv2-proto 1ms annealing	25.3$\pm$21%	**29.5$\pm$18%**	9.4$\pm$7.9%	**17.1$\pm$17%**	1.9%	**5.8%**	0.25%	**0.65%**

Without further improvements, the results would be a utility level of 2 variables with 3 bits of resolutions for LSS on D-Wave QA

Experimental results

	2 vars, 3bits/v		2 vars, 4bits/v		3 vars, 3bits/v		3 vars, 4bits/v	
	std	2's	std	2's	std	2's	std	2's
Adv-4.1	**22.1±6.3%**	21.2±25%	**4.5±3.4%**	2.7±3.3%	2.0%	**2.9%**	**0.12%**	≈ 0.01%
Adv2-proto 40μs annealing	na	na	na	na	2.0%	**2.7%**	0.12%	**0.19%**
Adv2-proto 1ms annealing	25.3±21%	**29.5±18%**	9.4±7.9%	**17.1±17%**	1.9%	**5.8%**	0.25%	**0.65%**

Without further improvements, the results would be a utility level of 2 variables with 3 bits of resolutions for LSS on D-Wave QA

The results really point at a **spectral gap issue**

- Next urgent step: mitigate the spectral gap issue and check if it improves

Conclusion and future work

- Contrary to intuition, Quantum Annealing (and other Quantum simulators) are much more versatile than initially thought (e.g. LSS)
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Future work:

- Think about generic ways of improving the spectral gap in target Hamiltonian
- Porting to other QPUs:
  - Work should start in early 2026-Q1 for Pasqal's Ruby QPU
  - Same for Lumy (Quandela)
  - if possible try IBM Quantum and IQM

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Merci

Thanks!

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