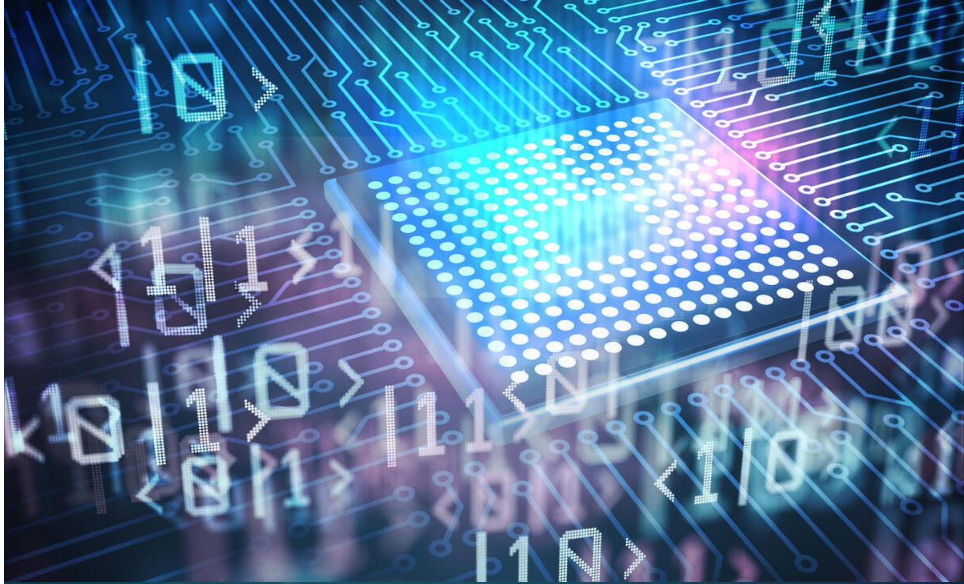
CSIRO

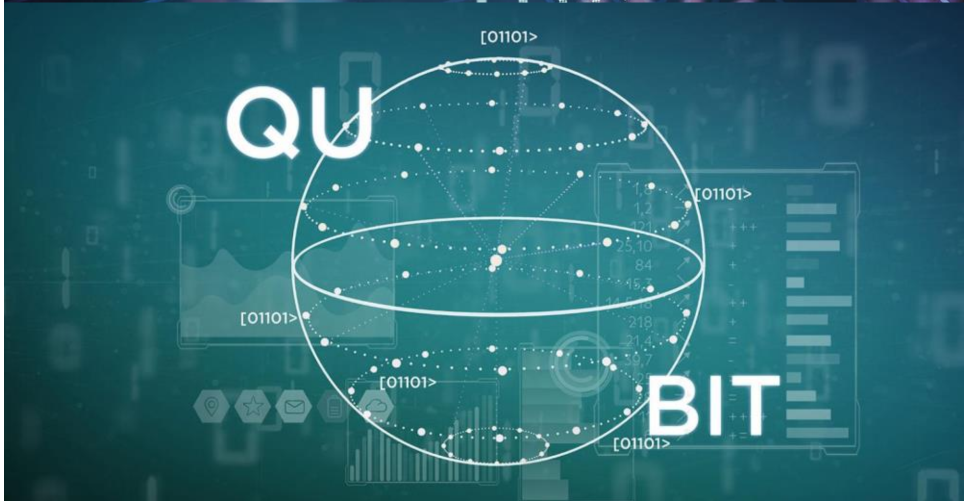
Applied Quantum Computing overview

- Quantum Annealing (QA) for optimization and Materials

Sam Yang, Tony Murphy, Peter Tyson, Clement Chu, Krzysztof Giergiel

CSIRO Manufacturing



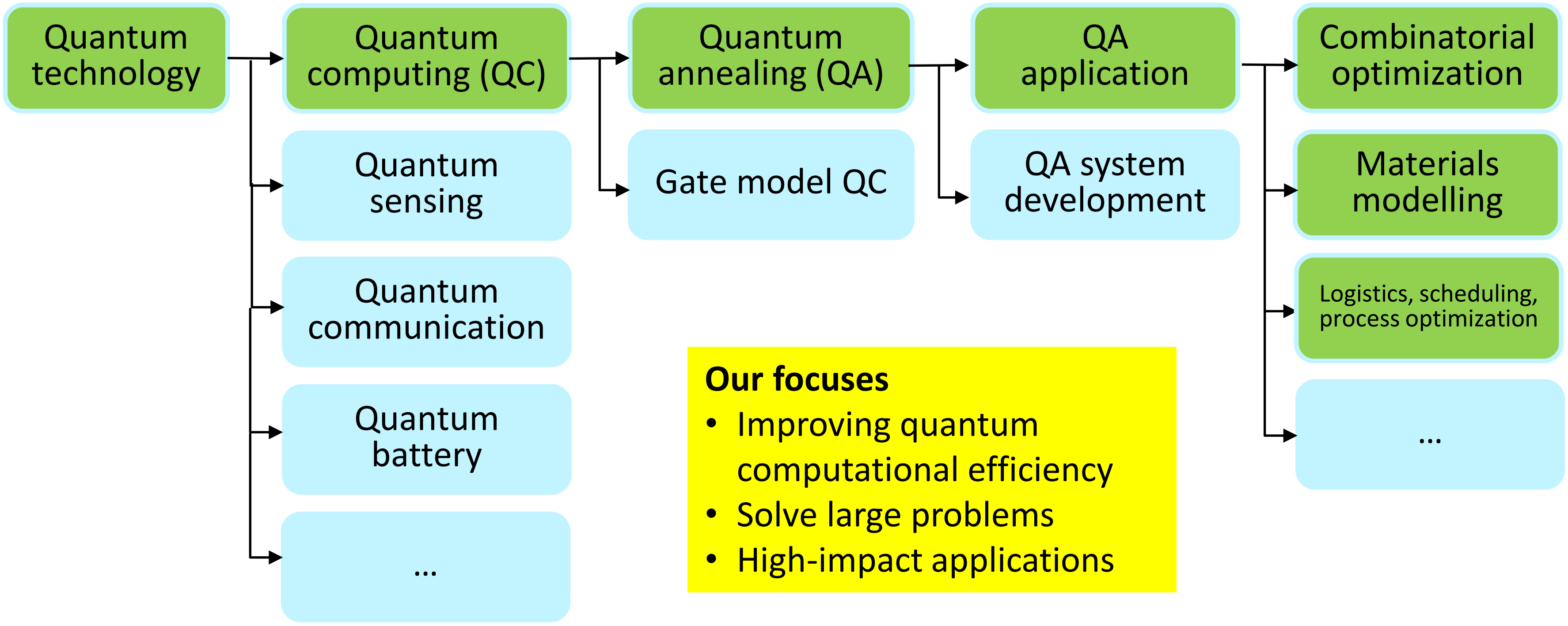


Contents

- Background: optimization, DCM, Ising spin-glass, QUBO
- Quantum annealing and simulated annealing
- Quantum computing error mitigation

Our applied quantum computing landscape

- **Research field & impact**



Our focuses
- Improving quantum computational efficiency
- Solve large problems
- High-impact applications

http://research.csiro.au/aqc

A simple optimization problem

- Four people: Xavier (x), Yolanda (y), Wanda (w), Zeke (z)
- Two rooms: 0 and 1
- Relations: x-y – friends, y-w – enemies, w-z – friends
- Objective: Locating people in 2 rooms such that friends are in the same room and enemies are not in the same room
- Numerical (binary) notation: x=0 – Xavier in room 0, x=1 = Xavier in room 1, etc.

x	y	z	w	objective
0	0	0	0	-2
0	0	0	1	-1
0	0	1	0	-2
0	0	1	1	-3
0	1	0	0	-2
0	1	0	1	-1
0	1	1	0	0
0	1	1	1	-1
1	1	0	0	-3
1	1	0	1	-2

- X-Y constraint: x+y-2xy. Same room 0, different room 1. That is, the objective function takes a lower value when Xavier and Yolanda are in the same room, and a higher value when they are in different rooms.
- W-Z constraint: w+z-2wz.
- Y-W constraint: negative of the above –y-w+2yw.
- Unconstrained objective function of the problem: x+y-2xy +w+z-2wz –y-w+2yw = x+z-2xy-2wz+2yw
- Optimal placement of people are achieved by adjust the binary values of x, y, w, z such that the objective function takes the minimum value.
- QUBO – quadratic unconstrained binary optimization
- Mathematically equivalent to Ising spin-glass formulation (0, 1) -> (-1, 1)
- Physical spins ↑, ↓
- Different weight for different constraints: : Lagrange multiplier or penalty factor
- Each room must have 2 people: $g*(x+y+z+w-2)^2$
- Each room can have no more than 2 people: $g*(x+y+z+w+p-2)^2$ - slack variables p
- Combinatorial optimization

DCM for lattice-style material microstructure modelling

- Data-constrained modelling (DCM, http://research.csiro.au/dcm is a method for determining the 3D distribution of materials with X-ray CT scans & statistical physics.
- $$T = \sum_{n=1}^{N} T_n \qquad T_n = \sum_{l=1}^{L} \left|\delta\mu_n^{(l)}\right|^{\beta=2} + E_n$$

  Objective function

  Linear absorption coefficient of material m with x-ray energy *l*

  $$\delta\mu_n^{(l)} = \sum_{m=0}^{M} \mu^{(m,l)} v_n^{(m)} - \hat{\mu}_n^{(l)} \Rightarrow 0 \qquad l = 1,2,\dots,L$$

  Number of X-ray beam energies (spectrums)

  X-ray CT reconstructed linear absorption coefficient for voxel n with X-ray energy *l*

  CT error for voxel *n* with beam energy *l*

  Volume fraction of material composition *m* in voxel *n* (multi-bit "Ising" spin s)

  $$\begin{cases} 0 \le v_n^{(m)} \le 1 \\ \sum_{m=0}^{M} v_n^{(m)} = 1 \end{cases} \qquad m = 0,1,2,\cdots,M;\ n = 1,2,\cdots,N$$

  Number of compositions *(M+1)*

  Number of voxels

  Strict constraint for each voxel

  Neighbouring interaction range

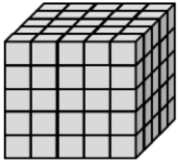
  Number of neighbouring voxels at distance *k*

  $$E_n = \sum_{m=0}^{M} S^{(m)} v_n^{(m)} + \sum_{k=0}^{K} \sum_{j=1}^{N^{(k)}} \sum_{m_1=0}^{M} \sum_{m_2=0}^{M} I_k^{(m_1,m_2)} \left(v_n^{(m_1)} v_{n+n_j^{(k)}}^{(m_2)}\right)^{\eta=1}$$

  Self energy for material composition *m* (applied magnetic field h)

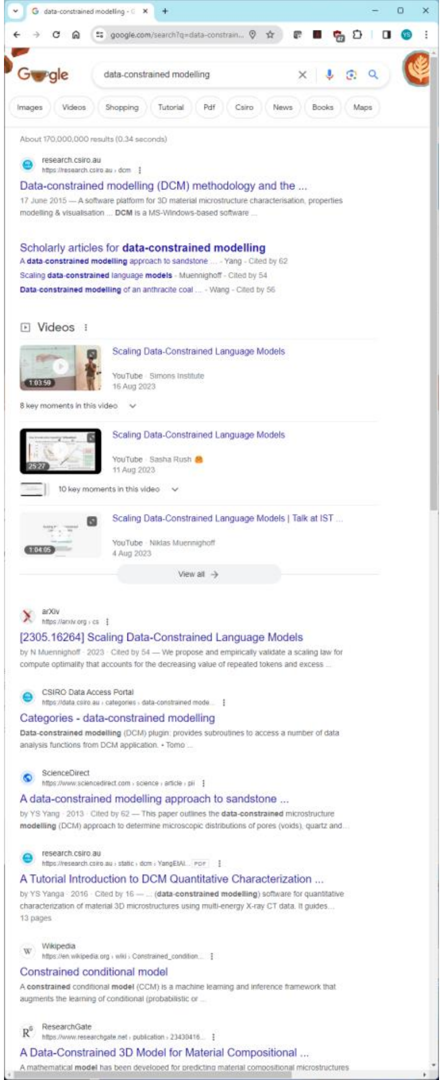
  Interaction energy between material compositions m_1 and m_2 at distance *k* (coupling energy between pairs of neighbouring spins J)

  Internal energy of voxel *n*. It is related to its own compositions and neighbouring voxels
- Typical size of the problem is N=1000^3 (academic, a billion) or N=4000^3 (industrial, 64 billions) voxels.
- Challenges include converging to local minima and computational efficiency – billions of voxels for a material sample.
- A problem is divided into sub-volumes for implementation on quantum annealers which have limited number of qubits.
- A sub-volume problem is expressed as Ising spin-glass / QUBO format for implementation on a quantum annealer



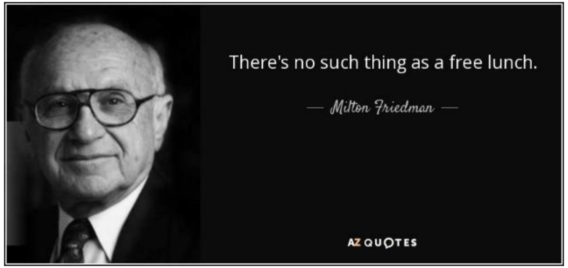
5x5x5 voxels sub-volume on a simple-cubic lattice / grid

$$\hat{T} = \sum_{<k,k_1>} \hat{J}_{\{k,k_1\}} s_k s_{k_1} + \sum_{k} \hat{h}_k s_k + \text{constant}$$



Community acceptance

- Advanced features are attractive
- Discounted price is more attractive
- Free offering is even more attractive



- Design complexity is free with additive manufacturing (3D printing)
  - ➢ Limitations in cost, productivity, porosity defect, distortion, fatigue life, corrosion resistance, …
- Parallel processing is free with quantum computing. e.g., 0.1ms to get a solution from a quantum annealer regardless of problem size
  - ➢ High qubit noise (~1%), limited number (<6,000) of qubits in a D-Wave Advantage QPU

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Classical versus quantum computers

- Programmable machine to manipulate physical quantities (observables): commonly electric voltage / current / fluid
- Bit: 0 or 1
- Binary & independent
- Billions or trillions of logical gates
- Error rate: 10^{-18}

- Programmable machine to manipulate quantum wave functions (collapsing to observables on completion): commonly superconducting current / photons /particle spins
- Qubit: a|0> + b|1>
- Superposition & entanglement
- 10s (gate model QC) or 1000s (QA) of qubits
- Error rate 10^{-3}

Quantum inspired classical simulators such as vector annealers?

(Combinatorial) Optimization computation: Simulated annealing versus quantum annealing

- Formulate the problem as computing the ground state of a Hamiltonian
- Ising spin-glass or QUBO – quadratic unconstrained binary optimization
- Perform multiple computations and select the solutions with the lowest energy
- “Independent / randomized” initial conditions for each computations
- Commonly used computing platform: Python with QPU cloud access

$$H = \sum_{\{k,k_1\}} \hat{J}_{\{k,k_1\}} s_k \, s_{k_1} + \sum_k \hat{h}_k \, s_k + \text{constant}$$

Simulated annealing (quantum inspired)

- Maximum entropy and minimum energy – minimizing free energy F= S – H/kT
- Start at high T and gradually lower it
- Classical logical gates
- Typical time per solution: 10 seconds
- Different implementations
- NEC vector annealer (100k qubits, Fujitsu Digital Annealer, Hitachi CMOS Annealer, Toshiba simulated bifurcator, …
- Local minima limited

Quantum annealing

- Adiabatic quantum computing / adiabatic theorem
  $H = H_0 + t{*}H_1$ (t: 0 → 1)
- Starting at ground state of H_0, gradually change t from 0 to 1.
- Qubits
- Typical time per solution: 0.1 millisecond
- Different qubit implementations
- D-Wave Systems (Advantage 5760 qubits, Advantage II 1200-7000 qubits), NEC quantum annealer (2030), QILIMANJARO QUANTUM TECH
- Qubit noise limited

Impact of qubit noise and local minima

- Solving a complex optimization problem may require large number of qubits / operations.
- Every qubit may be required to operate correctly to obtain a correct answer.
- In an ideal world, a computation is relatively insensitive to the problem size.
- High noise level for a physical qubit – order of 0.1-1%.
- Probability for correct answer decreases exponentially with the number of qubits. 100 qubits: $0.99^{100} = 0.37$; 1000 qubits: $0.99^{1000} = 4/100000$; 10000 qubits: $0.99^{10000} = 2 \times 10^{-44}$.
- Even if it converges to a minimum, it may only give a sub-optimal solution (local minima) rather than a true optimal solution (global minimum).
- Main stream thinking: using many (~ 1000) physical qubits to construct an error-corrected logical qubit

CSIRO SEMO technology & software

- An imperfect result from a quantum computer (such as a quantum annealer or simulator) is often not completely wrong. It contains (valuable) information about the correct answer (the true optimal solution).
- Using classical computing to mitigate errors – after measurements at completion of quantum computation.
- CSIRO has developed a patent-pending quantum computing spin-error mitigation for optimization (SEMO) technology to address the qubit noise and (to a degree) the local minima problems for solving combinatorial optimization problems with quantum/simulated annealers.
- The technology has been implemented as a SEMO Python dynamic module software – SEMO.pyd, with user-adjustable level of approximation.
- Four additional (essential) Python code lines are required to use SEMO:
  - `from SEMO import SEMO as SEMO`
  - `semo = SEMO(“xxxxxxxx-203d-42d2-a186-6f07c51c5d9c")`
  - `semo.SetupQUBO(qubo_coefficients)` or `semo.SetupIsing(linear_coefficients,quadratic_coefficients)`
  - `semo.DoErrorMitigation(variables, spins, energies)`
  - `semo.Help()`
  - `del semo`
- SEMO module is available now for CSIRO internal evaluation and testing

CSIRO SEMO technology evaluation with DCM on DWS Advantage

- Case study: binary image segmentation with data-constrained modelling (DCM, http://research.csiro.au/dcm).
- Randomly generated 3D cubit blocks ($1^3 – 10^3$) and with neighbouring coupling constant 0.1.
- For 512 (8x8x8) spins, QPU time speedup factors of 100,000 for SEMO I option 0 and 1 million for SEMO II option 2.
- For 1000 (10x10x10) spins and assuming the same exponential trend ($x^{1000}=(x^{500})^2$), the QPU time speedup factors would be ten billion SEMO I option 0 and one trillion for SEMO II option 2.
- The DCM problem with more than 1000 spins cannot be embedded on the DWS Advantage.
- With SEMO, QPU time increases *sub-linearly* – by a factor smaller than 100 with SEMO I option 0 and a factor smaller than 1.1 for SEMO II option 2, for problem size from 1 spin to 1000 spins.

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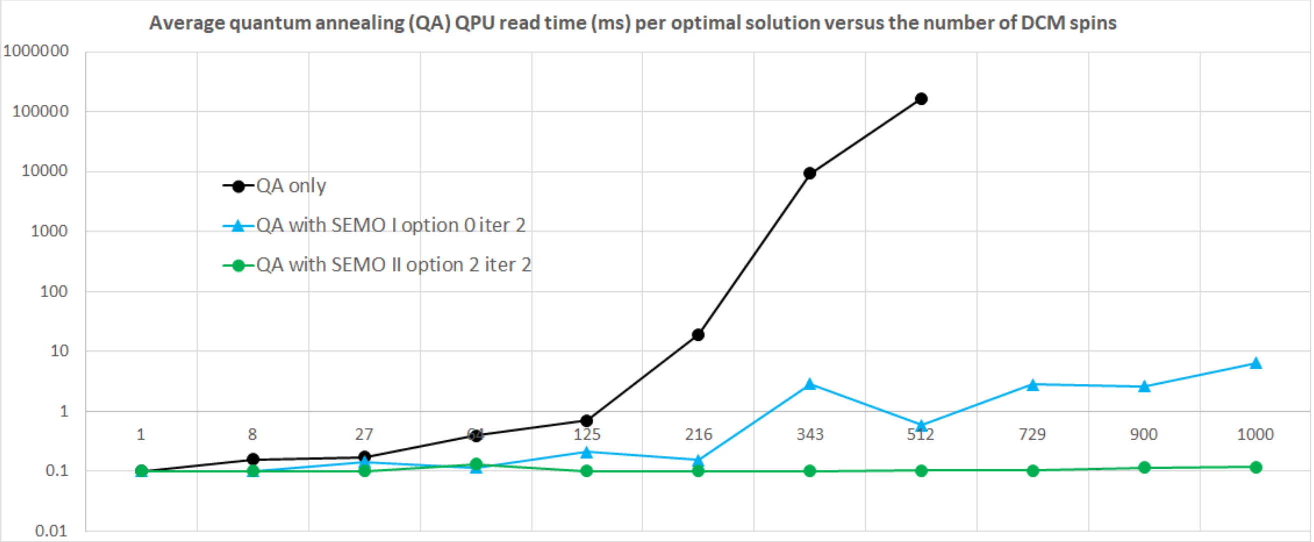

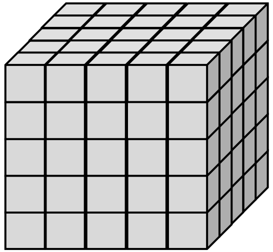

http://research.csiro.au/aqc

Summary

- Quantum annealing is for solving optimization problems
- Fundamental format is Ising spin-glass and QUBO (quadratic unconstrained binary optimization)
- Optimization objective function includes a weighted sum of constraints
- A range of problems can be formulated as the fundamental format
- Quantum annealers and quantum-inspired simulators are commercially available with 1000s to 100ks qubits
- Qubit noise and local minima are limiting factors
- CSIRO has a patent-pending solution for qubit errors and “local minima” issues

Thank you

Dr. Sam Yang
CSIRO Manufacturing
Principal Research Scientist

t: +61 3 9545 2759

e: sam.yang@csiro.au

Dr. Tony Murphy
CSIRO Manufacturing
Chief Research Scientist

t: +61 2 9413 7150

e: tony.murphy@csiro.au

w: http://research.csiro.au/aqc
e: appliedquantumcomputing@csiro.au