The next generation of techniques for quantum computing in continuous time

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EPSRC
Pioneering research and skills

A brief note about terminology

For the purposes of this talk:

- Adiabatic quantum computation (AQC) $\rightarrow$ *closed system* protocols where an eigenstate is maintained via the adiabatic theorem of quantum mechanics
- Quantum Annealing (QA) $\rightarrow$ *dissipation* from open system effects is the dominant mechanism

The terminology is not standardized and different groups may use these terms differently

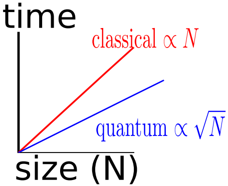
Why is a new generation of quantum algorithms necessary?

Early quantum devices are here

Before devices: proof-of-concept

- Algorithms with provable speedup
- As simple as possible to allow proofs
- Don't need real applications

- Heuristics not interesting $\rightarrow$ no way to test them



Now: real applications

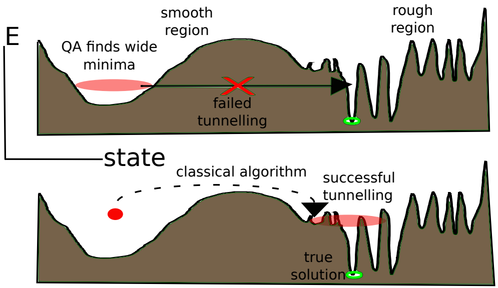
- Heuristics can be tested, don't need to be provable
- Need to take into account limitations of actual devices
- Real world problems

- Most 'provable' algorithms require too many resources

Image: public domain taken from wikimedia commons

Quantum is not a 'magic bullet'

Quantum protocols will be good at some things and bad at others



Optimisation Example: tunnelling suppressed by wide barriers

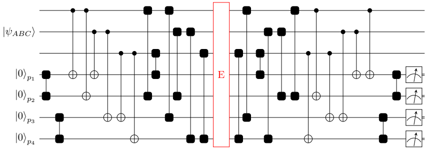
- Coherence limited so can't tunnel through wide barriers*
- Quantum algorithm only good at exploring 'rough' parts of energy landscape; quantum alone gets 'stuck' and fails
- But classical algorithms may be good at exploring smooth parts... hybrid quantum/classical algorithms

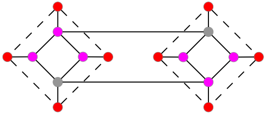
*Tunnelling through wide barriers could be interesting in highly coherent situations, see: arχiv:1807.04792

Gate model ~~versus~~ and continuous time

Gate model optimisation heuristics are very similar to continuous time evolution:

- Quantum approximate optimisation algorithm (QAOA) inspired by simulation of continuous time processes
- Variational quantum eigensolver (VQE) based on repeated measurements and changes $\rightarrow$ similar to thermal dissipation



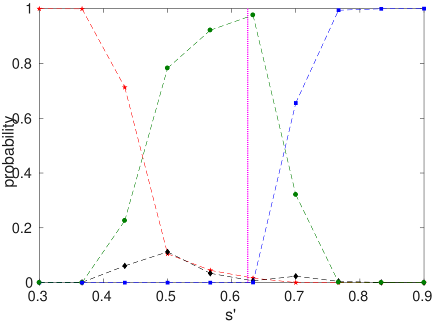


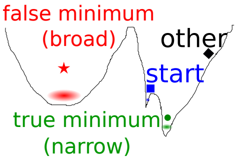
Large quantum annealers exist today:

- Testbed for quantum and hybrid quantum/classical heuristics
- Results can be ported to gate model setting as experimental platforms mature

Reverse annealing for quantum subroutines

- Start in candidate solution, search within range defined by $s' \in [0, 1]$ (smaller is longer range)
- Allows classical algorithm to guide local searches on D-Wave quantum annealers
- Figure is experimental data from a D-Wave device*





*For experimental details see my 2018 AQC talk (http://nicholas-chancellor.me/presentations.html) or come talk to me

Reverse annealing in algorithms*

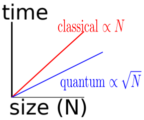
1. Start from one ground state to find other ground states (D-Wave whitpaper 14-1018A-A†)
   - Finding other GS 150x more likely then forward
2. Search locally around classical solution (arχiv:1810.08584†)
   - Start from greedy search solution
   - Speedup of 100x over forward annealing
3. Iterative search (arχiv:1808.08721†)
   - Iteratively increase search range until new solution found
   - Forward annealing could not solve any, reverse solved most
4. Quantum simulation(Nature 560 456–460 (2018)†)
   - Seed next call with result from previous
   - Seeding with previous state makes simulation possible
5. Monte Carlo and Genetic like algorithms (NJP 19, 2, 023024 (2017) and arχiv:1609.05875)
   - Transverse field parameter s' controls tradeoff between exploration and exploitation similar to temperature
   - Quantum analogues of many known classical algorithms
   - Genetic like composes guess from two or more known solutions

*† indicates experimental results

What does an early quantum advantage look like?

Old way of thinking:

Algorithm with known best classical scaling $\rightarrow$ QC performs better



- Not amenable to hybrid algorithms
- Scaling not known for important real world problems, we haven't even proven that $P \neq NP$!

More realistic:

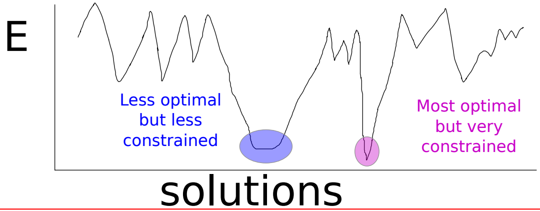
Meaningful improvement *in practice* by...

- finding more optimal solution than classical finds by itself,
- solving problem faster or using less energy,
- better sampling of a distribution,
- finding solutions which are better in some other way...

Enhancing Robustness of Solutions using reverse annealing

Using quantum annealers to find solutions which are robust in the sense that they can be adjusted to a modified problem definition at little or no energy cost

- Already known that annealers preferentially find good solutions which are ‘near’ other good solutions → leverage these effects algorithmically
- If a good solution is already known, can we use an annealer to trade optimality for robustness?



Funded by BP, NQIT, and EPSRC, work with Simon Benjamin group

bp

NQIT Networked Quantum Information Technologies

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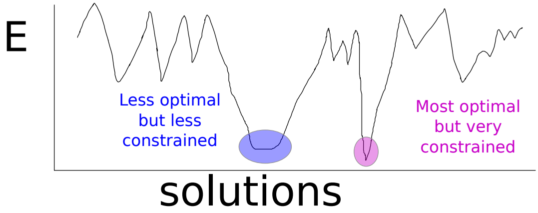
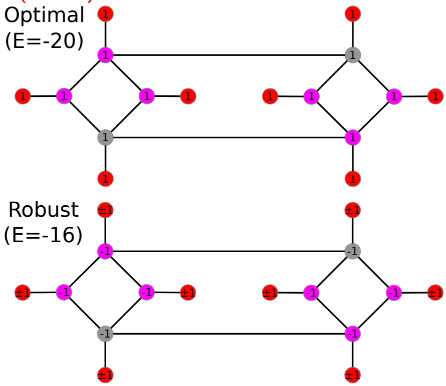
Why might we want this?

- Adjust solution if we later learn that our problem definition was slightly incorrect
- Penalty terms which are too expensive to encode on annealer could be implemented by adjustments in post-processing
  - Global non-linear constraints for instance are expensive to map
- Find ‘template’ solution which can be adjusted to solve many similar but not identical problems



A simple (motivational) example

Consider 16 qubit gadget from N. G. Dickson et. al. Nature Comm. 4, 1903 (2013) :



- a is the ground state but
- A D-Wave 2000Q with $1,280,000$ $5\mu s$ runs finds b $1,277,824$ times and a only 17 times

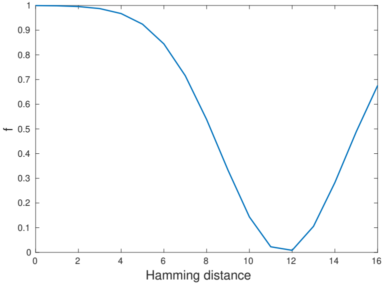
Simple test: add global penalty and do greedy search

Global penalty:

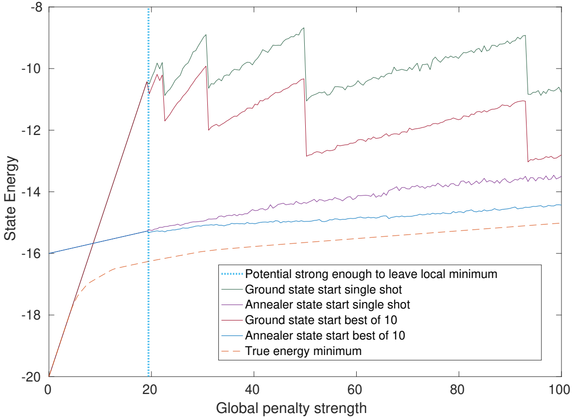
$$E(q) = E_{\text{Ising}}(q) + g\, f[\mathfrak{h}(q, r)]$$

where:

- q is a bitstring representing the state
- g is the strength of the penalty
- $\mathfrak{h}$ is Hamming distance
- r is a random bitstring
- f is a single variable function:



Starting in true ground state vs. state annealer finds



The large degeneracy in the state the annealer finds allows for much more effective adjustment → higher energy but more robust

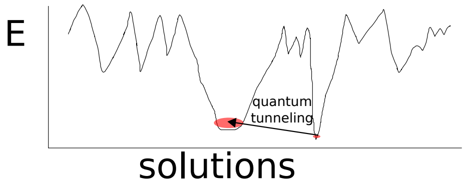
Reverse annealing to trade off optimality and robustness

Hypothetical situation:

- Already know the most optimal (planted) solution
- But we want more flexibility
- Are willing to 'pay' some optimality for a more flexible solution

Algorithm:

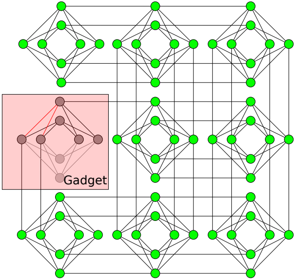
1. Start reverse annealing in planted solution
2. Search over a set range
3. Repeat many times
4. Keep most optimal solutions with certain robust features



Free variable gadgets (binary version)

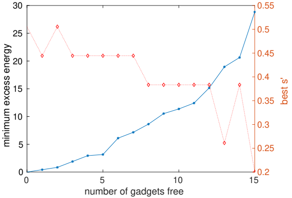
- Use planted solution method from Hen et. al. Phys. Rev. A 92, 042325 (2015) to make 'hard' problems with all -1 and all $+1$ ground state
- Before constructing replace some unit cells with 'free' variable gadgets
  - All variables fixed if 'outside' varibles agree
  - Become free (same energy for ± 1 values of some variables) if they do not (but energy unchanged)
  - Energy penalty because has to leave planted solution

Problem with planted solution (not shown)

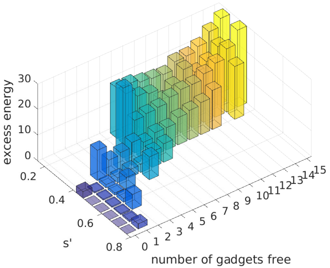


The tradeoff

What is the best excess energy we can find with a given number of gadgets free?

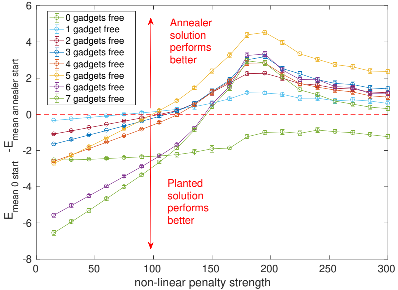


(smallest s' value taken in the event of a tie)



Putting new solutions to the test

- Choose $s' = 0.4444$ dataset $\rightarrow$ contains some of the best solutions
- Choose $10,000$ different instances of non-linear penalties
- Perform greedy search in each case and compare with planted solution
- Compare for different penalty strengths



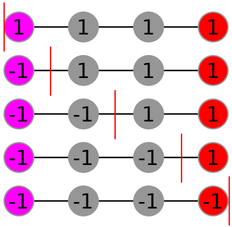
Crossover where annealer solution becomes the better choice

A more realistic version: integer variables

Concept of 'free' variables is a bit artificial much more natural for integer variables (broad versus narrow minima)

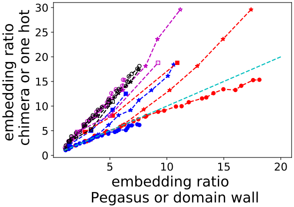
- Cumbersome to encode using traditional (one hot) method: N value integer variable $\rightarrow$ N qubit fully connected subgraph
- Better 'domain wall' encoding (see arχiv: 1903.05068)
  " " $\rightarrow$ $N-1$ qubit linearly connected subgraph

encoded value	qubit configuration
0	1111
1	-1111
2	-1-111
3	-1-1-11
4	-1-1-1-1



One slide aside: Domain wall encoding is a powerful tool for problem mapping

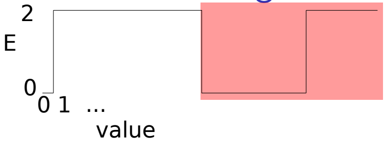
- Reduce number of qubits per variable by one
- Fewer connections within variable
- Structure tends to be better for embedding → technical reasons I won't discuss here see arχiv: 1903.05068



- Red and blue → comparisions of domain wall versus one hot
- magenta and black → effect of more advanced 'pegasus' hardware graph

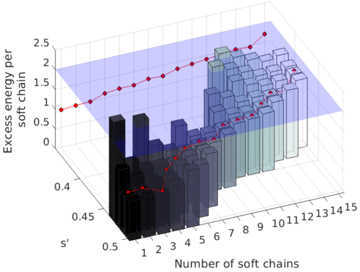
Domain wall encoding can make as much of a difference as rengineered hardware graph!

Finding robust solutions over integer variables



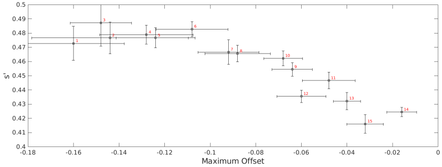
- Mixed integer/binary planted solution problem
- Unique minimum energy where binary part can be in lowest energy state
- Range over which it cannot, but has wider minima in red

Perform same experiment as for integer gadgets, chain is said to be 'soft' if domain wall is in wider minima

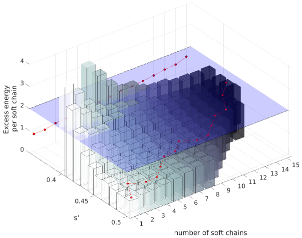


One more trick: anneal offsets

- Anneal different qubits by different amounts → more quantum fluctuations on the chains versus the other parts of the problem



Annealing less with smaller offsets useful if fewer soft chains desired

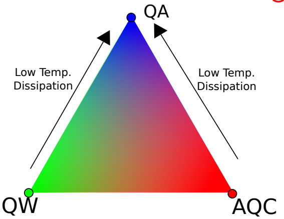


Quantum computing in continuous time

Three known ways in which continuous time quantum systems can solve problems, each has reverse annealing-like algorithm:

1. AQC (closed system) *slow transformation* $\rightarrow$ eigenstate maintained through adiabatic theorem of quantum mechanics Quant. Inf. Proc.10(1):33–52, (2011)
2. QA (open system) $\rightarrow$ low temperature dissipation finds low energy states reverse annealing relies on this dissipation
3. Quantum Walk (QW)$\rightarrow$ dynamics with a fixed Hamiltonian Phys. Rev. A **95**, 052309 (2017)*

Is there a method similar to reverse annealing which uses all three?



*Used to match energy, so subtly different than RA

Solving optimisation problems with QW*

Consider the following:

1. Transverse field Ising $H_d = -\sum_{i=1}^{n} \sigma_i^x$, $H_{\text{problem}} = \sum_{i=1}^{n} \sum_{j=1}^{n} J_{ij} \sigma_i^z \sigma_j^z$

$$H = \gamma\, H_d + H_{\text{problem}}$$

2. Start in ground state of H_d, $|\psi(t=0)\rangle = |\omega\rangle = \frac{1}{2^n} \sum_{i=1}^{2^n} |i\rangle$
3. By symmetry $\langle \omega \mid H_{\text{problem}} \mid \omega \rangle = 0$ $\therefore$ $\langle \psi(t=0) \mid H \mid \psi(t=0) \rangle = -\gamma\, n$
4. $\langle \psi(t>0) \mid H_d \mid \psi(t>0) \rangle \geq -\gamma\, n$ $\therefore$ by energy conservation $\langle \psi(t>0) \mid H_{\text{problem}} \mid \psi(t>0) \rangle \leq 0$ dynamics preferentially seeks out states with low energy w.r.t. H_{problem}

- Applied to Sherrington-Kirkpatric spin glass: arχiv:1903.05003 (see also: arχiv:1904.13339)
- Like extreme annealing schedule consisting of pause bracketed by instantaneous quenches

*Work with Viv Kendon and Adam Callison

Interpolating between AQC and QW

The energy conservation argument from the previous slide can be extended to any monotonic (closed system) quench

$$H(t) = A(t)\, H_d + B(t)\, H_{\text{problem}} \quad \frac{A(t)}{B(t)} \geq \frac{A(t+\delta t)}{B(t+\delta t)} \forall_t$$

Sketch of proof:

1. Trotterize time evolution: $A(t) \rightarrow A(t+\delta t)$ and $B(t) \rightarrow B(t+\delta t)$ and apply $|\psi(t+\delta t)\rangle = \exp(-iH(t)\delta t)|\psi(t)\rangle$ in separate steps
2. Rescale time so that Hamiltonian always resembles quantum walk $H_{eff}(\gamma(t)) = \gamma(t)\, H_d + H_{\text{problem}}$
3. In rescaled version $\gamma(t) \geq \gamma(t+\delta t) \therefore$ $\langle H_{eff}(\gamma(t))\rangle_{\psi(t)} - \gamma(t)\, n \geq \langle H_{eff}(\gamma(t+\delta t))\rangle_{\psi(t)} - \gamma(t+\delta t)\, n$
4. Because $\langle H_{eff}(\gamma(t))\rangle_{\psi(t)} \geq -\gamma(t)\, n \;\; \forall_t$, $\langle H_{\text{problem}}\rangle_{\psi(t)} \leq 0 \;\; \forall_t$

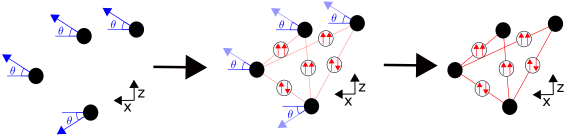
Biased driver Hamiltonian*

Define driver Hamiltonian using fields which are not (completely) transverse $H_d = \sum_{i=1}^{n} -\cos(\theta)\sigma_i^x - g_i \sin(\theta)\sigma_i^z$

- Start in ground state of H_d:
  $|\psi(t=0)\rangle = \bigotimes_{i=1}^{n} \frac{1}{\sqrt{2+2\,g_i\cos(\theta)}}[(1+g_i\cos(\theta))|0\rangle + \sin(\theta)|1\rangle]$
- Starting state biased toward classical bitstring g, $g_i \in \{-1,1\}$
- Closed system with monotonic sweep (including QW), time evolution improves the guess (on average):

$$\langle H_{\mathrm{problem}}\rangle_{\psi(t)} \leq \langle H_{\mathrm{problem}}\rangle_{\psi(0)}$$

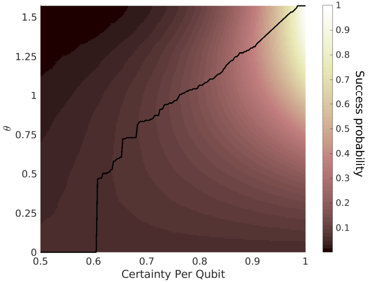
- Ground state is optimal solution so adiabatic theorem holds and dissipation can assist as well
  Can use AQC, QW and QA mechanisms simultaneously



*work with Laur Nita, Jie Chen, and Matthew Walsh. Note related work: arχiv:1906.02289 and Chinese Physics Letters, 30 **1** 010302

Preliminary Numerical Example *

- 10 qubit Sherrington-Kirkpatrick spin system
- Guess with bitwise certainty between 0.5 and 1
- Scan θ for QW to explore if biasing can help



- Hybrid strategy helps if over $\sim 60\%$ bitwise certainty
- Need to do more numerics, but encouraging

*courtesy of undergraduate project student Matthew Walsh

Take home messages

New algorithms and ways of thinking needed

- Existance of hardware changes what is interesting
- Hueristic and hybrid quantum/classical algorithms which solve real problems
- Quantum advantage can mean many things
  - Example: finding robust solutions

Gate model ~~versus~~ and continuous time

- Continuous time intuition useful for gate model heuristics
- Large annealers give opportunity to build intuition

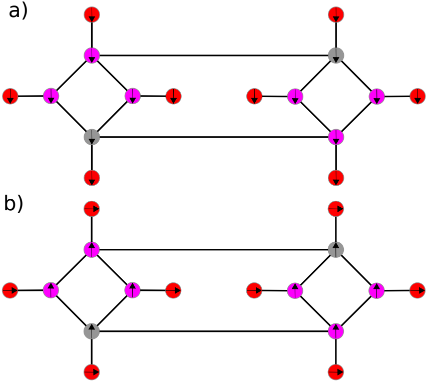
Multiple mechanisms in continuous time

- Hybrid subroutines which use multiple mechanisms at once
- Can prove advantage on average in closed system case

Supplemental slides

Constructing proof-of-principle Hamiltonian

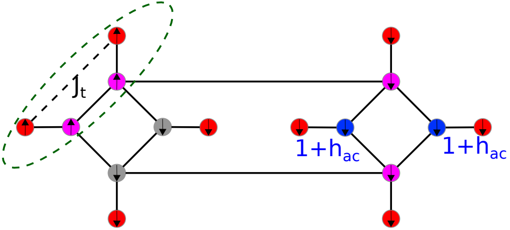
- Hamiltonians with features 1 and 2 are already known: free spin gadgets*
- Start with gadget from N. G. Dickson et. al. Nature Comm. 4, 1903 (2013)



- a: unique ground state (red, h=+1 violet h=-1)
- b: 256-fold degenerate excited state → false minimum

*See for instance: S. Boixo et. al. Nature Comm. 4, 3067 (2013)

Add local minimum and make tunable



- Starting state shown by arrows, ground state except for circled spins flipped blue field is in - direction
- J_t controls barrier between start state and ground state.
- h_{ac} controls the value of s_{cross}