Calibrating Simulations of Quantum Annealers for Predictive Models

Mike Zielewski, Keichi Takahashi,
Yoichi Shimomura, Hiroyuki Takizawa

TOHOKU UNIVERSITY

Cyberscience Center

Quantum Annealing (QA)

- Quantum metaheuristic for optimization problems
- System evolves under the time dependent Hamiltonian

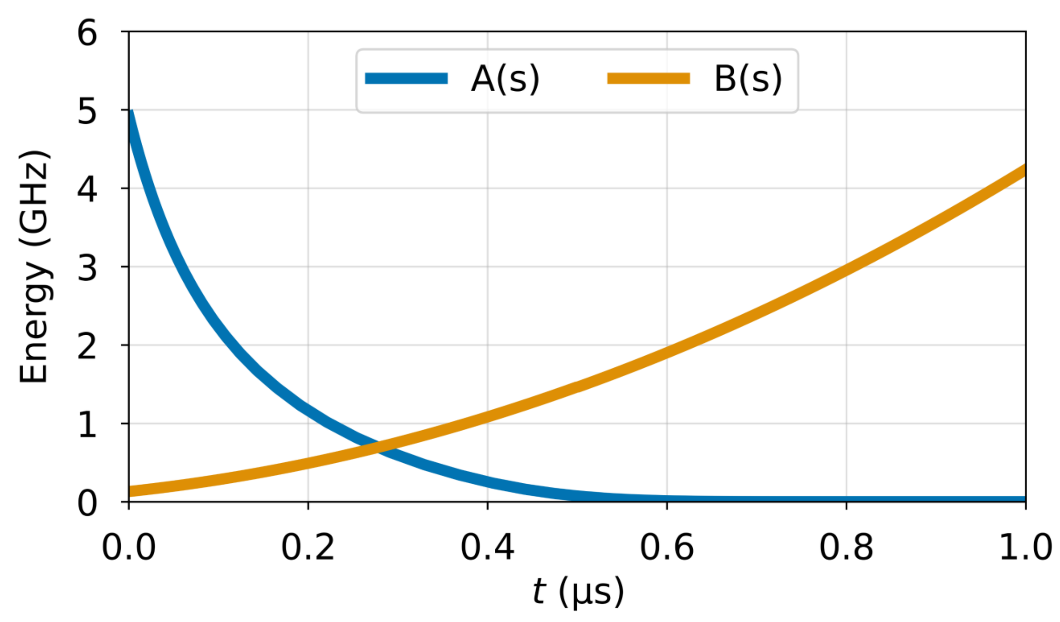
$$H(s) = A(s)H_D + B(s)H_P$$

H_D: quantum fluctuations, H_P: target problem,
s: annealing schedule

- Standard annealing schedule: $s(t) = t/t_a$

t: time, t_a: total time

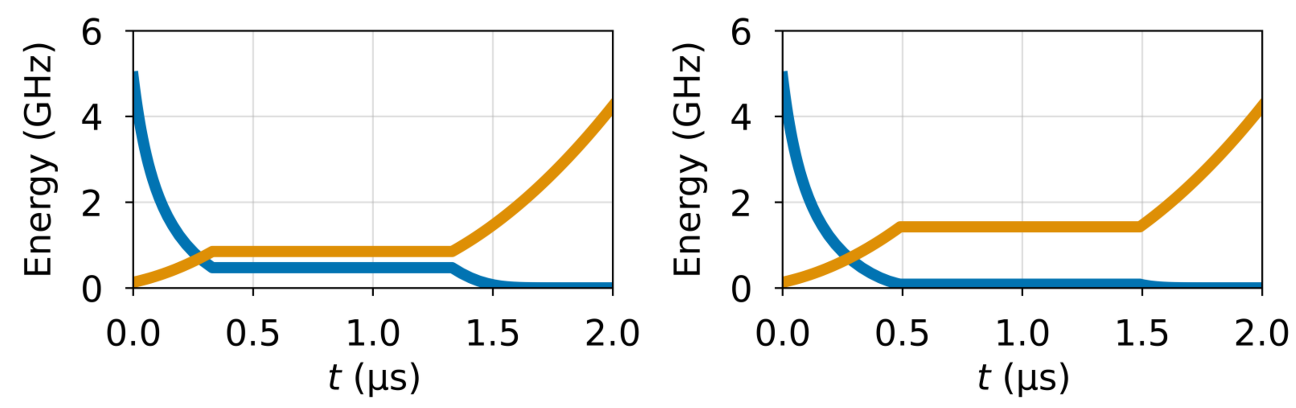
1µs forward annealing schedule

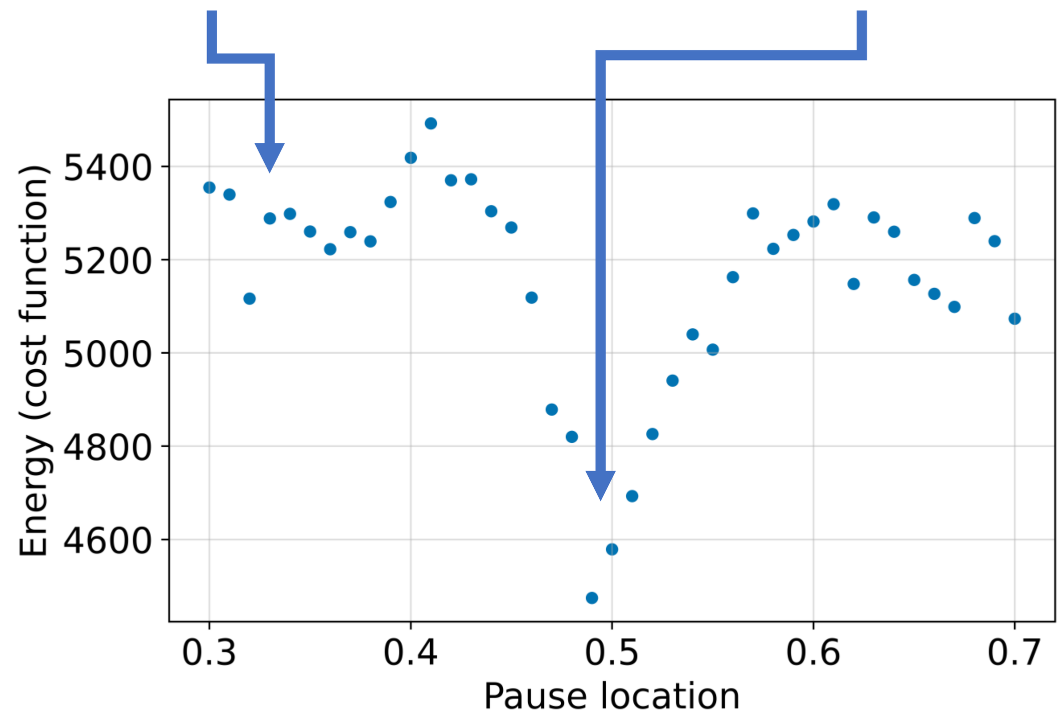


Pausing

- Annealing schedule modification where s is kept constant for a period of time
- May improve results depending upon pause location

1µs pause at $s = 0.33$ | 1µs pause at $s = 0.49$





- Problem and hardware properties, and other factors like embedding influence the optimal pause location

Spin-vector Monte Carlo with Transverse-field-dependent Updates (SVMC TF) [1]

- A classical model that represents qubits with angles $\in [0, \pi]$
- Angle updates are selected near the current angle, instead of being completely random
- As the transverse field weakens, the angle update range also becomes smaller, replicating the effects of freezeout
- Metropolis-Hastings style angle acceptance
- SVMC TF can replicate the effects of pausing in QA

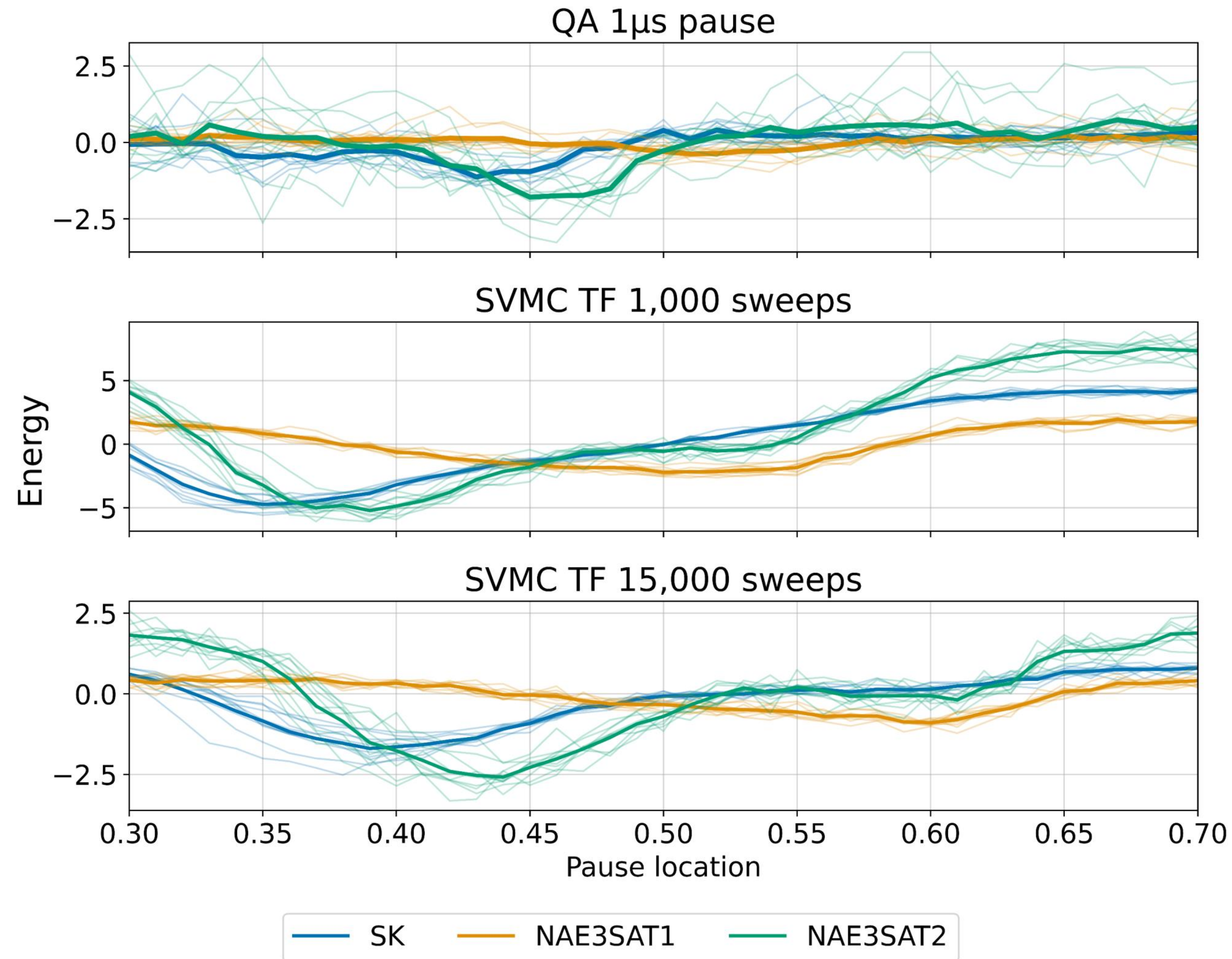
Motivation and Objective

- Our recent work combining SVMC TF and machine learning to predict optimal pause locations demonstrated improvements in multiple metrics [2]
- However, our proposal was unable to improve time-to-solution, indicating that the predicted optimal pause location was close to, but not exactly, the true value
- Root cause: annealer µs to SVMC TF sweeps ratio (1:10k)
- **What is a better approximation, is it problem dependent, and how can we find it with minimal annealer access time?**

Comparing Pausing in QA and SVMC TF

- The optimal pause location varies with problem type
  - SK – Sherrington Kirkpatrick model
  - NAE3SAT1/NAE3SAT2 – Not-all-equal 3-satisfiability with one and two clauses per variable, respectively

Average energy improvement from pausing



Distance from true optimal pause location

Problem type	Sweeps														
	1k	2k	3k	4k	5k	6k	7k	8k	9k	10k	11k	12k	13k	14k	15k
SK	.08	.06	.06	.06	.06	.05	.05	.04	.04	.05	**.03**	.04	**.03**	**.03**	.04
NAE3SAT1	**.01**	.03	.05	.05	.05	.07	.07	.07	.06	.07	.08	.08	.08	.07	.09
NAE3SAT2	.06	.05	.05	.05	.04	.03	.03	.03	.02	.03	.03	.02	.02	.02	**.01**

- No single µs to sweeps ratio works for all problems

Conclusions and Future Work

- Accurately simulating pausing with SVMC TF requires tuning the number of sweeps
- The value that leads to the highest correlation with quantum annealers varies significantly with problem type
- Accurate tuning can only be performed with access to a quantum annealer
- Future work: more efficient annealer access time utilization

Acknowledgments

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References

[1] "Comparing relaxation mechanisms in quantum and classical transverse-field annealing," *Phys. Rev. Appl.*, vol. 15, p. 014029, Jan 2021.
[2] "Efficient Pause Location Prediction Using Quantum Annealing Simulations and Machine Learning," *IEEE Access*, vol. 11, p. 104285, Sep 2023.