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Hybrid quantum annealing via molecular dynamics

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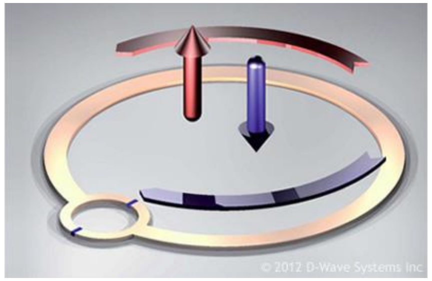
Tetsuo Hatsuda (RIKEN iTHEMS)

Joint iTHEMS – N3AS Meeting (2024.6.16-18)

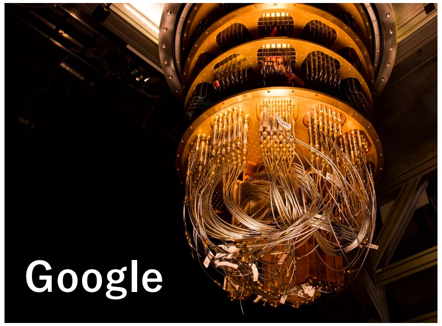


Superconducting Qubit (Quantum Bit)

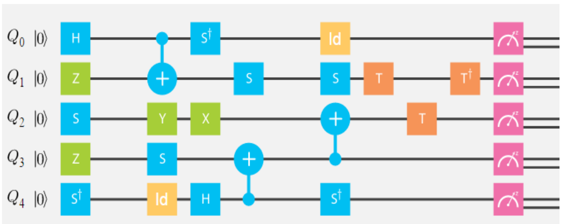
$$|\psi\rangle = \psi_0 |0\rangle + \psi_1 |1\rangle$$

Didital quantum computer
(Gate type)

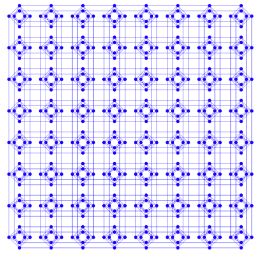
Analogue quantum computer
(Annealing type)

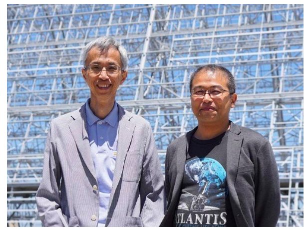


Feynman
(1981)



Equivalent under adiabatic time evolution



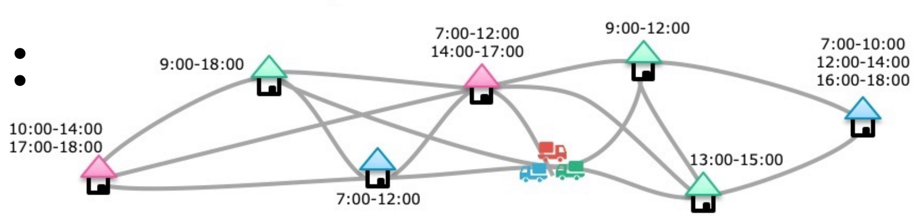


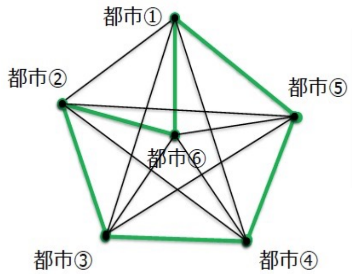
Nishimori & Kadowaki
(1998)

(review) Philipp Hauke et al 2020 Rep. Prog. Phys. 83 054401

Combinatorial optimization problems：

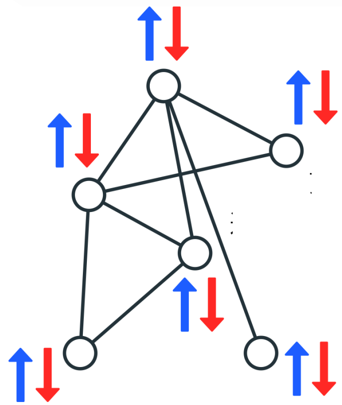
- Traveling salesman problem
- Vehicle routing problem
- Color-coding problem
- Portfolio in finance
  etc





Theorem：

Arbitrary combinatorial optimization problems can be mapped on the ground state search for Ising models with many-body interactions



$$\mathcal{H}_{\mathrm{Ising}}(s) = c_0 + \sum_{i}^{M} c_i s_i + \sum_{i<j}^{M} c_{ij} s_i s_j + \sum_{i<j<k}^{M} c_{ijk} s_i s_j s_k + \cdots + c_{12\cdots M} s_1 s_2 \cdots s_M$$

$$\mathcal{H}_{\text{Ising}}(s) = c_0 + \sum_{i}^{M} c_i s_i + \sum_{i<j}^{M} c_{ij} s_i s_j + \sum_{i<j<k}^{M} c_{ijk} s_i s_j s_k + \cdots + c_{12\cdots M} s_1 s_2 \cdots s_M$$

⇩ Auxiliary spins and constraints

Ising model with two-body interactions

$$\mathcal{H}_{\text{Ising}}(s) = \frac{1}{2}\sum_{i \neq j}^{N} J_{ij} s_i s_j + \sum_{i=1}^{N} h_i s_i,$$

Quantum anealing (Kadowaki-Nishimori)

$$\mathcal{H}_{\text{QA}}(\sigma;\tau) = A(\tau)\left[-\sum_{i=1}^{N} \sigma_i^x\right] + B(\tau)\left[\frac{1}{2}\sum_{i \neq j}^{N} J_{ij} \sigma_i^z \sigma_j^z + \sum_{i=1}^{N} h_i \sigma_i^z\right],$$

Optimization problem in 2^N dim ($N > 1000$) in NISQ eta ⇒ hybrid quantum annealing

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Hybrid quantum annealing via molecular dynamics

Hirotaka Irie[1,2]✉, Haozhao Liang[3,4], Takumi Doi[2,3], Shinya Gongyo[2,3] & Tetsuo Hatsuda[2]

A novel quantum–classical hybrid scheme is proposed to efficiently solve large-scale combinatorial optimization problems. The key concept is to introduce a Hamiltonian dynamics of the classical flux variables associated with the quantum spins of the transverse-field Ising model. Molecular dynamics of the classical fluxes can be used as a powerful preconditioner to sort out the frozen and ambivalent spins for quantum annealers. The performance and accuracy of our smooth hybridization in comparison to the standard classical algorithms (the tabu search and the simulated annealing) are demonstrated by employing the MAX-CUT and Ising spin-glass problems.

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Hybrid Quantum Annealing (HQA) with MD

Energy landscape in full 2^N dimension
Molecular dynamics (MD) for classical magnetic flux

$$\mathcal{H}_{\mathrm{MD}}(\varphi, p; \tau) = \alpha(\tau) \sum_{i=1}^{N} \left(\frac{p_i^2}{2} + V(\varphi_i) \right) + \beta(\tau) \left[\frac{1}{2} \sum_{i \neq j}^{N} J_{ij} \varphi_i \varphi_j + \sum_{i=1}^{N} h_i |\varphi_i| \varphi_i \right]$$

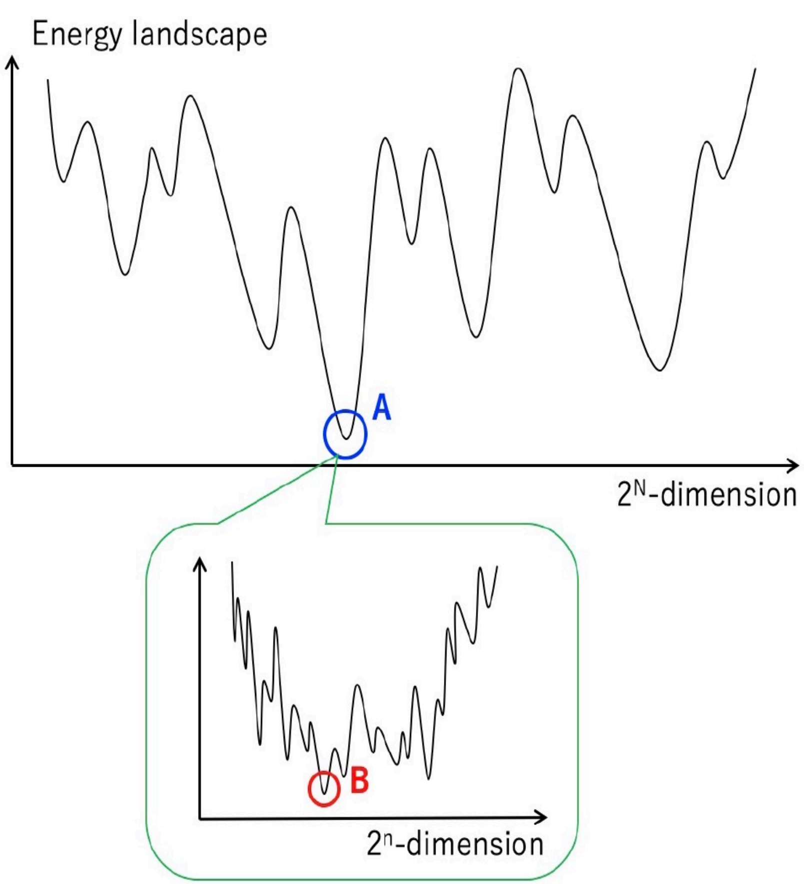
N=10,000

Seamless and automatic dimensional reduction

n=100

Energy landscape in reduced 2^n dimensions
Quantum annealing (QA) for Ising spin

$$\mathcal{H}_{\mathrm{QA}}(\sigma; \tau) = A(\tau) \left[-\sum_{i=1}^{n} \sigma_i^x \right] + B(\tau) \left[\frac{1}{2} \sum_{i \neq j}^{n} J_{ij} \sigma_i^z \sigma_j^z + \sum_{i=1}^{n} h_i \sigma_i^z \right]$$



CPU

GPU

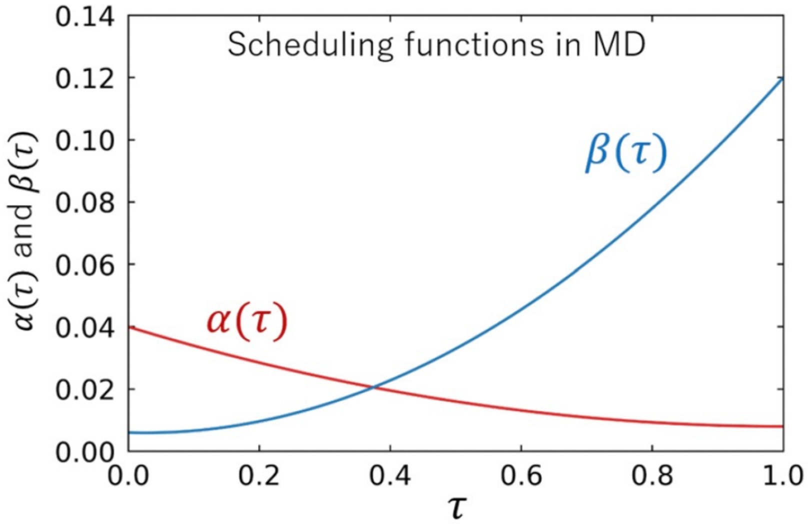
QPU

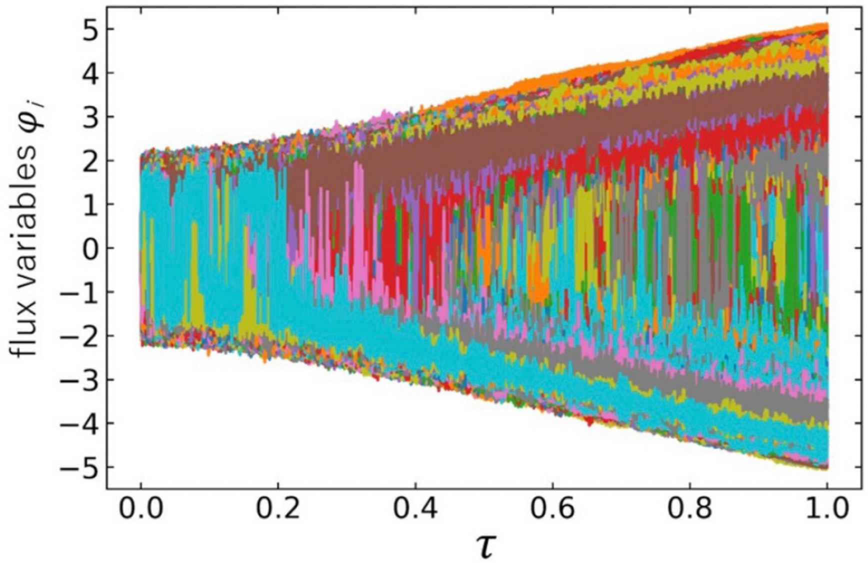
Molecular Dynamics

$$g\,\frac{d\varphi_i}{d\tau} = \frac{\partial \mathcal{H}_{\mathrm{MD}}(\varphi, p; \tau)}{\partial p_i}, \qquad g\,\frac{dp_i}{d\tau} = -\frac{\partial \mathcal{H}_{\mathrm{MD}}(\varphi, p; \tau)}{\partial \varphi_i},$$

$$\mathcal{H}_{\mathrm{MD}}(\varphi, p; \tau) = \alpha(\tau) \sum_{i=1}^{N} \left(\frac{p_i^2}{2} + V(\varphi_i) \right) + \beta(\tau) \left[\frac{1}{2} \sum_{i \neq j}^{N} J_{ij} \varphi_i \varphi_j + \sum_{i=1}^{N} h_i |\varphi_i| \varphi_i \right],$$

N=10,000



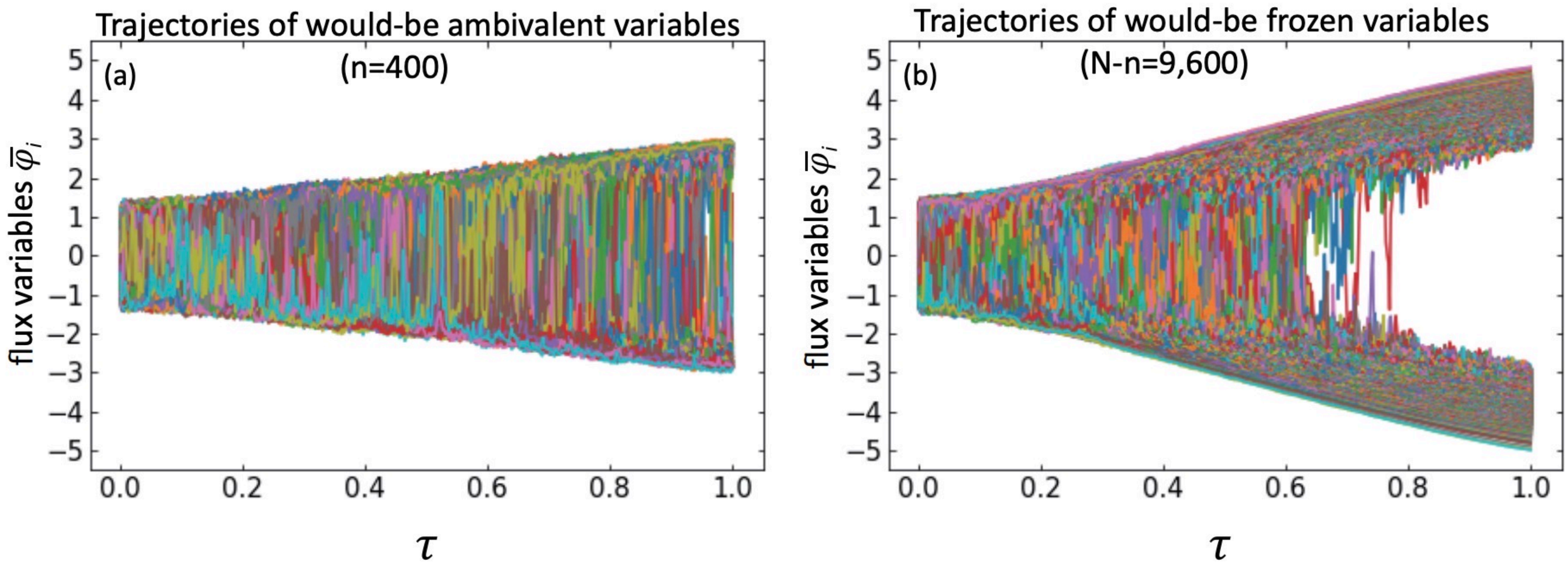


Molecular Dynamics

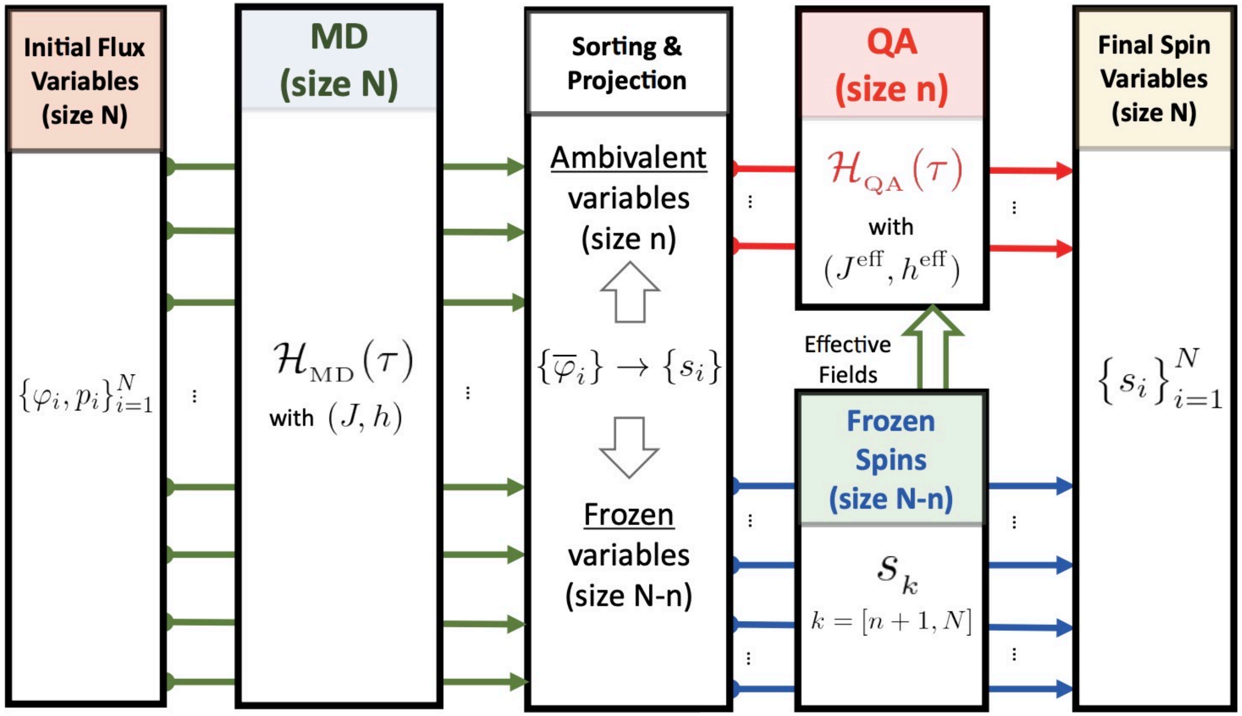
$$g\,\frac{d\varphi_i}{d\tau} = \frac{\partial \mathcal{H}_{\mathrm{MD}}(\varphi, p; \tau)}{\partial p_i}, \qquad g\,\frac{dp_i}{d\tau} = -\frac{\partial \mathcal{H}_{\mathrm{MD}}(\varphi, p; \tau)}{\partial \varphi_i},$$

$$\overline{\varphi}_i(\tau) \equiv \frac{1}{\delta}\int_{\tau-\delta}^{\tau} d\tau'\,\varphi_i(\tau'),$$

$$\left|\overline{\varphi}_{1'}(\tau=1)\right| \le \left|\overline{\varphi}_{2'}(\tau=1)\right| \le \cdots \le \left|\overline{\varphi}_{n'}(\tau=1)\right| \le \cdots \le \left|\overline{\varphi}_{N'}(\tau=1)\right|$$



Molecular Dynamics (MD) → Quantum Annealing (QA)



$$\mathcal{H}'_{\mathrm{Ising}}(s) = \frac{1}{2}\sum_{i' \neq j'}^{n} J^{\mathrm{eff}}_{i'j'} s_{i'} s_{j'} + \sum_{i'=1}^{n} h^{\mathrm{eff}}_{i'} s_{i'}$$

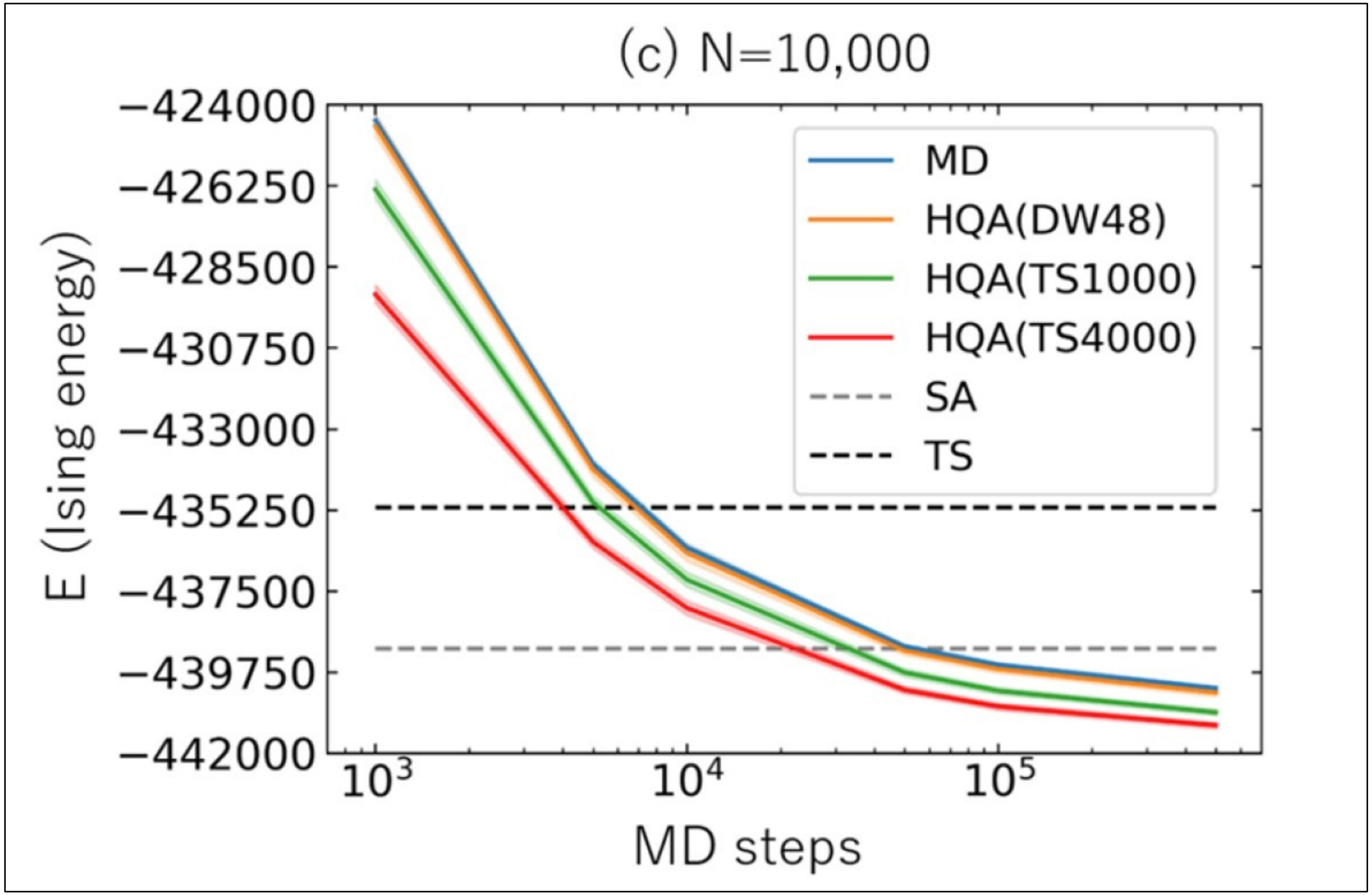
$$J^{\mathrm{eff}}_{i'j'} = J_{i'j'}, \quad h^{\mathrm{eff}}_{i'} = h_{i'} + \sum_{k'=n+1}^{N} J_{i'k'} s_{k'}, \quad (i', j' = 1, 2, \ldots, n).$$

Ising spin glass problem

$$\mathcal{H}_{\mathrm{Ising}}(s) = \frac{1}{2}\sum_{i\neq j}^{N} J_{ij} s_i s_j + \sum_{i=1}^{N} h_i s_i$$

$-1 \leq J_{ij} \leq +1$

$-2 \leq h_i \leq +2$



MD: Molecular Dynamics

HQA: Hybrid

SA: Simulated Annealing

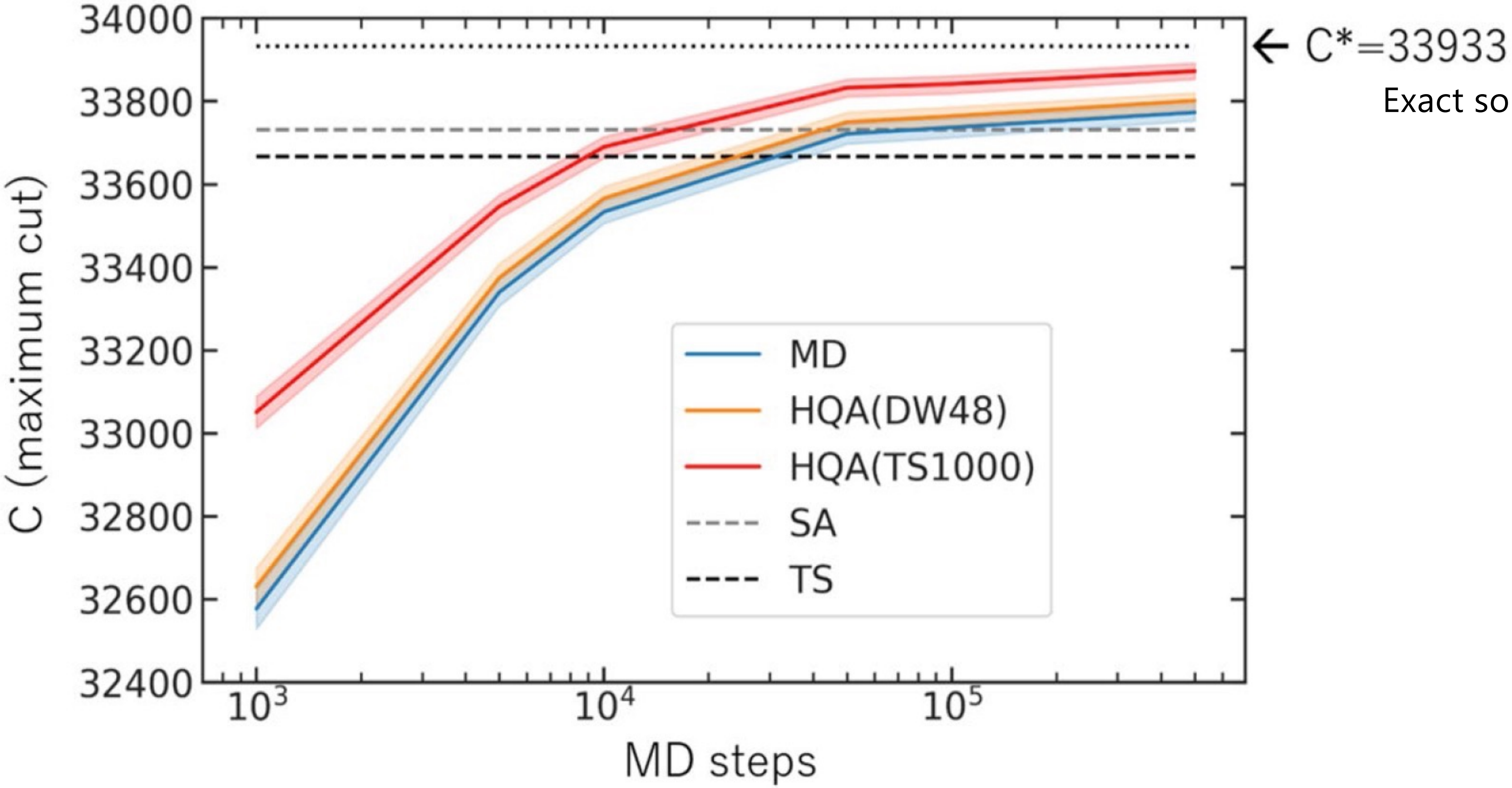
TS: Tabu Search

MAX-CUT problem

$$\mathcal{H}_{\text{Ising}}(s) = \frac{1}{2}\sum_{i\neq j}^{N} J_{ij}s_i s_j$$

$$J_{ij} = \pm 1$$

N=2000



Summary

- Quantum annealing：

  as classical optimizer → real-world applications

  as quantum simulator → basic science applications

- HQA with MD

  the fastest hybrid method for MAX-CUT problem
  at the time of 2021.

- Future

  better mathematical foundation on the error

  Ising model → Potts model

  quantum application???