Hybrid Quantum Annealing via Molecular Dynamics

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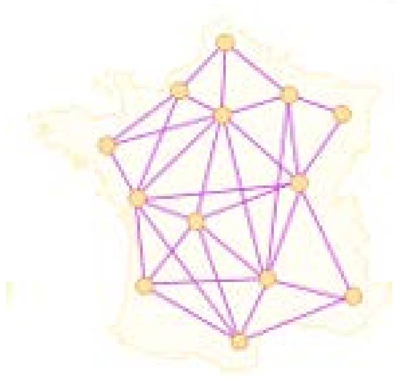
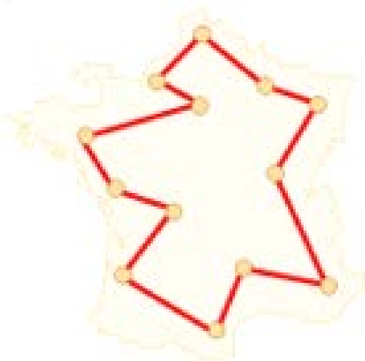
Challenge: combinatorial optimization problem

- Large scale combinatorial optimization problems are ubiquitous and their solutions have significant impact on science and society

Travelling salesperson problem (TSP)

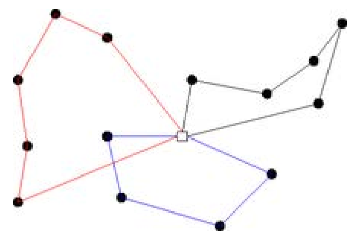




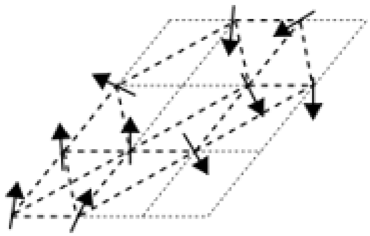
Find a shortest path which visits each city once and returns to the original city

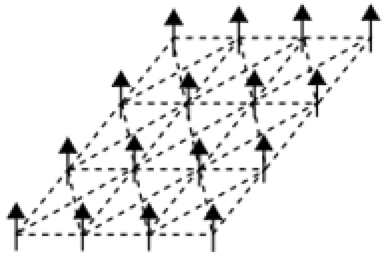
Vehicle routing problem (VRP)

(more generalization...)



Ising spin-glass model





Find a solution which minimizes the energy

(Figs from Wikipedia)

How to solve combinatorial optimization problems?

- Quantum Computing, in particular, Quantum Annealing (QA) is expected to be a powerful solution

Kadowaki-Nishimori (1998)

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

Trivial Hamiltonian　　　　Target Hamiltonian

$$A(\tau_i) \gg B(\tau_i), \quad A(\tau_f) \ll B(\tau_f)$$

Exploit quantum fluctuations instead of, e.g., thermal fluctuations in usual simulated annealing

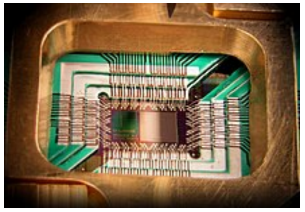
D-wave

- Rapid progress in QA hardware

but remains to be NISQ device
(noisy intermediate-scale quantum device)

N-qubit → ~$\sqrt{N}$-qubit
for fully-connected problem

2007: 16 qubit
2011: 128 qubit
2013: 512 qubit
2015: 1152 qubit
2017: 2048 qubit
2020: 5640 qubit
2023: 7000+ qubit
~24



How to solve combinatorial optimization problems?

- Effective use of classical computer is also crucial in NISQ-era

  Quantum-classical hybrid solver

  iterative use of QA solver from outer classical solver — Chancellor ('17), Okada et al. ('19)

  find persistent vars by multiple use of classical solver — Chardaire et al. ('15), Karimi- et al. ('17)

  New idea awaited!

  Classical-only solvers also in active development

  Coherent Ising machine (optical), CMOS annealing machine (SA/MA), Digital Annealer (SA)

  Simulated bifurcation machine (Molecular-Dynamics (MD)), ...

  In particular, MD is beneficial in scalability/performance but sys err introduced

  c.f. Quantum computer w/ gate-type qubits

  Suitable for more general problems

  #qubit = 5 ('16) → 27 ('19) → 433 ('22) → 4000+ ('25) [IBM]

  "Quantum supremacy" (google, '19): 200 sec (quantum) vs 10,000yrs (classical)

  (but 10,000yrs → 2.5days (IBM, '19) → 300sec (Liu+, '21) in classical)

We now consider the Ising spin problem

$$\mathcal{H} = \frac{1}{2}\sum_{i\neq j}^{N} J_{ij}\sigma_i^z\sigma_j^z + \sum_{i=1}^{N} h_i\sigma_i^z$$

How can we exploit the advantages of each of classical and quantum computers?

Molecular Dynamics (MD) to mimic QA

Quantum annealing (QA)

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

H (transverse) H (Ising)

$$\tau = [0,1] \qquad A(0) \gg B(0), \quad A(1) \ll B(1)$$

If $BJ_{ij} \leftrightarrow \beta J_{ij}|\varphi_i\varphi_j|$

$Bh_i \leftrightarrow \beta h_i|\varphi_i\varphi_i|$

Molecular Dynamics (MD)

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

H (+/- oscillation) ~ H (Ising)

φ_i : continuous flux variable

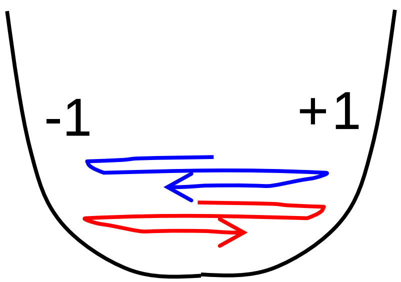
$$V(\varphi) = \varphi^M \quad (M = 4, 6, \cdots)$$

$$\tau = [0,1] \qquad \alpha(0) \gg \beta(0), \quad \alpha(1) \ll \beta(1)$$

Molecular Dynamics (MD) to mimic QA

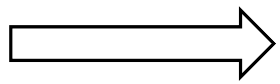
$$\mathcal{H}_{\rm MD}(\varphi, p; \tau) = \alpha(\tau) \sum_{i=1}^{N} \left(\frac{p_i^2}{2} + V(\varphi_i) \right) + \beta(\tau) \left[\frac{1}{2} \sum_{i \neq j}^{N} J_{ij} \varphi_i \varphi_j + \sum_{i=1}^{N} h_i |\varphi_i| \varphi_i \right]$$

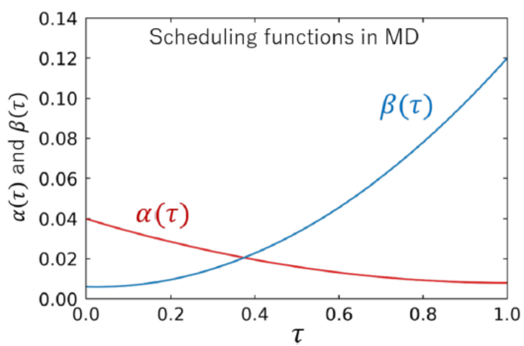
init cond: $\varphi_i(0) = 0, \quad p_i(0) = \pm 1$ (random)

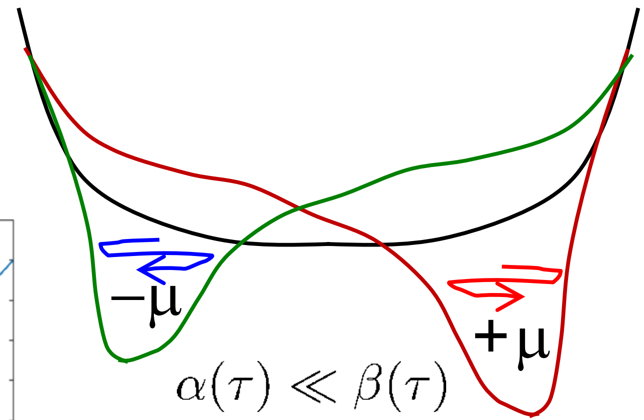


$\alpha(\tau) \gg \beta(\tau)$

$\tau \sim 0$



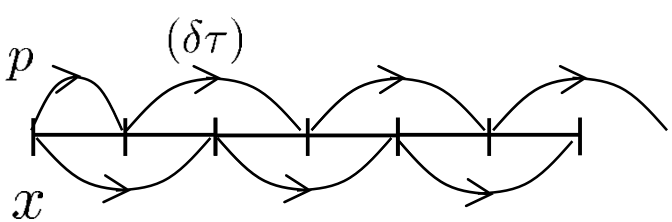




$\alpha(\tau) \ll \beta(\tau)$

$\tau \sim 1$

We solve MD by leap-frog method



- 2nd-order prec: $\mathcal{O}((\delta\tau)^2)$ err
- symplectic & time-reversal
  (if Hamiltonian does not have explicit τ-dep)

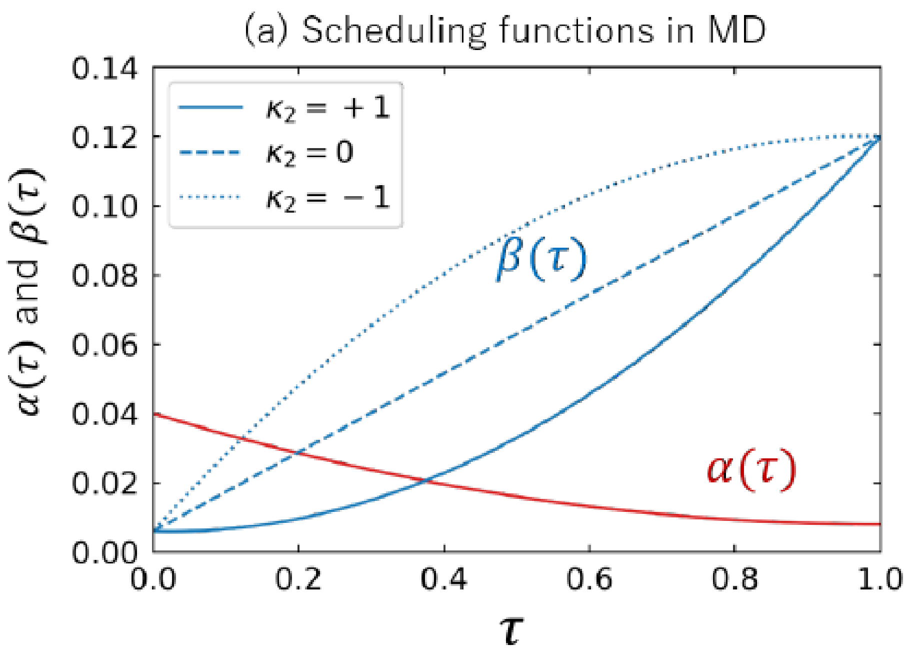
Our MD could be better than other MD solvers w/ artificial +/- barrier

(It can be improved by higher-prec solver)

Adiabaticity in MD

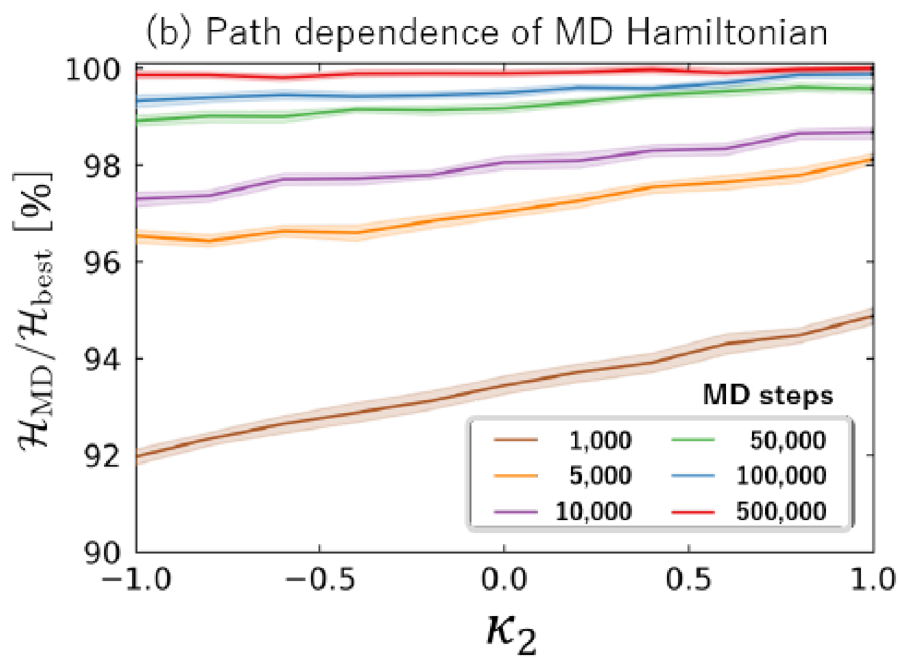
In the case of QA (AQC), it is guaranteed that the system is the ground state thanks to the quantum adiabatic theorem

In the case of MD, there is no such guarantee, so we make numerical check



$$\beta(\tau) = \beta_f\left(\tau + \kappa_1(1-\tau) + \kappa_2\tau(\tau-1)\right)$$

Test w/ Ising spin-glass, N=10,000
single instance, 10 initial condition



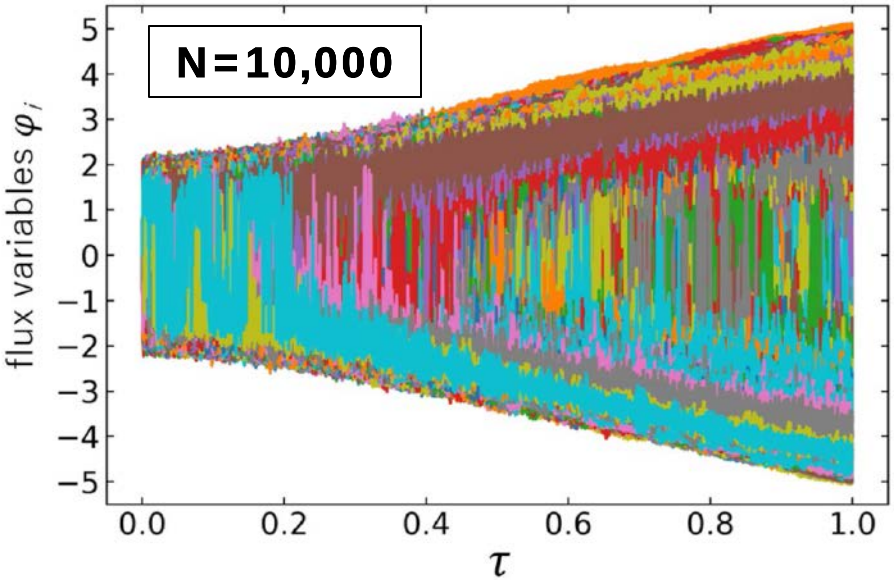
Final value of MD Hamiltonian H(τ=1) is indep of schedule function, in particular for finer MD step

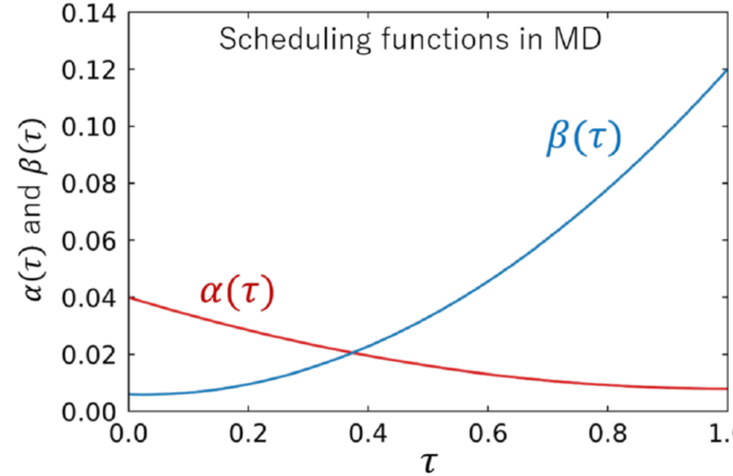
➔ Good Adiabaticity

Test of MD for Ising spin grass problem

$N = 10,000, \quad -1 \le J_{ij} \le +1, \quad -2 \le h_i \le +2$

$(\delta\tau)^{-1}_{\mathrm{MD}} = 50,000$





We observe a tendency that variables fall into two (+ or -) categories

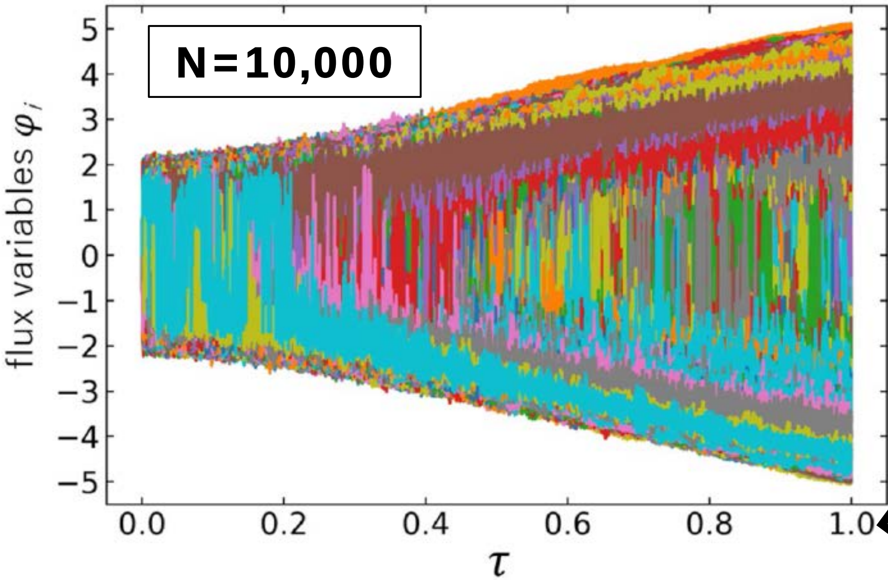
➔ MD works rather well

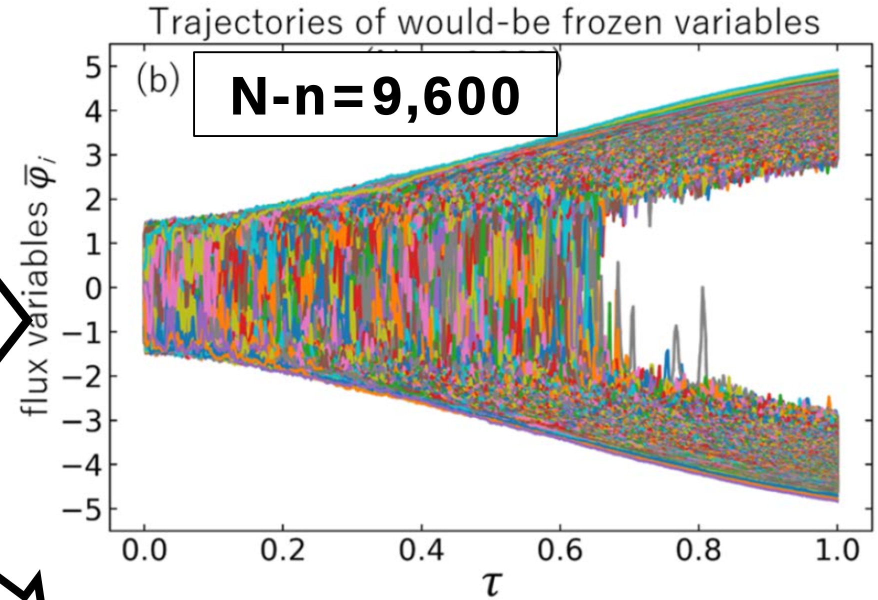
However, it takes additional long-time for "all" variables to be settled down

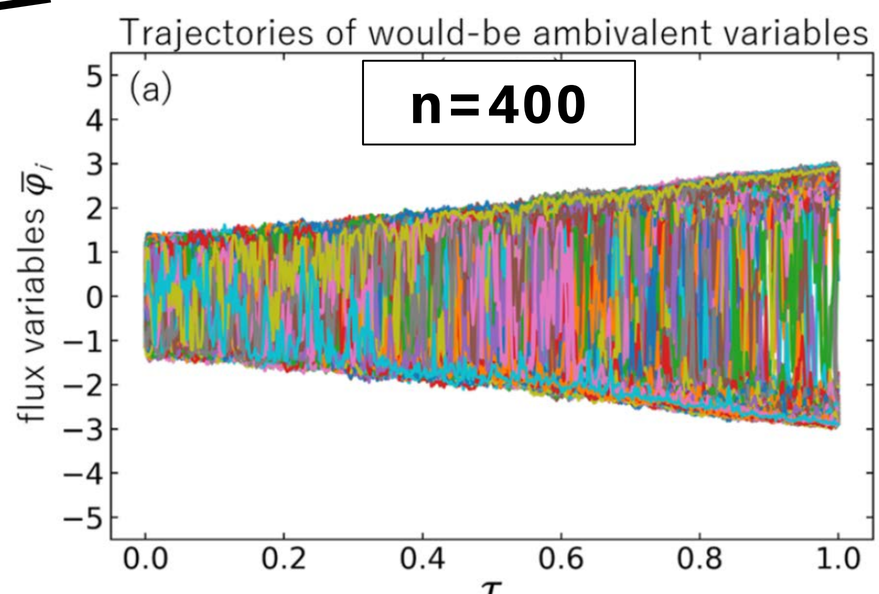
Correspondence between QA and MD $(BJ_{ij} \leftrightarrow \beta J_{ij}|\varphi_i\varphi_j|, \ Bh_i \leftrightarrow \beta h_i|\varphi_i\varphi_i|)$
can be recovered only when $|\varphi_i| \to \mu$ for all i

➔ systematic error from the non-zero distribution of variables

“Hierarchy” in variables



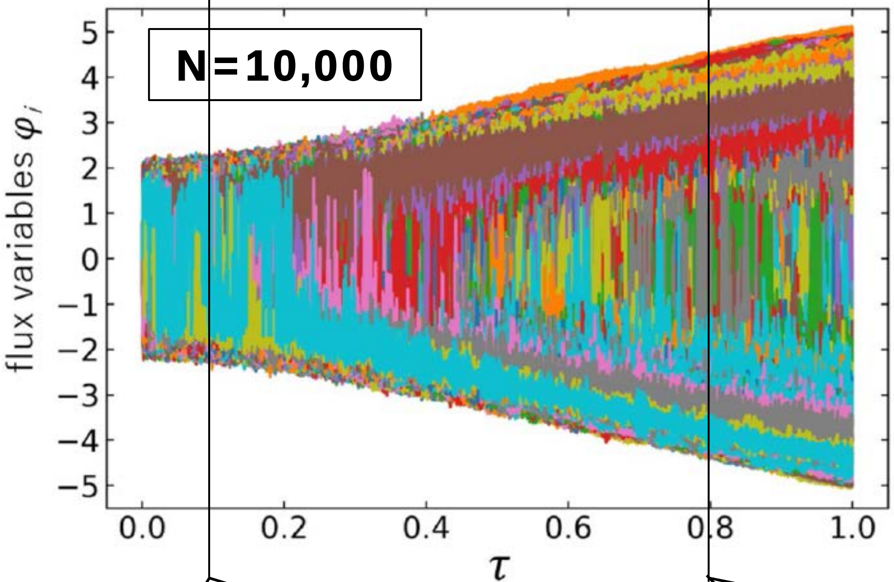




Are all variables subject to similar “difficulty to solve” ?
➔ No!

Among N=10,000 variables,
only 400 vars are “ambivalent”,
while 9,600 vars are almost “frozen”

“Hierarchy” in variables



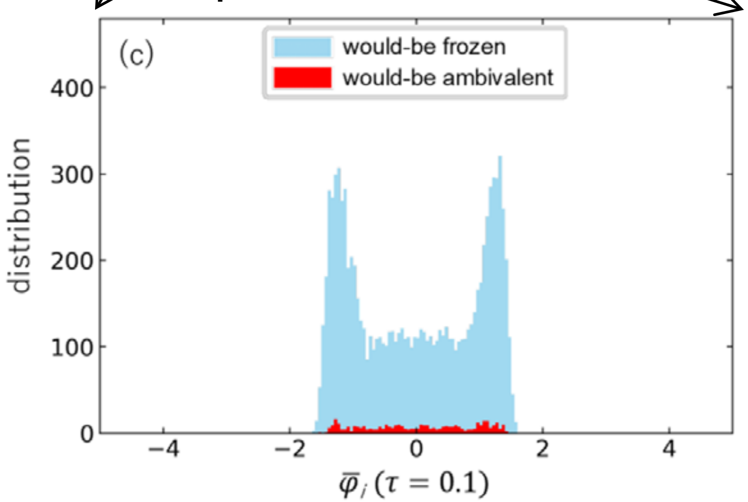
Our MD is good at extracting small-sized “difficult problem” from large-sized problem

where we define time-averaged vars

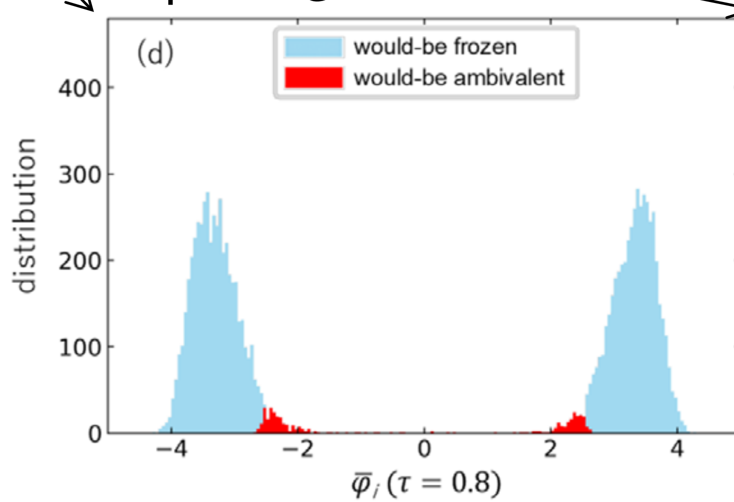
$$\overline{\varphi}_i(\tau) \equiv \frac{1}{\delta}\int_{\tau-\delta}^{\tau} d\tau' \varphi_i(\tau')$$

and sort them w.r.t. $|\overline{\varphi}_i(\tau = 1)|$

snapshot @ τ=0.1

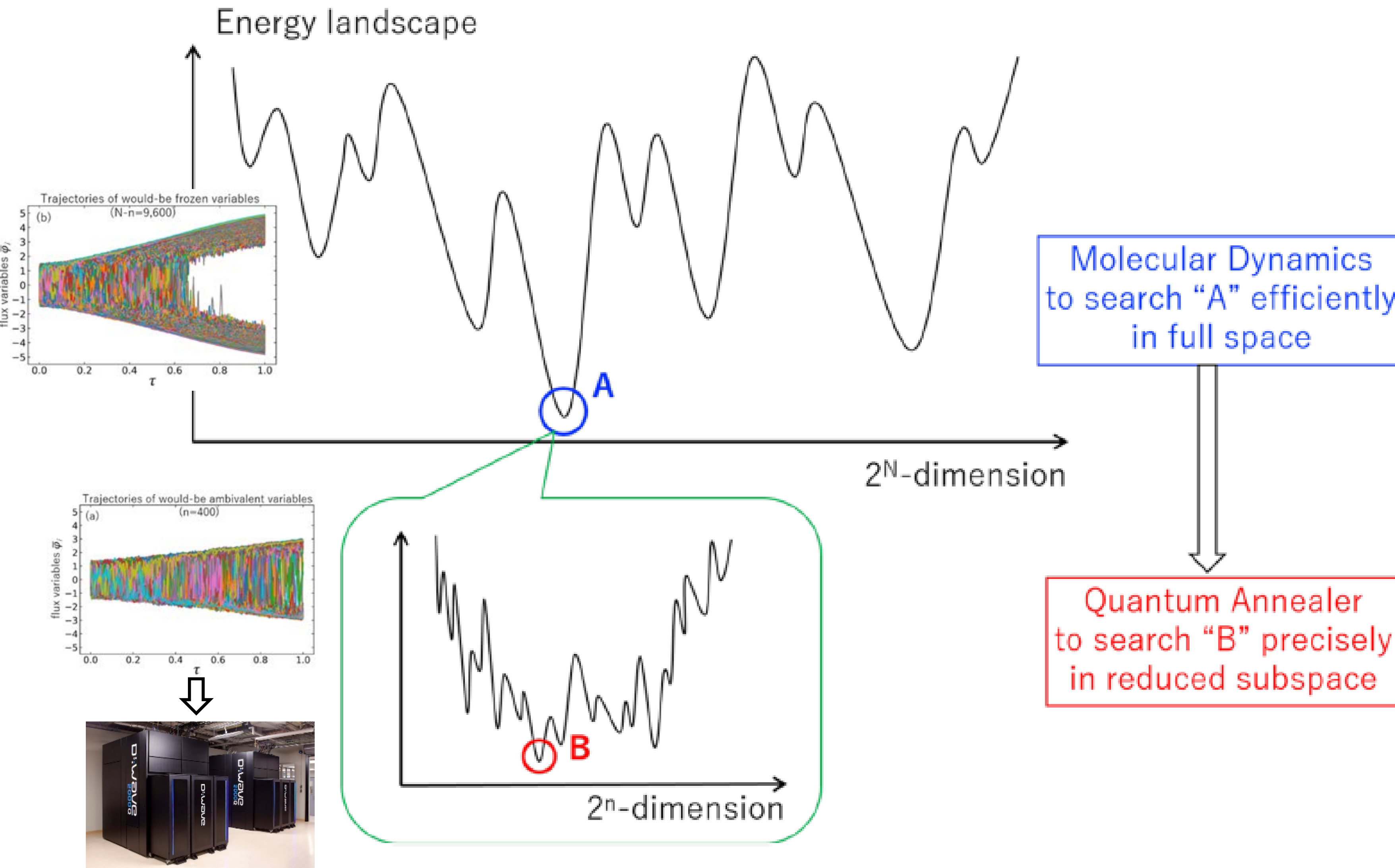


snapshot @ τ=0.8

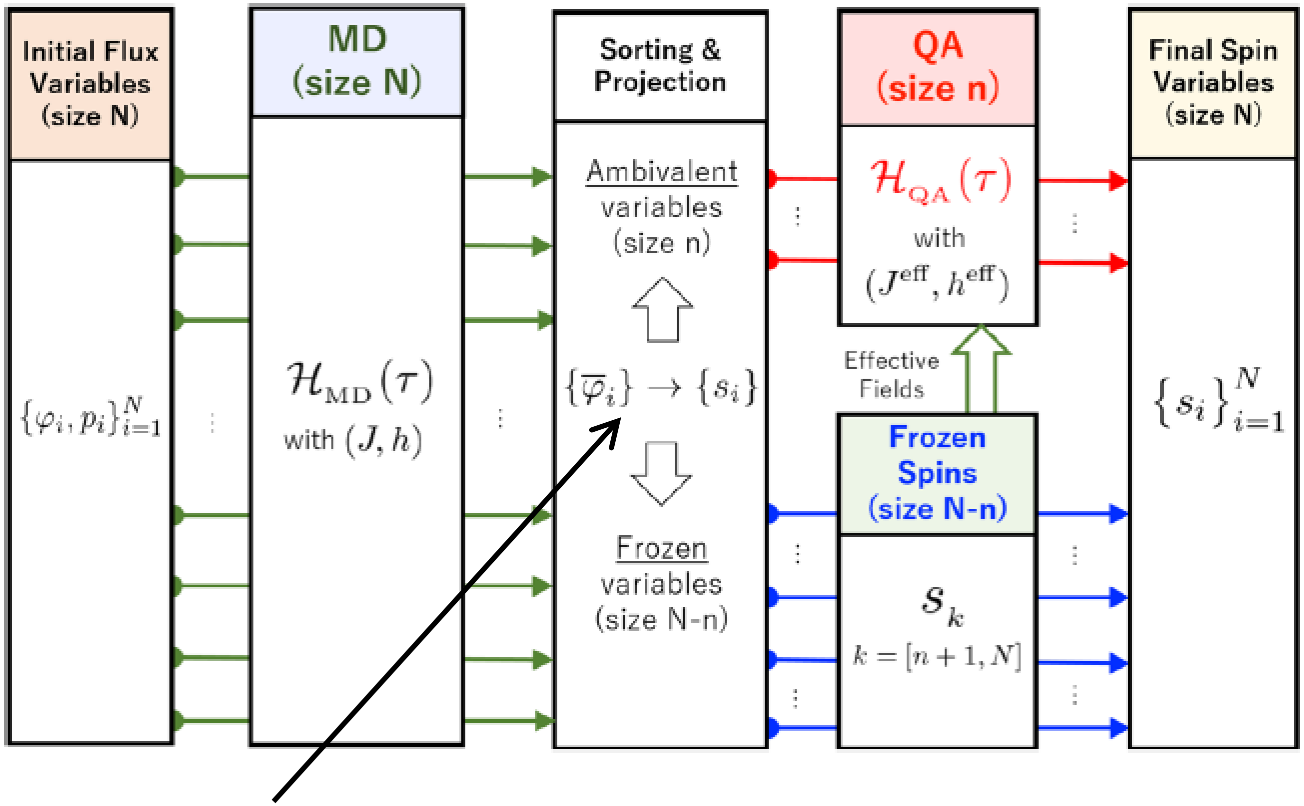


Hybrid Quantum Annealing (HQA) via MD

New Idea: **use classical MD as preconditioner for quantum annealing**



Flowchart of Hybrid Quantum Annealing (HQA)



We sort w.r.t. continuous time-averaged variables at τ=1,

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

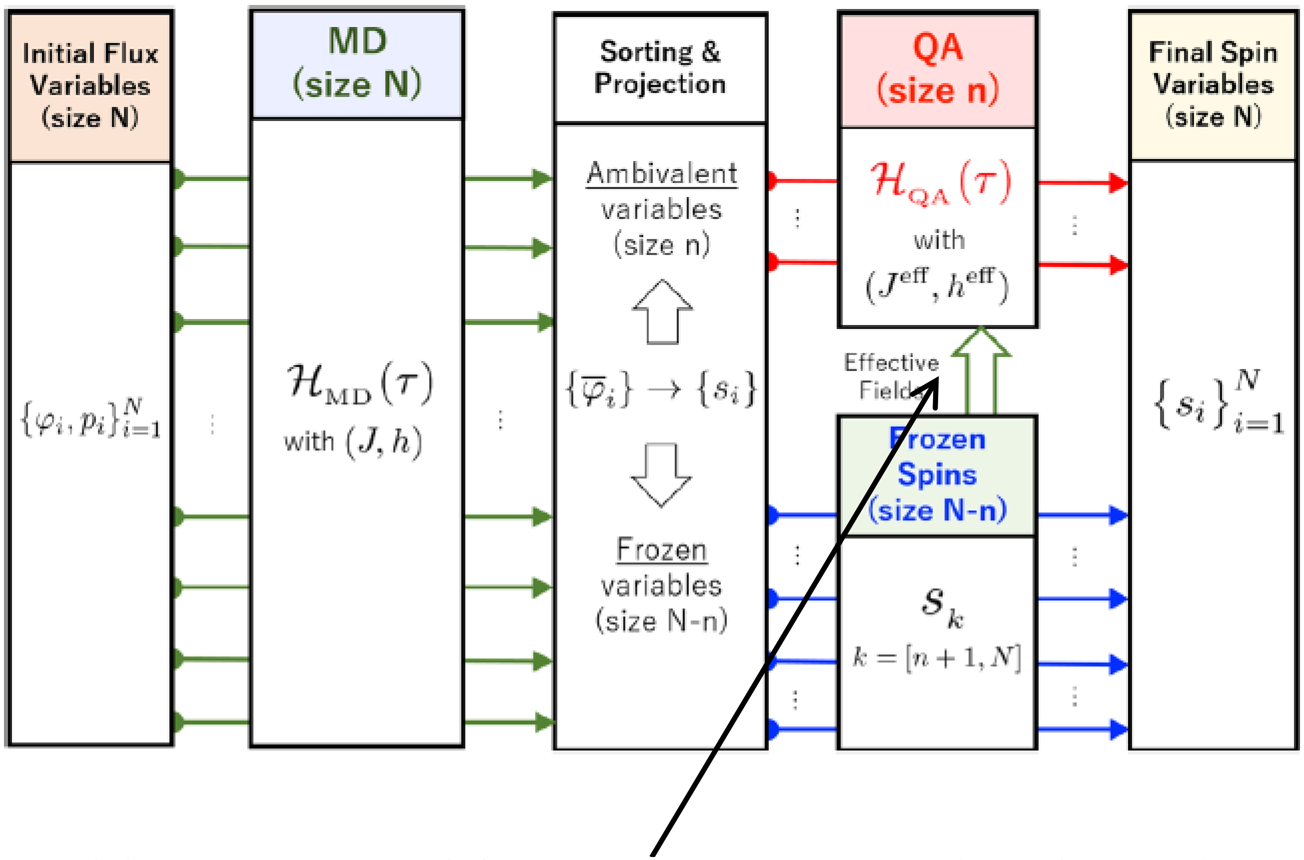
$$i' = 1, 2, \cdots, n \ (\text{ambivalent}) \quad k' = n+1, n+2, \cdots, N \ (\text{frozen})$$

and then project frozen variables to discrete spin variables

$$s_{k'} = \text{sgn}\left(\overline{\varphi}_{k'}(\tau = 1)\right)$$

→ we can avoid “continuous-vars” sys err (if frozen spins are correct)

Flowchart of Hybrid Quantum Annealing (HQA)



$$\mathcal{H}'_{\rm Ising}(s) = \mathcal{H}_{\rm Ising}(s|s_{k'=n+1,\cdots,N} : \text{frozen}) - (\text{const.})$$

$$= \frac{1}{2}\sum_{i'\neq j'}^{n} J^{\rm eff}_{i'j'} s_{i'} s_{j'} + \sum_{i'=1}^{n} h^{\rm eff}_{i'} s_{i'}$$

$$J^{\rm eff}_{i'j'} = J_{i'j'} \qquad h^{\rm eff}_{i'} = h_{i'} + \sum_{k'=n+1}^{N} J_{i'k'} s_{k'} \qquad (i', j' = 1, 2, \cdots, n)$$

Numerical Results of
Hybrid Quantum Annealing (HQA)

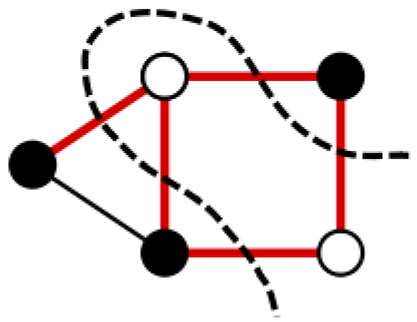
MAX-CUT problem

Consider an undirected graph

$$\mathcal{G} = (\mathcal{V}, \mathcal{E})$$

$\mathcal{V}$: vertices

$\mathcal{E}$: edges w/ weight $\{w_{ij}\}_{(ij)\in\mathcal{E}}$



(Fig from wiki)

Problem:

Find a partition of vertices into 2 sets, $\mathcal{V} = \mathcal{V}_+ \cap \mathcal{V}_-$

which maximizes the sum of weights w_{ij} connecting 2 sets

$$C \equiv \sum_{i\in\mathcal{V}_+, j\in\mathcal{V}_-} w_{ij}$$

Equivalent to minimizing the energy in Ising spin-glass model

$$C(s) = \frac{1}{2}\sum w_{ij}(1 - s_i s_j) = -\frac{1}{2}H_{\text{Ising}}(s) + C_0 \qquad (s_i = \pm 1)$$

$$H_{\text{Ising}}(s)\Big|_{J_{ij}=w_{ij}, h_i=0} = \frac{1}{2}\sum_{i\neq j} J_{ij} s_i s_j$$

MAX-CUT problem

We consider 2000-node complete graph (K_{2000})

w/ random weights $J_{ij} = \pm 1$ & ensemble (instance) average

(we use 100 instances)

Classical solver to be benchmarked

SA (simulated annealing)

TS (tabu search)

MD-only

Parameters are optimized w/ comp cost of SA, TS >~ HQA

(Others) SBM: simulated bifurcation machine

CIM: coherent ising machine

(Cost could be different)

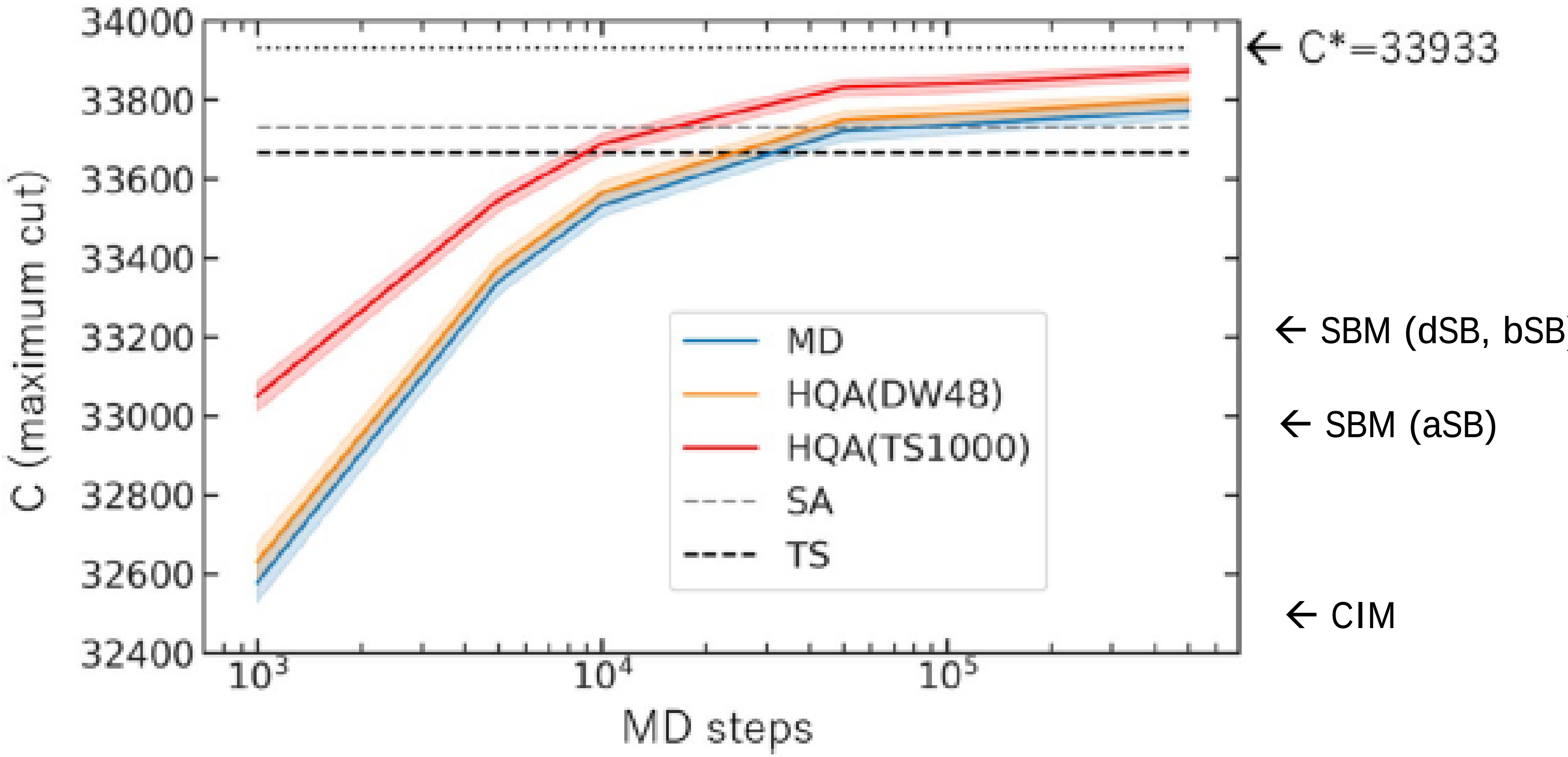
HQA

HQA (DW48) : HQA w/ n= 48 subsystem solved by D-wave

HQA (TS1000) : HQA w/ n=1000 subsystem solved by TS

Dominant cost is MD-part

HQA for MAX-CUT problem (K_{2000})



Comp cost of SA, TS is ~> 10^6 MD

MD-only is better than SA, TS
HQA is even better, achieving ~0.2% accuracy

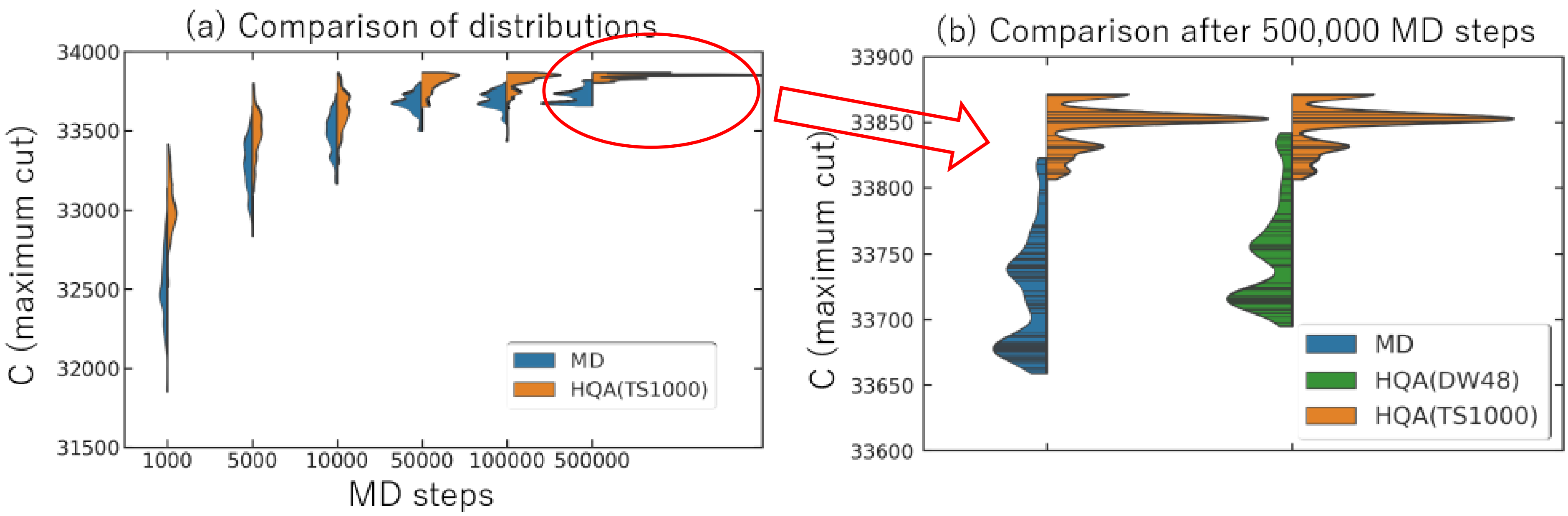
SA requires ~x10 cost to achieve the same accuracy

HQA exhibits significant improvement

Initial condition dep of MD, HQA (for MAX-CUT problem)

Initial condition of MD: $\varphi_i(0) = 0, \quad p_i(0) = \pm 1(\mathrm{random})$

Study the dependence from single instance & 100 initial conditions



More #MD-steps → better results & sharper distribution
HQA achieves even better results & shaper distribution

HQA for Ising spin-glass problem

We consider N=1,000, 2,000 and 10,000 systems

w/ random parameters & ensemble (instance) average

$-1 \leq J_{ij} \leq +1, \quad -2 \leq h_i \leq +2$ w/ uniform distribution

(we use 100 instances)

Classical solver to be benchmarked

SA (simulated annealing)

TS (tabu search)

MD-only

Comp cost of SA, TS is ~> 10^6 - 10^7 MD and thus >~ HQA

Parameters are optimized

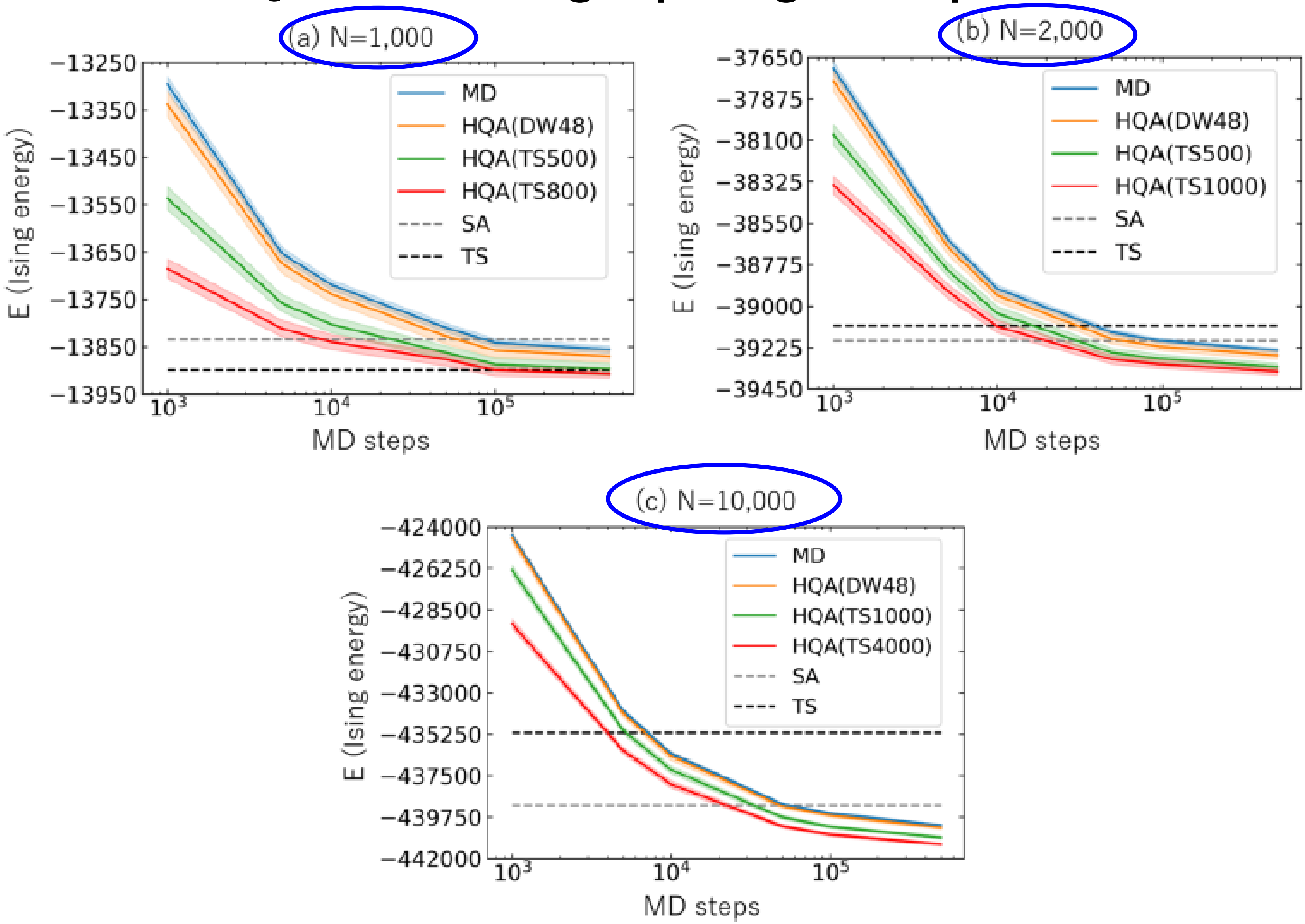
HQA

HQA (DW48) : HQA w/ n= 48 subsystem solved by D-wave

HQA (TS-XXX) : HQA w/ n=XXX subsystem solved by TS

Dominant cost is MD-part

HQA for Ising spin-glass problem



HQA exhibits significant improvement

SA requires ~ x100 cost to achieve MD-only accuracy (N=10,000)

Summary

- Hybrid Quantum Annealing (HQA) via Molecular Dynamics
  - New quantum-classical hybrid scheme
    to solve combinational optimization problem
  - MD can serve as a powerful preconditioner for QA
    - “frozen” / “ambivalent” variables can be identified
    - ➔ “difficult problem” in reduced subspace extracted from full space
    - (NISQ-era) QA solver to search a fine solution in reduced subspace
  - HQA achieves better performance/accuracy than classical SA/TS
    - Larger improvement for a larger system
    - The same concept to extract hierarchy in variables can be utilized
      w/ any other solver combinations

- Future
  - Extension to binary variables, multi-valued variables
  - More theoretical clarification for classical MD