Track Reconstruction for Future Colliders with Quantum Algorithms

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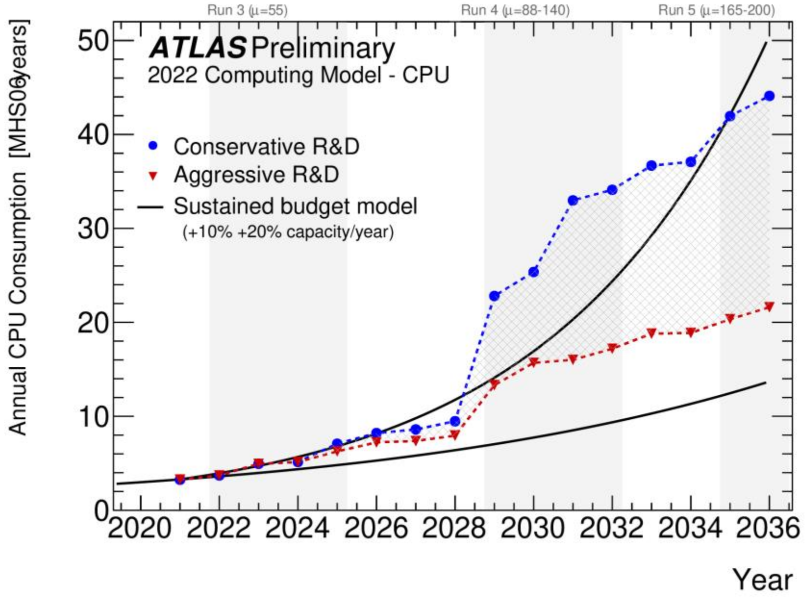
Track Reconstruction at LHC & HL-LHC



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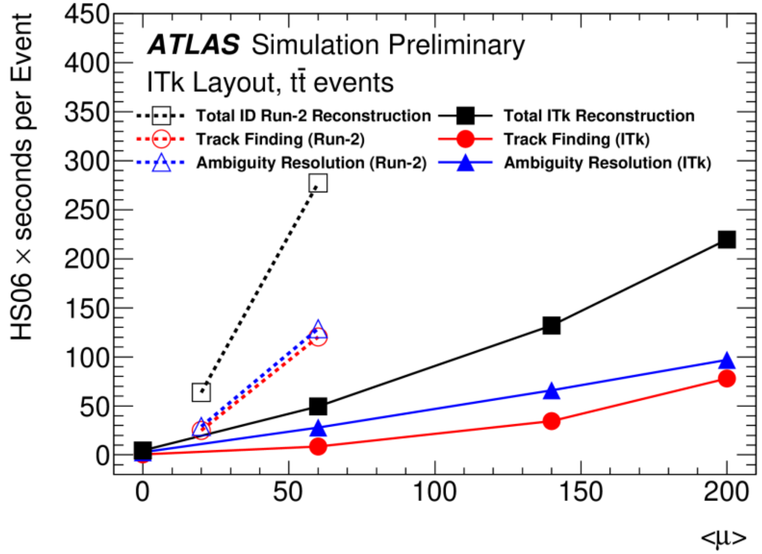
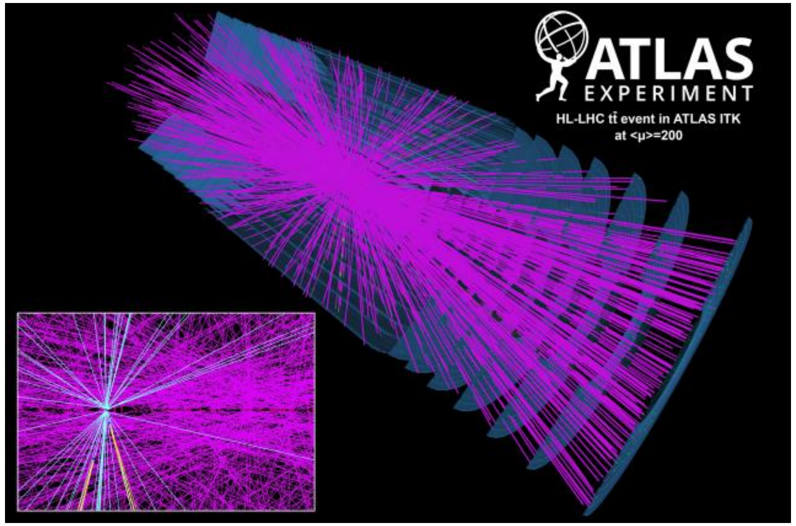


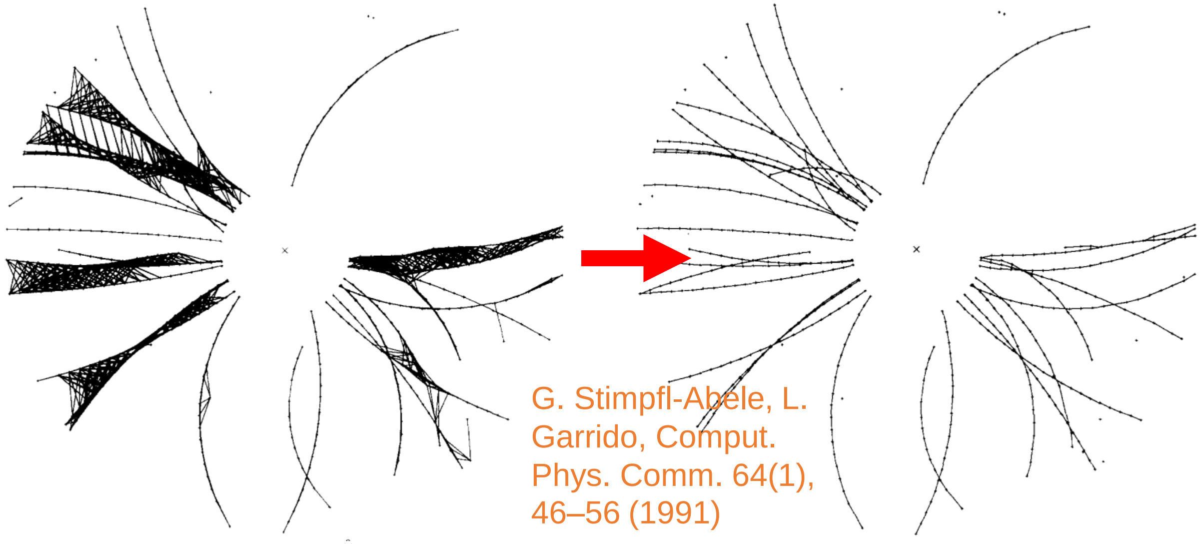


- At the HL-LHC, **[CPU time will increase exponentially with more pileup]**, leading to increase in annual computing cost by a factor of 10-20.
- **Tracking in the most CPU-consuming reconstruction task.**
- GPU & ML-based approaches are actively investigated, but **quantum algorithms may also bring in innovations.**

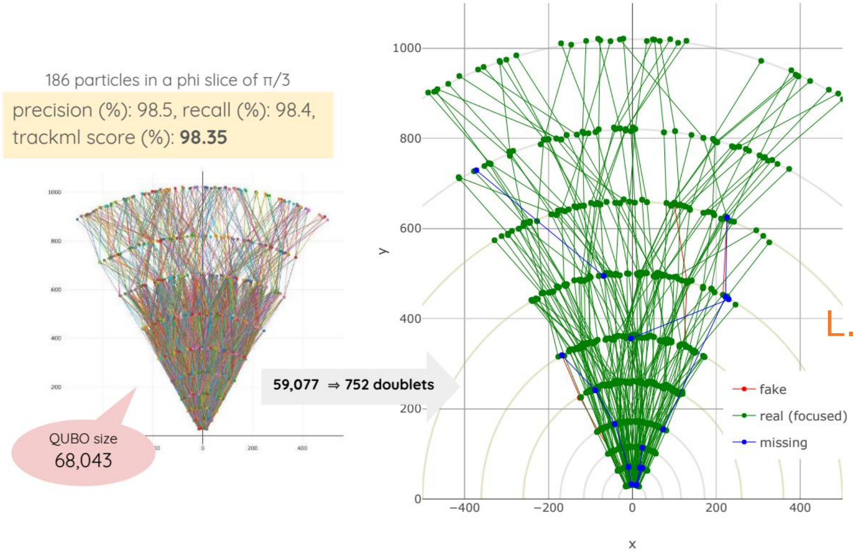
	Run 1	Run 2	HL-LHC
μ	21	40	150-200
Tracks	~280	~600	**~7-10k**

Tracking as Optimization Problem

- **Tracking as an optimization problem: a global approach to reconstruct tracks in one-go.** (↔iterative approach: Combined Kalman Filter)
- **Stimple-Abele & Garrido (1990):** simulated annealing w/ all potential doublets generated with some cuts applied & pursue a binary classification task (i.e. solve an Ising/QUBO problem) to determine which ones should be kept.
- **Modern quantum computing versions:** quantum annealers w/ doublets (A. Zlokapa et al.) & triplet-based (F. Bapst et al.) approaches; quantum gate machines (L. Funcke et al., etc.)



G. Stimpfl-Abele, L. Garrido, Comput. Phys. Comm. 64(1), 46–56 (1991)



L. Linder

Quantum Computers

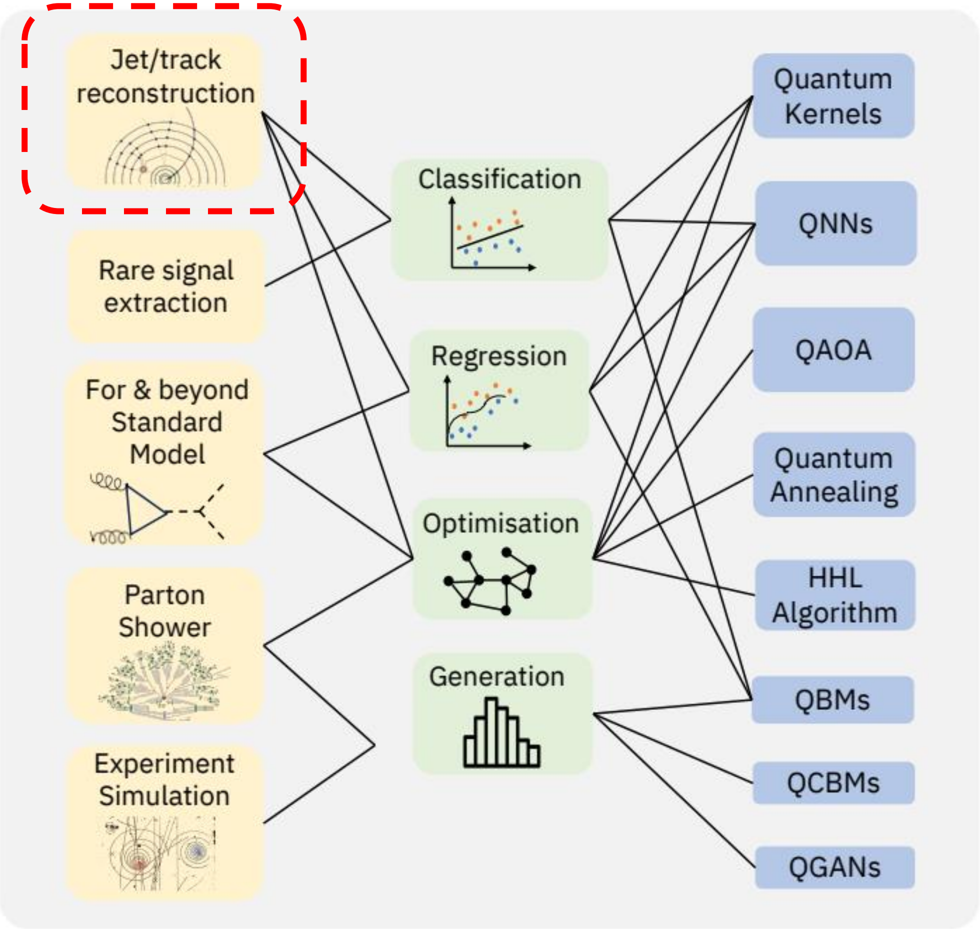
Quantum Annealing

- Utilizes adiabatic quantum evolution to seek for the ground state of a Hamiltonian
  → Only applicable to optimization problems
- Adopted only by D-Wave Systems.

Quantum Gates

- Utilizes quantum logic gates
- General purposed
- IBM, Google, Xanadu, IonQ, Origin Quantum, QuantumCTek, etc.

Both as well as quantum-inspired approaches have been actively investigated in HEP



QC4HEP White Paper

Scope of This Talk

1. Tracking w/ Quantum Gate Computer

- **H. Okawa**, "Charged particle reconstruction for future high energy colliders with Quantum Approximate Optimization Algorithm," Springer Communications in Computer and Information Science, 2036 (2024) 272–283, arXiv:2310.10255

2. Tracking w/ Quantum-Annealing-Inspired Algorithm

- **H. Okawa**, Q.-G. Zeng, X.-Z. Tao, M.-H. Yung, "Quantum Annealing Inspired Algorithms for Track Reconstruction at High Energy Colliders," arXiv:2402.14718 (2024).

QUBO Formulation w/ Triplets

- Tracks are formed by connecting silicon detector hits: e.g. triplets (segments w/ 3 hits).
- Doublets/triplets are connected to reconstruct tracks & it can be regarded as a **quadratic unconstrained binary optimization (QUBO) / Ising** problem.

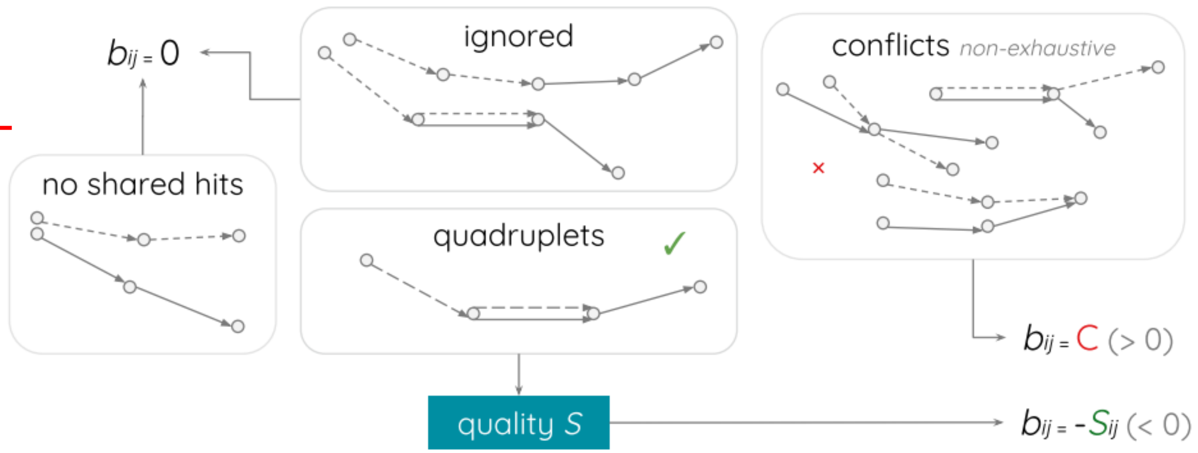
$$O(a,b,T) = \underbrace{\sum_{i=1}^{N} a_i T_i}_{\text{Quality of triplets}} + \underbrace{\sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j}_{\text{Compatibility b/w triplet pairs}}$$

$$a_i = \alpha \left(1 - e^{\frac{|d_0|}{\gamma}}\right) + \beta \left(1 - e^{\frac{|z_0|}{\lambda}}\right),$$

b_{ij} = 0 (if no shared hit), 1 (if conflict)
= $-S_{ij}$ (if two hits are shared)

$$S_{ij} = \frac{1 - \frac{1}{2}(|\delta(q/p_{Ti}, q/p_{Tj})| + max(\delta\theta_i, \delta\theta_j))}{(1 + H_i + H_j)^2},$$

F. Bapst et al. Comp. Soft. Big Sci. 4 (2019) 1.

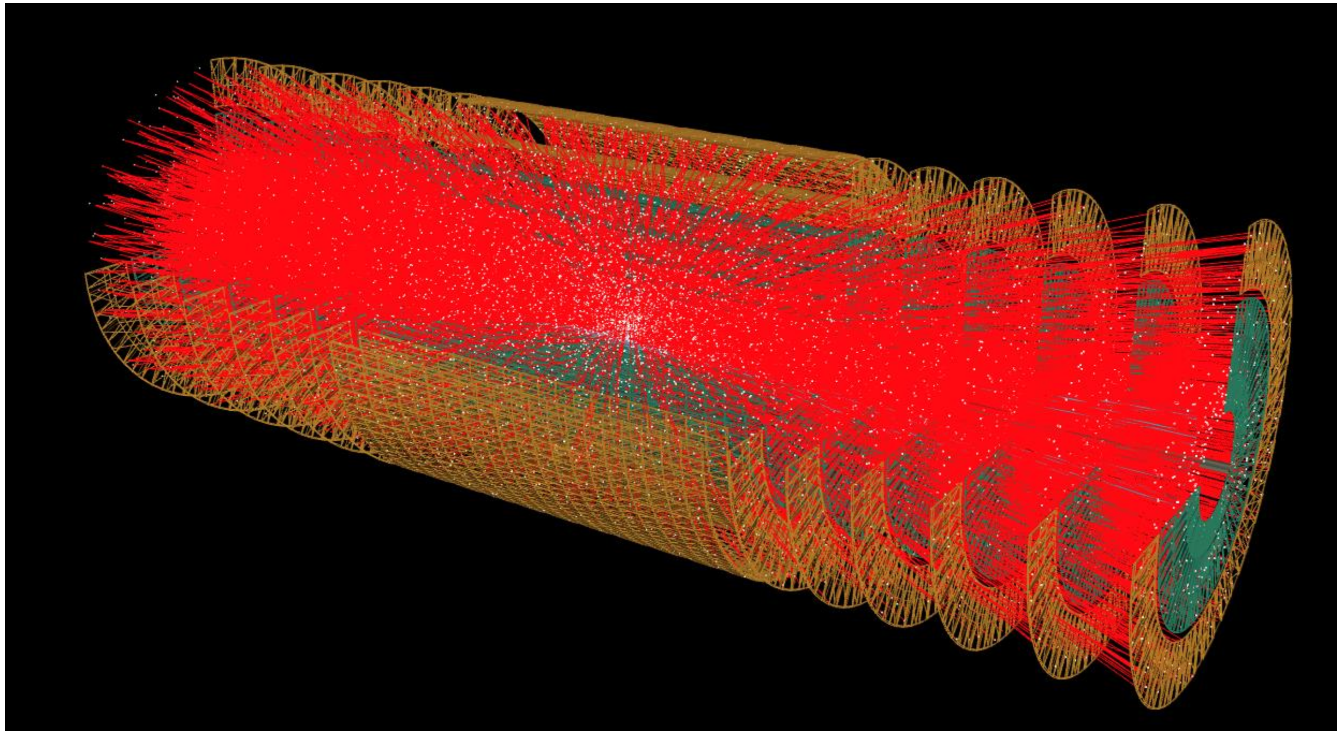


Minimizing QUBO is equivalent to searching for the ground state of the Hamiltonian.

Dataset (TrackML)

- TrackML is an open-source dataset prepared for TrackML Challenges (two competitions hosted by CERN & Kaggle).
- It is **designed w/ HL-LHC conditions (200 pileup) & run w/ fast simulation (e.g. noise, inefficiency, parametrized material effects, etc.)**
- Only tracks w/ p_T>1 GeV in the barrel are considered.
- QUBO is computed event by event using hepqpr-qallse framework.

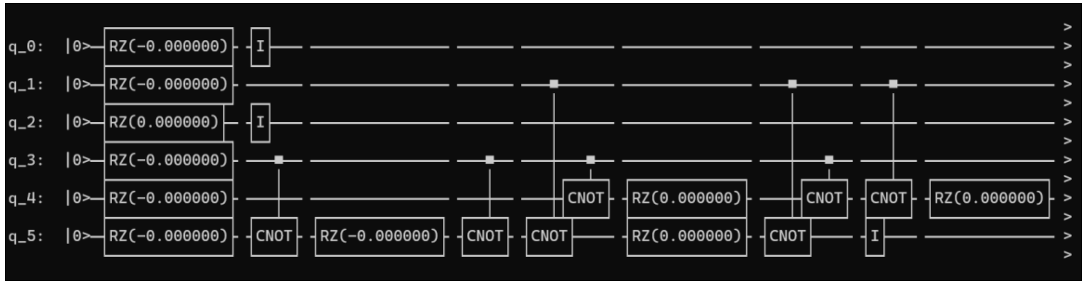
Amrouche, S., et al., arXiv:1904.06778 (2019);
Amrouche, S., et al., Comput. Softw. Big Sci. 7(1), 1 (2023)



Thanks to Andreas Salzburger for suggestions and discussions!

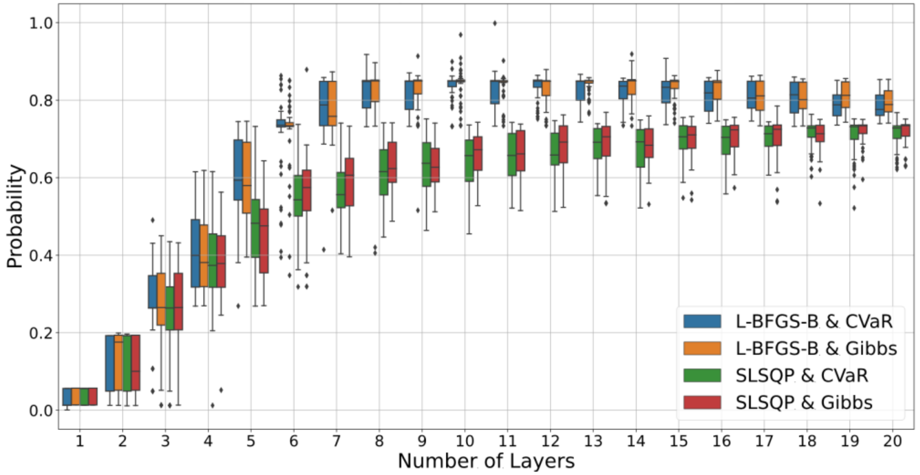
H. Okawa, Springer Communications in Computer and Information Science, 2036 (2024) 272–283, arXiv:2310.10255

1. Quantum Gate Approach

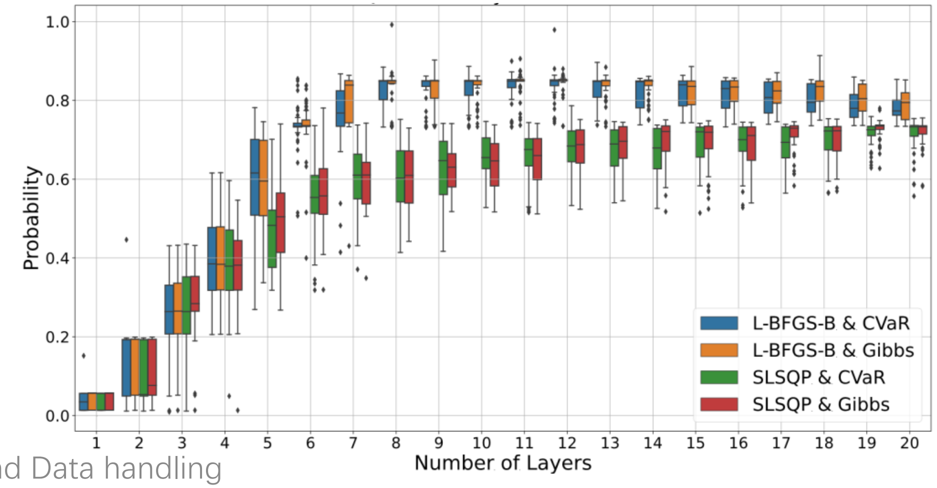


- Used Quantum Alternative Operator Ansatz (QAOA) in pyqpanda-algorithm by Origin Quantum.
- # of layers, loss function & optimizer are optimized.
- Used quantum simulator as well as 6-qubit Origin Quantum hardware (Wuyuan).
- Accuracy reaches ~100% for >=4 layers (as multiple measurements are pursued)
- No sign of performance degradation in hardware for <=20 layers

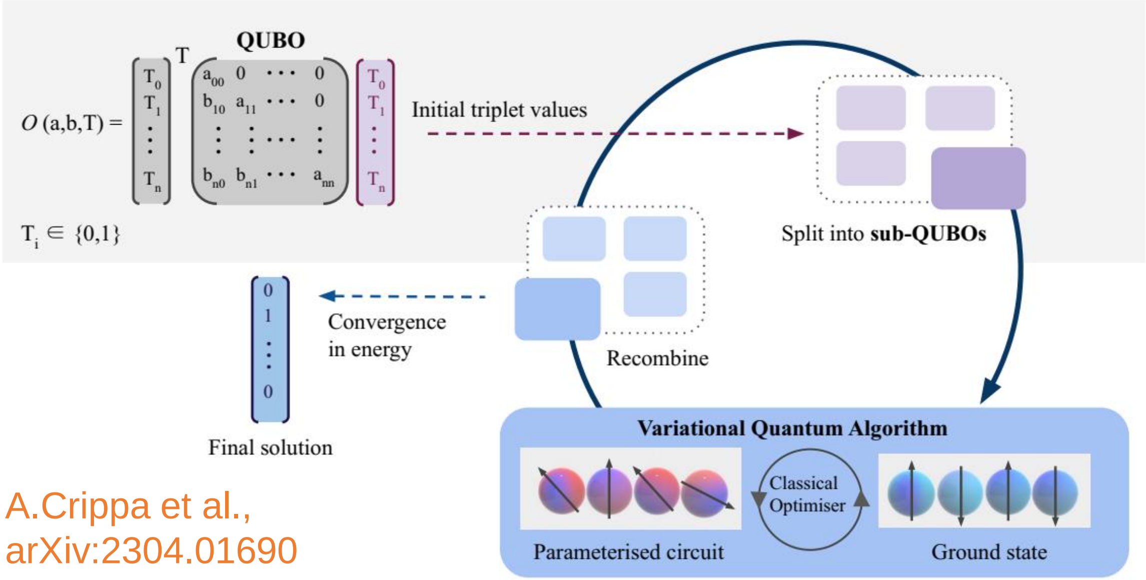
Quantum Simulator



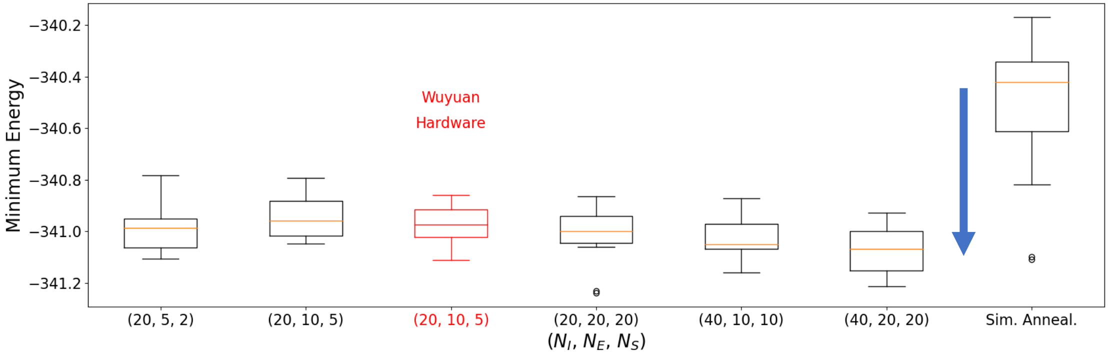
Wuyuan Hardware



Sub-QUBO Method

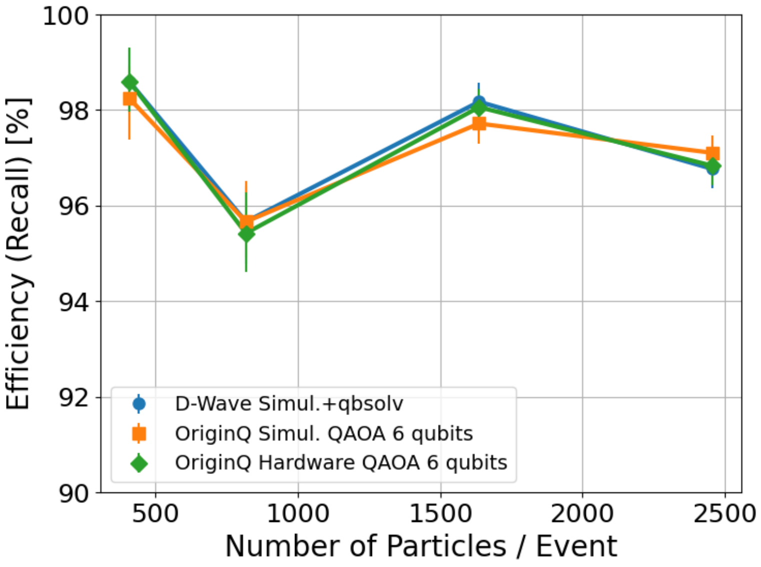


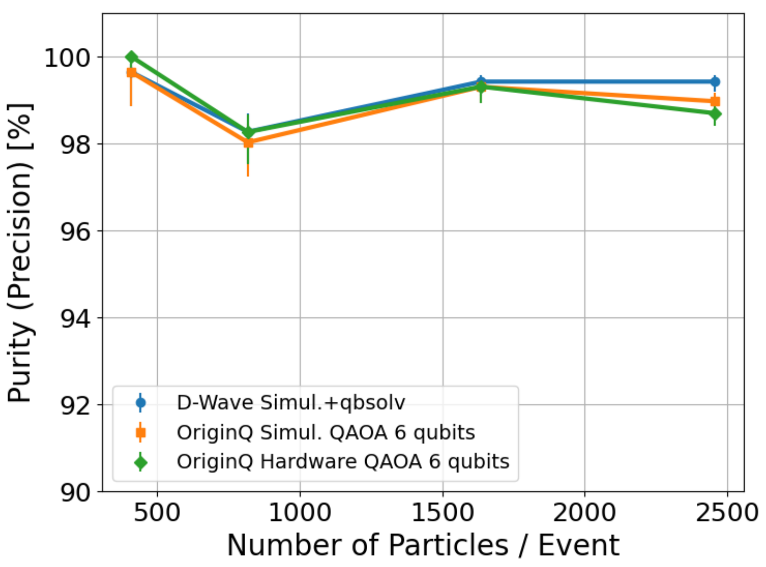
A.Crippa et al., arXiv:2304.01690

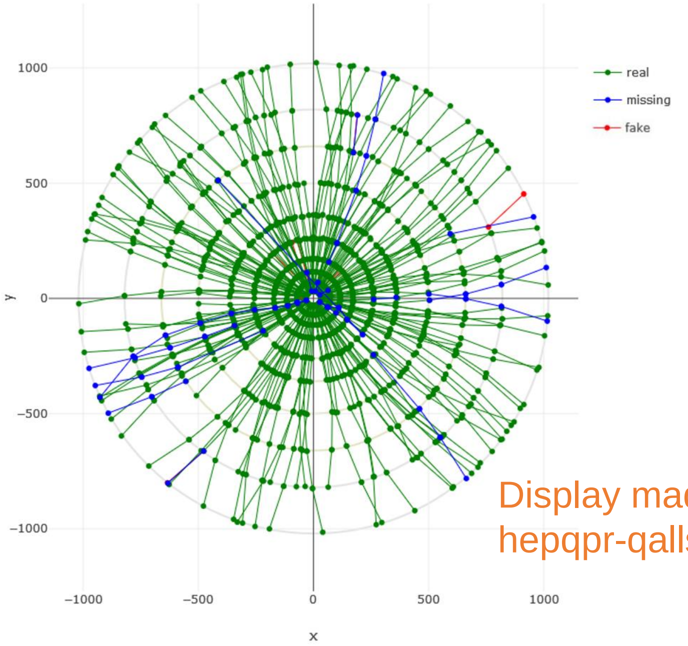


- Number of triplet candidates determines number of qubits required → **~O(10²x10²~10⁵x10⁵)**
  HL-LHC conditions do not fit into the current scale of quantum annealing & gate computers
- QUBO is split into sub-QUBOs of size 6x6 to match with OriginQ hardware.
- **Theoretically-robust sub-QUBO method using multiple solution instances** is adopted (Y. Atobe, M. Tawada, N. Togawa, IEEE Trans. Comp. 71, 10 (2022) 2606) → known to outperform empirical methods like qbsolv

WIP: Triplet Efficiency & Purity







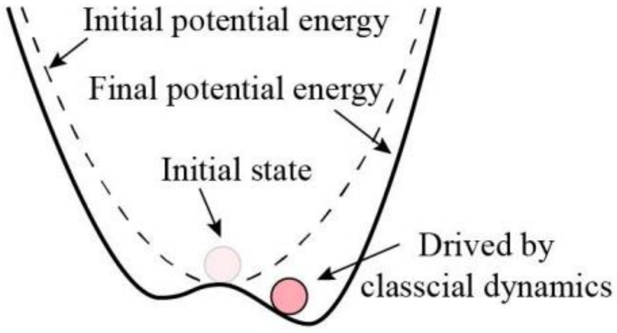
Display made w/ hepqpr-qallse

$$\text{Efficiency} = \frac{TP}{TP+FN} = \frac{\#\text{ of matched reconstructed doublets}}{\#\text{ of true doublets}},$$

$$\text{Purity} = \frac{TP}{TP+FP} = \frac{\#\text{ of matched reconstructed doublets}}{\#\text{ of all reconstructed doublets}},$$

- QAOA+sub-QUBO provides **compatible performance as the previous quantum annealing studies.**
- **No sign of degradation in the real hardware**
- This is the 1st tracking w/ QAOA, theoretically robust sub-QUBO & Chinese quantum computer

2. Quantum Annealing Inspired Algorithms



Quantum inspired algorithm

- "Quantum-inspired" algorithms search for minimum energy through the **classical time evolution of differential equations:** simulated annealing, simulated bifurcation (SB), simulated coherent Ising machine, etc.
- **SB in particular can run in parallel unlike simulated annealing**, in which one needs to access the full set of spins & not suitable for parallel processing

Simulated Bifurcation (SB)

- **adiabatic Simulated Bifurcation (aSB)**

$$\dot{x}_i = \frac{\partial H_{\mathrm{SB}}}{\partial y_i} = \Delta y_i, \qquad \dot{y}_i = -\frac{\partial H_{\mathrm{SB}}}{\partial x_i} = -[\boxed{Kx_i^2} - p(t) + \Delta]x_i + \xi_0 \sum_{j=1}^{N} J_{ij} x_j$$

- **ballistic Simulated Bifurcation (bSB)**

$$\dot{x}_i = \frac{\partial H_{\mathrm{SB}}}{\partial y_i} = \Delta y_i, \qquad \dot{y}_i = \frac{\partial H_{\mathrm{SB}}}{\partial x_i} = (p(t) - \Delta)x_i + \xi_0 \sum_{j=1}^{N} J_{ij} x_j$$

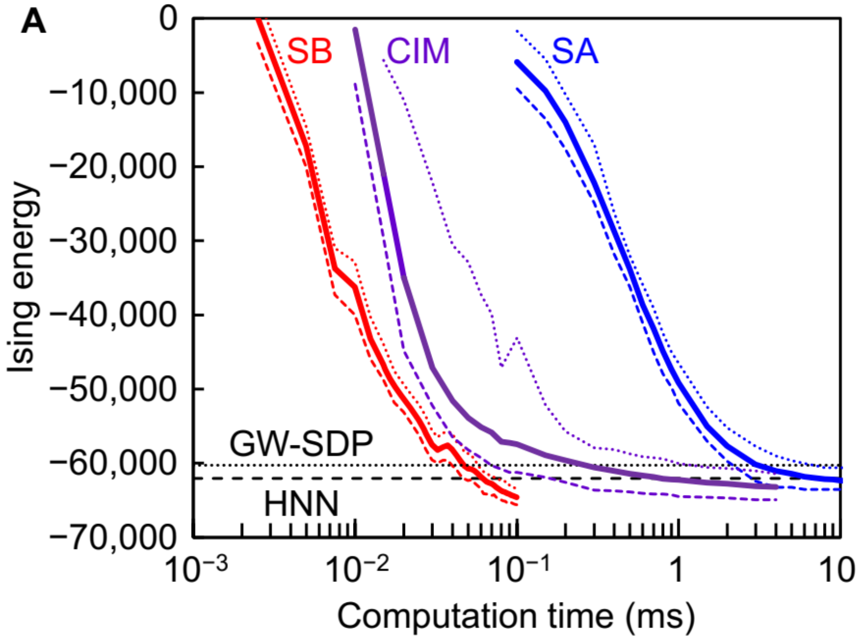
- **discrete Simulated Bifurcation (dSB)**

$$\dot{x}_i = \frac{\partial H_{\mathrm{SB}}}{\partial y_i} = \Delta y_i, \qquad \dot{y}_i = \frac{\partial H_{\mathrm{SB}}}{\partial x_i} = (p(t) - \Delta)x_i + \xi_0 \sum_{j=1}^{N} \boxed{J_{ij}\mathrm{sign}(x_j)}$$

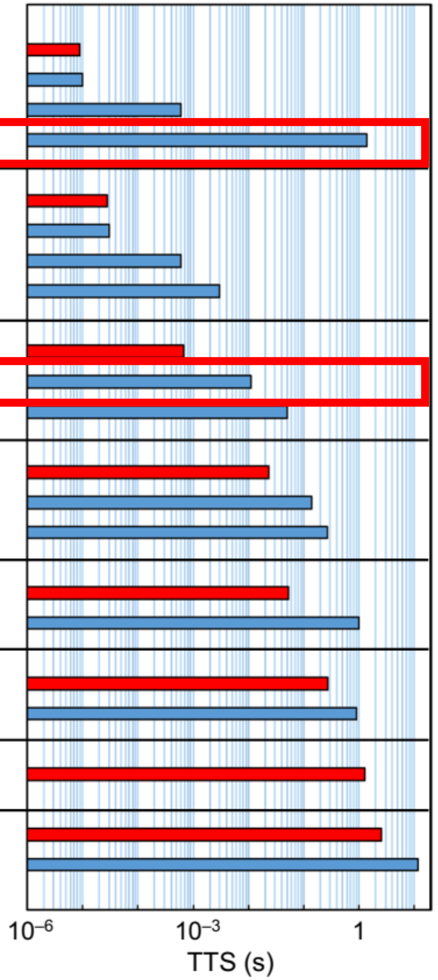
M.H. Yung

Simulated Bifurcation

Goto et al., Sci. Adv. 2019; 5: eaav2372
Goto et al., Sci. Adv. 2021; 7: eabe7953

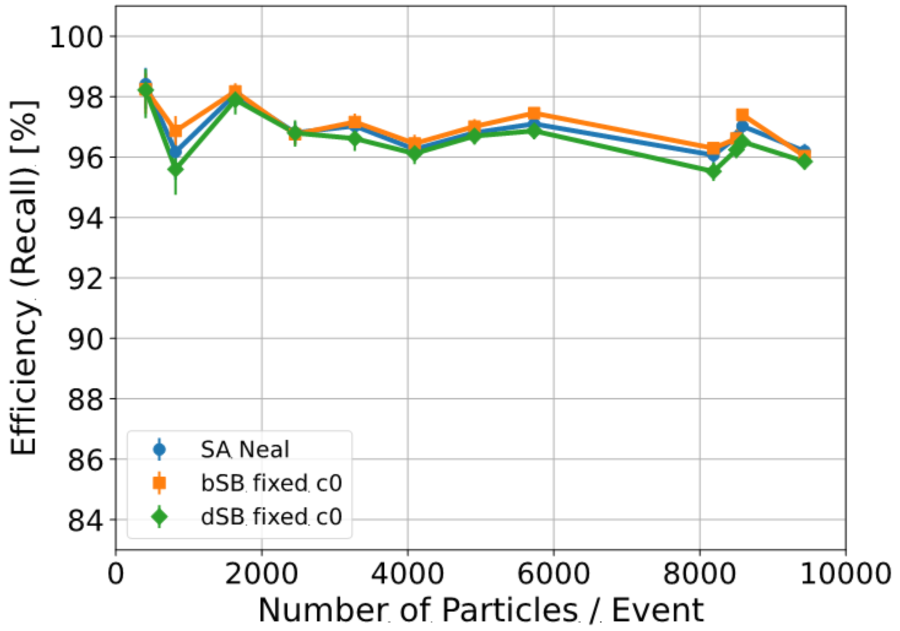


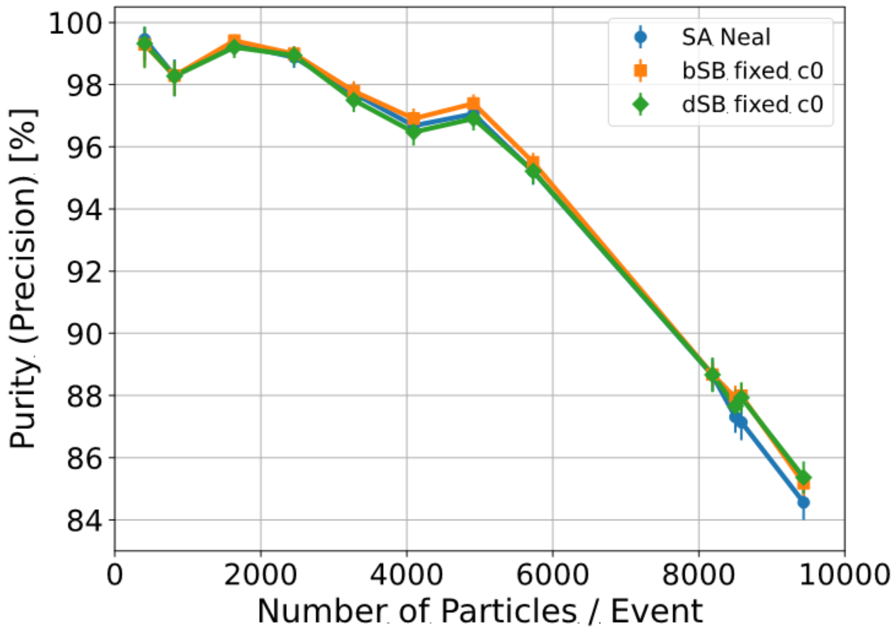
N	Connectivity	$J_{i,j}$	Machine	TTS
60	All-to-all	{±1}	**dSBM** RBM CIM QA	**9.2 μs** 10 μs 0.6 ms 1.4 s
100	All-to-all	{±1}	**dSBM** RBM SimCIM CIM	**29 μs** 30 μs 0.6 ms 3.0 ms
200	Sparse (Degree 3)	{0, −1}	**dSBM** QA CIM	**0.70 ms** 11 ms 51 ms
700	All-to-all	{±1}	**dSBM** SimCIM DA	**25 ms** 0.14 s 0.27 s
1024	All-to-all	{±1}	**dSBM** DA	**55 ms** 1 s
1024	All-to-all	16 bits $\{-2^{15}+1, \ldots, 2^{15}-1\}$	**dSBM** DA	**0.29 s** 0.9 s
2000 (K_{2000})	All-to-all	{±1}	**dSBM**	**1.3 s**
2000 (G22)	Sparse (1%)	{0, −1}	**dSBM** SimCIM	**2.7 s** 12 s



- **Simulated bifurcation is known to outperform other quantum-inspired algorithms as well as quantum annealing (QA) for some problems**
- Simulated Coherent Ising Machine (CIM) had largely degraded performance in our study, so is not presented.

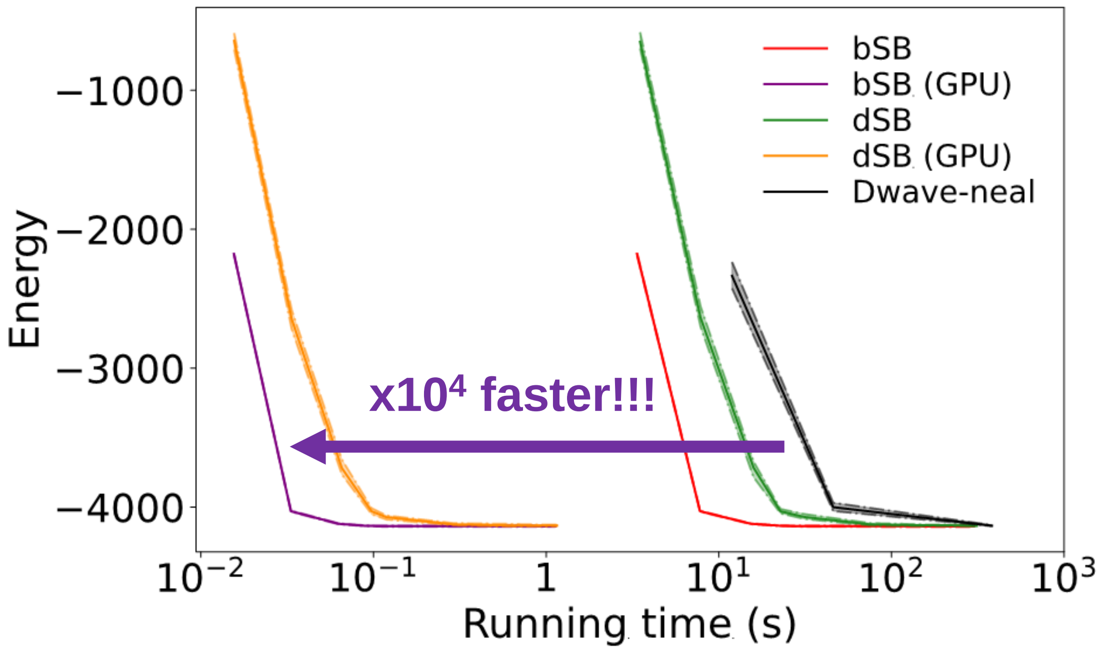
Track Efficiency & Purity w/ QAIA





- Simulated bifurcation provides **compatible or slightly better performance than D-Wave Neal.**
- **Track efficiency stays over 95%** for all dataset up to the highest HL-LHC conditions
- Purity degrades with track multiplicity but **>90% for <6000 particles, >84% even for ~10000 particles**.

Computation Speed



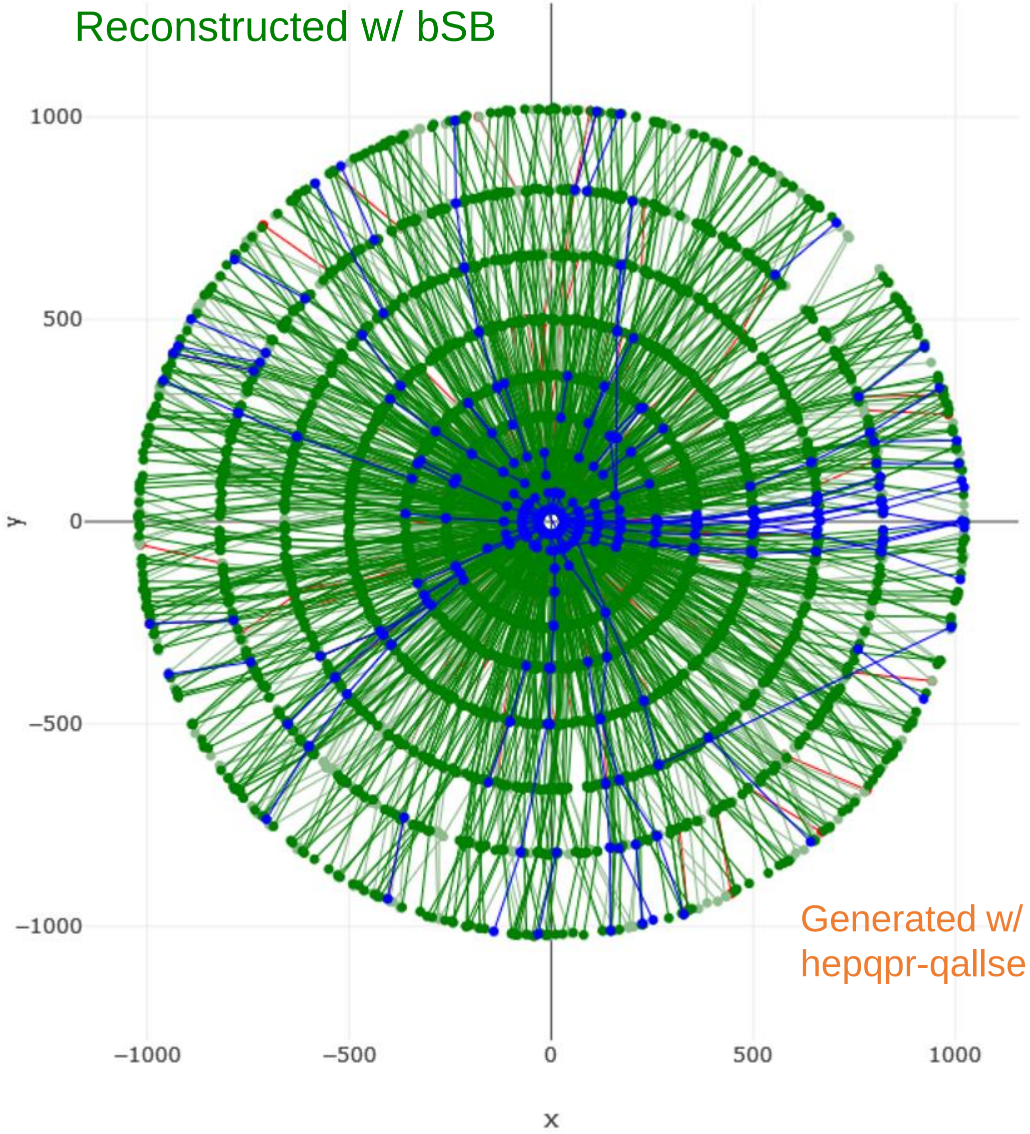
Only 1 CPU/GPU used respectively

Data Information		Time to target [s]				
# of particles	QUBO size	bSB	bSB (GPU)	dSB	dSB (GPU)	D-Wave Neal
409	778	0.007	0.021	0.032	0.092	0.060
818	1431	0.012	0.019	0.293	0.478	0.169
1637	2904	0.012	0.019	0.293	0.478	0.169
2456	4675	0.014	0.017	–	–	0.479
3274	6945	0.032	0.022	–	–	1.229
4092	10295	0.005	0.022	0.015	0.065	0.030
4912	14855	0.027	0.016	–	–	2.165
5730	22022	0.109	0.042	–	–	3.853
8187	67570	0.488	0.028	–	–	404.297
8500	78812	1.899	0.108	–	–	785.732
8583	80113	1.321	0.067	–	–	93.782
9435	109498	3.884	0.140	–	–	1366.808

- Ballistic simulated bifurcation provides **4 orders of magnitude speed-up (23min → 0.14s) from D-Wave Neal** at most **(D-Wave qbsolv is even 2 orders of magnitude slower than Neal)**.
  → More speed-up expected with larger data size.
- Unlike D-Wave Neal, **simulated bifurcation can effectively run w/ multiple processing, GPU & FPGA → Perfect match with HEP computing environment!!**

Summary

- Tracking is the highest CPU-consuming reconstruction task in the HL-LHC era.
- Improvement of existing methods & classical ML methods are bringing in improvement, but another leap from quantum machine learning would be highly exciting.
- Presented recent results on the quantum tracking using two complementary approaches: using a quantum-gate computer (w/ QAOA+subQUBO) or quantum-annealing inspired algorithms.
- Quantum Gate approach: promising tracking performance from the real quantum hardware; **1st tracking w/ QAOA, theoretically robust sub-QUBO & Chinese quantum computer**
- Quantum-inspired approach: **four orders of magnitude speed-up** at most (more speed-up expected w/ larger dataset) & **can already be considered for implementation**. This is the **1st application of simulated bifurcation in HEP!**
- Further studies are ongoing. Stay tuned!



Thank you for listening!

Backup

References to Previous Studies

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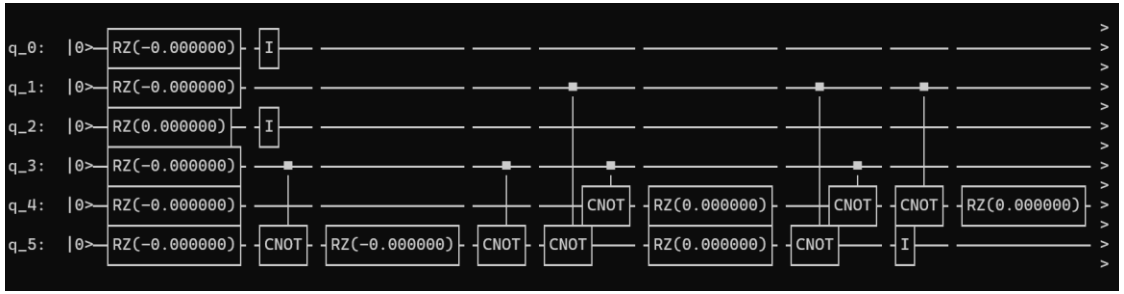
- Magano, D., et al.: Quantum speedup for track reconstruction in particle accelerators. Phys. Rev. D 105(7), 076012 (2022) https://doi.org/10.1103/PhysRevD.105.076012

QAOA in Origin Quantum (本源)

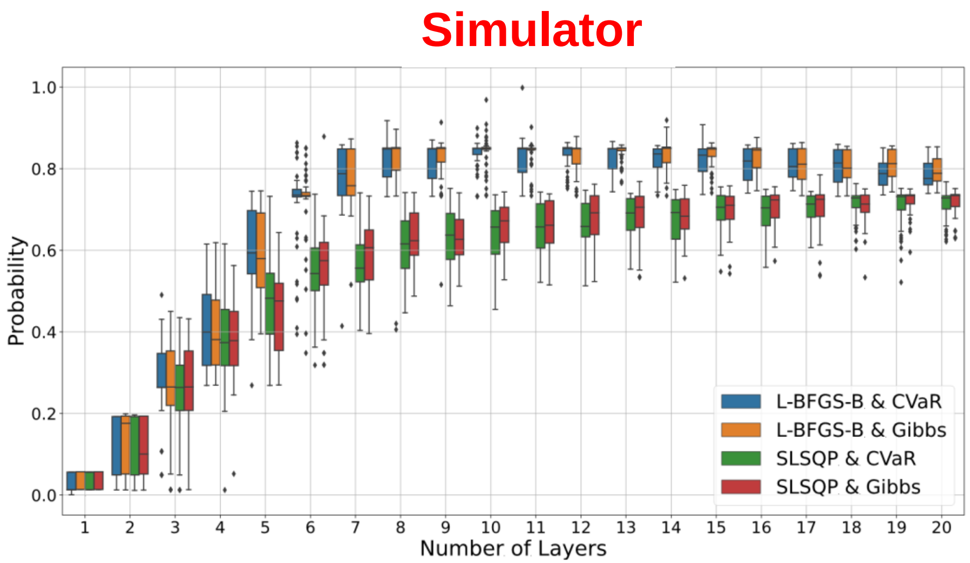
- QAOA solves binary optimization problem. Library in pyqpanda-algorithm by Origin Quantum.
- Adopts **Quantum Alternative Operator Ansatz** for QAOA.

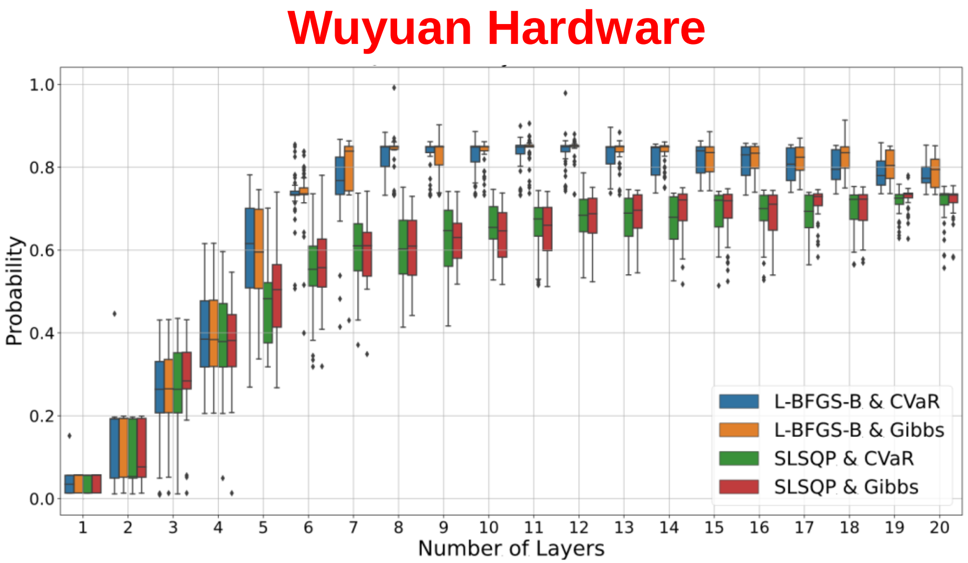
An example of circuits from the actual run



- Can utilize CVaR loss function (P. Barkoutsos et al., Quantum, 2020, 4: 256) or Gibbs optimization
- **6 qubit machine (Wuyuan 悟源)** is used for the real hardware computation in this talk.

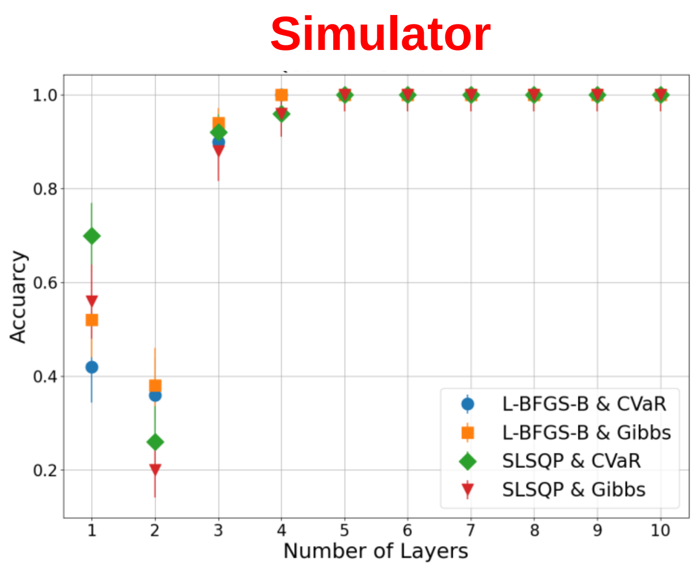
QAOA Optimization

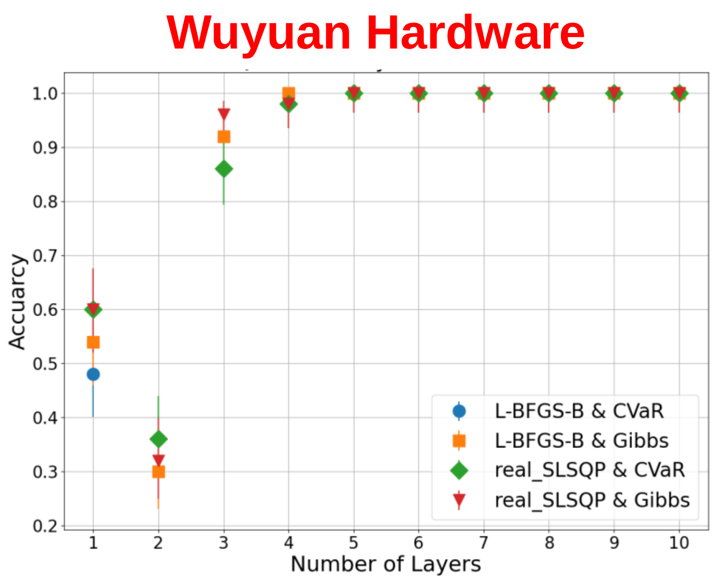




- **QAOA does not perform well w/ shallow layers, but provides good performance with more layers. Compatible performance b/w hardware & simulator.**
- L-BFGS-B optimizer is better than SLSQP. TNC has degraded performance & not shown here.
- No significant difference w/ CVaR or Gibbs loss function.
- **Probability saturates around 7 layers for L-BFGS-B cases.**

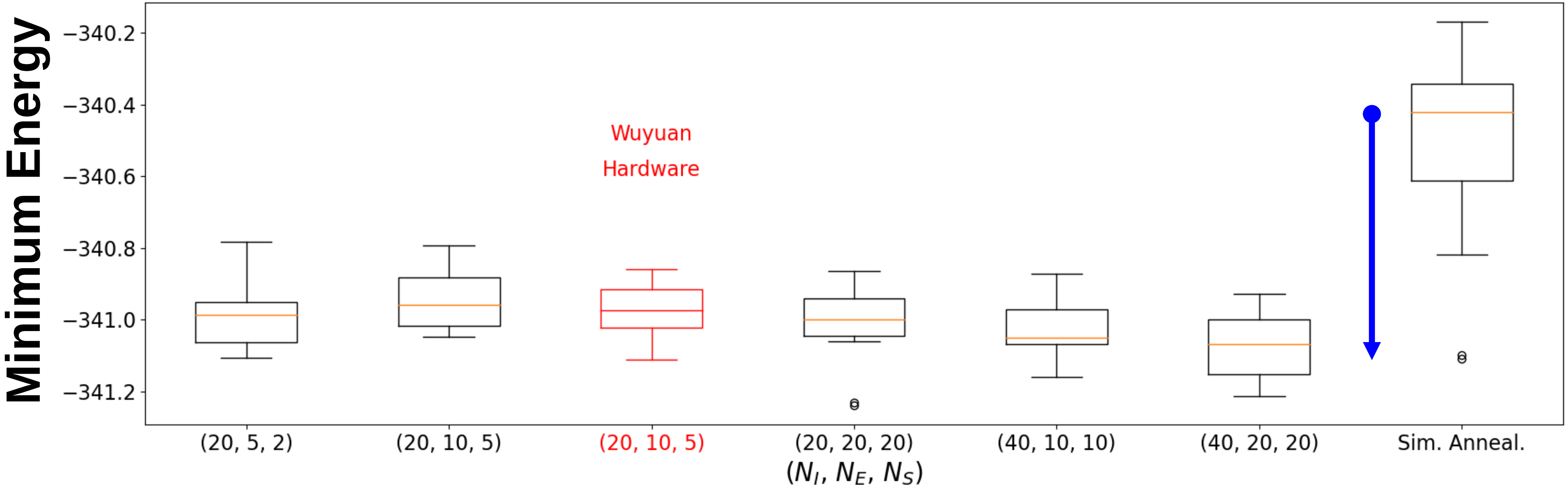
QAOA Accuracy





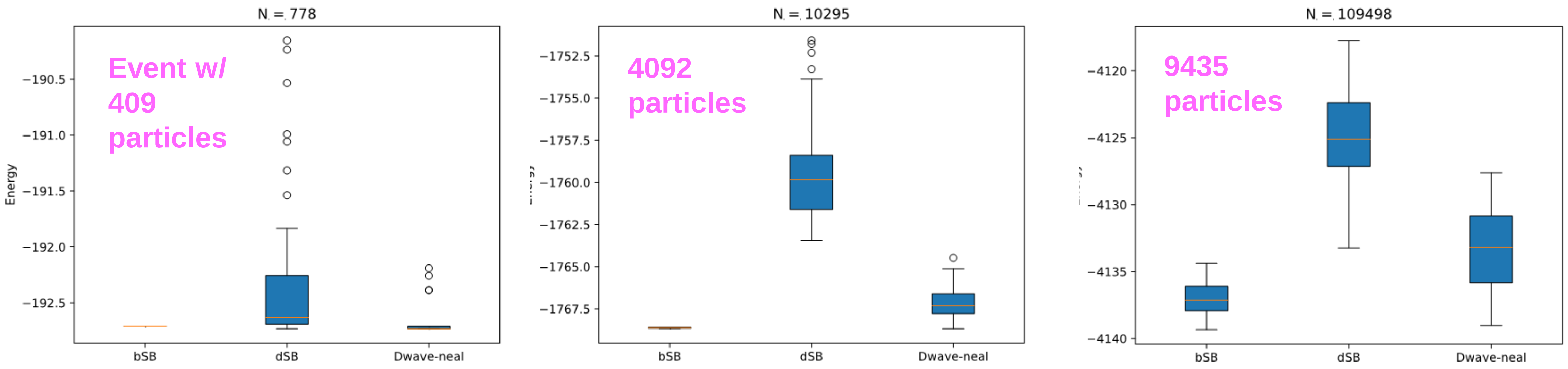
- **Note that the probability is NOT the accuracy of QAOA.**
- A single job runs multiple measurements, ranks the answers by probability & select the highest probability state as answer.
- **The accuracy already reaches 100% within the statistical uncertainty at 5 layers.**
- For further studies, a conservative choice of 7 layers is used.

Preliminary sub-QUBO Results



- Ran measurements to compare the performance and stability. 7 layers used in QAOA.
- No significant dependence on sub-QUBO model parameters (N_I, N_E, N_S) & **compatible performance between OriginQ simulator & actual hardware!**
- **Visible improvement w/ sub-QUBO compared to the simulated annealing only!**

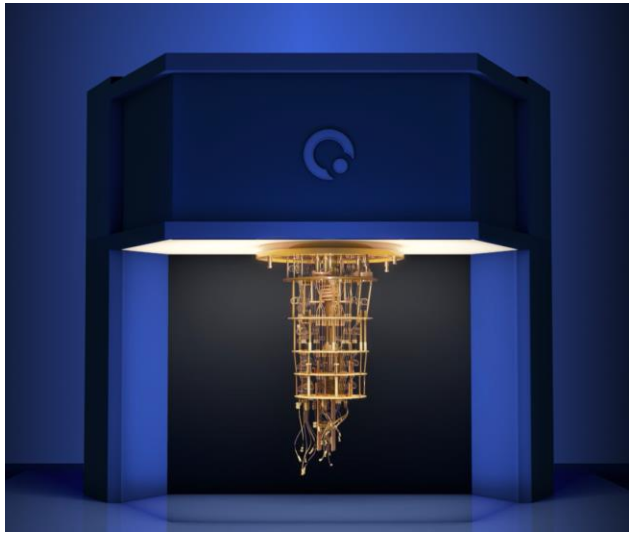
Mimimum Ising Energy Prediction



- Originally proposed adiabatic simulated bifurcation (aSB) is largely outperformed by new versions, so not shown here. D-Wave Neal is shown as a simulated annealing benchmark.
- **Ballistic simulated bifurcation (bSB) provides the best prediction of minimum energy with the least fluctuation**.
- Discrete simulated bifurcation (dSB) is not as good as the other two, but the impact on the reconstruction performance is not significant (next slide)

Origin Quantum

From Origin Quantum website



- Using superconductors.
- Free hardware available last year: 6 (悟源) & 12 qubits (悟空)
- 72 qubit machine available this year.

Origin Quantum

From Origin Quantum website

OriginQ Wukong -72-qubit QPU state

Last Update Time: Jul 18, 2024 23:54:54

Basic Information

queue	Latest calibration time	Latest calibration qubits	Latest calibration couplers	history calibration Info
0	Jul 18, 2024 23:54:54	/	/	View all

T1	T2*	BasicQGate	MaxLayers	MaxShots
14.84 µs(Avg)	1.85 µs(Avg)	U3、CZ	500	65535

Data view

Single-qubit Two-qubit

Qubit	Frequency	T1	T2*	ReadoutFidelity	ReadoutFidelity F0/F1	SingleGateFidelity
q0	4313	18.64	2.10	0.8696	0.9094/0.8298	0.9978
q1	4660	10.49	1.30	0.8824	0.933/0.8318	0.9978
q2	4107	20.68	0.94	0.4995	0.9628/0.0362	0.9987
q3	4180.919	10.81	3.09	0.8888	0.9042/0.8734	0.9973
q5	4094	7.18	1.21	0.9228	0.9302/0.9154	0.9975

Map view

The average SingleGateFidelity is 0.9973

0.9953 0.9988

The average CZ GateFidelity is 0.9597

0.8846 0.9985

$$QUBO = \sum_i a_i x_i + \sum_{i>j} b_{ij} x_i x_j$$

Multiple Solution Instances

- 3 parameters (N_I, N_E, N_S) in this sub-QUBO method.
- Extract N_I quasi-optimal solutions from full-QUBO classically.
- Randomly select N_S solution instances from N_I.
- Focus on particular binary variable x_i. Rank them in accordance to how much they vary over N_S solution instances. Highly varying x_i will be included in the sub-QUBO model.
- Pick-up process of N_S solution from quantum computing is repeated N_E times & N_E sub-QUBO models are considered.
- Returns a pool of N_I solutions & the best solution will be chosen.

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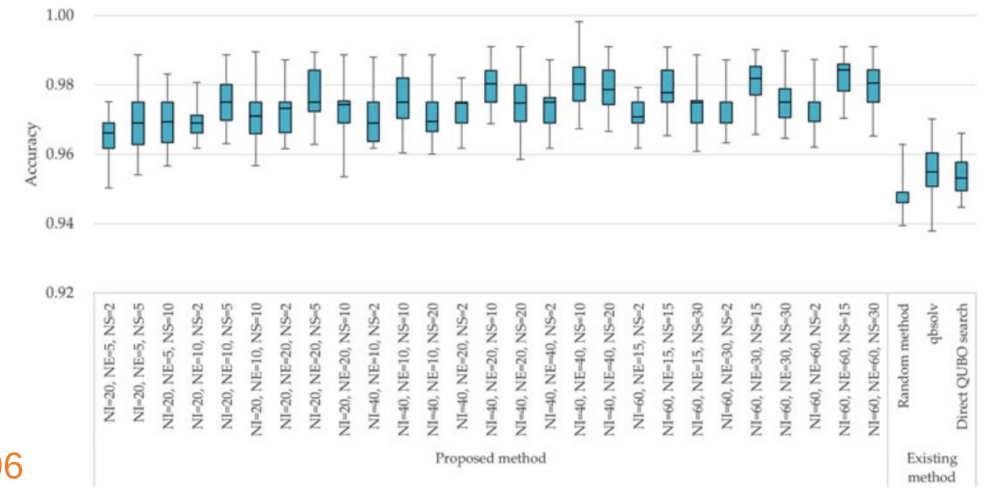
Sub-QUBO Methods

Algorithm 2. Proposed Hybrid Annealing Method

procedure PROPOSED METHOD WITH MULTI-INSTANCES
  for $(i = 1; i \leq N_I; i++)$ **do**
    $X_i \leftarrow$ Initialize(QUBO)
    Pool $\leftarrow$ AddInstancePool(Pool, X_i)
  $X_{best} \leftarrow$ FindBest(Pool)
  while not converged **do**
    for $(i = 1; i \leq N_I; i++)$ **do**
      $X_i \leftarrow$ Optimize(QUBO, X_i)
        ▷ Using a classical computer
    for $(i = 1; i \leq N_E; i++)$ **do**
      $X_1, X_2, \cdots, X_{N_S} \leftarrow$ SelectInstance(Pool, N_S)
      for $(j = 1; j \leq n; j++)$ **do**
        for $(k = 1; k \leq N_S; k++)$ **do**
          $c_j \leftarrow c_j + x_{k,j}$
        $d_j \leftarrow |c_j - \frac{N_S}{2}|$
      subQUBO $\leftarrow$ Extract(ArgSort($d_1, d_2, \cdots, d_n$), m, X_t)
      $X' \leftarrow$ Optimize(subQUBO, X_t)
        ▷ Using an Ising machine
      Pool $\leftarrow$ AddInstancePool(Pool, X')
    $X_{best} \leftarrow$ FindBest(Pool)
    Pool $\leftarrow$ ArrangeInstancePool(Pool, N_I)
  return $f(X_{best}), X_{best}$

Algorithm 4. Qbsolv[10]

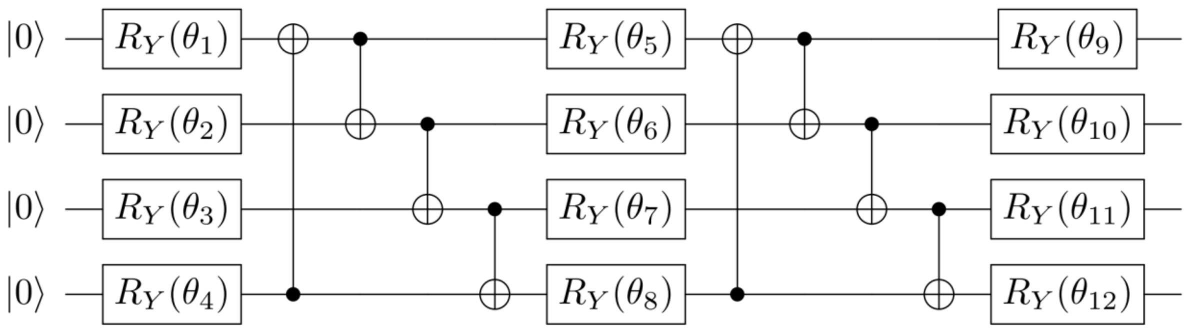
procedure QBSOLV
  $X \leftarrow$ Initialize(QUBO)
  $X_{best} \leftarrow$ TabuSeach(QUBO, X)
  index $\leftarrow$ OrderByImpact(QUBO,X_{best})
  while not converged **do**
    for $(i = 0; i < \text{Size(QUBO)}; i+ = \text{Size(subQUBO)})$ **do**
      subQUBO $\leftarrow$ Decompose(QUBO,
        index[$i : i$+Size(subQUBO)-1], X_{best})
      subX $\leftarrow$ Optimize(subQUBO, X_{best})
      X[index[$i : i$+Size(subQUBO)-1]] $\leftarrow$ subX
    $X \leftarrow$ TabuSearch(QUBO, X)
    index $\leftarrow$ OrderByImpact(QUBO, X)
    if $f(X) < f(X_{best})$ **then**
      $X_{best} \leftarrow X$
  return $f(X_{best}), X_{best}$



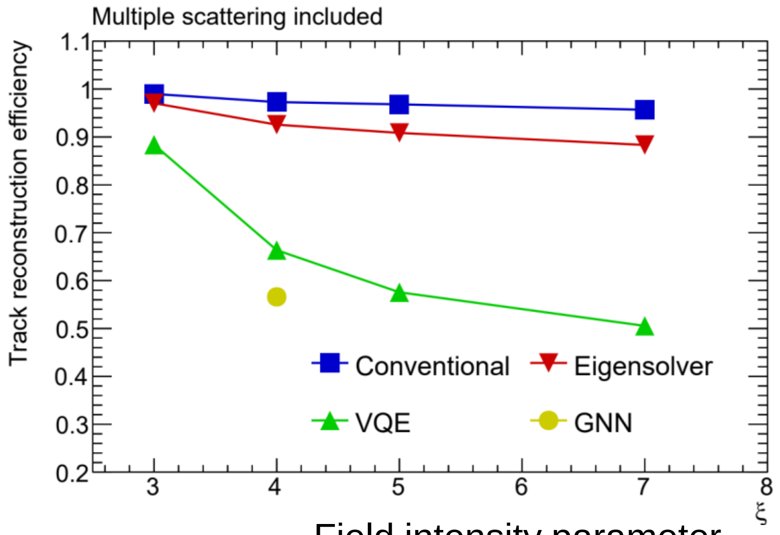
Y. Atobe, M. Tawada, N. Togawa, IEEE Trans. Comp. 71, 10 (2022) 2606

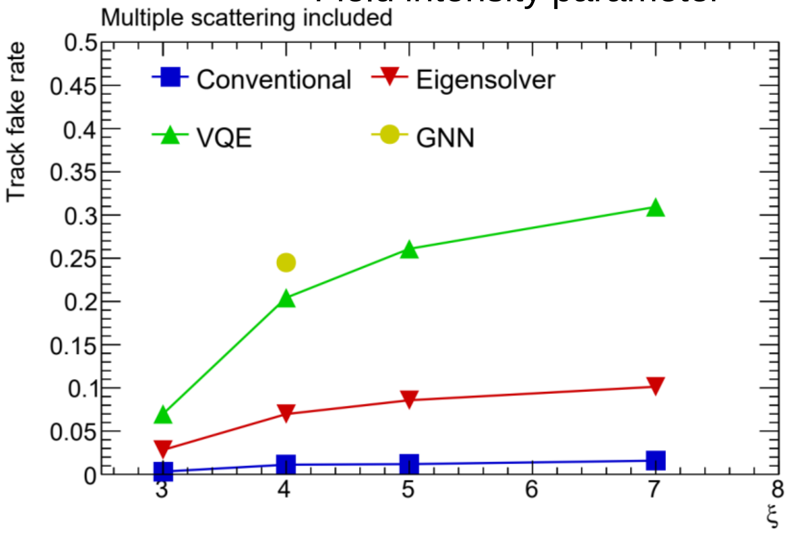
L.Funcke, T.Hartung, B.Heinemann, K.Jansen, A.Kropf, S.Kühn, F.Meloni, D.Spataro, C.Tüysüz, Y.C.Yap, https://arxiv.org/abs/2202.06874

Previous Results from LUXE



- Tracking successfully ran w/ quantum & classical benchmarks
- Classical GNN performance is limited by the training dataset size
- Room for improvement for both GNN & quantum tracking (optimization ongoing)



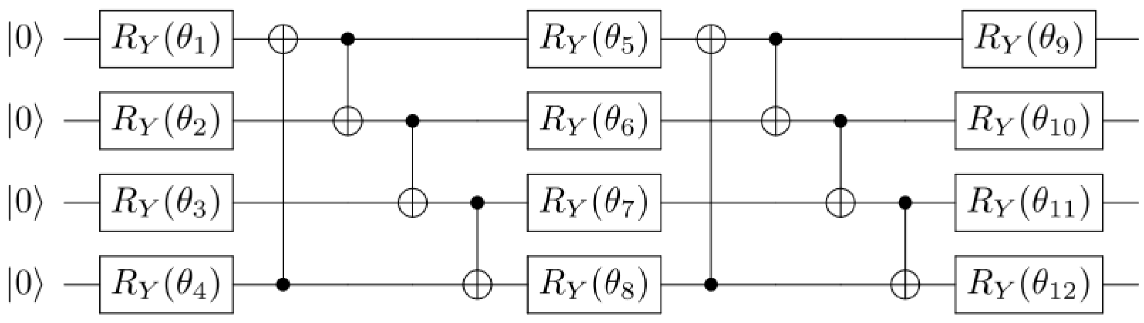


Gate-based Approach: VQE

- QUBO can be mapped to Ising Hamiltonian and be solved using Variational Quantum Eigensolver (VQE) or Quantum Approximate Optimization Algorithm (QAOA) w/ quantum gates.

$$\mathcal{H} = -\sum_{n=1}^{N}\sum_{m<n} \bar{b}_{nm}\sigma_n^x\sigma_m^x - \sum_{n=1}^{N} \bar{a}_n \sigma_n^x$$

- DESY team considered VQE: TwoLocal ansatz w/ R_Y gates & circular CNOT entangling pattern w/ IBM
- Performance compatible w/ classical traditional method.



Only 4 qubits drawn for simplicity