Jet Reconstruction with Quantum-Annealing-Inspired Algorithms

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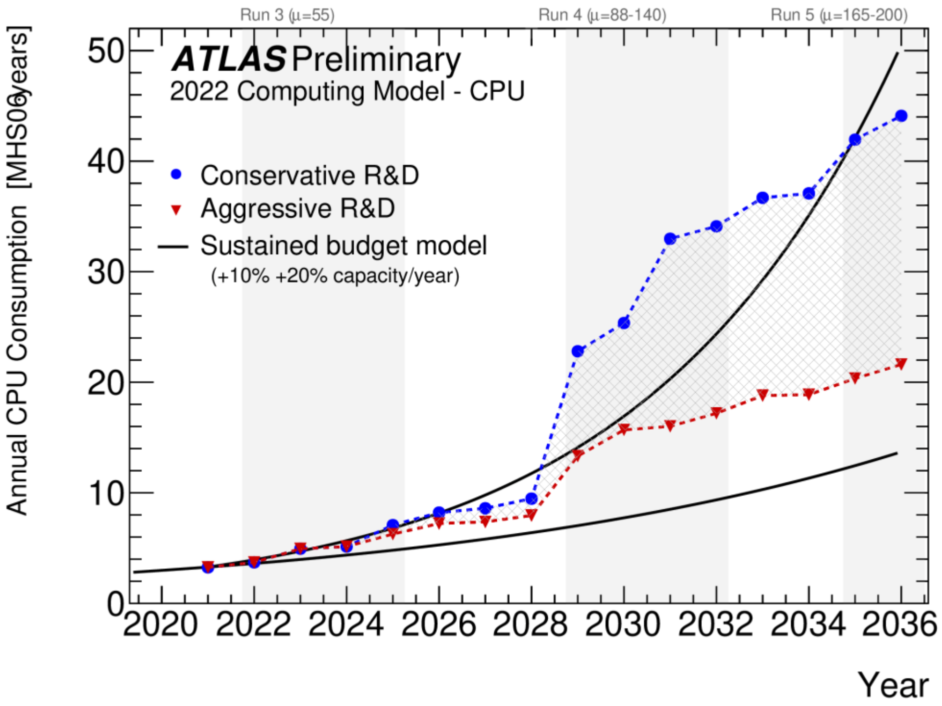
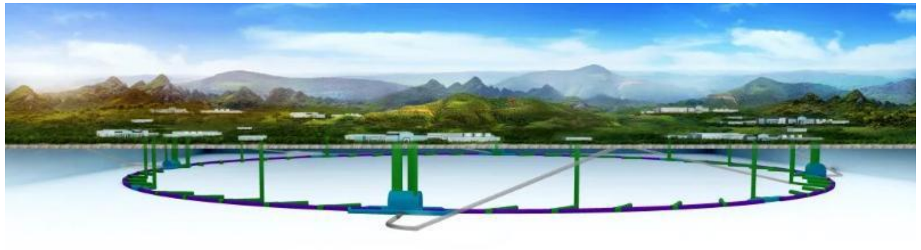
Work in collaboration with Xian-Zhe Tao, Qing-Guo Zeng, Man-Hong Yung
(Shenzhen Institute for Quantum Science and Engineering [IQSE]) arXiv:2410.14233

Picture credits: Qianhui Shi, Yan Liang

Reconstruction at Future Colliders





- **At HL-LHC & CEPC Z-pole operation, we will enter the exa-byte era.**
- At the HL-LHC, CPU time exponentially increases with pileup, leading to increase in annual computing cost by x10-20.
- **CEPC Z-pole data taking may experience similar computing challenges.**
- **Along w/ detector simulation, reconstruction is very CPU-consuming.**
- **We may benefit from quantum algorithms.**

Quantum Approaches

Quantum Gates

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

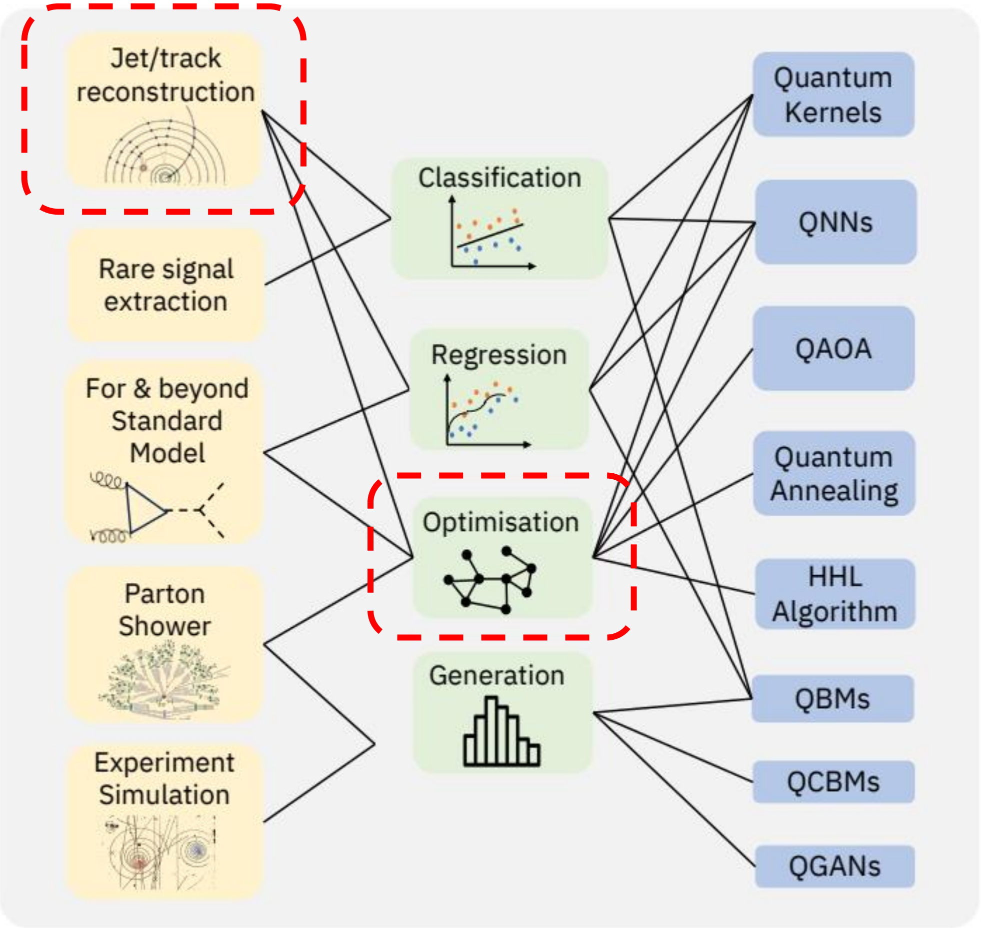
Ising machines

Quantum Annealing

- Uses adiabatic quantum evolution to search for the ground state of a Hamiltonian
  → Only applicable to optimization problems
- Implemented in D-Wave Systems.

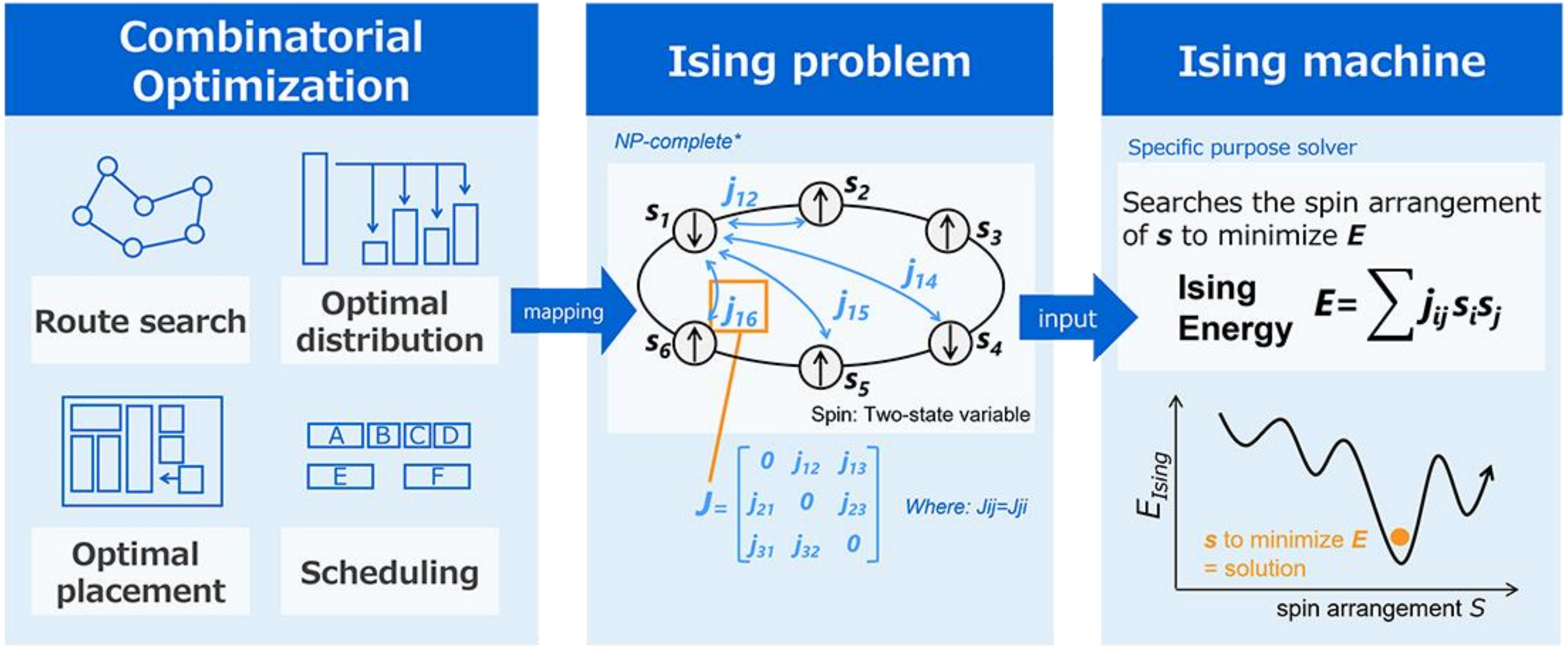
Quantum-Inspired ← Scope of this talk

- Inspired by quantum annealing.
- Simulated annealing, simulated coherent Ising machine, simulated bifurcation, etc.



QC4HEP White Paper

Combinatorial Optimization Problem

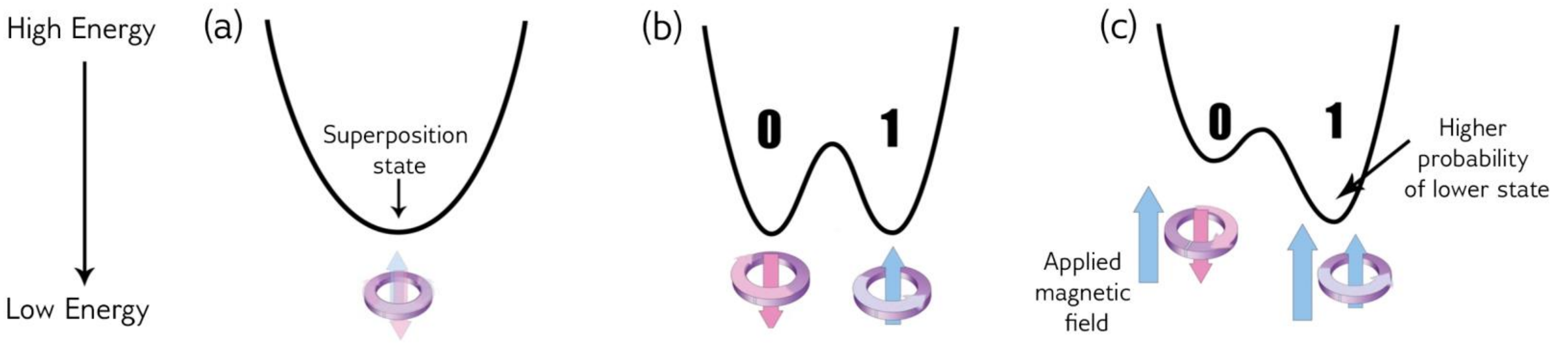


- Combinatorial optimization problems are non-deterministic polynomial time (NP) complete problem: no efficient algorithm exists to find the solution.
- They can be mapped to **Ising (or quadratic unconstrained binary optimization; QUBO) problems**. The ground state of an Ising Hamiltonian is designed to provide the answer.
  - Ising [±1 spins], QUBO [0/1 binaries]. They can easily be converted to each other (backup).
- **Track & jet reconstruction can also be formulated as Ising/QUBO problems.**

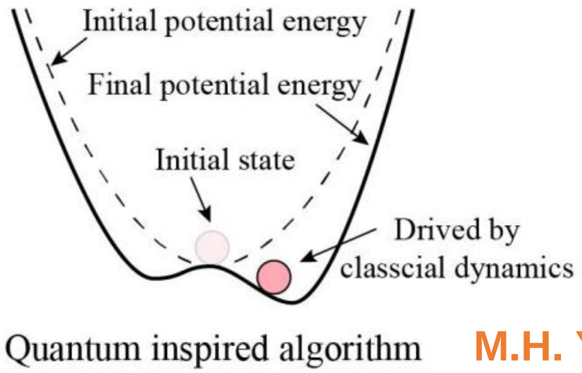
Quantum-Annealing-Inspired Algorithms (QAIAs)

Quantum Annealing

From D-Wave



Quantum-inspired



M.H. Yung

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

Simulated Bifurcation (SB)

➤ adiabatic Simulated Bifurcation (aSB)

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

➤ ballistic Simulated Bifurcation (bSB)

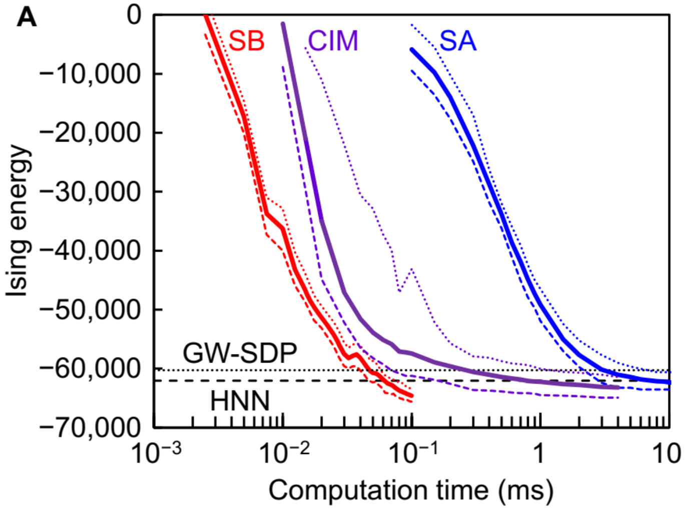
$$\dot{x}_i = \frac{\partial H_{SB}}{\partial y_i} = \Delta y_i, \qquad \dot{y}_i = \frac{\partial H_{SB}}{\partial x_i} = (p(t) - \Delta)x_i + \xi_0 \sum_{j=1}^{N} J_{ij} x_j$$

➤ discrete Simulated Bifurcation (dSB)

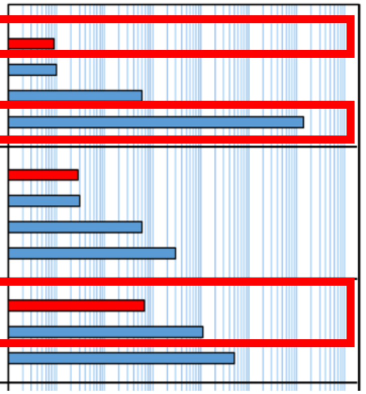
$$\dot{x}_i = \frac{\partial H_{SB}}{\partial y_i} = \Delta y_i, \qquad \dot{y}_i = \frac{\partial H_{SB}}{\partial x_i} = (p(t) - \Delta)x_i + \xi_0 \sum_{j=1}^{N} J_{ij} \mathrm{sign}(x_j)$$

Simulated Bifurcation (SB)

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**	**9.2 μs**
			RBM	10 μs
			CIM	0.6 ms
			QA	1.4 s
100	All-to-all	{±1}	**dSBM**	**29 μs**
			RBM	30 μs
			SimCIM	0.6 ms
			CIM	3.0 ms
200	Sparse (Degree 3)	{0, −1}	**dSBM**	**0.70 ms**
			QA	11 ms
			CIM	51 ms

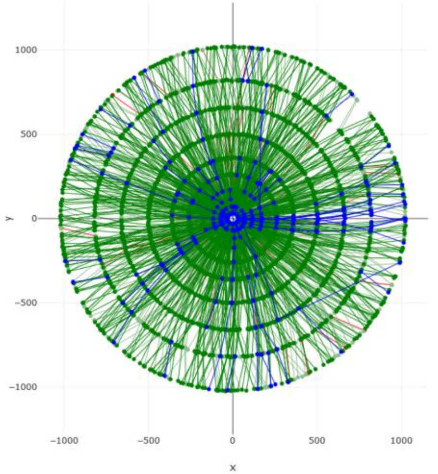


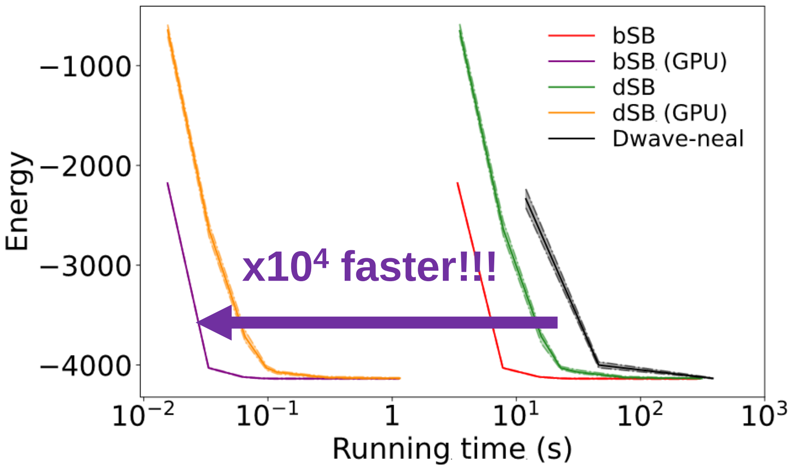
Q.G. Zeng et al., Comm. Phys. (2024) 7:249

Graph size	Algorithm	Hardware	Time(s)
	TTN	CPU 1 core	5.62
	Brute-force search[46]	GPU Titan V	$>10^{48}$
4 × 4 × 8	Exact belief propagation[13]	CPU 1 core	~0.96
	QA[13]	D-Wave	~0.05
	bSB	CPU 1 core	0.12
	bSB	GPU Tesla V100	<0.001
	TTN	CPU 1 core	32400
	TTN[44]	GPU Tesla V100	84
8 × 8 × 8	Brute-force search[46]	GPU Titan V	$>10^{190}$
	Exact belief propagation[13]	CPU 1 core	~2880
	dSB	CPU 1 core	17.64
	dSB	GPU Tesla V100	<0.68

- **SB is known to outperform other quantum-inspired algorithms as well as quantum annealing (QA) for some problems**
- **Our previous study: track reconstruction w/ SB → 4 orders of magnitude speed-up from SA.**

H. Okawa, Q.G. Zeng, X.Z. Tao, M.H. Yung, Comput. Softw. Big Sci. 8, 16 (2024)





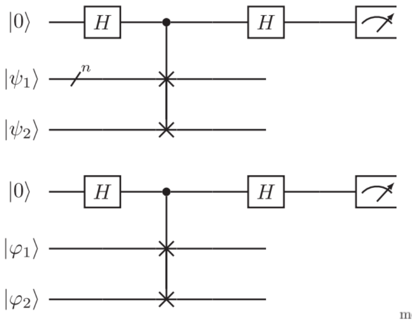
Previous Jet Reco. Studies (Sequential)

- Jet reconstruction is a clustering problem. Quantum algorithms may bring in acceleration.
- A few algorithms were considered to replace the traditional iterative calculation. Expected to bring in speed-up, but still at a conceptual stage.

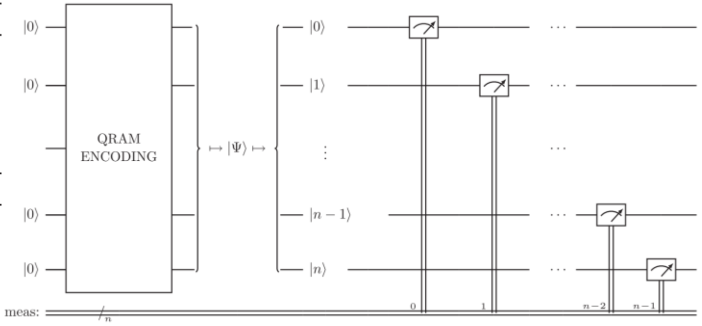
Quantum K-means，Quantum Affinity Propagation (AP)，Quantum k_t

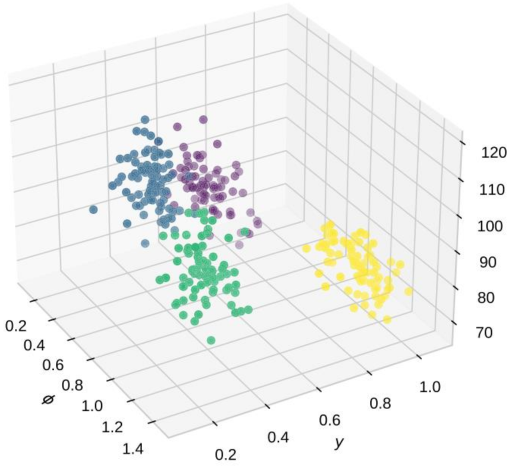
J.J. Martinez de Lejarza, L. Cieri, G. Rodrigo, PRD 106 036021 (2022)

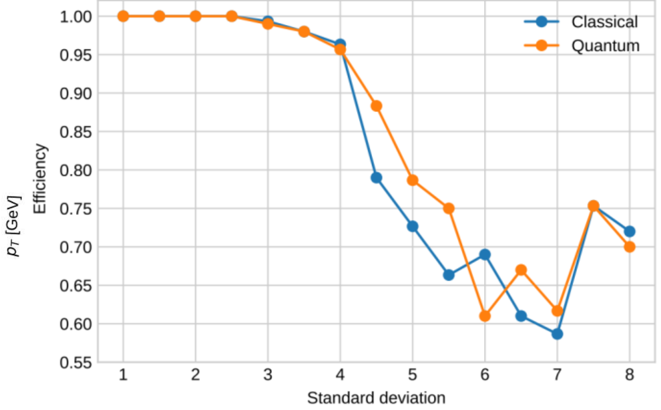
Computes distance in Minkowski space



Assigns each particle to the nearest centroid





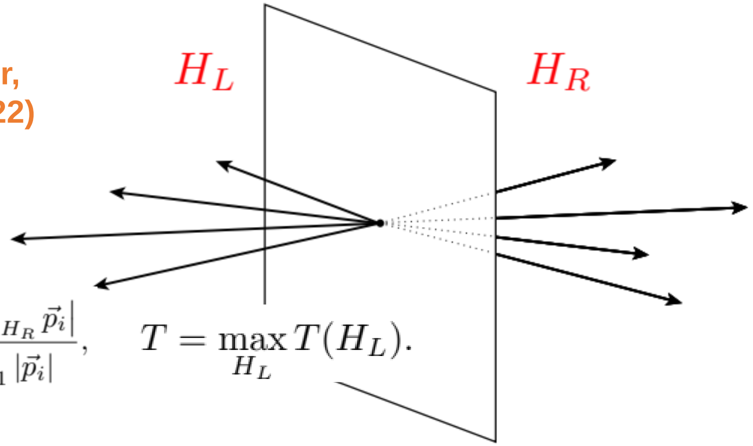


- Similar studies： Grover search **A. Wei, P. Naik, A.W. Harrow, J. Thaler, PRD 101, 094015 (2020)**, quantum K-means **D. Pires, P. Bargassa, J. Seixas, Y. Omar, arXiv:2101.05618 (2021).**

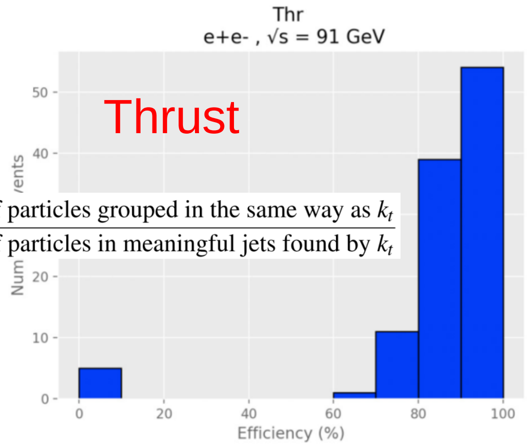
Previous Jet Reco. Studies (Global/QUBO)

Quantum Annealing (Thrust or Angle-based)

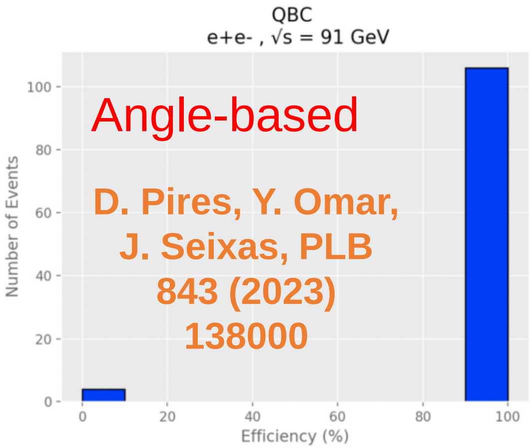
A. Delgado, J. Thaler, PRD 106, 094016 (2022)



$$T(H_L) = \frac{2\left|\sum_{i\in H_L}\vec{p}_i\right|}{\sum_{i=1}^{N}|\vec{p}_i|} = \frac{2\left|\sum_{i\in H_R}\vec{p}_i\right|}{\sum_{i=1}^{N}|\vec{p}_i|}, \qquad T = \max_{H_L} T(H_L).$$



$$\varepsilon = \frac{\#\text{ of particles grouped in the same way as } k_t}{\#\text{ of particles in meaningful jets found by } k_t}$$

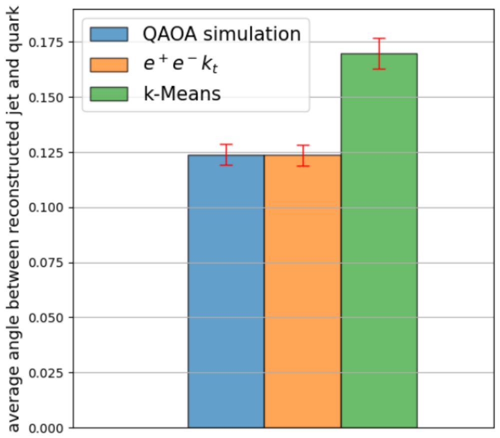


D. Pires, Y. Omar, J. Seixas, PLB 843 (2023) 138000

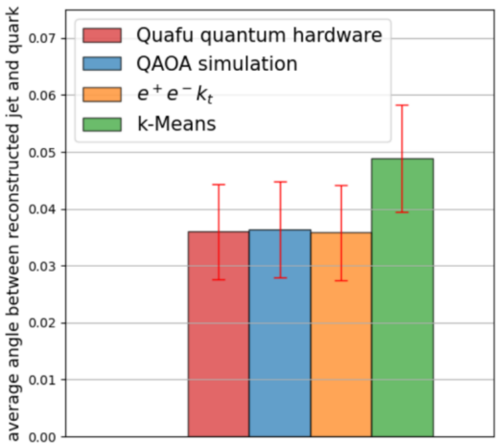
Quantum Gates (e.g. QAOA)

Y. Zhu et al., arXiv:2407.09056

30-particle data ($e^+e^- \rightarrow ZH \rightarrow \nu\nu ss$)



6-particle data ($e^+e^- \rightarrow ZH \rightarrow \nu\nu ss$)



- Jet reconstruction can also considered as a QUBO problem, but **fully-connected QUBOs are very difficult to solve.**
- Angle-based method has better performance than the Thrust-based method, but **does not work for multijet (N_{jet}>2) events so far.** [D. Pires et al.]
- QAOA approach is only tested with significantly downsized dataset (6, 30 particles) [Y. Zhu et al.]

QUBO Formulation in This Study

QUBO Formulation

$$O_{\text{QUBO}}^{\text{multijet}}(x_i) = \sum_{n=1}^{n_{\text{jet}}} \sum_{i,j=1}^{N_{\text{input}}} Q_{ij} x_i^{(n)} x_j^{(n)} + \lambda \sum_{i=1}^{N_{\text{input}}} \left(1 - \sum_{n=1}^{n_{\text{jet}}} x_i^{(n)}\right)^2,$$

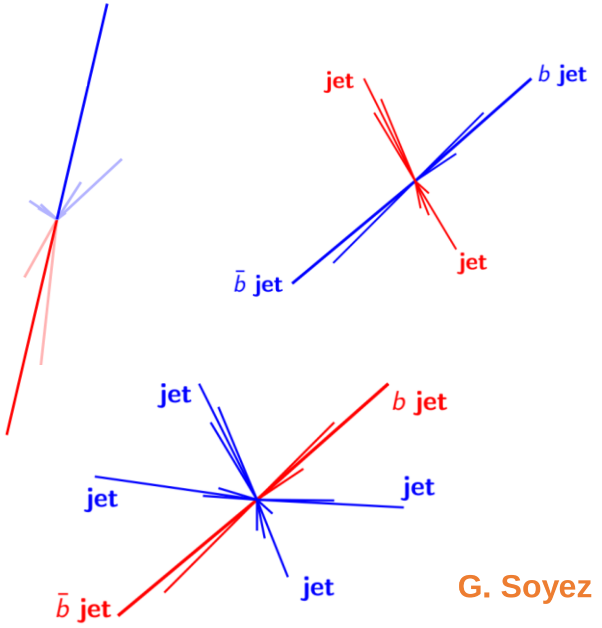
Defines distances b/w jet constituents

Avoids double-assignment of jet constituents

$$Q_{ij} = 2\min(E_i^2, E_j^2)(1 - \cos\theta_{ij}).$$ **[ee-k_t distance]**

$$Q_{ij} = -\frac{1}{2}\cos\theta_{ij}$$ **[angle-based]**

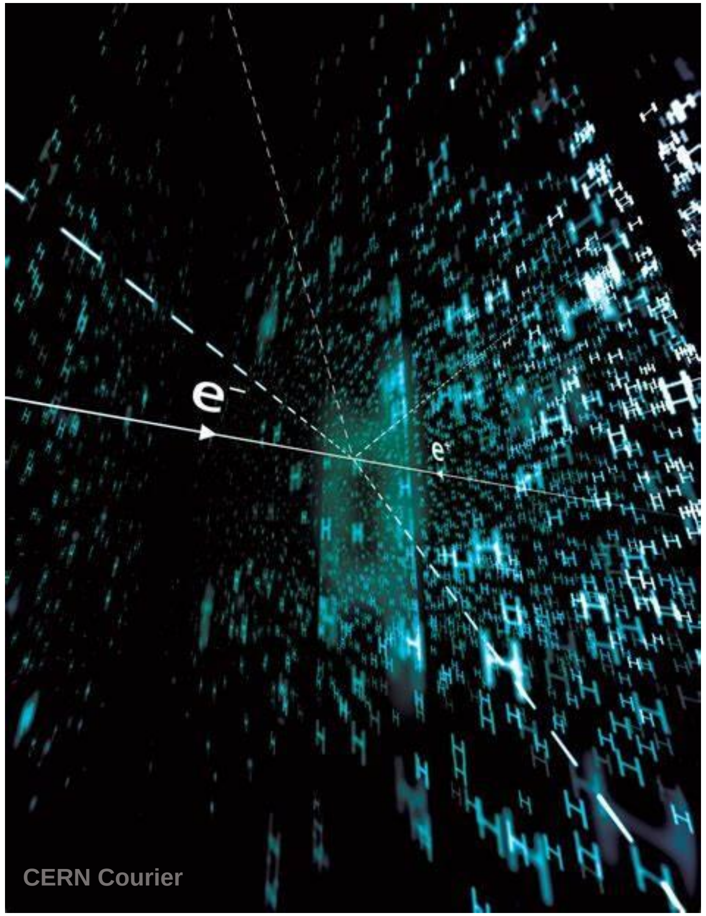
D. Pires, Y. Omar, J. Seixas, PLB 843 (2023) 138000



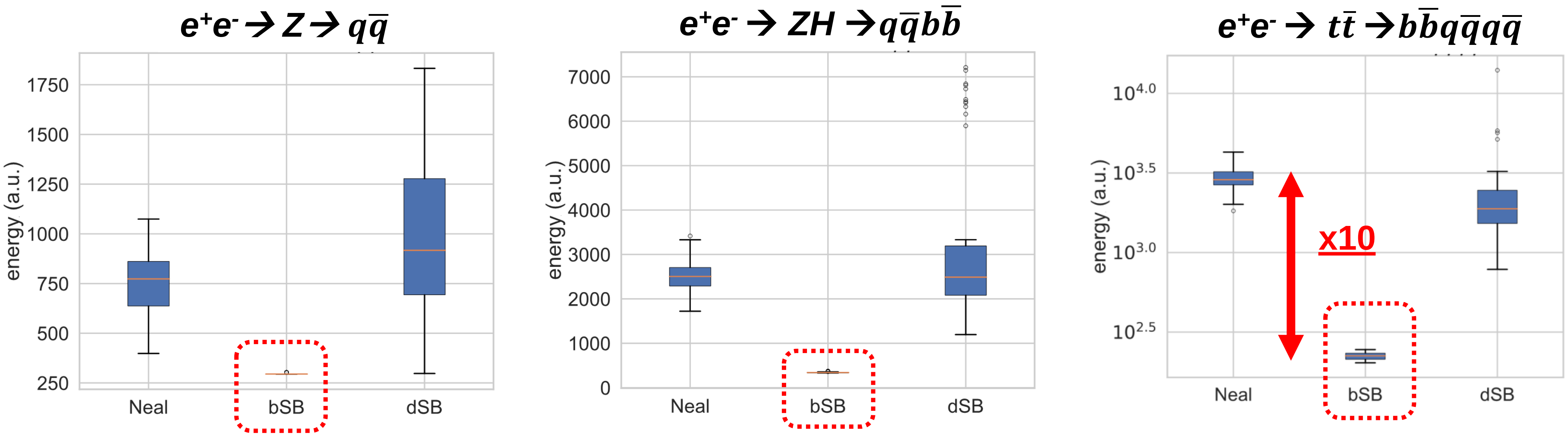
- **<u>Exclusive jet finding (n_{jet} fixed) with the ee-k_t algorithm</u>** is considered → the baseline at CEPC & other e+e- future Higgs factories.
- **We adopt the same ee-k_t distance in the QUBO formulation. <u>This QUBO is designed for general jet multiplicity beyond dijet</u>.** → $x_i^{(n)}=1$ means the i-th jet constituent belongs to the n-th jet.
- The angle-based method is also shown for comparison **[D. Pires et al PLB 843 (2023) 138000].**

Dataset

- Three sets of e+e- collision events are generated to consider various jet multiplicity:
  - $Z \rightarrow q\bar{q}$ (√s=91 GeV, 2 jets),
  - $ZH \rightarrow q\bar{q}b\bar{b}$ (√s=240 GeV, 4 jets)
  - $t\bar{t} \rightarrow b\bar{b}q\bar{q}\bar{q}q$ (√s=360 GeV, 6 jets)
- **Delphes card with the CEPC 4th-detector concept** is used for the fast simulation.
  → Thanks to Gang Li, Shudong Wang and Xu Gao for feedback!
- Jets are reconstructed from **the particle flow candidates**.



Ising Energy Prediction

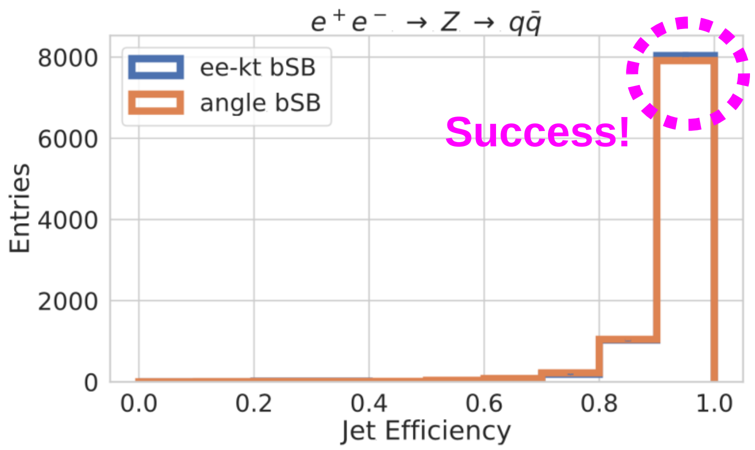


- **Fully-connected QUBOs are difficult to solve**; it is known that quantum annealing hardware is not good at solving them so far.
  - This is in contrast to track reconstruction, in which the QUBOs are largely sparse.
- **Ballistic SB (bSB) predicts energy lowest with the smallest fluctuation.**
- **Performance is especially outstanding for 6-jet QUBOs → bSB can find x10 lower minimum energy for the all-hadronic $t\bar{t}$ events!**

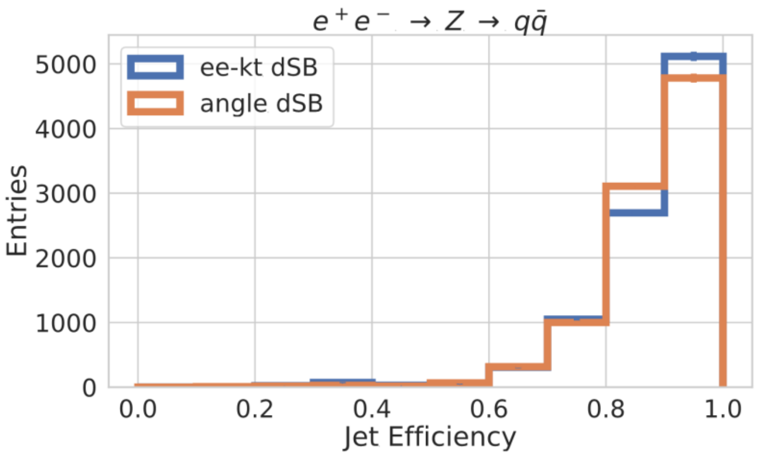
Efficiency ($Z \rightarrow q\bar{q}$: 2 jets)

$$\varepsilon = \frac{\text{\# of particles grouped in the same way as } k_t}{\text{\# of particles in meaningful jets found by } k_t}$$

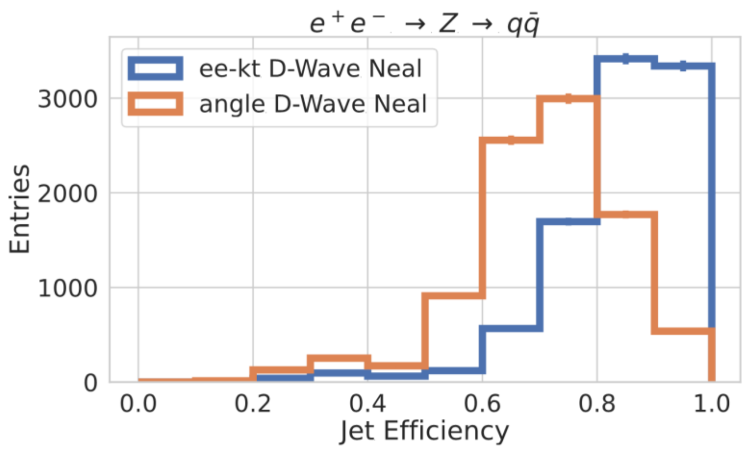
bSB



dSB



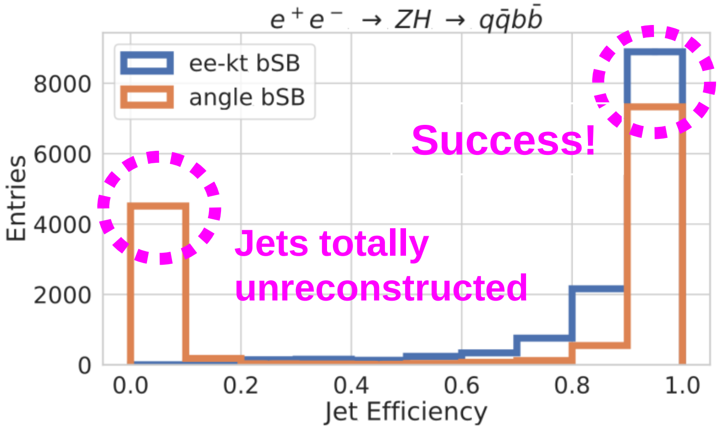
D-Wave Neal



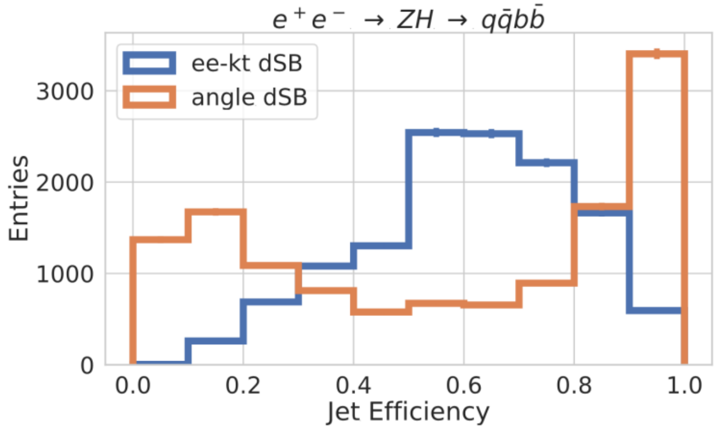
- Most jet reconstruction w/ quantum approaches adopts the above-defined efficiency as performance metric; i.e. compatibility of jet assignment w/ the traditional ee-k_t jet finding.
- **bSB provides the highest efficiency. D-Wave Neal has visibly degraded performance already in dijet events. dSB also has lower efficiency than bSB.**
- **The ee-k_t approach performs better than the angle-based method for all cases.**

Efficiency ($ZH \rightarrow q\bar{q}b\bar{b}$: 4 jets)

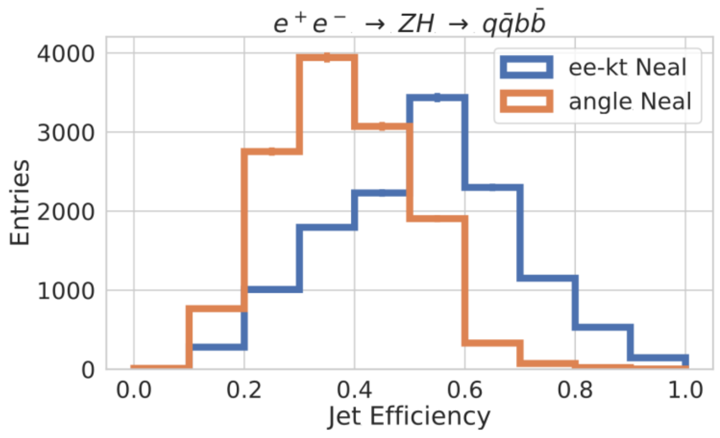
bSB



dSB

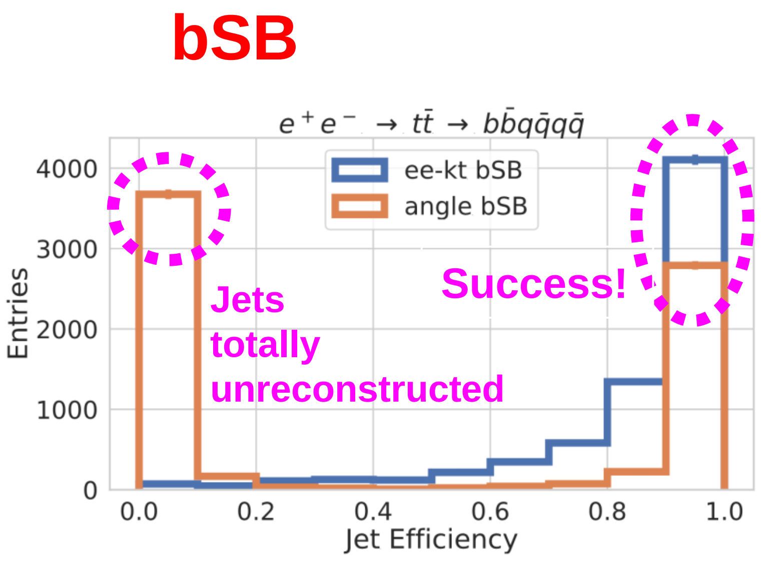


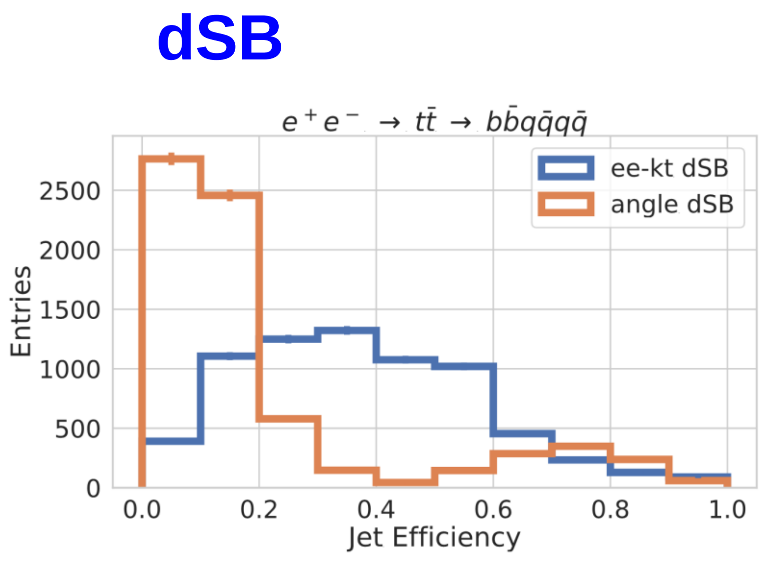
D-Wave Neal

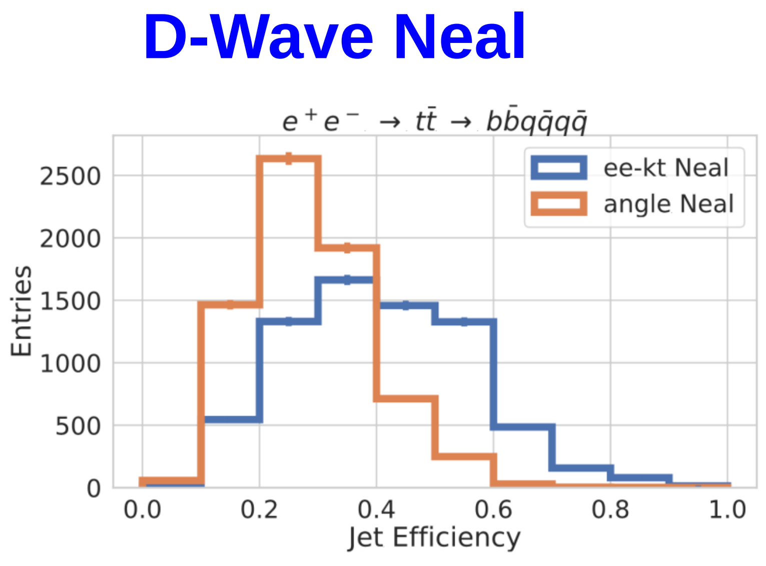


- **Angle-based method does not work for N_{jet}>2; many jets are missed and/or jet constituents are unreasonably assigned.** Angles are inappropriate for multijet conditions.
- **dSB & D-Wave Neal cannot reconstruct jets properly regardless of the distance adopted → because of the non-optimal predicted energy**
- **Only bSB w/ ee-k_t distances maintains reasonable performance.**

Efficiency ($t\bar{t} \rightarrow b\bar{b}q\bar{q}q\bar{q}$: 6 jets)



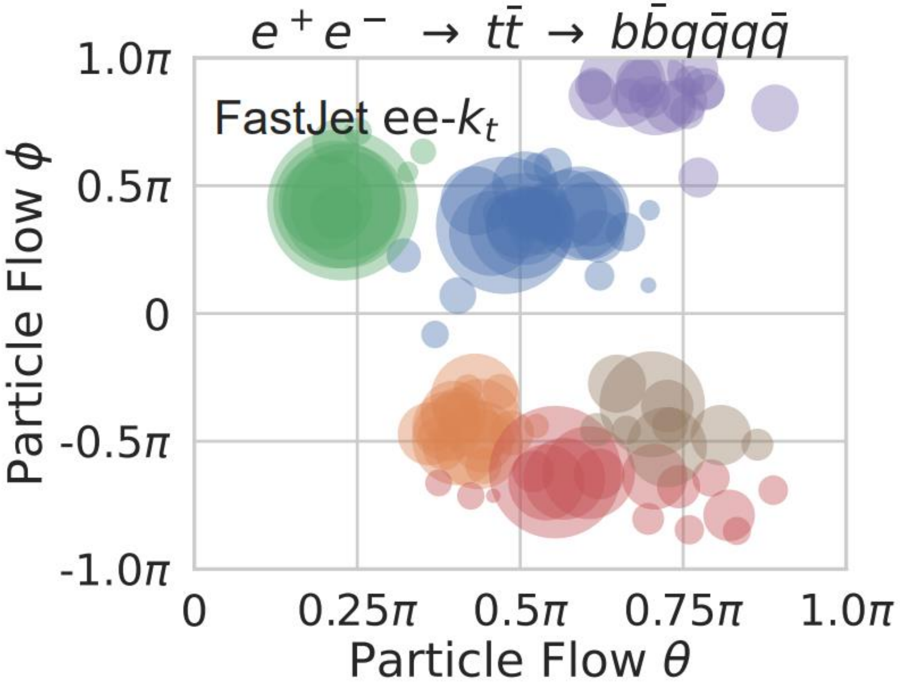




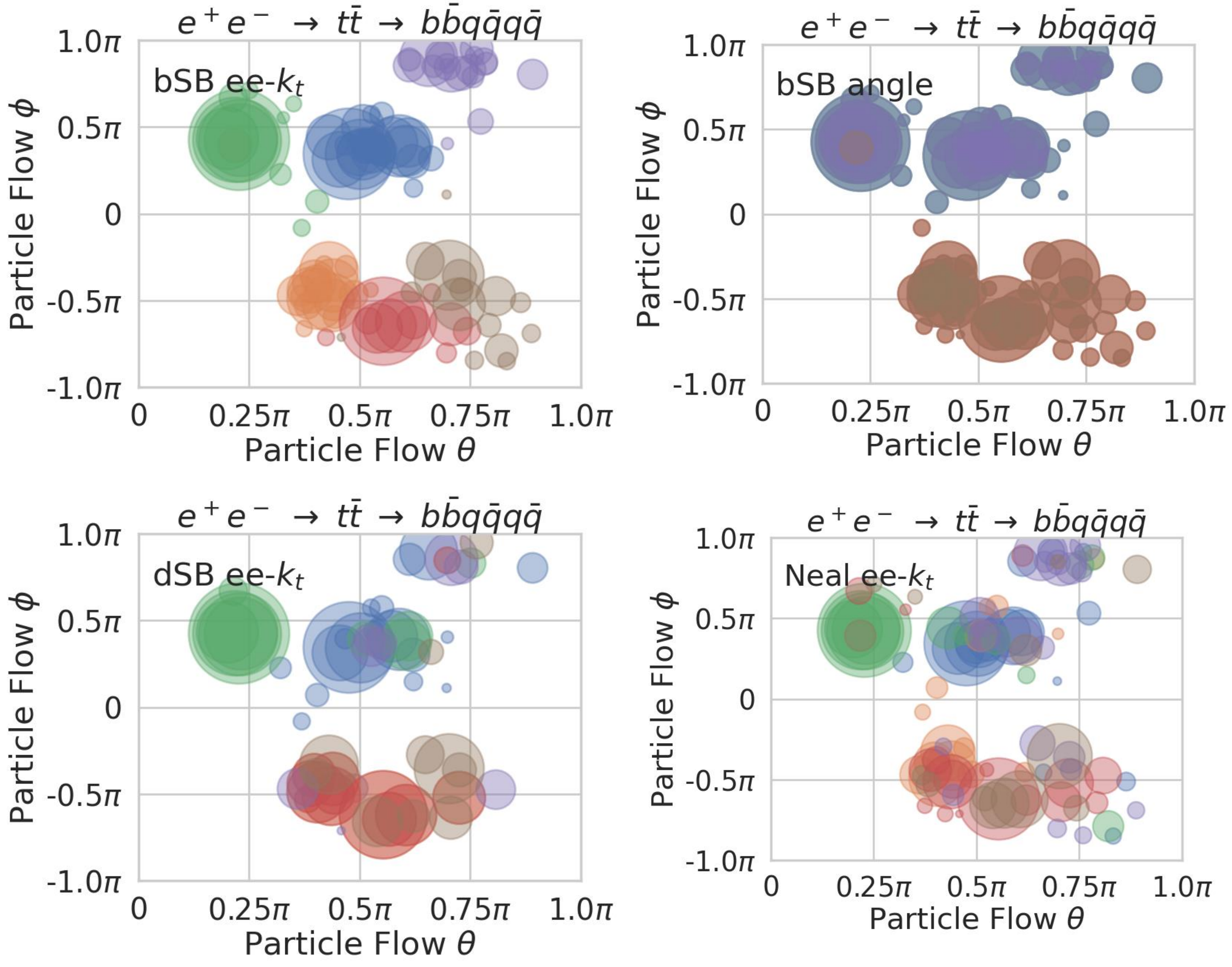
- Angle-based method does not work for $N_{jet}>2$; angles are very likely inappropriate for dense conditions. **The trend is more apparent in ttbar events than the ZH.**
- **dSB & D-Wave Neal cannot reconstruct jets properly regardless of the distance adopted → because of the non-optimal predicted energy**
- **Only bSB w/ ee-k_t distances maintains reasonable performance.**

Event Displays ($t\bar{t}$)

Baseline (FastJet)

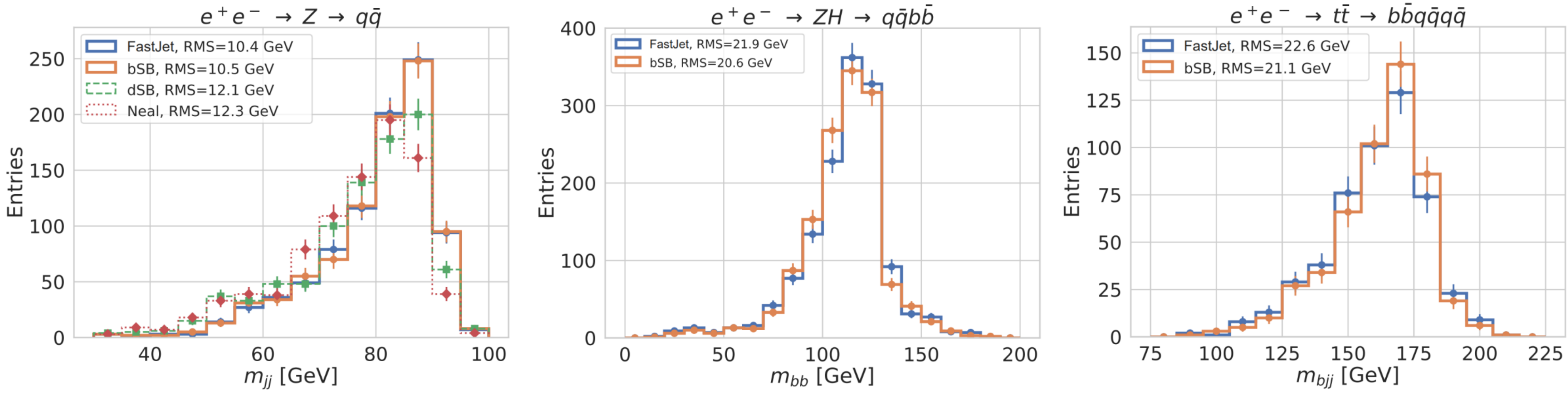


QAIAs



- **Only bSB w/ ee-k_t QUBO can reasonably reconstruct all jets.**
- **Other approaches misses some jets and/or PFlows are totally mixed up.**

Impact on Invariant Mass

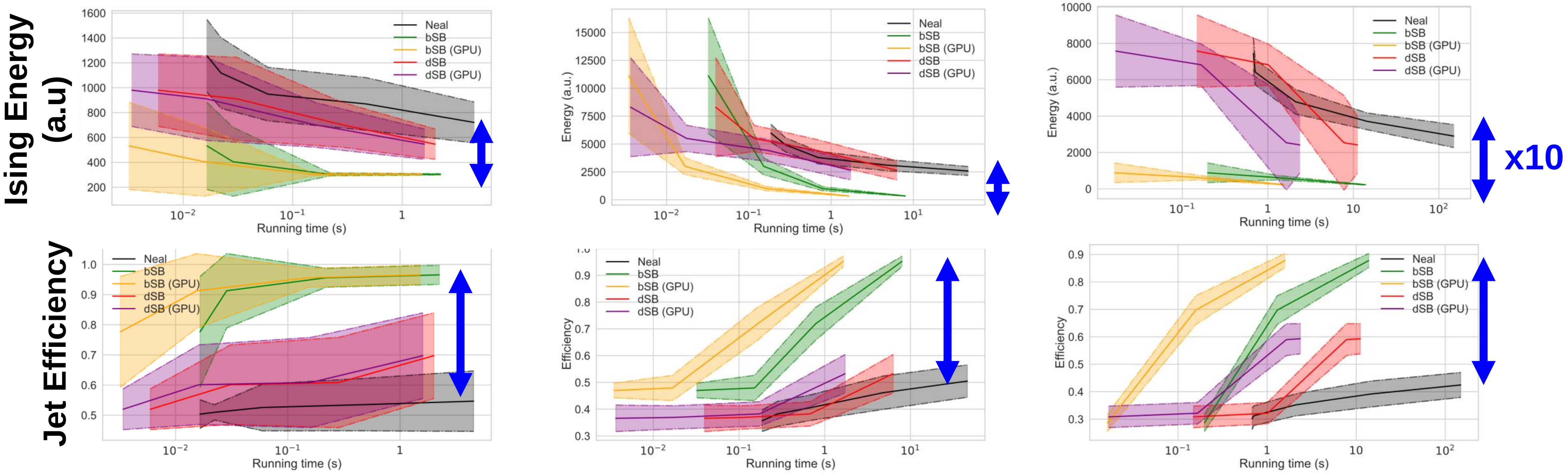


- **As <u>FastJet is NOT the 'TRUE' answer</u>, resemblance to it is not the decisive performance metric.** → Z, Higgs and top quark mass resolutions are evaluated.
- **<u>bSB improve mass resolution for multijet! (& comparable resolution for Z)</u>**
- **dSB & Neal already has ~20% degradation in Z mass resolution & unable to properly reconstruct jets in multijet events (thus not shown for ZH & $t\bar{t}$)**

Computation Speed

Only 1 CPU/GPU used

$e^+e^- \to Z \to q\bar{q}$ $e^+e^- \to ZH \to q\bar{q}b\bar{b}$ $e^+e^- \to t\bar{t} \to b\bar{b}q\bar{q}q\bar{q}$



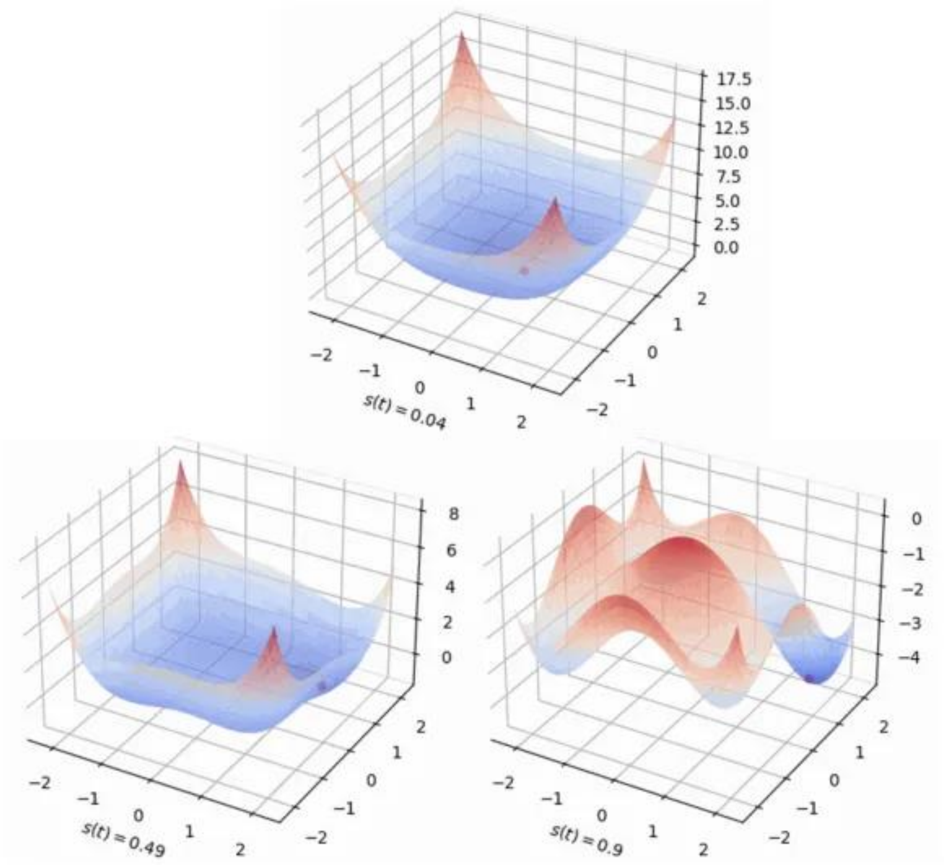
- **Ising solvers usually continue to improve energy prediction w/ running time.**
- **<u>bSB significantly outperforms dSB & Neal</u> (& an order of maganitude speed-up w/ GPU)**
- **D-Wave Neal is trapped in a local minimum (x10 worse energy prediction for $t\bar{t}$). dSB is slower in energy convergence & less successful than bSB for energy prediction.**

Summary

- Jet reconstruction can be formulated as an Ising/QUBO problem.
- Its QUBOs are fully-connected; notoriously difficult to solve (e.g. w/ quantum annealers), leading to failure in multijet reconstruction in the existing studies.
- A set of quantum-annealing-inspired algorithms (QAIAs) is considered. Important findings are:

1. **A QAIA, i.e. ballistic simulated bifurcation (bSB) can reasonably predict ground state energy even for multijet → First successful demonstration of multijet reconstruction w/ a QUBO approach.**
2. **QUBO design is also important:** angle-based QUBOs do not work for multijet, but ee-k_t-distanced QUBOs can successfully reconstruct multijet events.
3. **Jet reconstruction w/ bSB & ee-k_t QUBOs provides slightly improved energy resolution.**

- This algorithm may have potential use cases at CEPC: not just for offline jet reconstruction but also for triggers during the Z-pole operation.
- Further studies (especially on the speed-up) are ongoing.



Thank you for listening!

Backup

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Applications to Track Reconstruction

- 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.

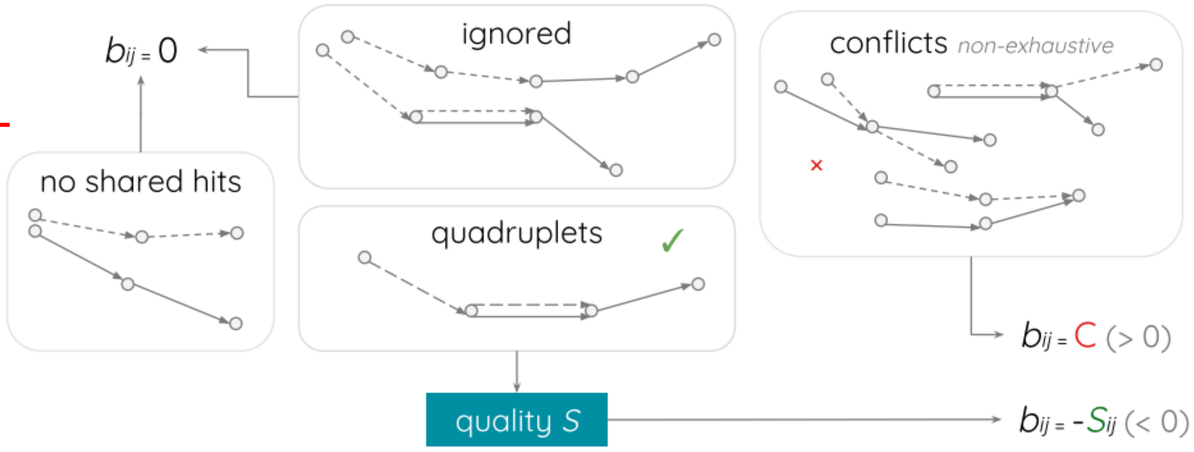
$$O(a,b,T) = \underbrace{\sum_{i=1}^{N} a_i T_i}_{\text{Quality of triplets}} + \underbrace{\sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j}_{\text{Compatibility b/w triplet pairs}}$$

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

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.



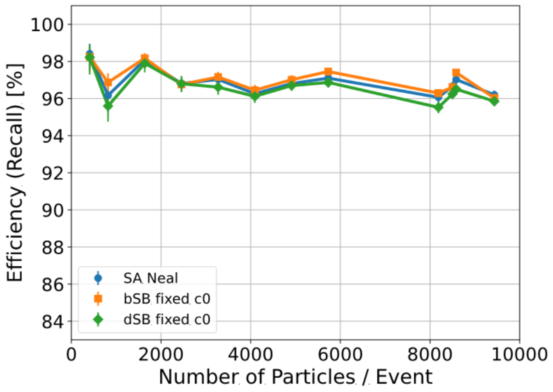
Minimizing QUBO is equivalent to searching for the ground state of the Hamiltonian.

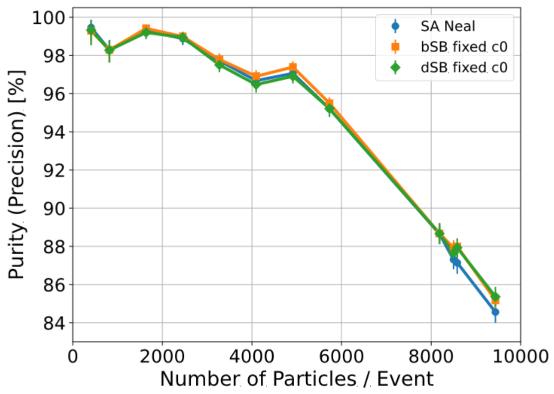
H. Okawa, Q.G. Zeng, X.Z. Tao, M.H. Yung,
Springer Comput. Softw. Big Sci. 8, 16 (2024)

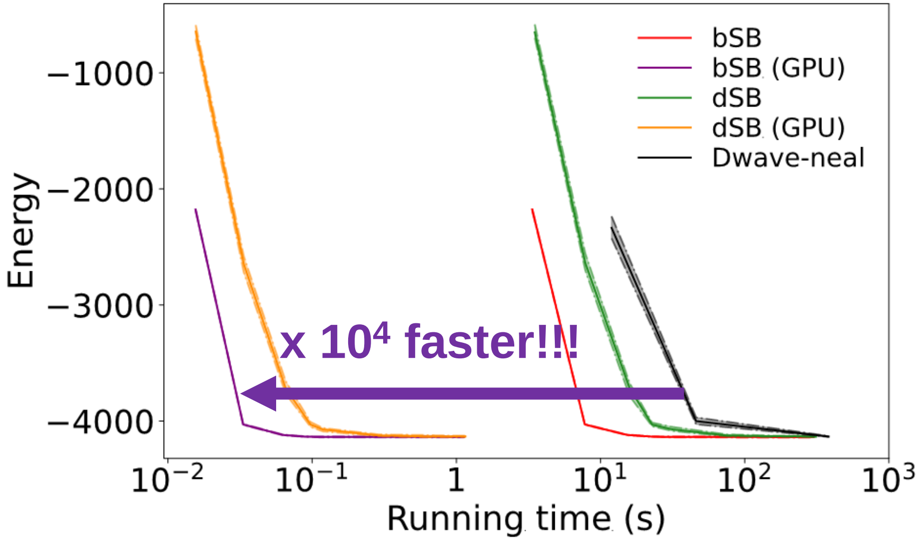
Applications to Track Reconstruction

- QAIAs provide promising performance for the HL-LHC conditions; efficiency>95%, purity>85%.
- **bSB is ~10000 times faster than D-Wave Neal** for the largest TrackML dataset.
- Currently under consideration for ongoing experiments.

No limitations on # of qubits, being a classical algorithm







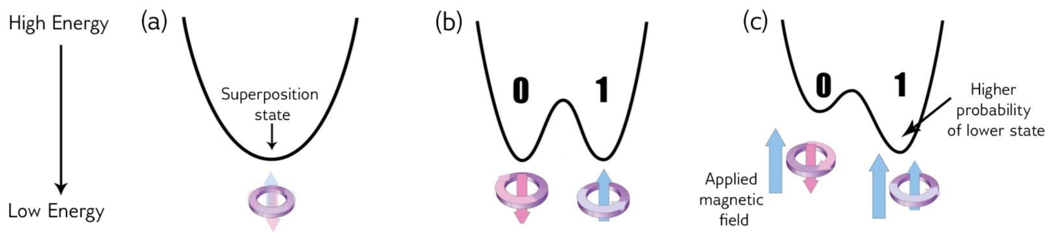
Used MindsporeQuantum
Only 1 CPU or GPU (23min→0.13s)

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

Quantum Approaches

Quantum annealing

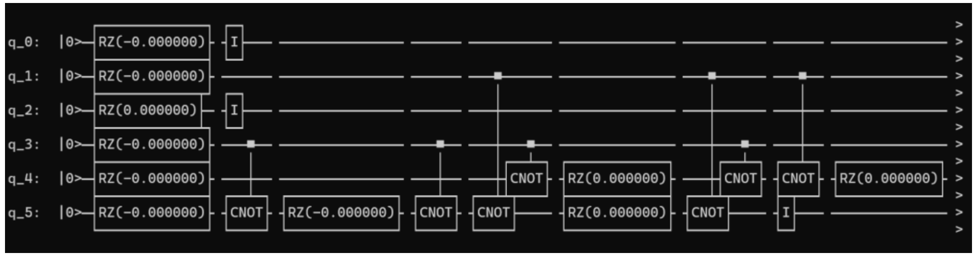
From D-wave website



- Quantum annealer looks for the global minimum of a given function with quantum tunneling.
- D-Wave currently provides 5000+ qubit service.
- Pros: High number of qubits available, although not all qubits are available for fully connected graphs (only a few hundred qubits)
- Cons: Unable to access the actual hardware from China.

Quantum Gates

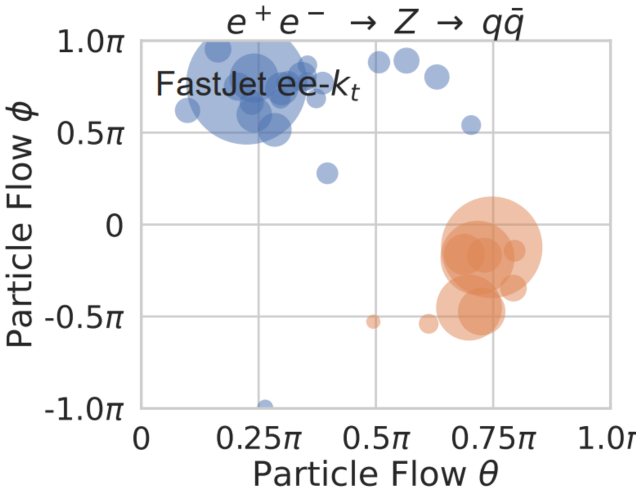
QAOA circuit implemented in Origin Quantum



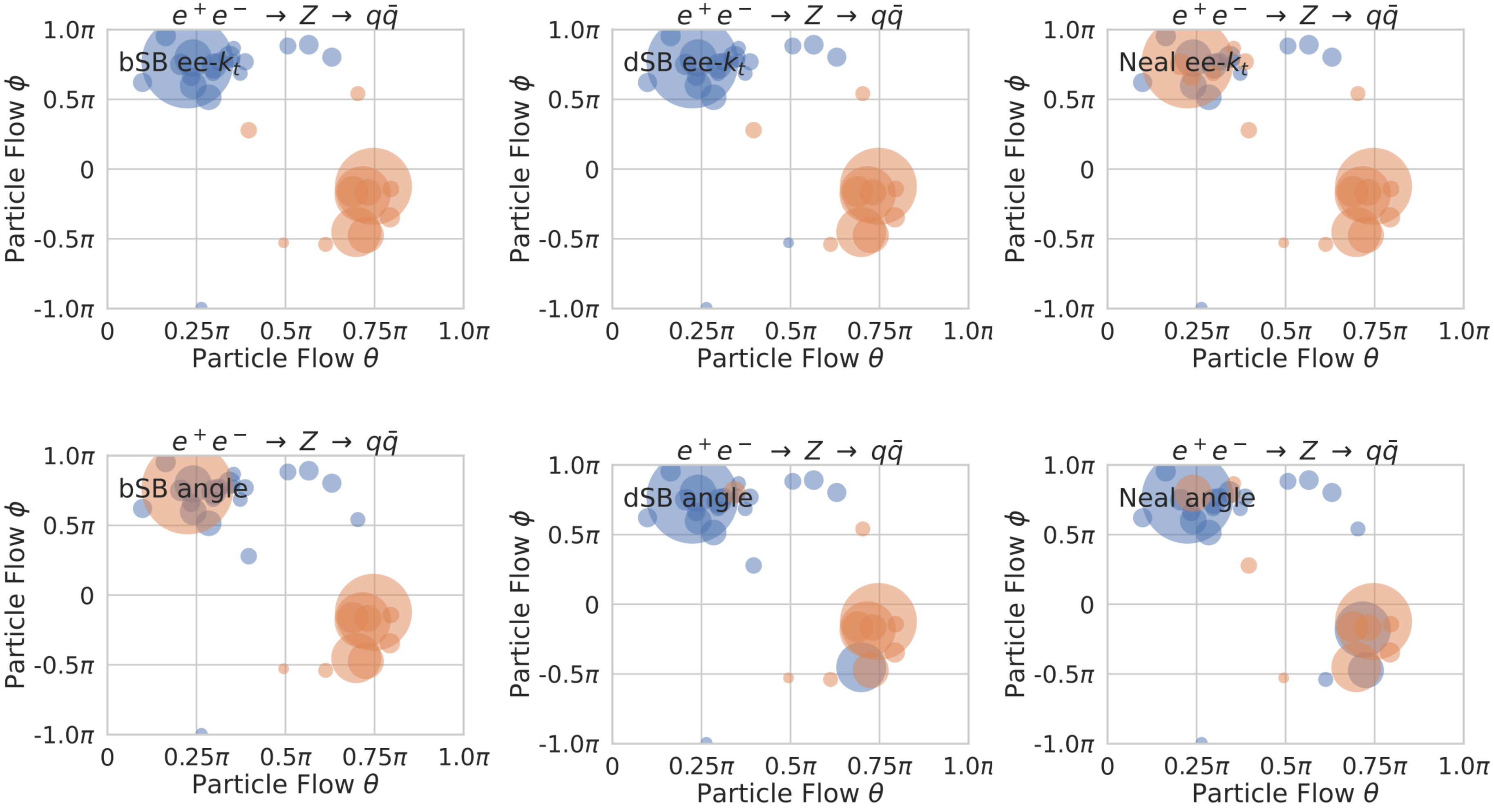
- Quantum gate machines are universal, and can also solve Ising problems with variational circuits: e.g. Variational Quantum Eigensolver (VQE), Quantum Approximate Optimization Algorithm (QAOA), etc.
- Pros: Universal computing, a few platforms available in China
- Cons: Number of qubits is much less than quantum annealing

Event Displays (Z)

Baseline (FastJet)

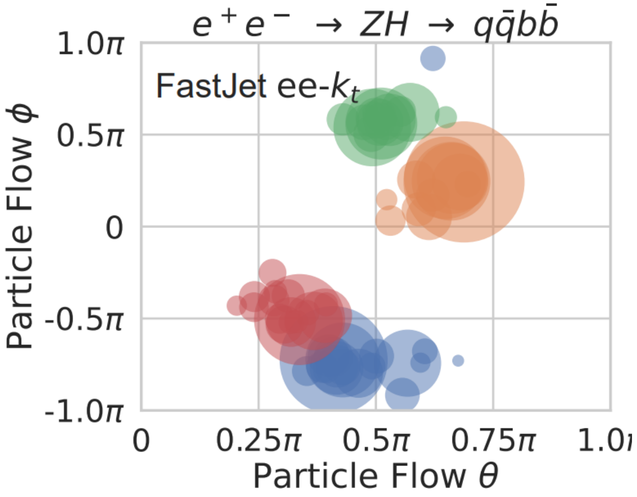


QAIAs

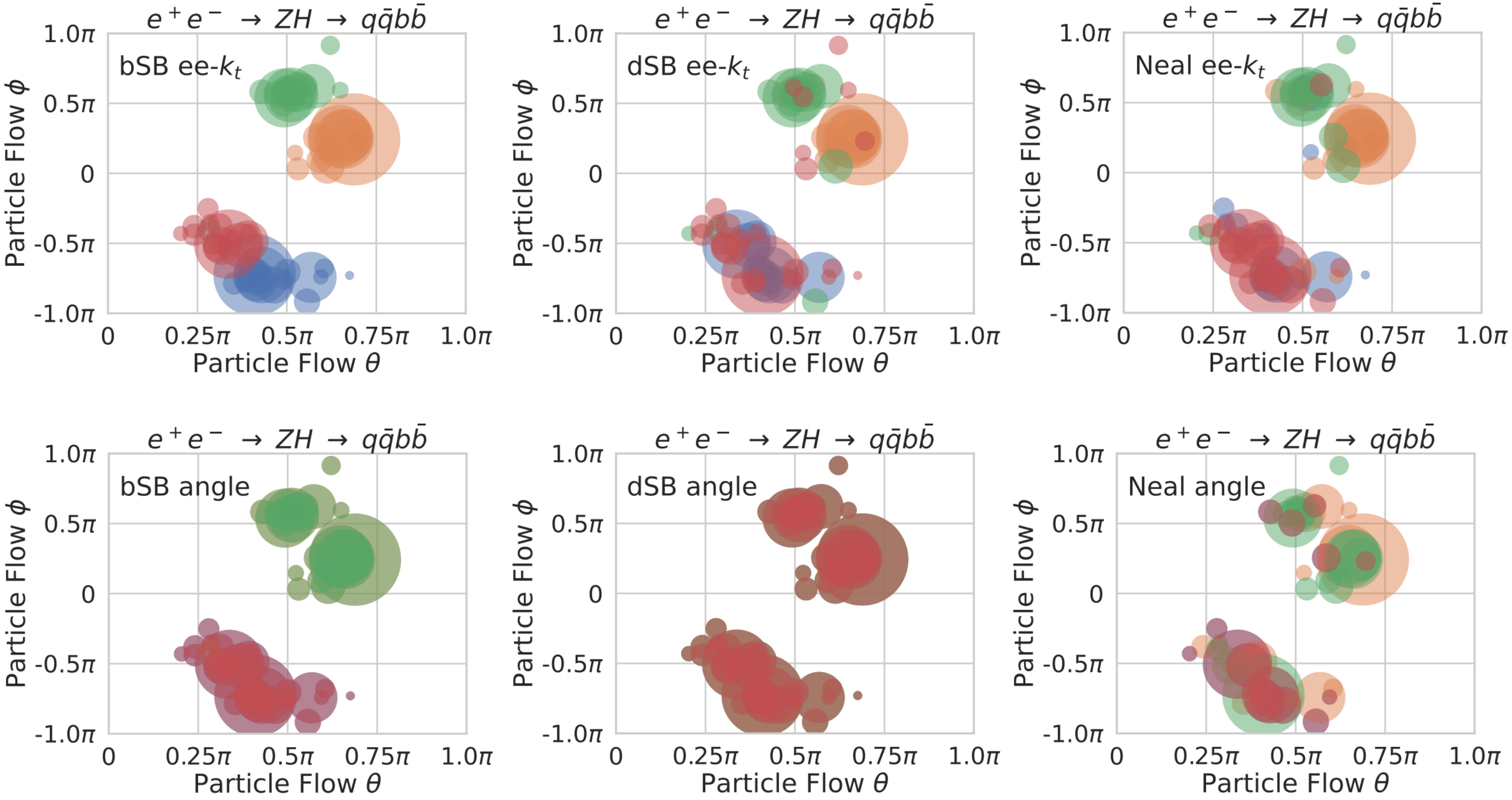


Event Displays (ZH)

Baseline (FastJet)



QAIAs

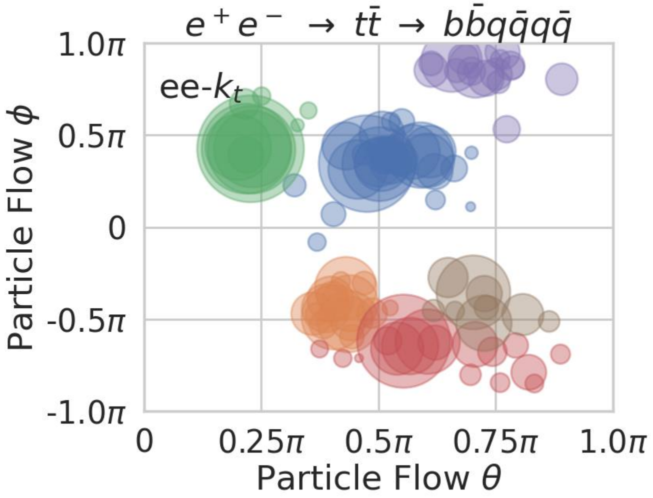


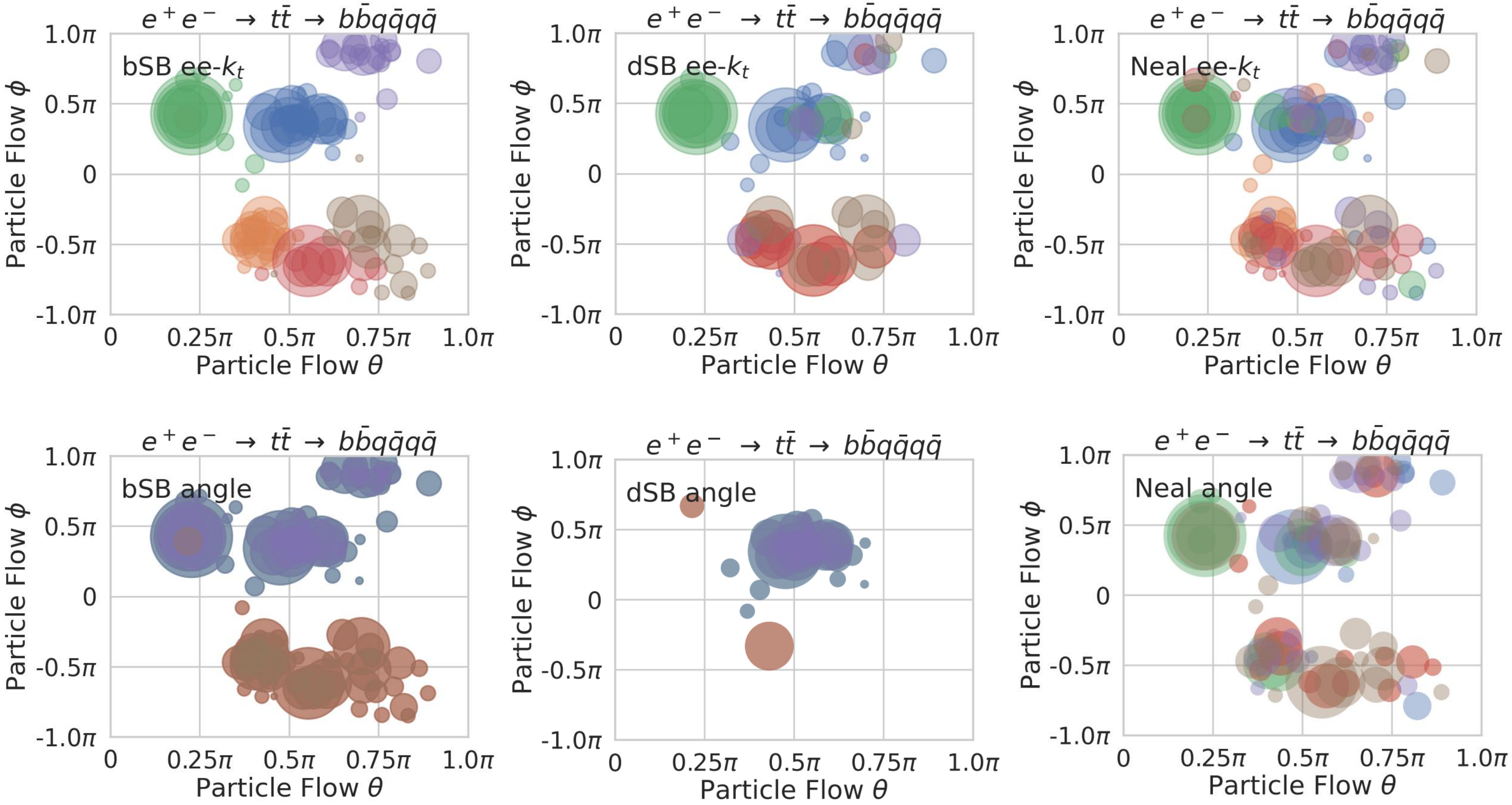
- **Only bSB w/ ee-kt QUBO can reasonably reconstruct all jets**
- **Other approaches misses some jets and/or PFlows are totally mixed up.**

Event Displays ($t\bar{t}$)

QAIAs

Baseline (FastJet)





- **Only bSB w/ ee-kt QUBO can reasonably reconstruct all jets.**
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QUBO ↔ Ising Conversion

$$O_{\mathrm{QUBO}}(s_i) = \sum_{i,j=1}^{N_{\mathrm{input}}} Q_{ij} s_i s_j, \quad \leftrightarrow \quad H(x_i) = \frac{1}{2} \sum_{ij}^{N} J_{ij} x_i x_j + \sum_{i}^{N} h_i x_i,$$

$$x_i \longleftrightarrow 2s_i - 1$$

$$J_{ij} \longleftrightarrow \frac{Q_{ij}}{2}$$

$$h_i \longleftrightarrow \frac{\sum_j Q_{ij}}{2}$$

Simulated Bifurcation (SB)

aSB

$$\begin{aligned}
\dot{x}_i &= \frac{\partial H_{\mathrm{aSB}}}{\partial y_i} = a_0 y_i \\
\dot{y}_i &= -\frac{\partial H_{\mathrm{aSB}}}{\partial x_i}, \\
&= -\left[x_i^2 + a_0 - a(t)\right] x_i + c_0 h_i + c_0 \sum_{j=1}^{N} J_{ij} x_j, \\
H_{\mathrm{aSB}} &= \frac{a_0}{2} \sum_{i=1}^{N} y_i^2 + V_{\mathrm{aSB}} \\
V_{\mathrm{aSB}} &= \sum_{i=1}^{N} \left(\frac{x_i^4}{4} + \frac{a_0 - a(t)}{2} x_i^2 \right) \\
&\quad -c_0 \sum_{i=1}^{N} h_i x_i - \frac{c_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} x_i x_j,
\end{aligned}$$

bSB

$$\begin{aligned}
\dot{x}_i &= \frac{\partial H_{\mathrm{bSB}}}{\partial y_i} = a_0 y_i \\
\dot{y}_i &= -\frac{\partial H_{\mathrm{bSB}}}{\partial x_i}, \\
&= -\left[a_0 - a(t)\right] x_i + c_0 h_i + c_0 \sum_{j=1}^{N} J_{ij} x_j, \\
H_{\mathrm{bSB}} &= \frac{a_0}{2} \sum_{i=1}^{N} y_i^2 + V_{\mathrm{aSB}} \\
V_{\mathrm{bSB}} &= \frac{a_0 - a(t)}{2} \sum_{i=1}^{N} x_i^2 - c_0 \sum_{i=1}^{N} h_i x_i - \frac{c_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} x_i x_j \\
&\quad \text{(when } |x_i| \le 1 \text{ for all } x_i\text{)}, \\
&= \infty \quad \text{(otherwise)}.
\end{aligned}$$

dSB

$$\begin{aligned}
\dot{x}_i &= \frac{\partial H_{\mathrm{dSB}}}{\partial y_i} = a_0 y_i \\
\dot{y}_i &= -\frac{\partial H_{\mathrm{dSB}}}{\partial x_i}, \\
&= -\left[a_0 - a(t)\right] x_i + c_0 h_i \\
&\quad + c_0 \sum_{j=1}^{N} J_{ij} \operatorname{sgn}(x_j), \\
H_{\mathrm{dSB}} &= \frac{a_0}{2} \sum_{i=1}^{N} y_i^2 + V_{\mathrm{aSB}} \\
V_{\mathrm{dSB}} &= \frac{a_0 - a(t)}{2} \sum_{i=1}^{N} x_i^2 - c_0 \sum_{i=1}^{N} h_i x_i \\
&\quad - \frac{c_0}{2} \sum_{i=1}^{N} \sum_{j=1}^{N} J_{ij} x_i \operatorname{sgn}(x_j) \\
&\quad \text{(when } |x_i| \le 1 \text{ for all } x_i\text{)} \\
&= \infty \quad \text{(otherwise)},
\end{aligned}$$