基于量子退火启发的重建算法

IHEP ML workshop and ML group kick-off, 2024年10月16日

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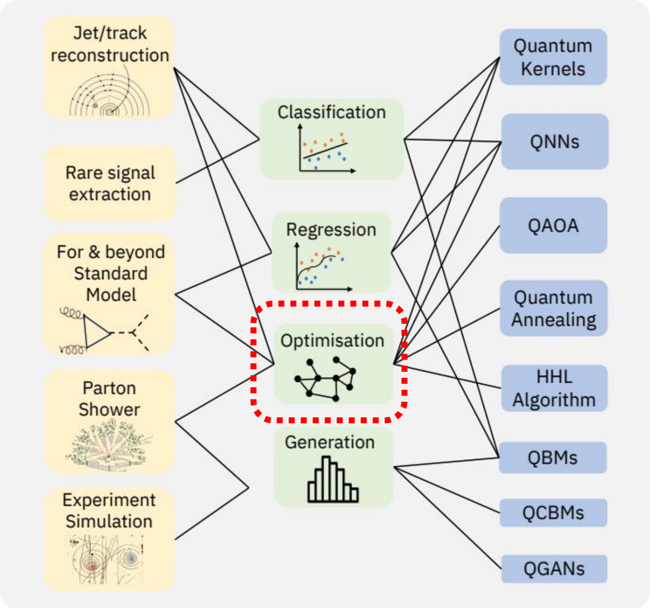
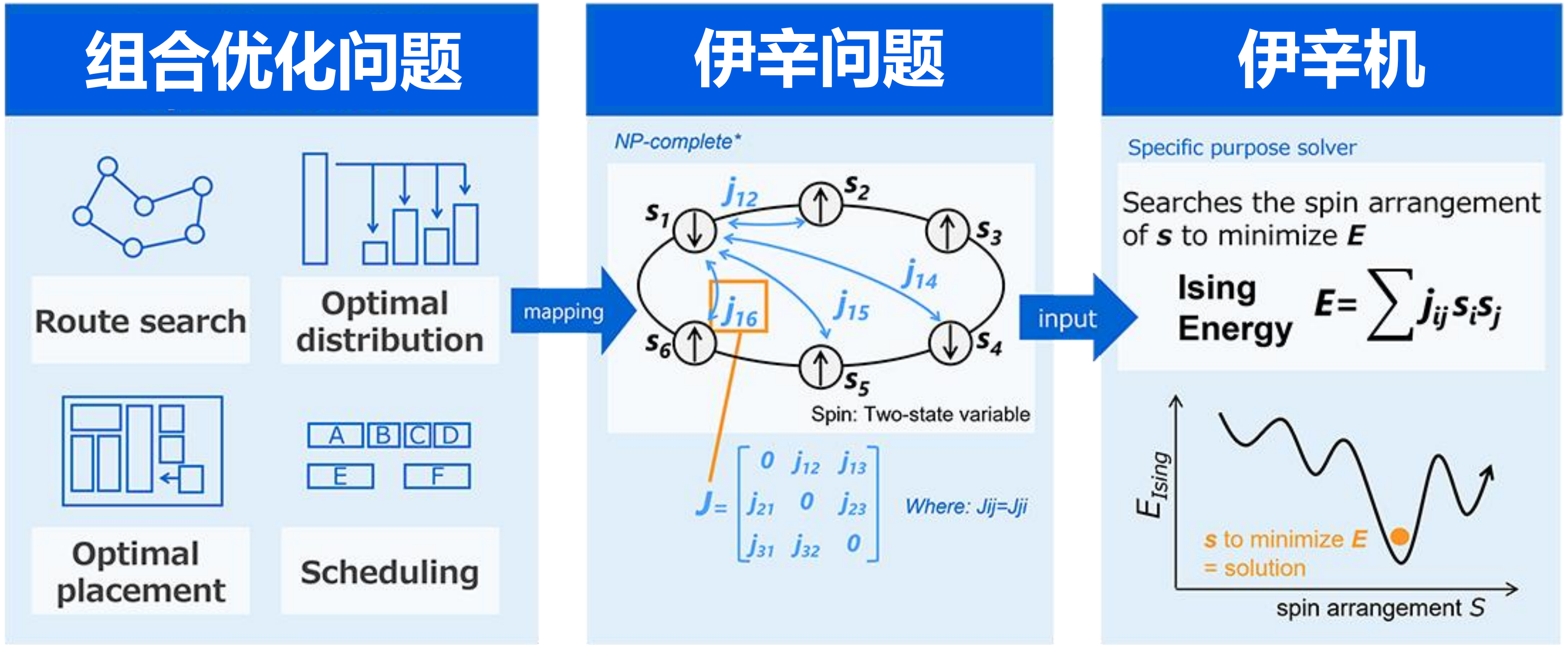
组合优化问题

翻译来©TOSHIBA





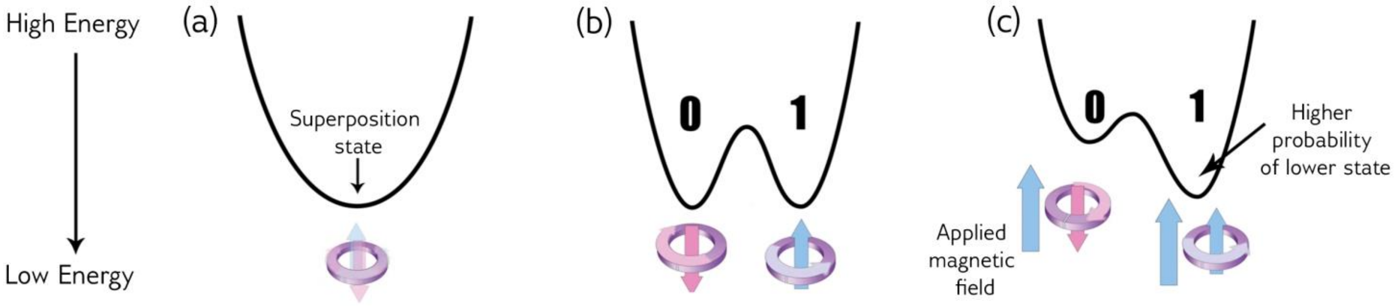
- **组合优化问题是非确定性多项式(NP)完全问题→不能确定是否在多项式时间内找到答案。**
- 可以表示为伊辛问题。社会中的许多应用。伊辛机在合理的时间内求解绝对或近似的基态。
- **在高能物理中，径迹和喷注重建等许多任务也可以表述为伊辛问题。**

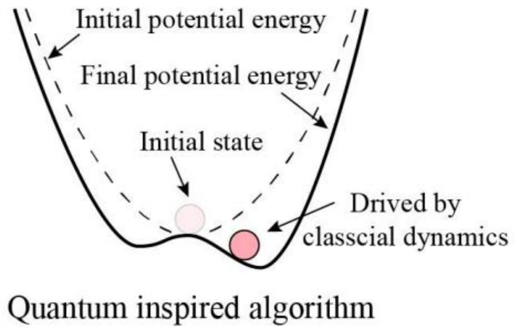
量子退火启发算法

量子退火 (Quantum Annealing [QA])

量子退火启发算法 (QA-Inspired Alg.)

From D-wave website





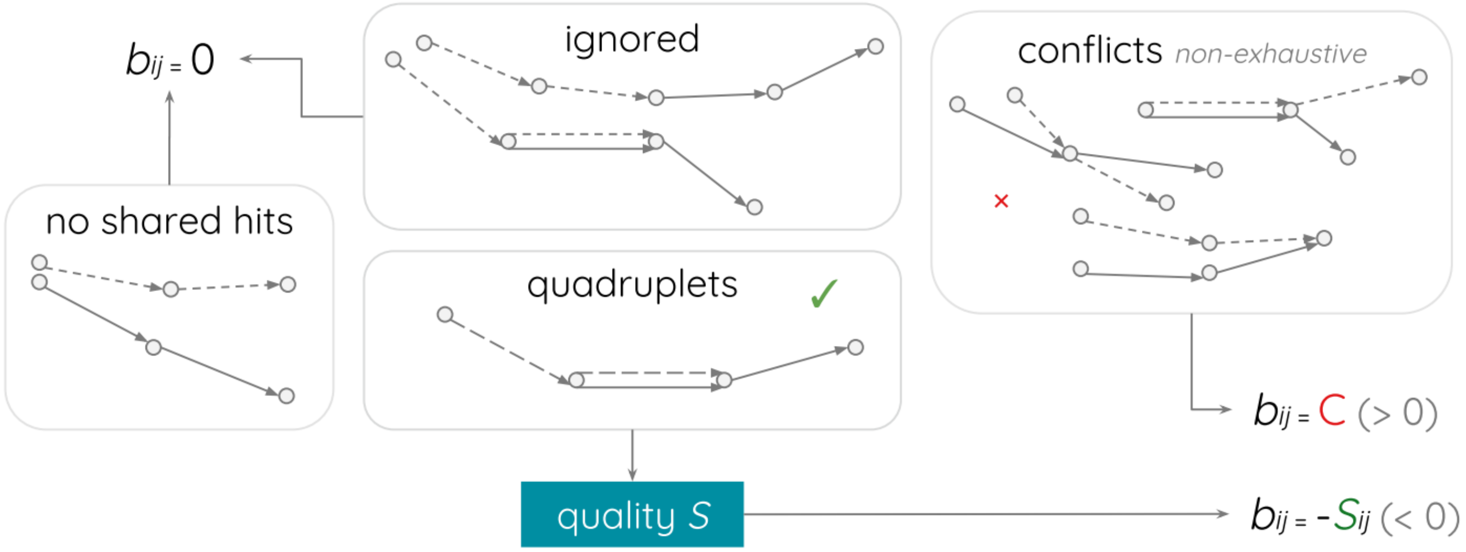
Graph size	Algorithm	Hardware	Time(s)
	TTN	CPU 1 core	5.62
	Brute-force search[46]	GPU Titan V	$>10^{48}$
4 × 4 × 8	Exact belief propagation[13]	CPU 1 core	~0.96
	QA[13]	D-Wave	~0.05
	bSB	CPU 1 core	0.12
	bSB	GPU Tesla V100	<0.001
	TTN	CPU 1 core	32400
	TTN[44]	GPU Tesla V100	84
8 × 8 × 8	Brute-force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

- **量子退火启发算法通过微分方程的经典时间演化寻找伊辛哈密顿量的最小能量**（模拟退火 simulated annealing，模拟分叉算法 simulated bifurcation等）
- 与模拟退火不同，模拟分叉算法可以并行运行
- 对于一些问题，**模拟分叉算法优于量子退火**

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

径迹重建为组合优化问题

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



$$O(a,b,T) = \sum_{i=1}^{N} a_i T_i + \sum_{i}^{N} \sum_{j<i}^{N} b_{ij} T_i T_j$$

Quality of triplets

Compatibility b/w triplet pairs

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

$$T_i, T_j \in \{0, 1\}$$

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

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

- 径迹重建可以作为一个组合优化问题。
- 伊辛哈密顿量的设计方式是正确答案给出的最低能量。
  →可以直接使用量子退火机！(和量子退火启发算法)
- 量子门也可以用：变分量子算法(VQE)，量子近似优化算法(QAOA)来解决组合优化问题

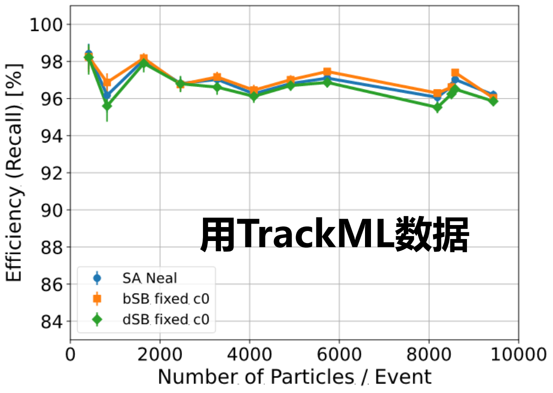
H. Okawa, Springer Communications in Computer and Information Science, 2036 (2024) 272–283, arXiv:2310.10255

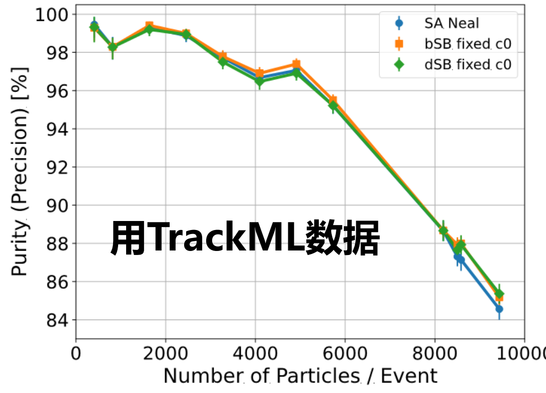
大川英希 [高能所], 曾庆国, 陶贤哲, 翁文康 [深圳量子院/南科大],
Springer Comput. Softw. Big Sci. 8, 16 (2024)

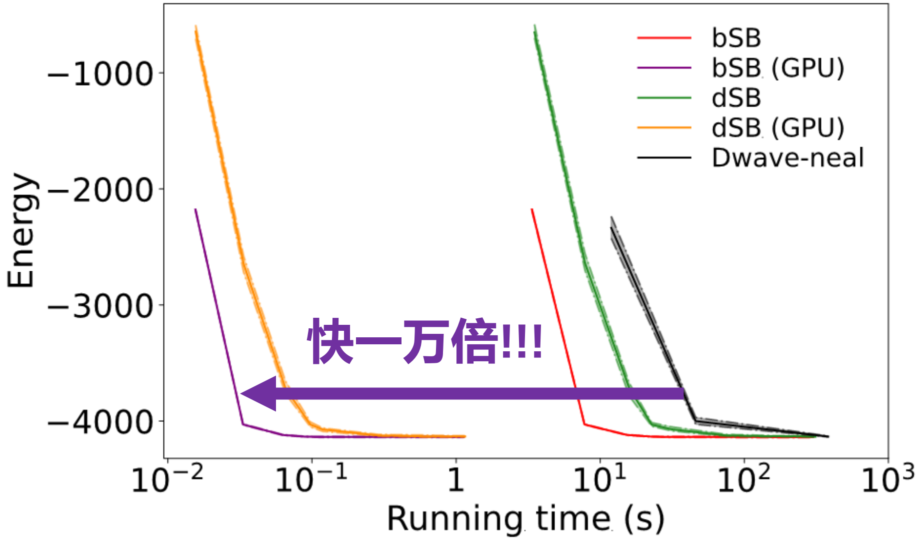
量子启发算法的潜力！

没有量子比特数的限制，可以处理巨大数据！

- **全球首次在高能物理中使用模拟分叉算法。**径迹重建性能很好(在HL-LHC最稠密条件，还保持效率>95%，纯度>85%)
- **比模拟退火算法快一万倍！这不是未来的算法，而是在正在运行的实验上就可以使用！(LHC, BESIII等)**







代码在华为MindsporeQuantum
只用一个CPU或GPU (23分钟→0.13秒)

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

喷注重建为组合优化问题

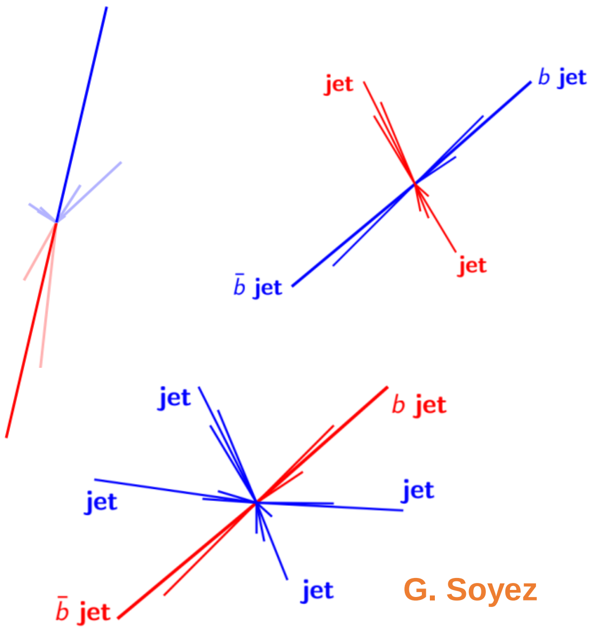
喷注重建QUBO

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

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

$$Q_{ij} = -\frac{1}{2}\cos\theta_{ij}$$ **[基于角度]**

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



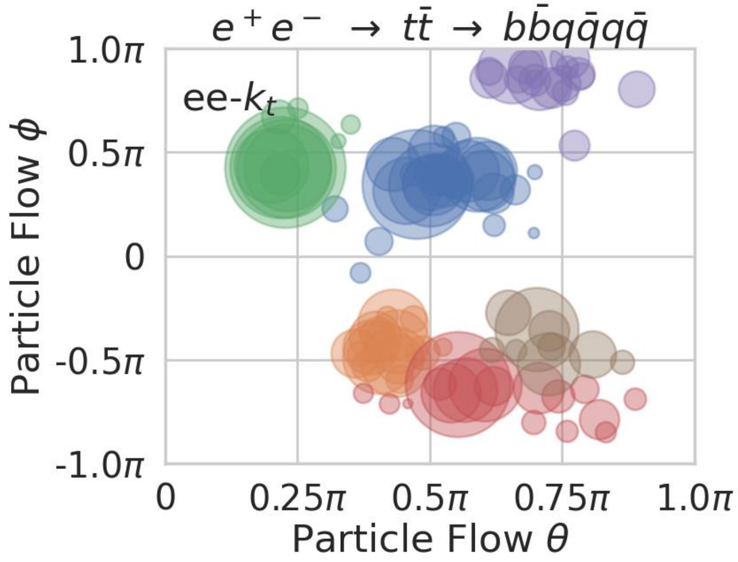
G. Soyez

- **考虑exclusive喷注重建（在事例的喷注数固定的）。在CEPC等**e+e-对撞机的标准方法。
- **喷注重建QUBO成分完全连接，非常难用真实量子退火器解决（A. Delgado, J. Thaler, PRD 106, 094016 (2022)）**
- **D. Pires等使用的角度算法 → 对双喷注事例没问题，但多喷注事例中性能很差**
- 我们采用ee-k_t距离和使用量子退火启发算法以重建多喷注事例。

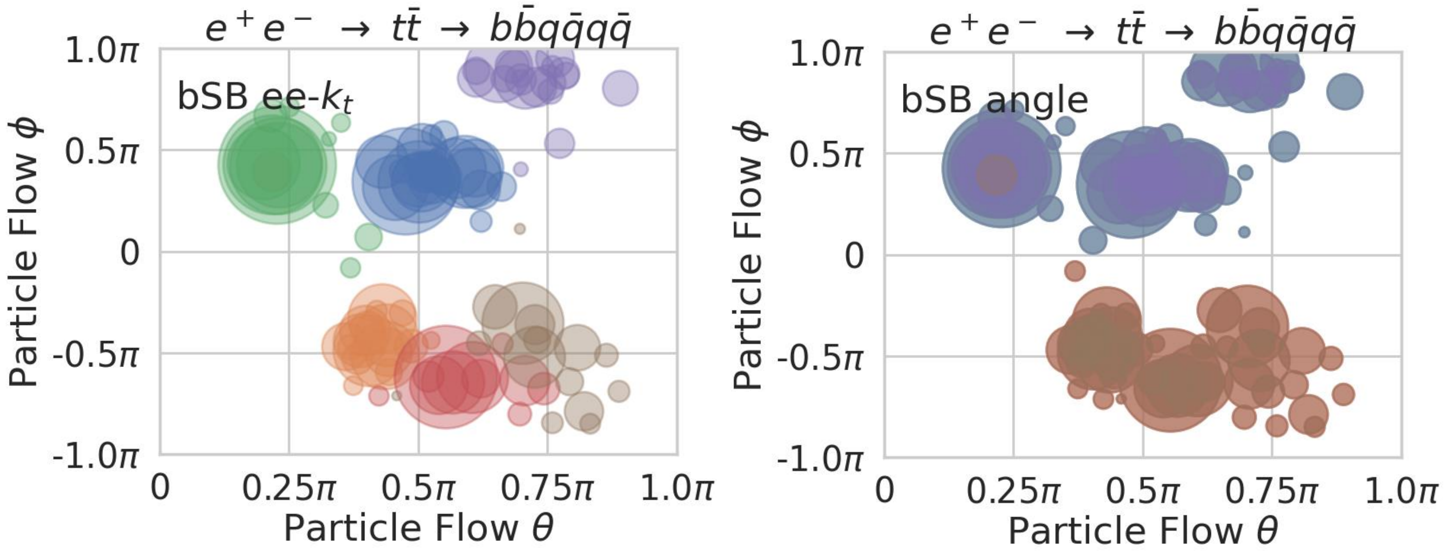
多喷注重建

大川英希 [高能所], 陶贤哲,曾庆国, 翁文康 [深圳量子院/南科大],
论文准备中

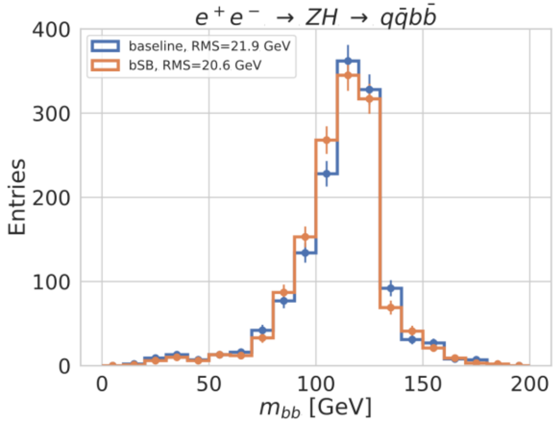
传统方法 (FastJet)

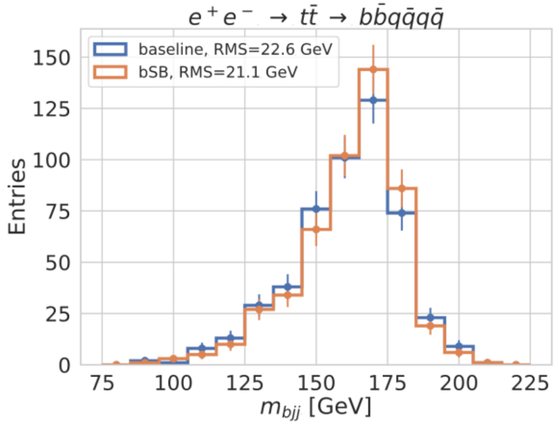


弹道模拟分叉算法



- **弹道模拟分叉算法和ee-kt距离可以解决多喷注重建！（模拟退火不能）**
- **<u>全球首次成功用QUBO重建多喷注事例。</u>**
- **比FastJet质量分辨率也比较改善了。**



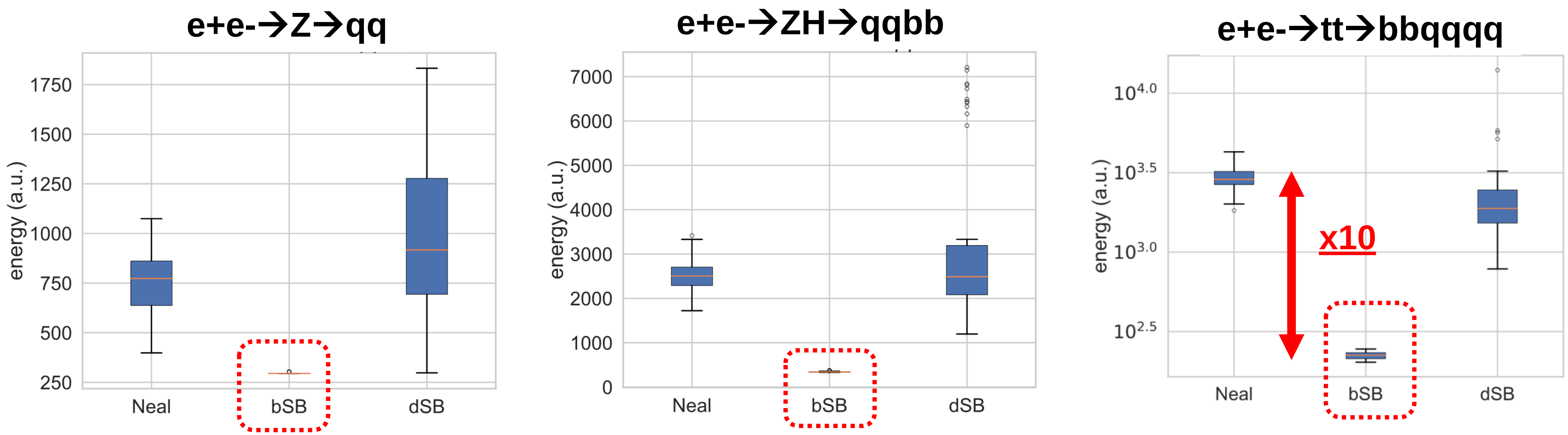


总结

- 未来的对撞机会进入exabyte数据时代，需要巨大的计算资源。 重建是最消耗计算资源的计算任务之一。
- 我们热切期待有新的数据处理方法来应对这一挑战。
- 量子退火启发算法，尤其是模拟分叉算法对“比特数量”几乎没有限制，可以直接处理超大规模（比特数目可达上亿）的数据集。
    - 此外，与模拟退火不同，模拟分叉算法除了能够在CPU上运行，也可在GPU和FPGA实现并行加速
- 量子机器学习还没有进入实践阶段，但量子启发算法已经开始提供创新！这两种类型的研究都必须进行。
- 请期待进展!

备份

Ising Energy Prediction

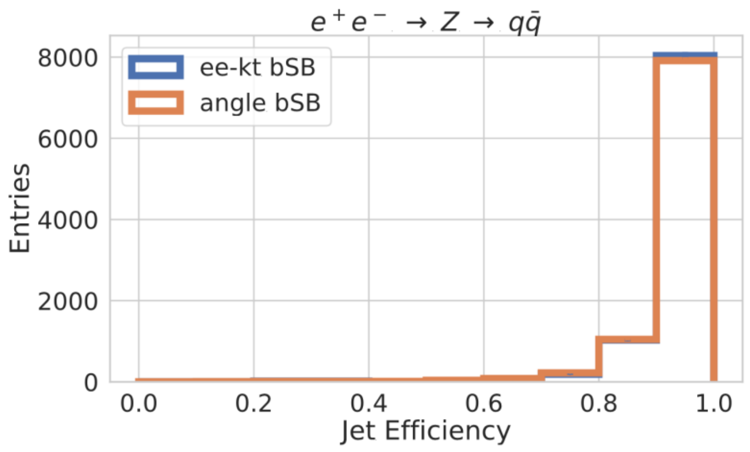


- **Fully-connected QUBOs are difficult to solve**; it is known that quantum annealing hardware is not good at solving them so far.
  - This is in contract to track reconstruction, in which the QUBOs are largely sparse.
- **Ballistic SB (bSB) predicts energy lowest with the smallest fluctuation.**
-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

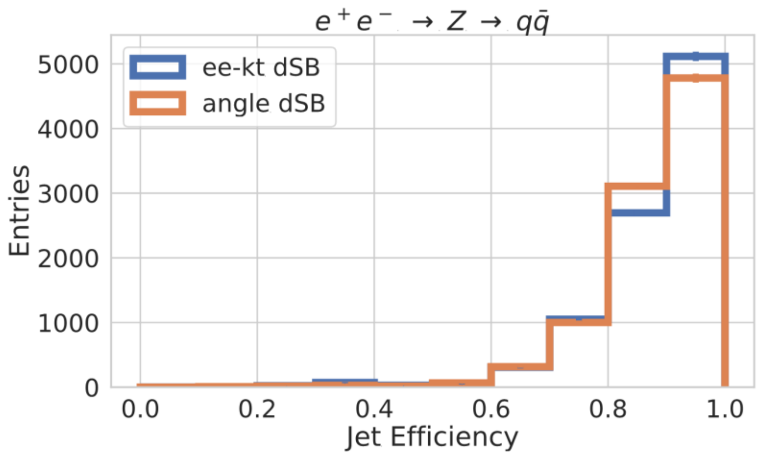
Efficiency (Z→qq: 2 jets)

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

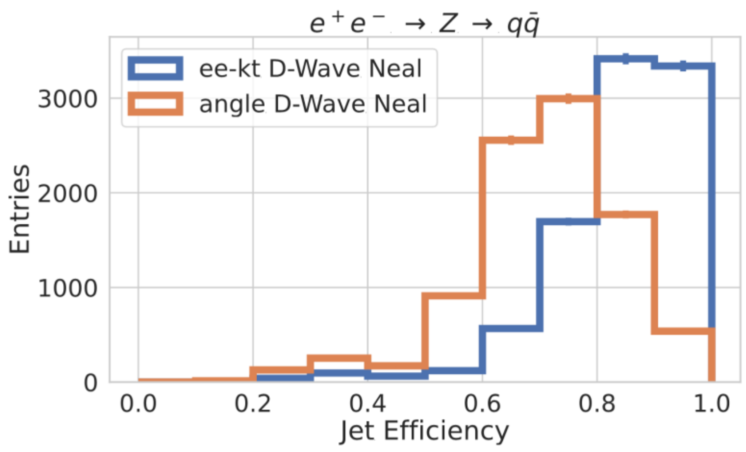
bSB



dSB



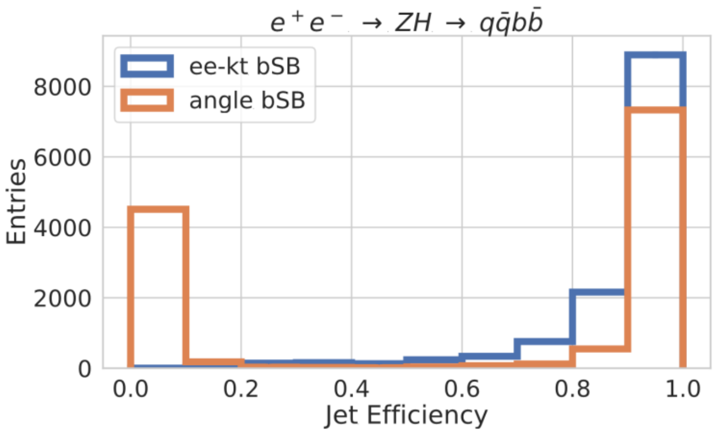
D-Wave Neal



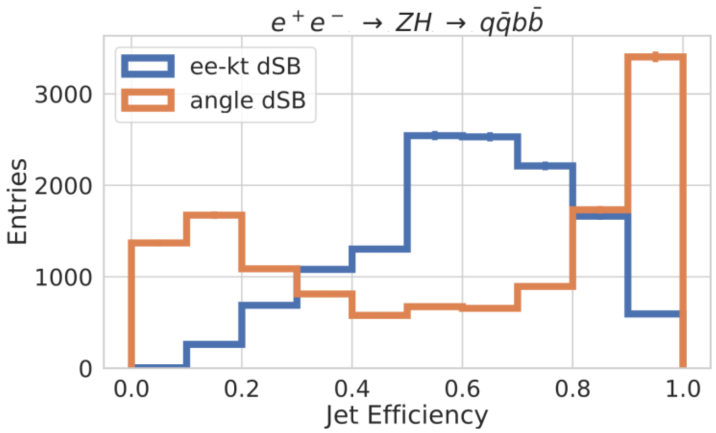
- Most jet reconstruction w/ quantum approaches adopts the above-defined efficiency as performance metric; i.e. compatibility of jet assignment w/ the traditional ee-k_t jet finding.
- **bSB provides the highest efficiency. D-Wave Neal has visibly degraded performance already in dijet events. dSB also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

Efficiency (ZH→qqbb: 4 jets)

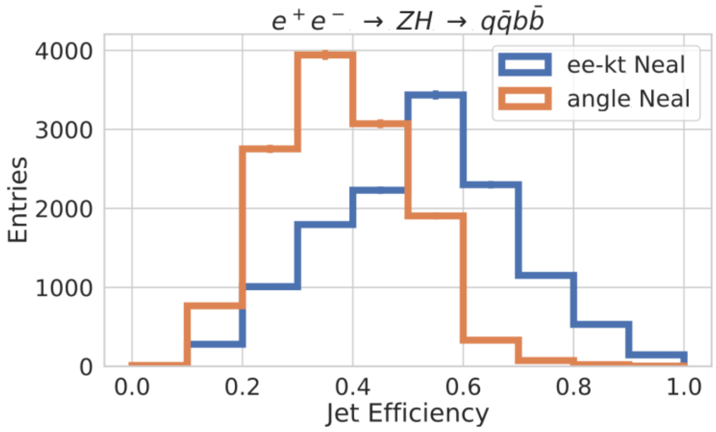
bSB



dSB



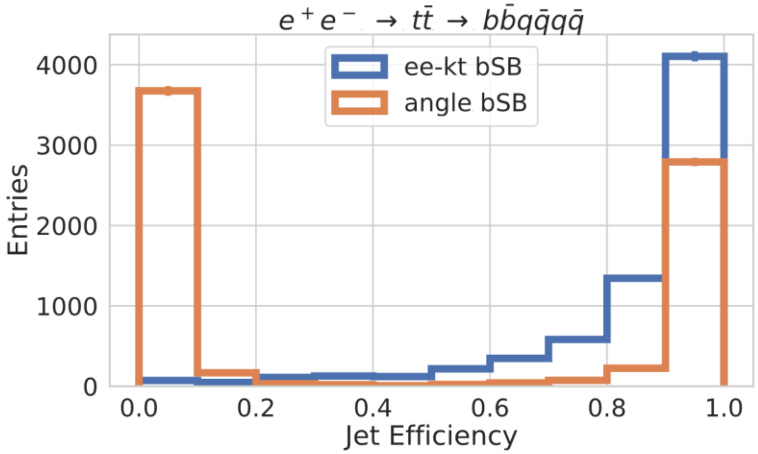
D-Wave Neal



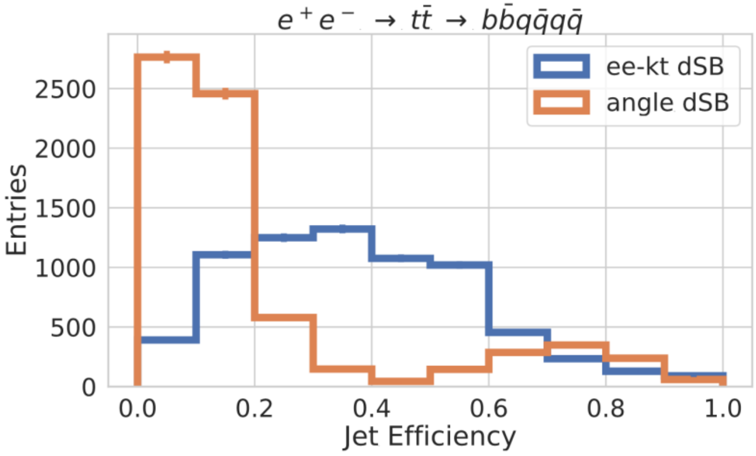
- **Angle-based method does not work for N_{jet}>2**; angles are very likely inappropriate for multijet conditions.
- **dSB & D-Wave Neal cannot reconstruct jets properly regardless of the distance adopted → because of the non-optimal predicted energy**
- **Only bSB maintains reasonable performance.**

Efficiency (tt→bbqqqq: 6 jets)

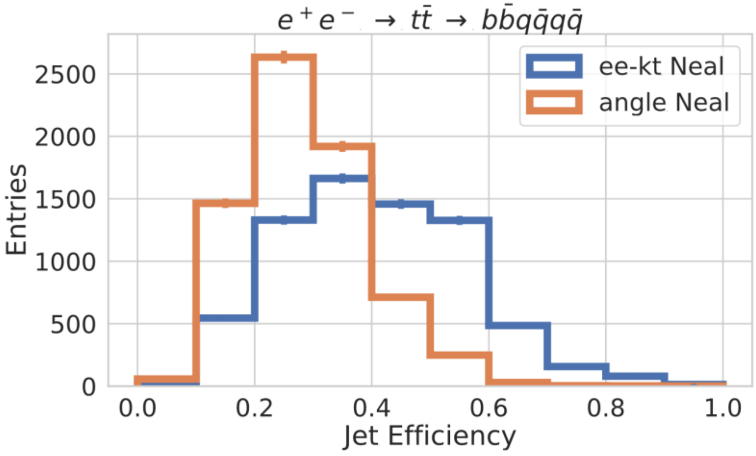
bSB



dSB



D-Wave Neal

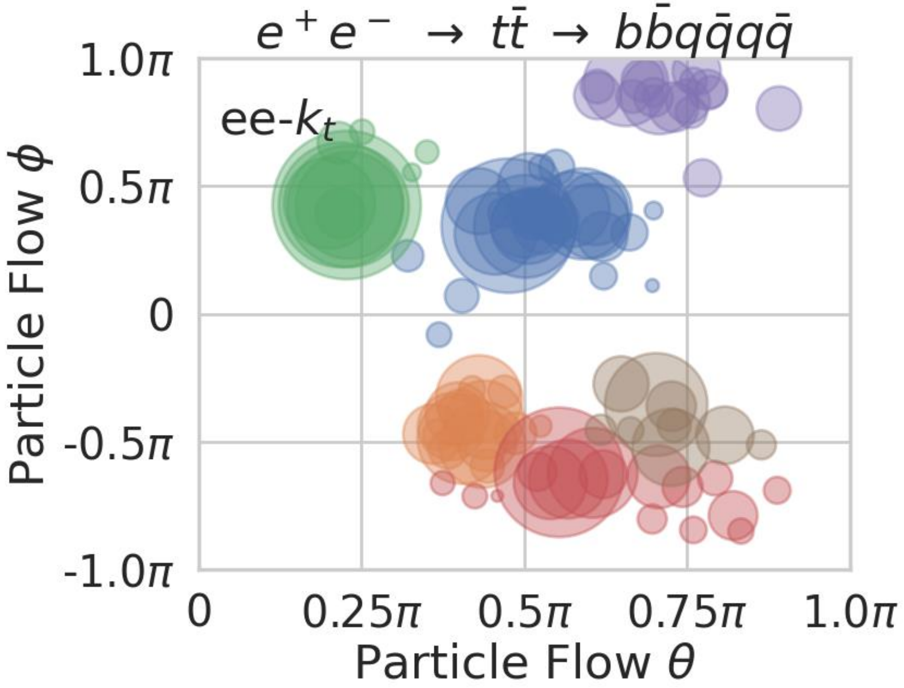


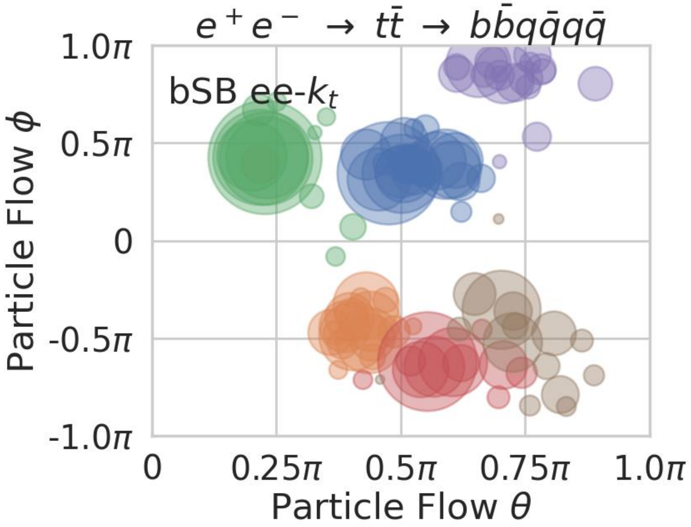
- Angle-based method does not work for $N_{jet}>2$; angles are very likely inappropriate for dense conditions. **The trend is more apparent in ttbar events than the ZH.**
- **dSB & D-Wave Neal cannot reconstruct jets properly regardless of the distance adopted → because of the non-optimal predicted energy**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

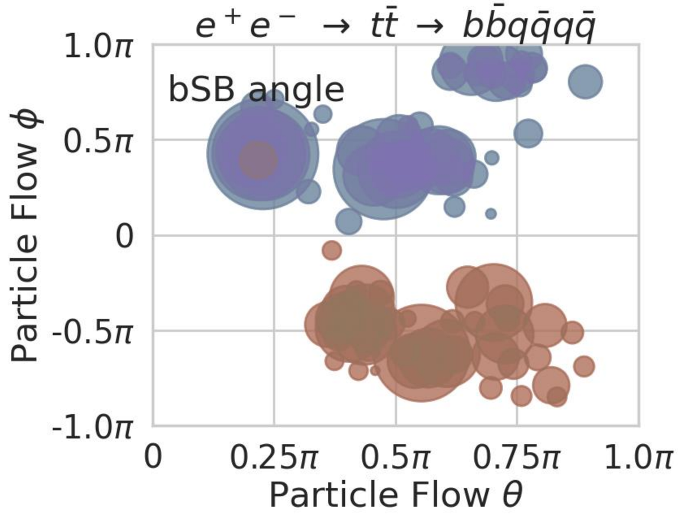
Event Displays

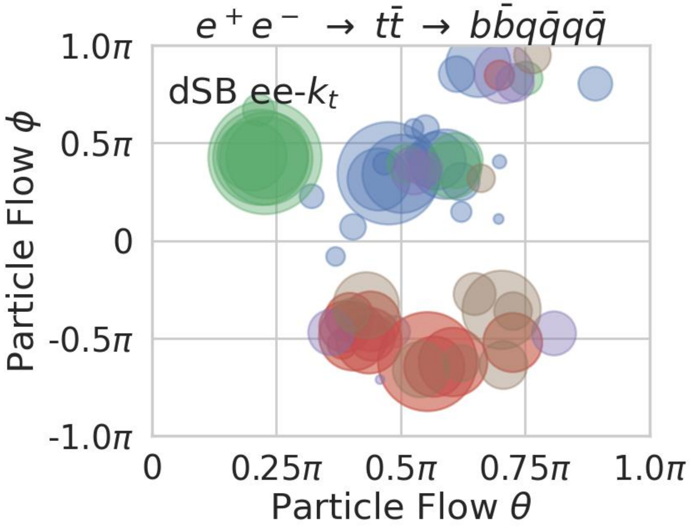
QAIAs

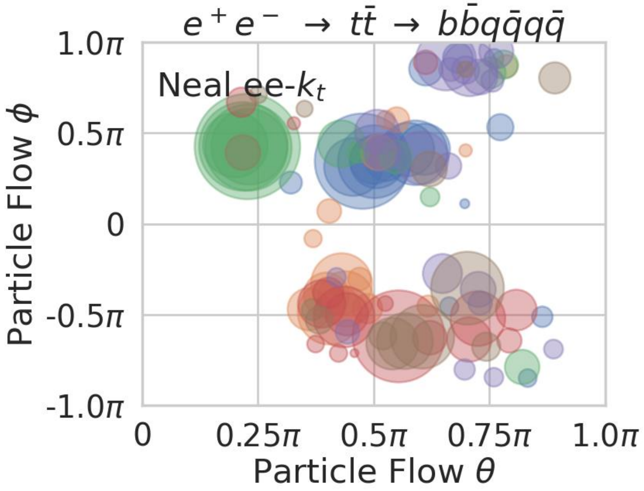
Baseline (FastJet)











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