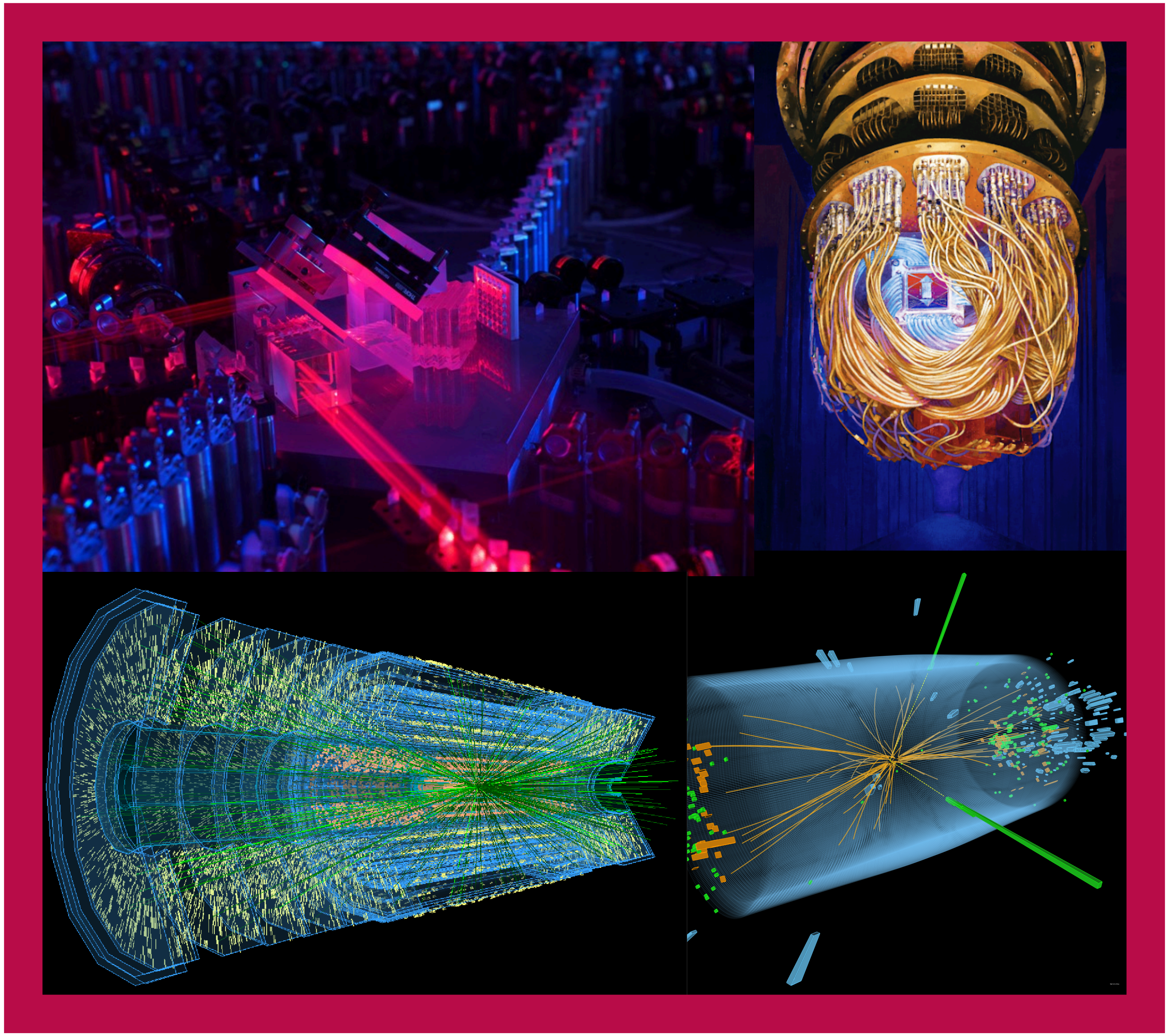
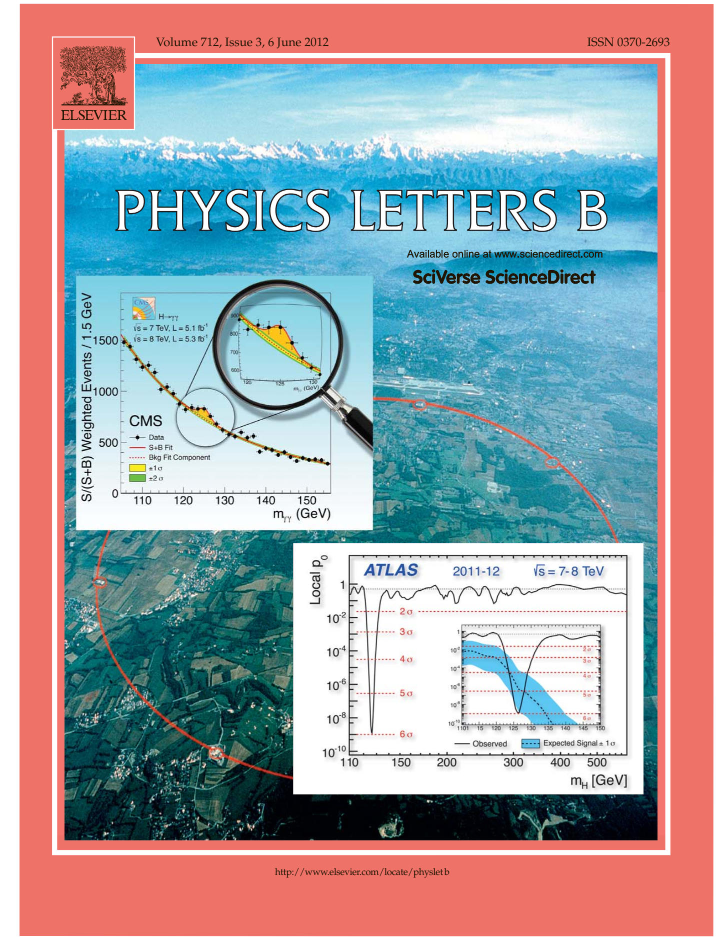
Ideas for applications of quantum computing to particle physics at the LHC

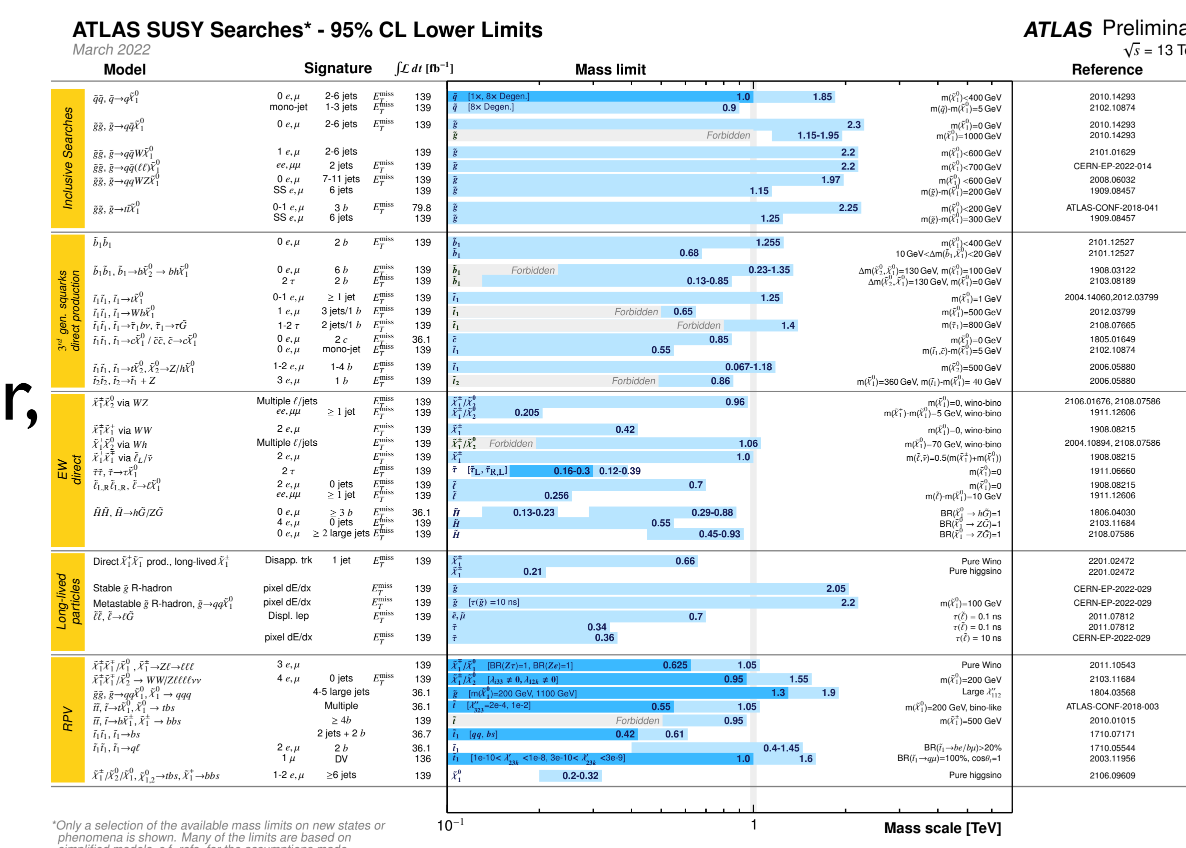


Heather M. Gray, Humboldt Kolleg 2022, Kitzbühel

Introduction

- As we've already heard in a number of talks this week, we've had a remarkable harvest of physics results from the LHC
  - In particular, the discovery and study of the **Higgs boson**
  - Also many detailed measurements of the **Standard Model**
- However, so far, despite some hints, no conclusive evidence for **physics beyond the Standard Model**
- Run 3, which is expected to double the available dataset, is starting now, however, all eyes are on the upgrade to the LHC, the High-Luminosity LHC (HL-LHC), currently scheduled to start in 2029



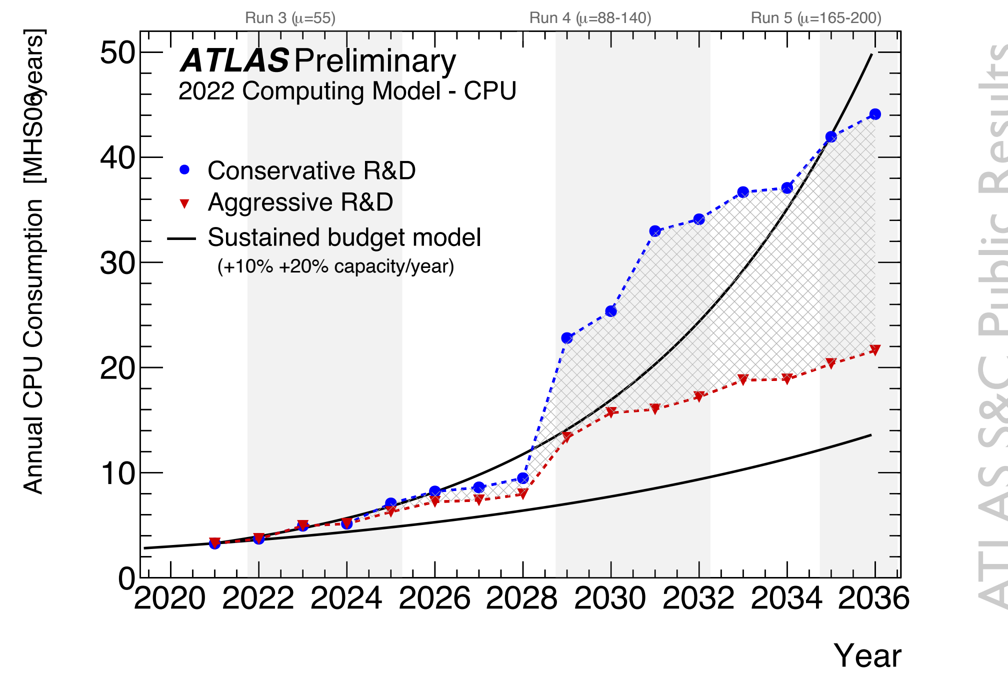


ATLAS SUSY Summary Plots

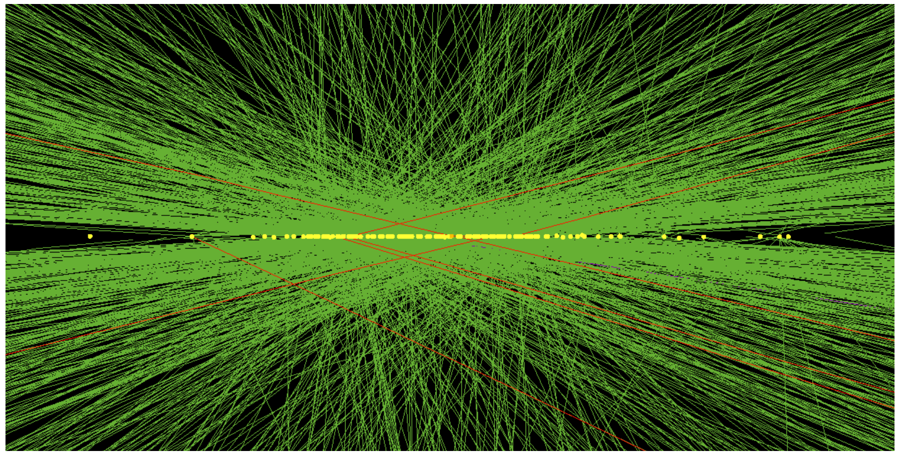
The Software and Computing Challenge at the HL-LHC and Beyond

- The HL-LHC will be an exciting time for particle physics, e.g. for ATLAS/CMS
    - **5-7x** increase in luminosity (LHC upgrade)
    - **4-5x** increase in event size (new detectors)
    - **10x** increase in event rate (trigger upgrade)
- However, **flat computing budgets** mean that the current computing would fall short of needs
- Requires **new techniques** and **new ideas** to close this gap
- The problem will be far worse at **future colliders** such as FCC-hh with up to 1000 (!) additional collisions (pile up) per bunch crossing

HL-LHC Computing Challenge



Pile up

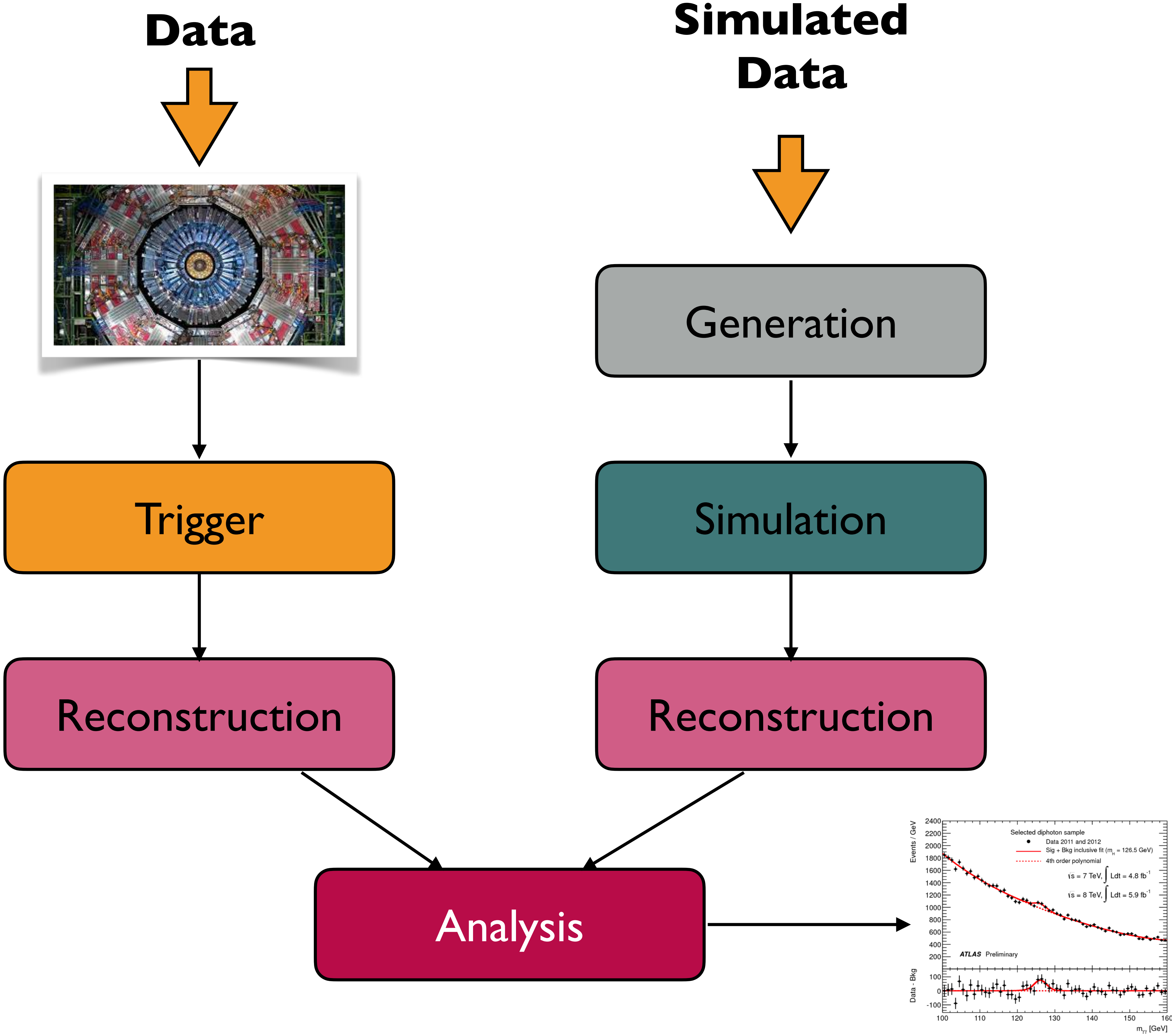


proton-proton collision vertex

Why Quantum Computing?

- Initial ideas for quantum computing date back **40 years** (Benioff, Feynman, Manin, etc,)
  - Use quantum mechanical processes to **simulate quantum mechanical systems**
- Further interest was stimulated by the invention of **quantum algorithms** in the early 1980's with the promise of solutions to intractable problems on quantum computers (Shor, Grover, etc)
  - Exponential information storage
  - Revolutionize cryptography
  - Solutions to unsolved (classical) problems
- Most recently quantum computing has been in the news in regards to **quantum advantage** (supremacy)
  - Google, IBM, Jiuzhang
- Quantum computing is likely at the peak of its hype cycle
  - *How might quantum computing be useful for high-energy physics?*

Typical Data Flow for HEP Experiments



Many Potential Applications

- **Generation/Simulation**
  - MC generation, e.g. correlations in parton shower*
  - QCD*

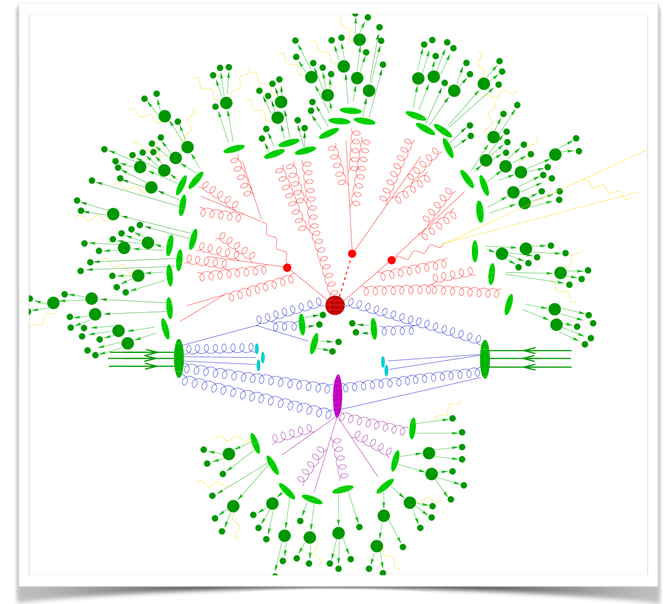
theory

- **Reconstruction**
  - Particle tracking
  - Calorimeter clustering
- **Analysis**
  - Higgs analyses
  - SUSY searches
  - Predominantly **quantum machine learning** (QML)

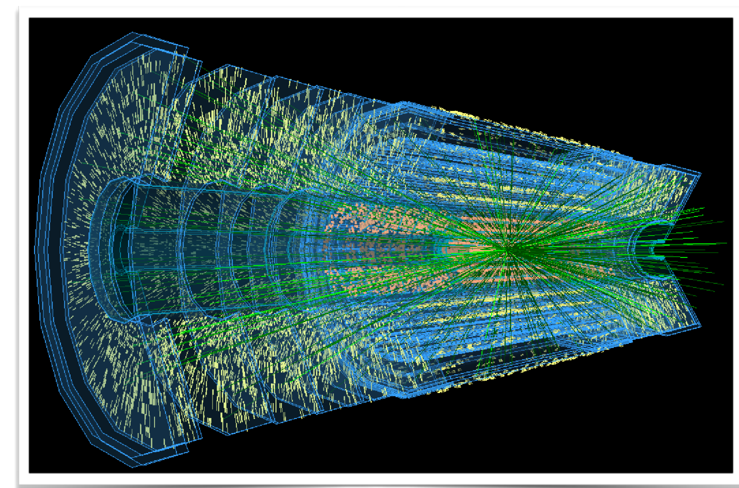
experiment

*Covered in other talks

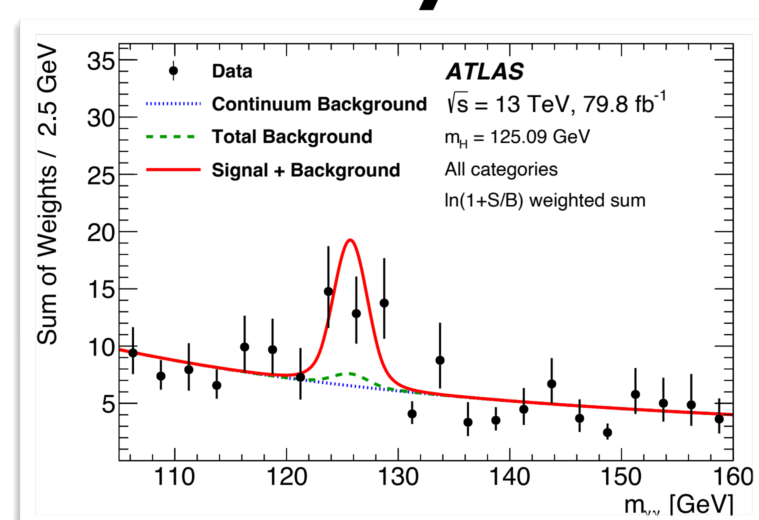
Simulation



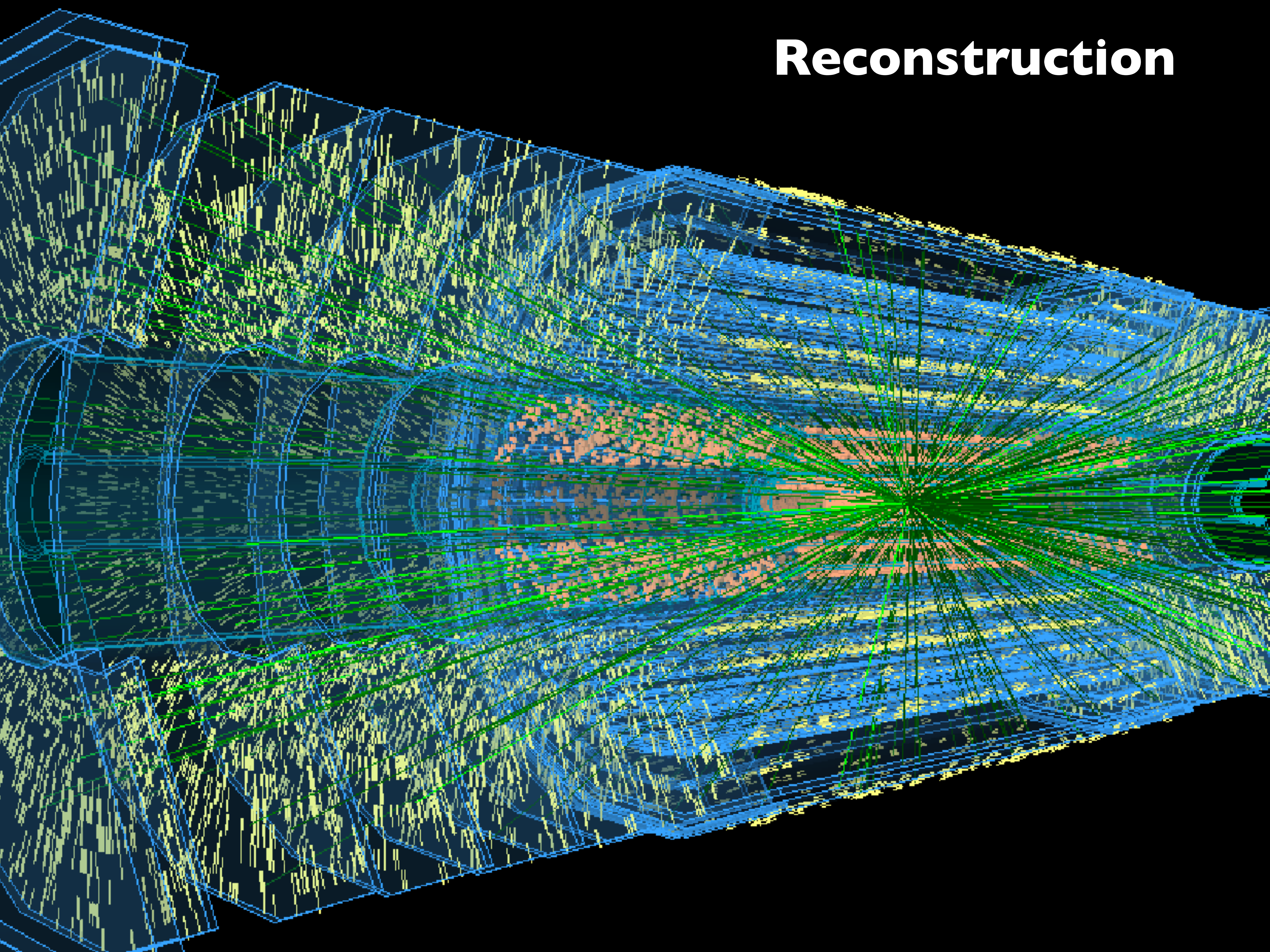
Reconstruction



Analysis



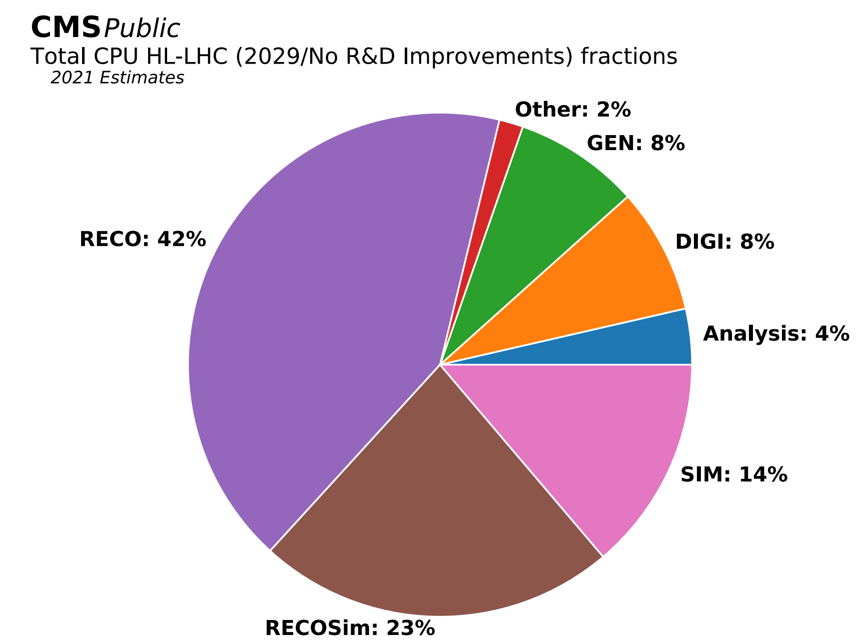
Reconstruction



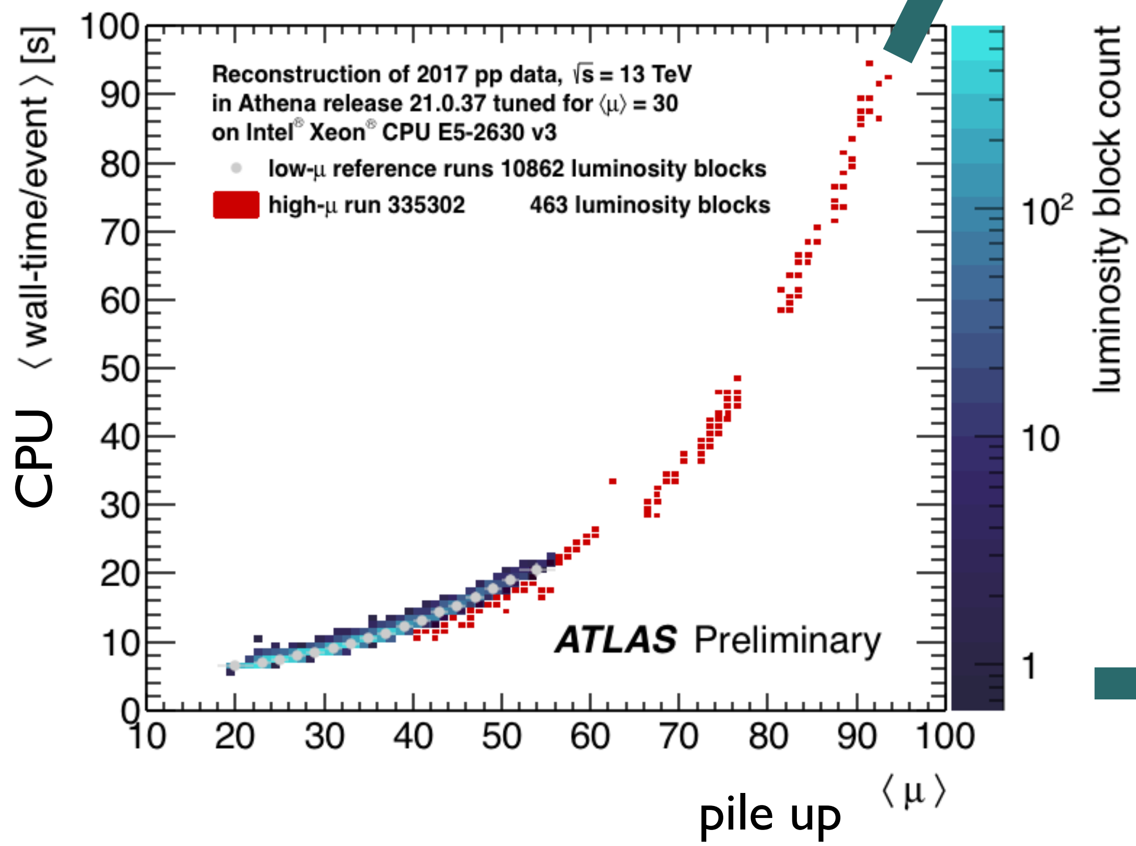
Reconstruction

- Reconstruction algorithms process the real or simulated **detector output** to produce **physics objects** for analysis
- By 2030, reconstruction could take up to 40% of CPU requirements due to increasing pile up (additional pp collisions)

CMS Computing Needs (no R&D)



CMS Computing Results



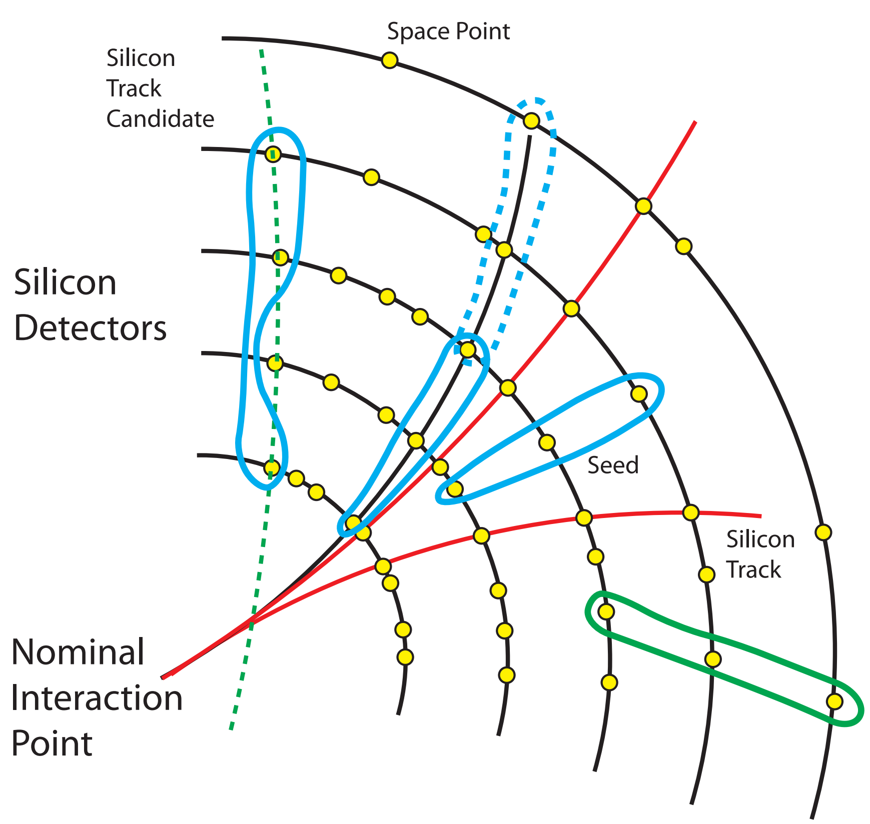
Track reconstruction is expected to have a large CPU burden at the HL-LHC … and even greater at future pp colliders

Can we develop better algorithms using quantum computers?

HL-LHC: μ= 140-200

Tracking Algorithms: Current Approaches

- Methods for track finding can be classified as either global or local
  - **Global**: Treat all measurements simultaneously
    - Hough, Legendre transforms, Hopfield networks, Graph Neural Networks
  - **Local**: Process measurements sequentially
    - track road, track following, Kalman Filter

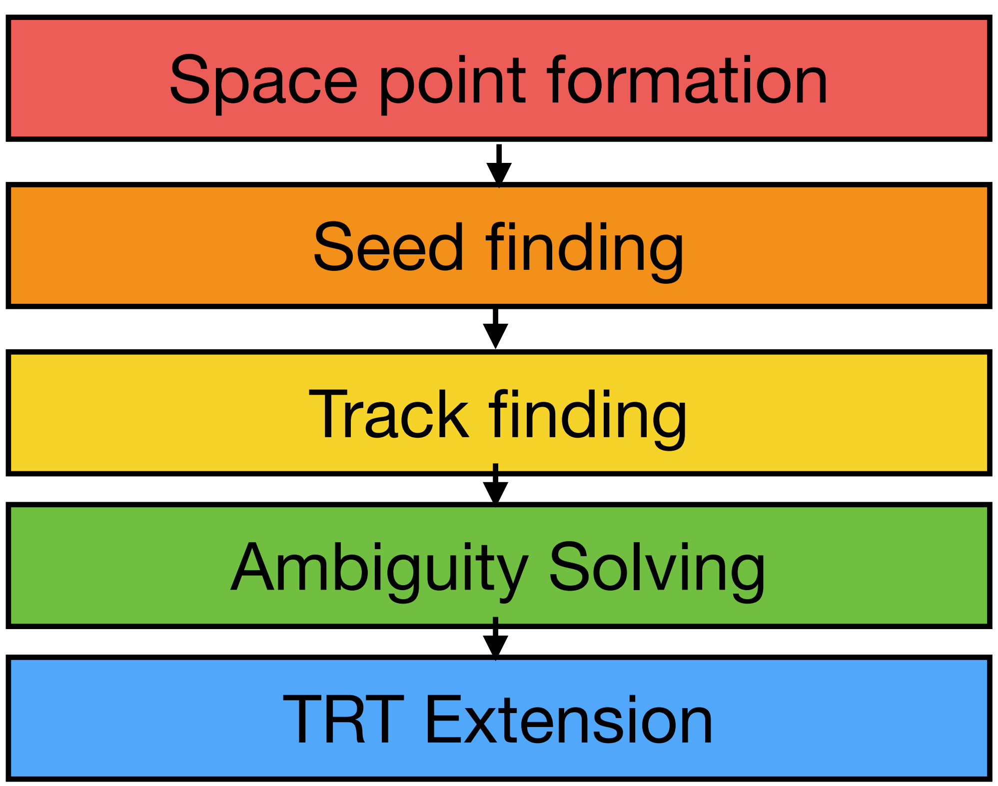


See e.g. Strandlie and Fruhwirth, Track and vertex reconstruction: From classical to adaptive methods for a review

Tracking Algorithms: Current Approaches

- Tracking algorithms at the LHC generally follow a multi-step local track following algorithms based on the Kalman filter
- Local algorithms can be parallelized (e.g. multithreaded, GPU), but execution time scales with the number of tracks
- Tracking is a key element of events **reconstruction**, but increasingly also in the **trigger** especially with the advent of even more specialized tracking detectors for triggering

Example track reconstruction sequence (ATLAS)



Track reconstruction in the CMS trigger for HL-LHC

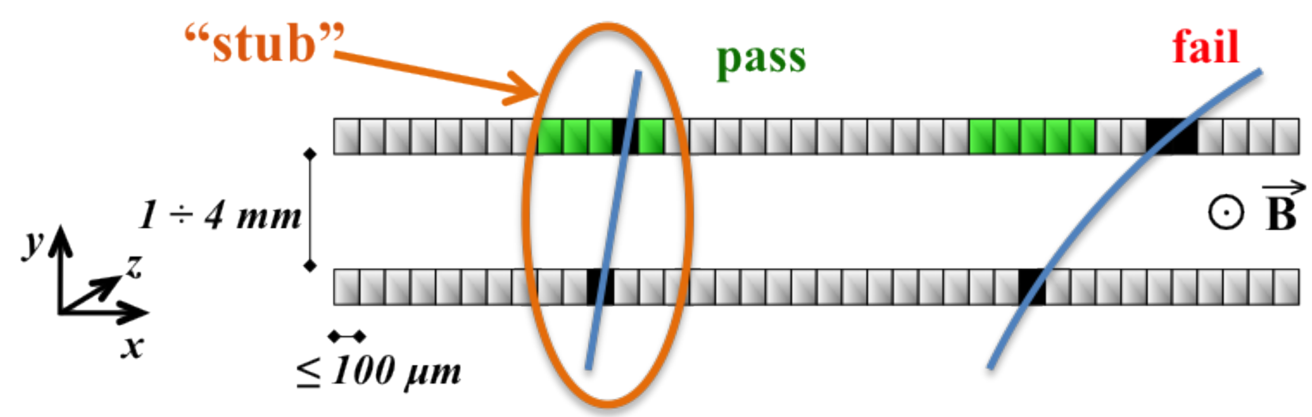
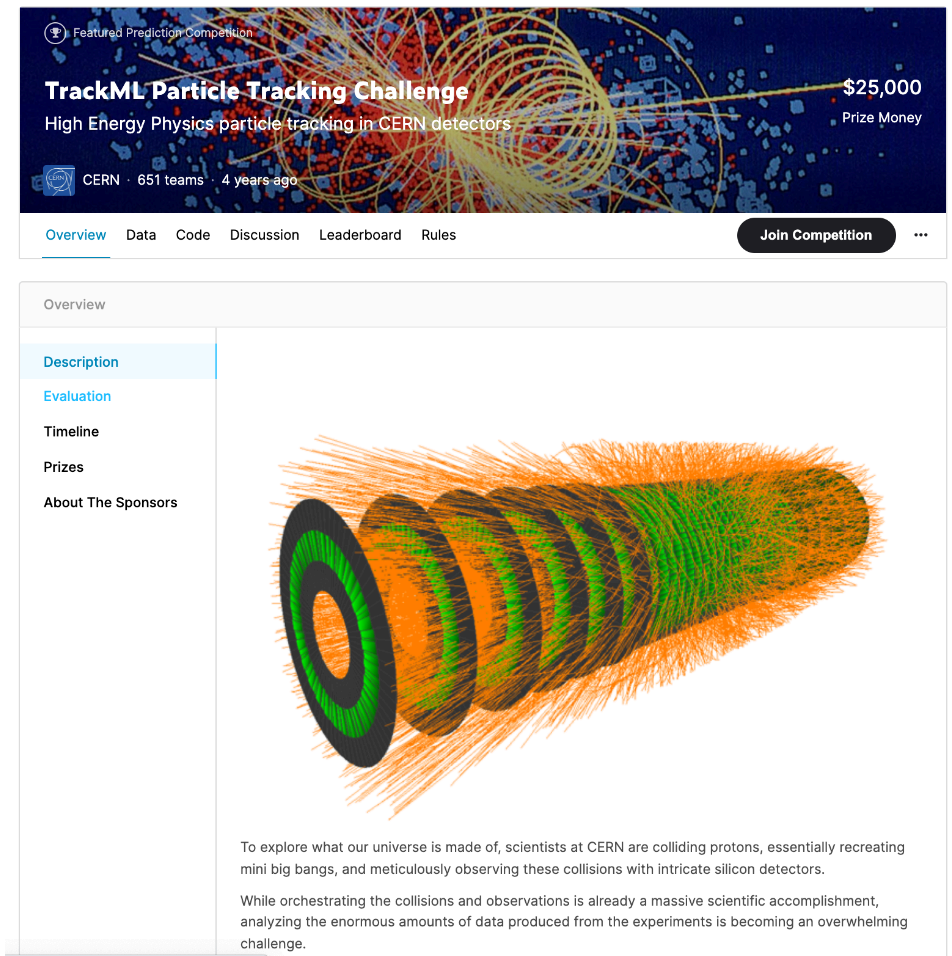


Image Credit: Louise Skinnari

Tracking on Quantum Computers

- Several groups have explored tracking algorithms for quantum computers
  - Berkeley/LBNL + Tokyo, DESY, METU+CERN+Caltech
- Algorithms have been developed for **quantum annealers** and **digital quantum computers**
- Almost all studies here use the trackML dataset
  - Open dataset produced for a tracking machine learning challenge (i.e. see if ML experts can develop better tracking algorithms)
- Many restrict the multiplicity and/or focus on the central detector region and/or high p_T



TrackML on kaggle

Amrouche et al, TrackML Accuracy Stage

U.S. DEPARTMENT OF ENERGY

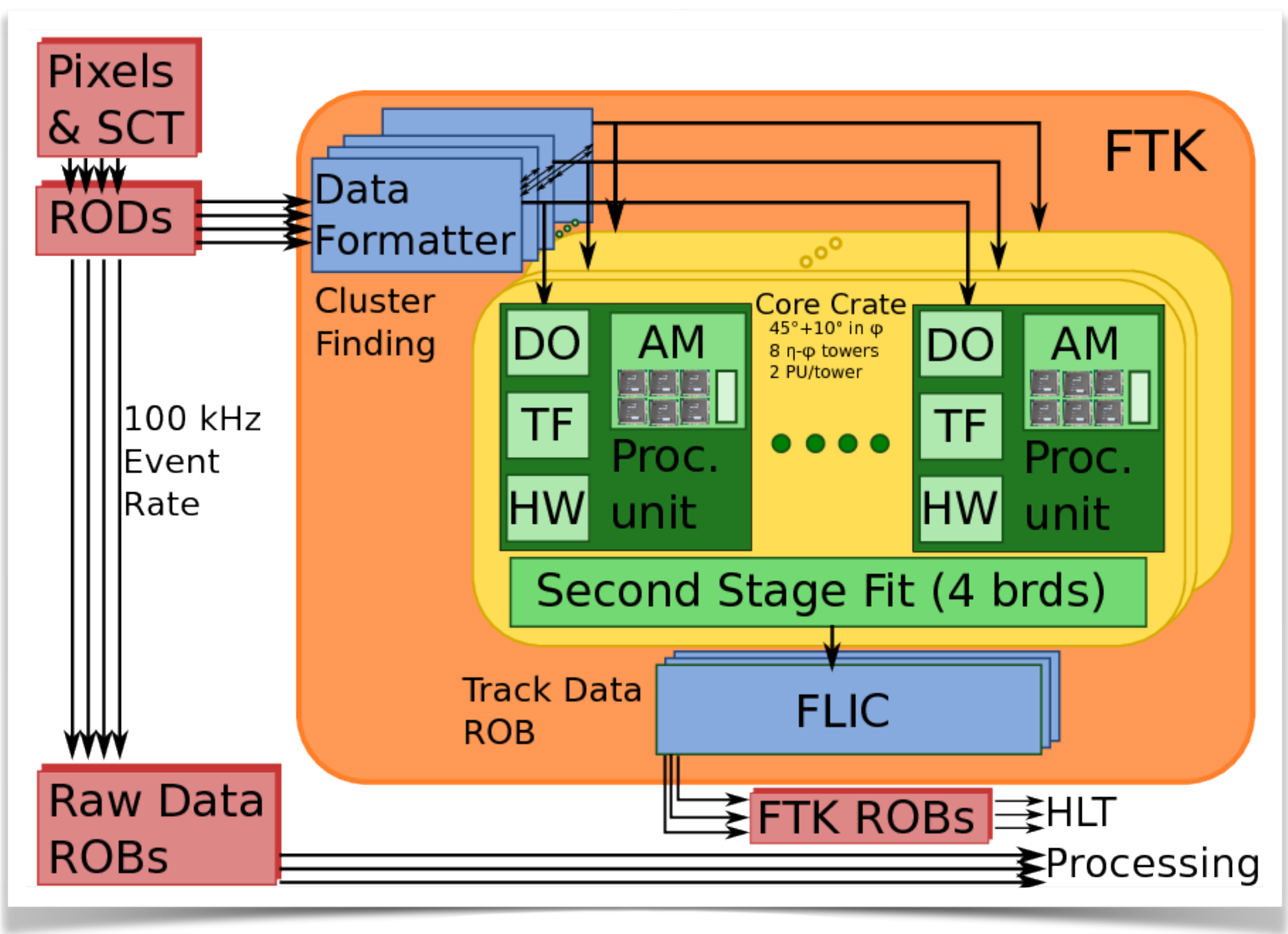
Office of Science

Algorithm 1: Quantum Associative Memory (QuAM)

Shapoval and Calafiura, arXiv:1902.00498

Tracking with Associative Memory

- Store possible track patterns directly in hardware
  - Instead of running algorithms to reconstruct tracks, look up patterns of hits
  - Avoids **combinatorial scaling**
  - Can be sensitive to changes in detector conditions
- Technique considered for hardware track triggers, e.g. Fast Track Trigger (FTK) design for ATLAS



Quantum Associative Memory

- Theoretically proven asymptotic advantages of circuit-based QC
  - Optimal* recall of unstructured memories
  - Optimal memory capacity

Strategy

- Memorize N patterns by assembling a quantum superposition of the basis states:

$$|\Xi\rangle = \sum^{N} \alpha_i |\xi^i\rangle, \qquad \alpha_i \in \mathbb{C} \quad \wedge \quad N \leqslant 2^n \quad \wedge \quad \sum^{N} |\alpha_i|^2 = 1$$

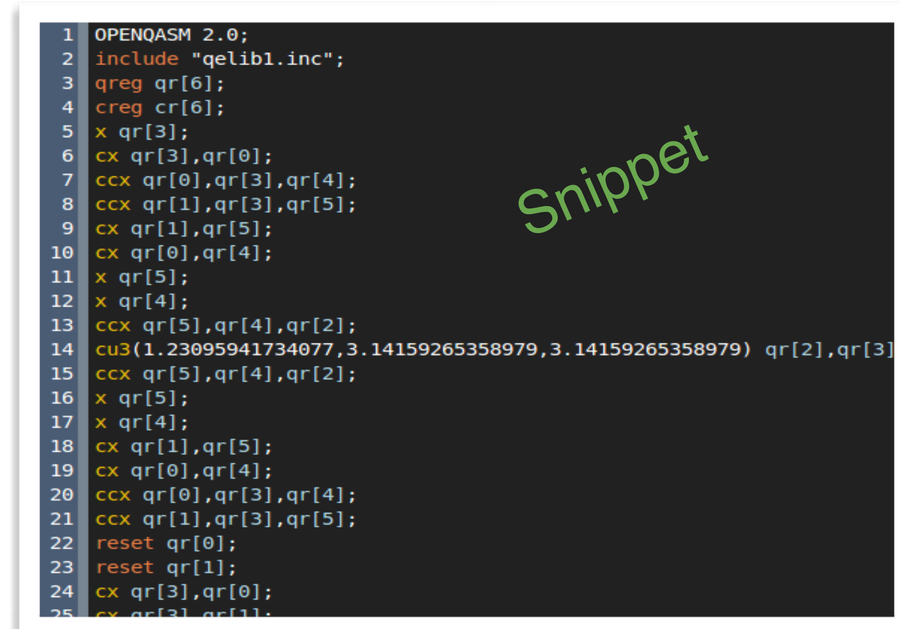
- Apply generalized Grover's algorithm to amplify the amplitude of a pattern being recalled.
- Measure memory

*an algorithm is optimal if no other algorithm can outperform it by more than a constant factor

Implementation

- Developed QuAM circuit generators implementing the Trugenberger's initialization and generalized Grover's algorithms
  - Open-source quantum computing platform, Qiskit
- Supported backends
  - IBM QE cloud-based quantum chips [5Q Yorktown/Tenerife, 14Q Melbourne, 20Q Tokyo]
  - Local/remote noisy simulators

Storage QuAM

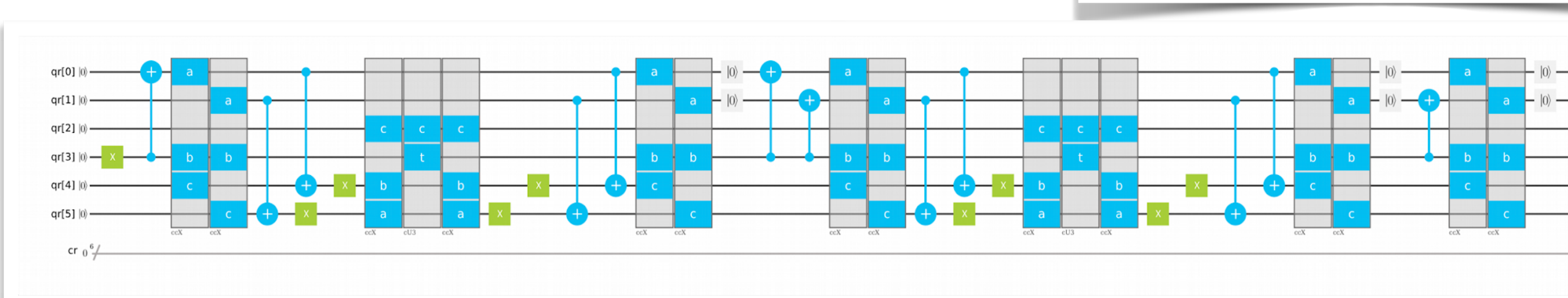


```
OPENQASM 2.0;
include "qelib1.inc";
qreg qr[6];
creg cr[6];
x qr[3];
cx qr[3],qr[0];
ccx qr[0],qr[3],qr[4];
ccx qr[1],qr[3],qr[5];
cx qr[1],qr[5];
cx qr[0],qr[4];
x qr[5];
x qr[4];
ccx qr[5],qr[4],qr[2];
cu3(1.23095941734077,3.14159265358979,3.14159265358979) qr[2],qr[3]
ccx qr[5],qr[4],qr[2];
x qr[5];
x qr[4];
cx qr[1],qr[5];
cx qr[0],qr[4];
ccx qr[0],qr[3],qr[4];
ccx qr[1],qr[3],qr[5];
reset qr[0];
reset qr[1];
cx qr[3],qr[0];
```


Retrieval QuAM

```
s qr[5];
h qr[5];
cx qr[4],qr[5];
h qr[5];
s qr[5];
h qr[4];
h qr[5];
x qr[4];
x qr[5];
h qr[5];
cx qr[4],qr[5];
h qr[5];
x qr[4];
x qr[5];
h qr[4];
h qr[5];
h qr[5];
cx qr[4],qr[5];
h qr[5];
```


Example: complete circuit for **storing** one 2-bit pattern

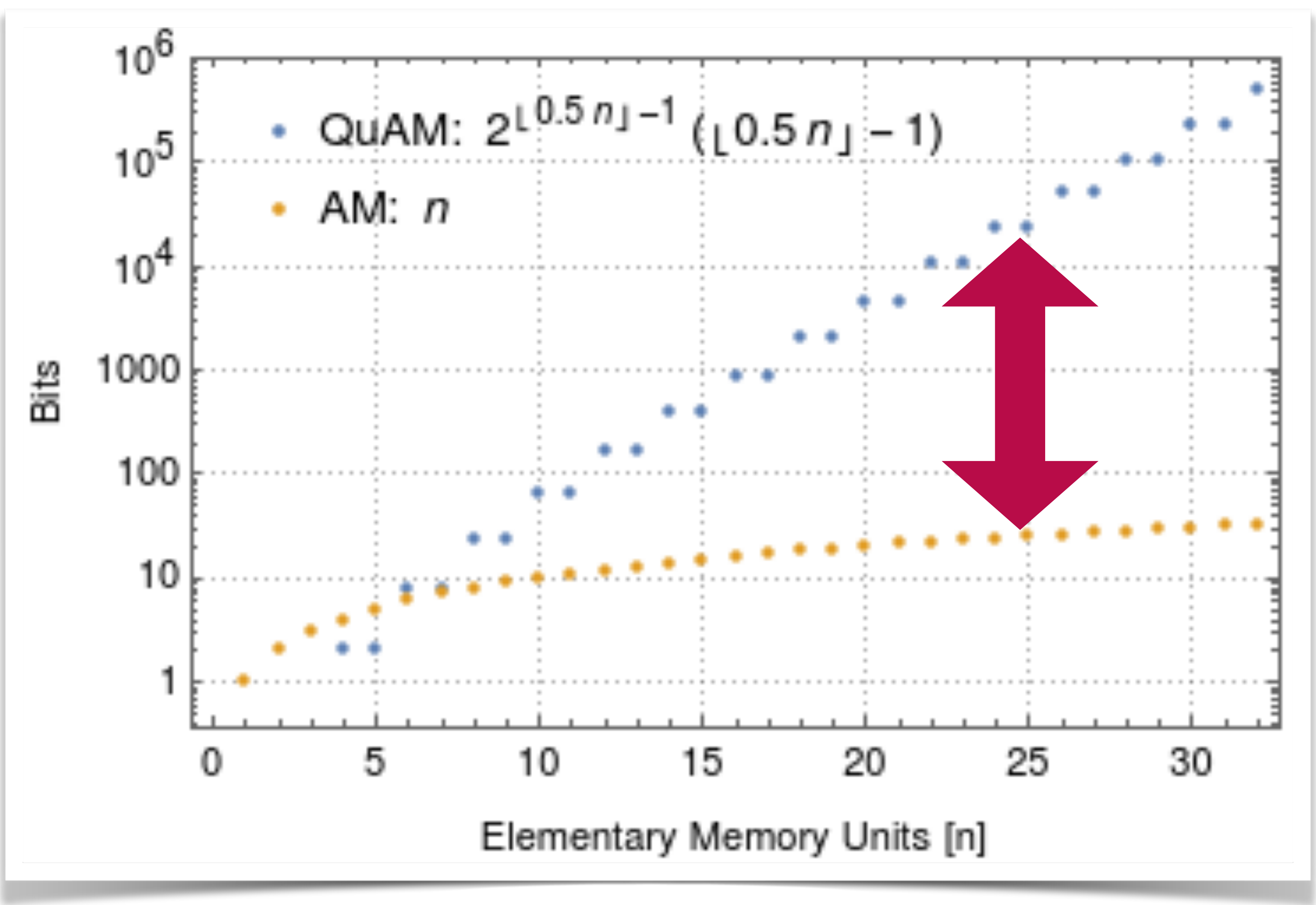


C.A Trugenberger, Probabilistic Quantum Memories. PRL 87, 6 (2001)   arXiv:1902.00498

Storage Capacity

Exponential storage capacity (2d)
Requires 2(d+1) qubits to operate

Detector hit identifier (bits)	8	16	32
8 hit track pattern (bits)	64	128	256
QuAM register (qubits)	130	258	514
QuAM capacity (patterns)	$\sim 10^{19}$	$\sim 10^{38}$	$\sim 10^{77}$



cf: 10^{78}-10^{82} atoms in the known universe

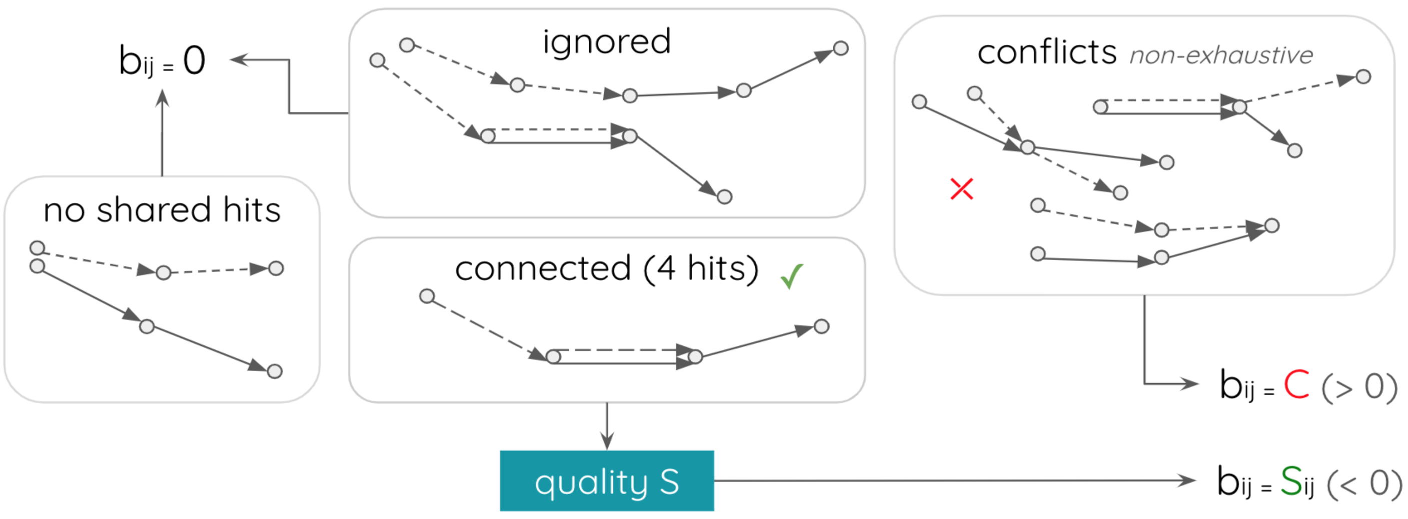
Algorithm 2
Quantum Annealing

Bapst et al, arXiv:1902.08324

https://github.com/derlin/hepqpr-qallse

Offline: Quantum Annealing

- Formulate track reconstruction as an **energy minimization problem**
    - Use quantum annealers from D-Wave to find the minimum
- Global algorithm
    - Execution time ~independent of the number of tracks
- Formally, express problem as a Quadratic unconstrained binary optimization (QUBO)
    - Inspired from *, but use triplets of hits instead of doublets as the qubits
    - Encode the quality of the triplets based on physics properties.
    - Pair-wise connections b act as constraints (>0) or incentives (<0)
    - To minimize objective function, select best triplets to form track candidates

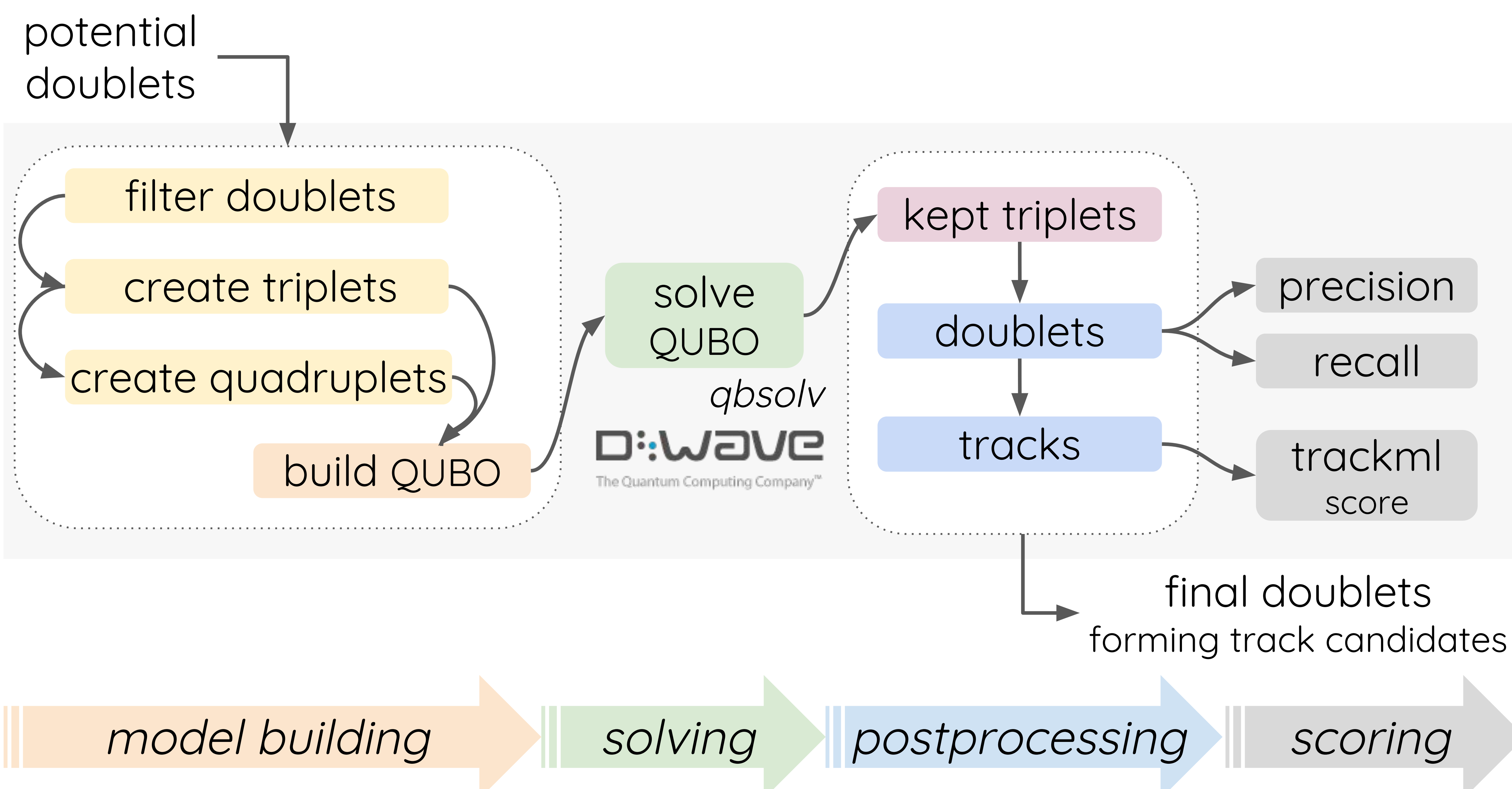


*Stimpfl-Abele & Garrido, Fast track finding with neural networks

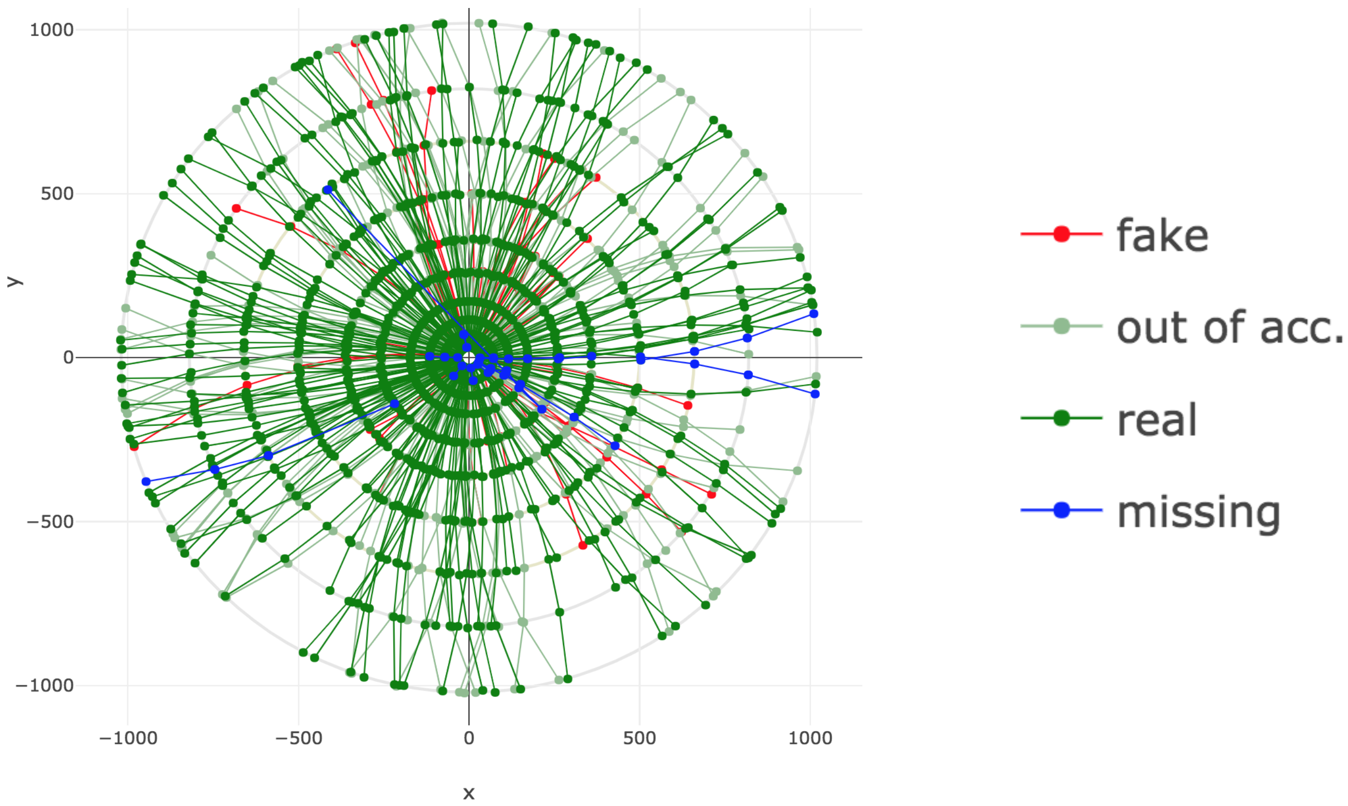
Implementation

arXiv:1902.08324

- Dataset: simplified TrackML dataset, focus on barrel, 1+ GeV, at least 5 hits
  - Toy dataset, but representative of expected conditions at the HL-LHC
- QUBO solvers: qbsolv (D-Wave + simulation), neal (classical)
- D-Wave 2X (1152 qubits), D-Wave 2000Q (2048 qubits)

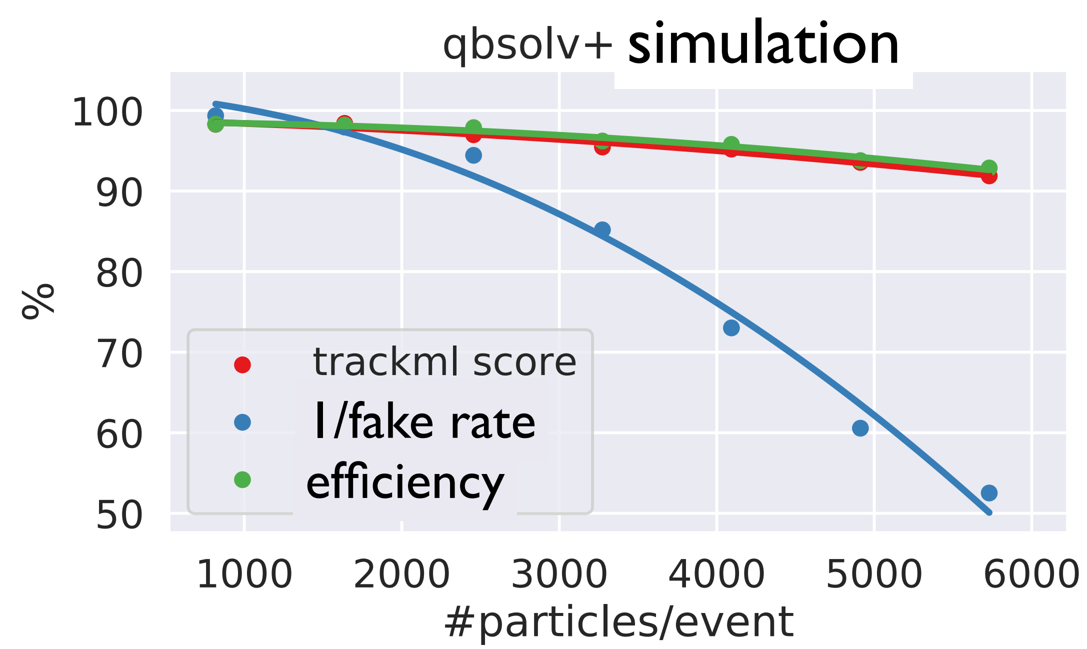


Performance



Doublets for a dataset of 2456 particles and 16855 hits

Physics performance as a function of occupancy using a D-Wave 2X (qbsolv).

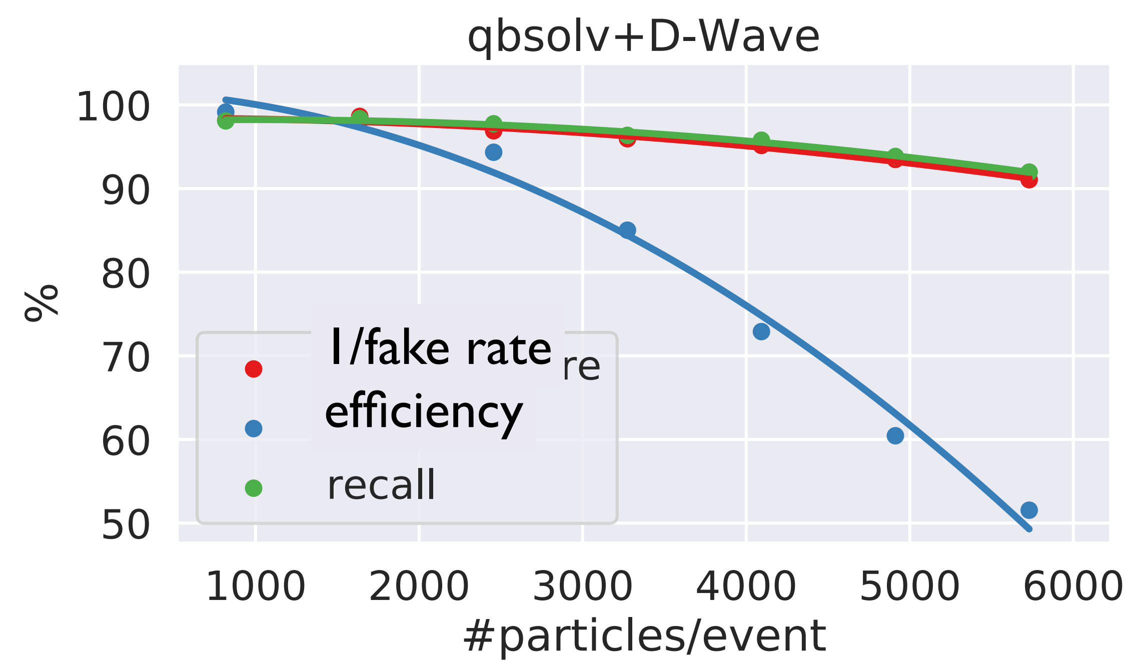


Timing

building: 0-20 min

solving: 0-12s (sim), **0-56 min** (D-Wave*)

*important time overhead with D-Wave due to use of queues

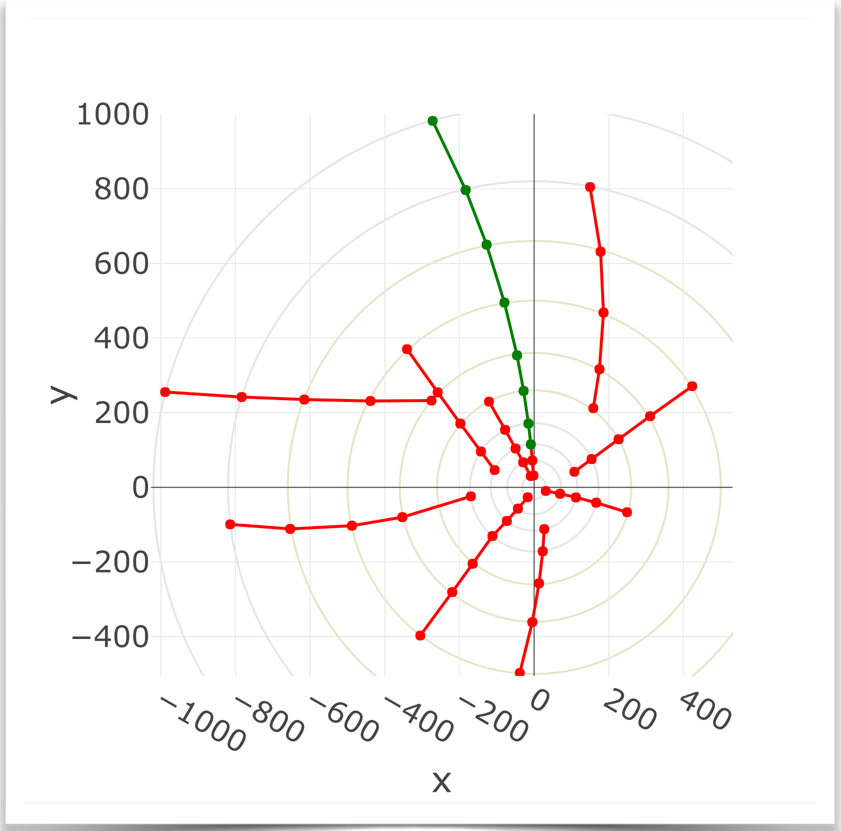


arXiv:1902.08324

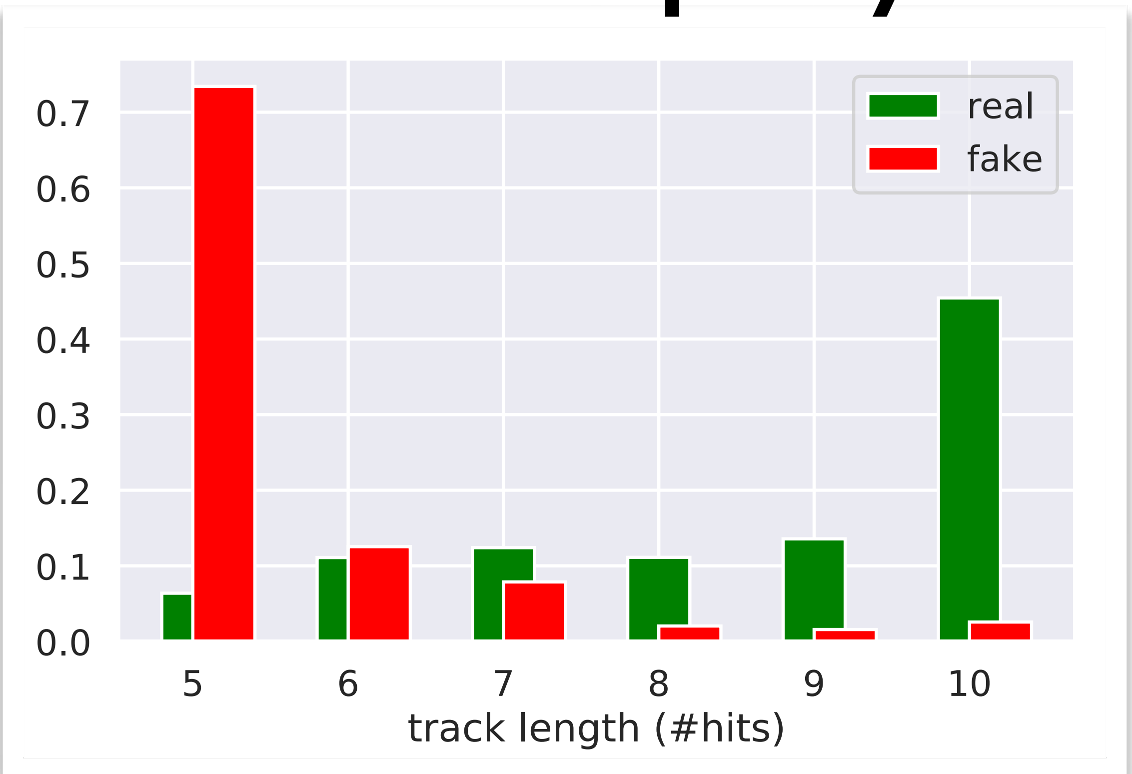
Reducing Fakes

arXiv:1902.08324

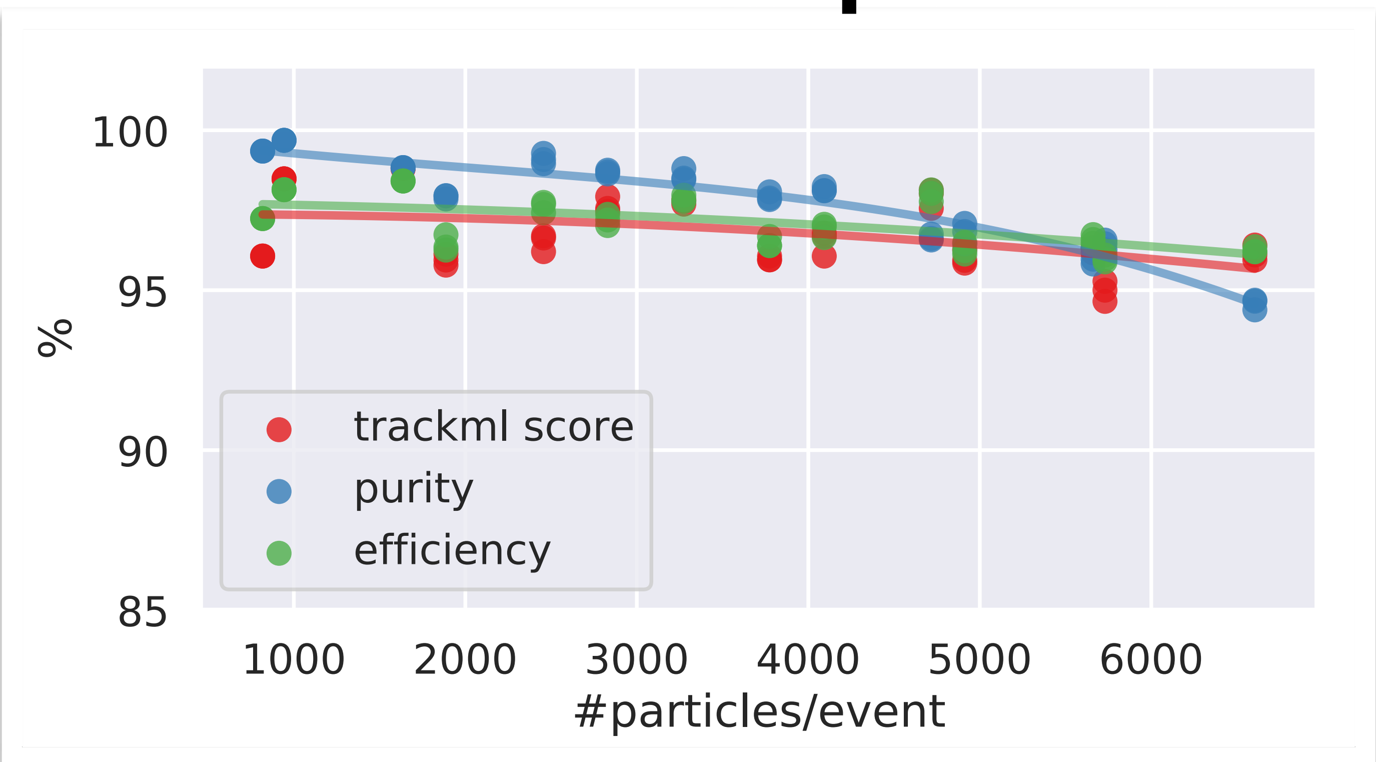
- At multiplicities approaching the HL-LHC, fake contribution becomes significant
- Methods to **reduce fakes**
  - tighten track quality requirements
  - refining conflict & bias terms, e.g. including vertex assumptions



Track quality

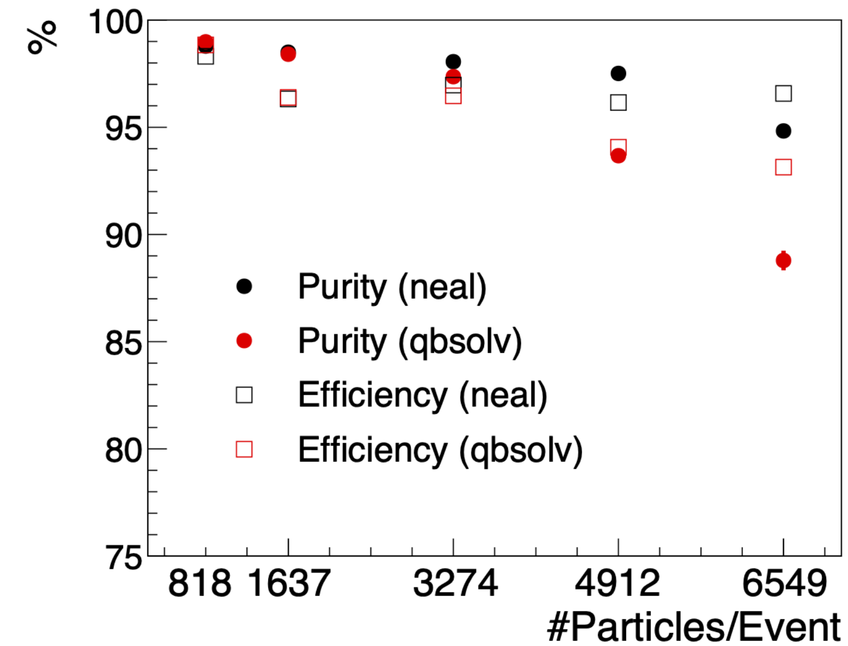


Vertex assumptions



Further performance optimizations

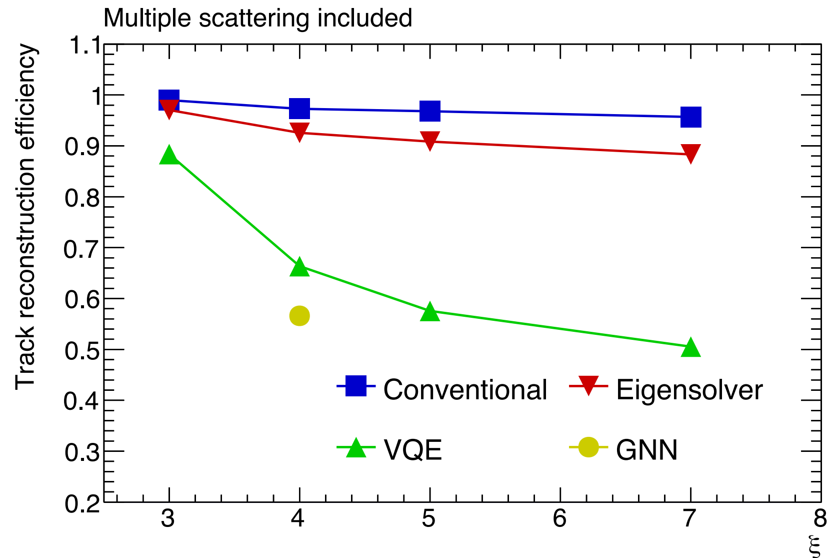
- Further improvement of the purity of the algorithm
  - Extend to expected HL-LHC multiplicities
- Study performance using the **Fujitsu Digital Annealer**
  - Annealing time is independent of the number of tracks
  - Superior performance to DWave
- Recently initial studies for the LUXE experiment, Funcke et al

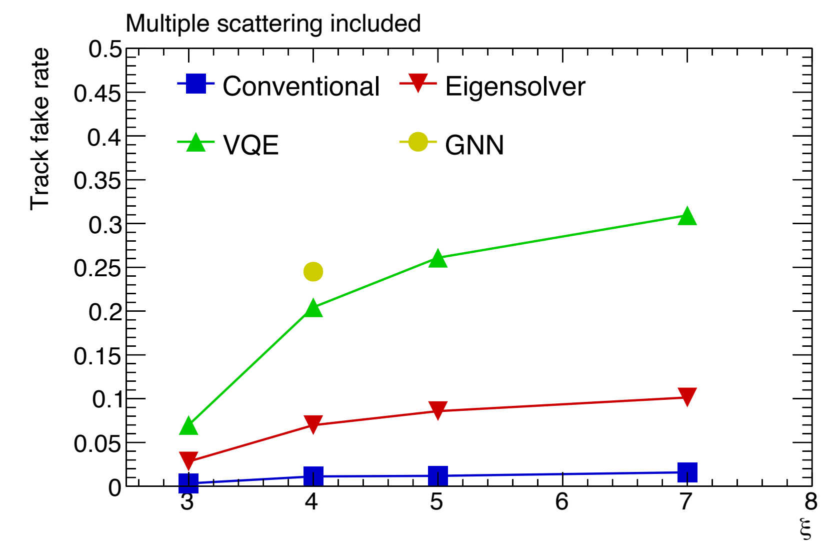


Saito et al

Density [%]	N_{slice}	DA [sec]		neal [sec]
		CPU time	Anneal time	total time
5	46	0.09	0.29	0.27
10	68	0.15	0.42	0.66
20	71	0.22	0.44	1.29
40	74	0.52	0.45	2.46
60	73	0.94	0.45	4.29
80	74	1.79	0.46	7.49
100	74	3.73	0.45	12.87

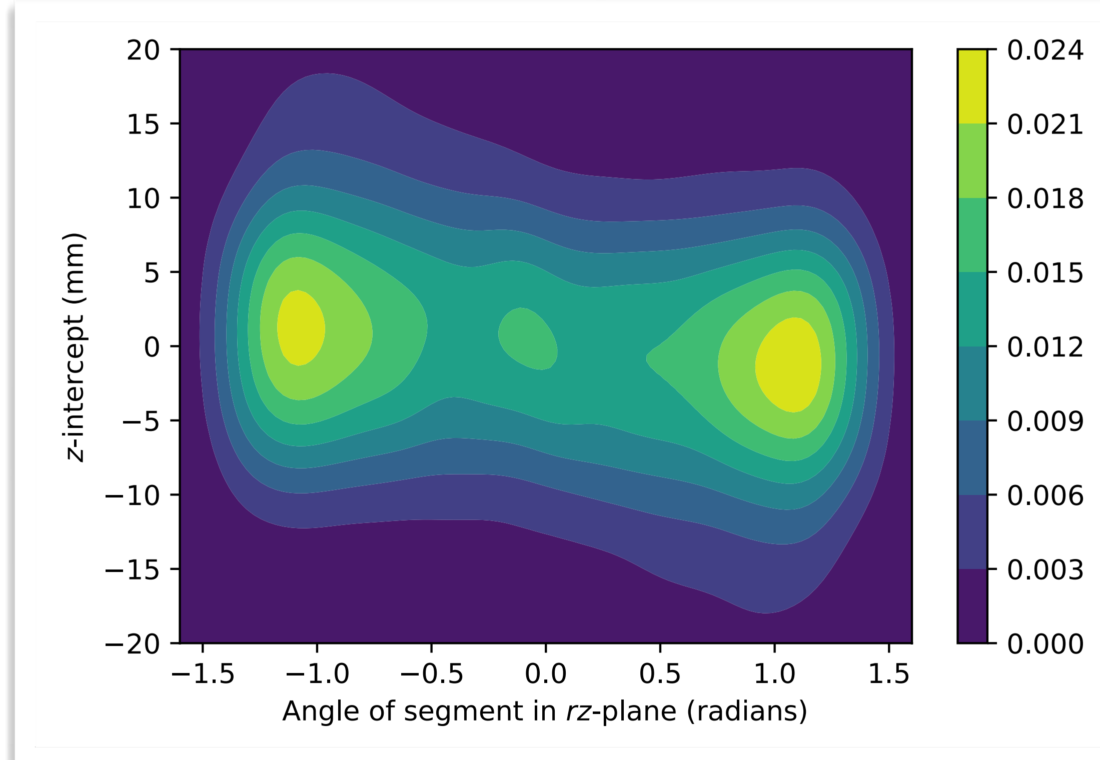
LUXE

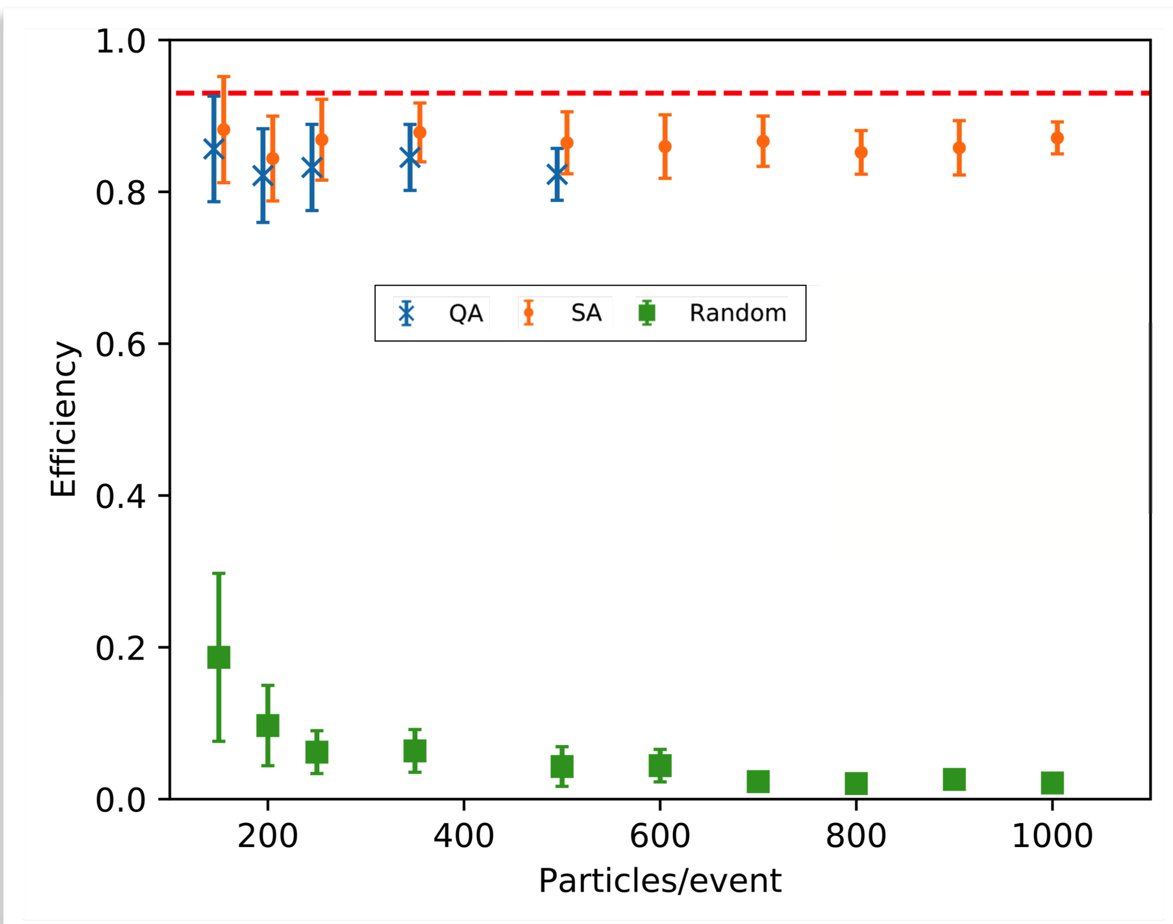


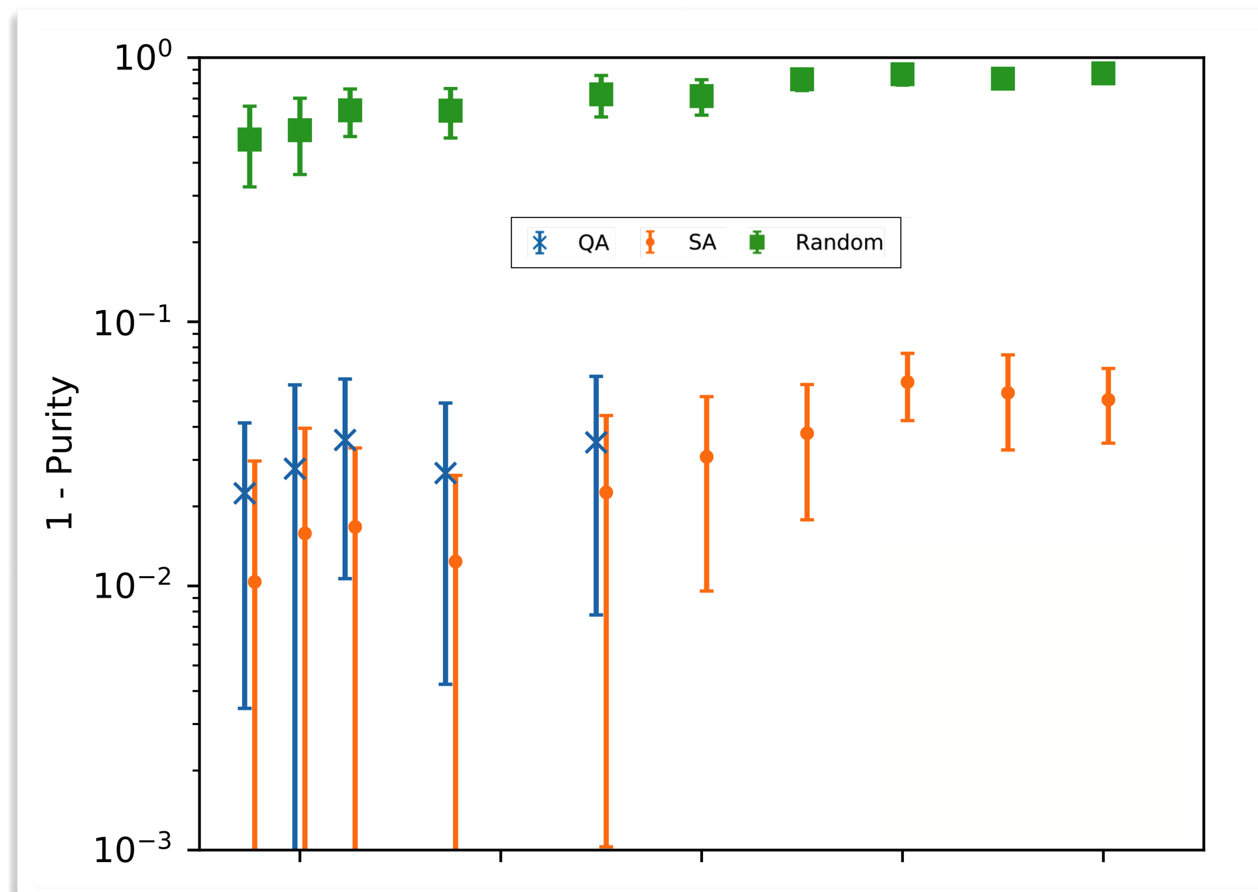


Quantum Annealing

- An independent implementation of quantum annealing using Hopfield networks for tracking from Zlokapa et al, arXiv: 1908.04475
- KDE to estimate connection probability for a pair of hits





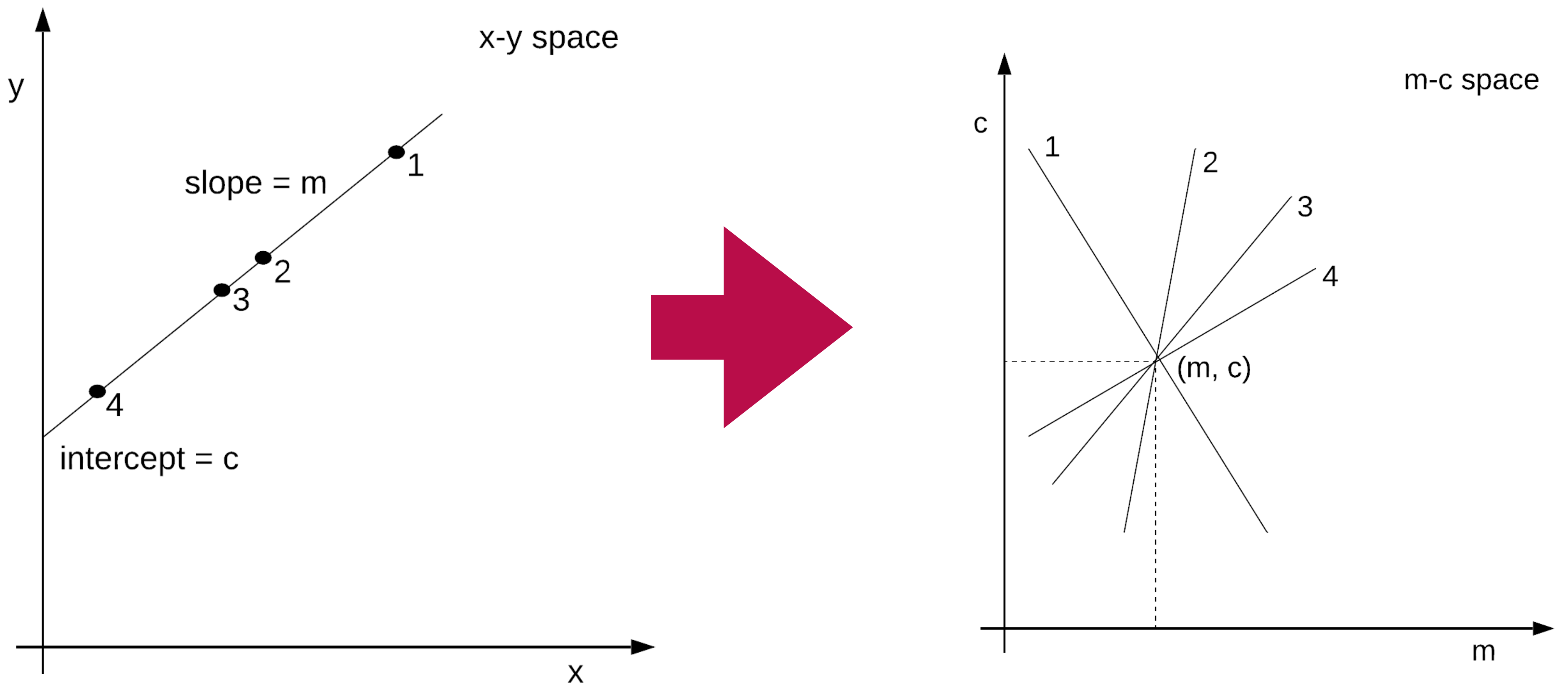


Zlokapa et al, arXiv: 1908.04475

Algorithm 3
Quantum Hough Transform

Preliminary study

Quantum Hough Transform



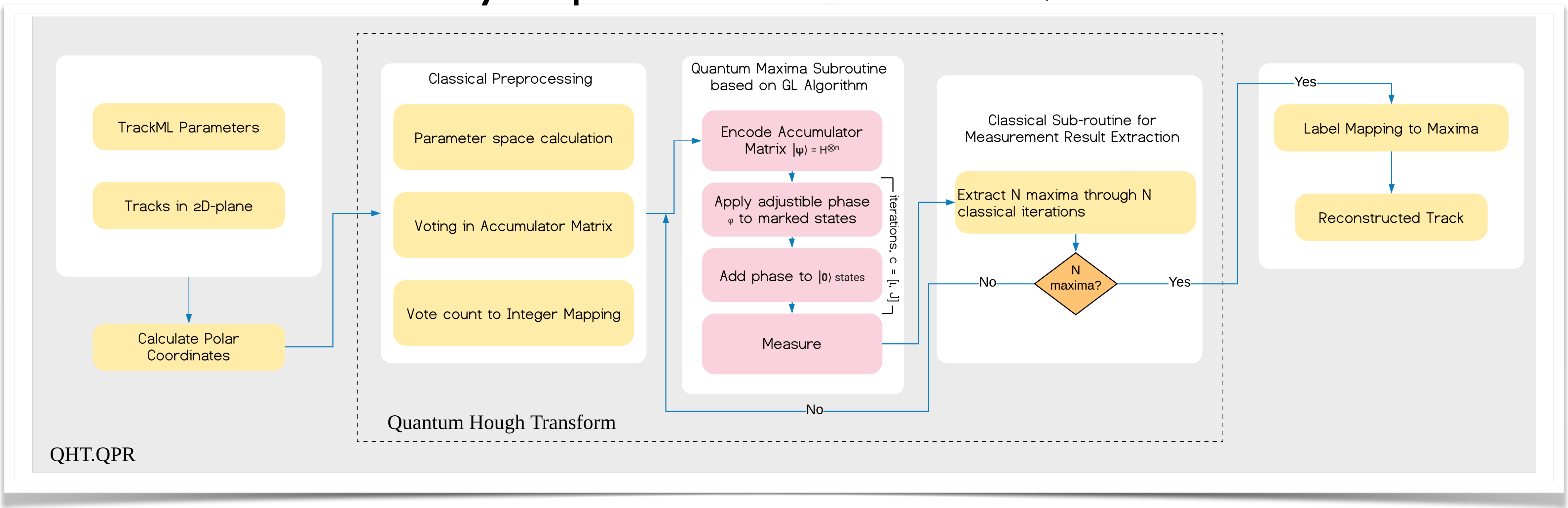
P.V.C. Hough (1962), R.O. Dude, P.E. Hart (1972), D.H. Ballard (1980)

Slide Credit: A. Yadav

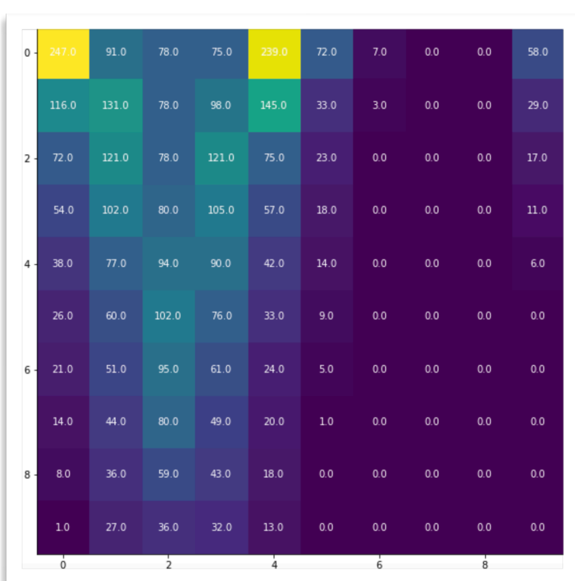
Implementation & Preliminary Results

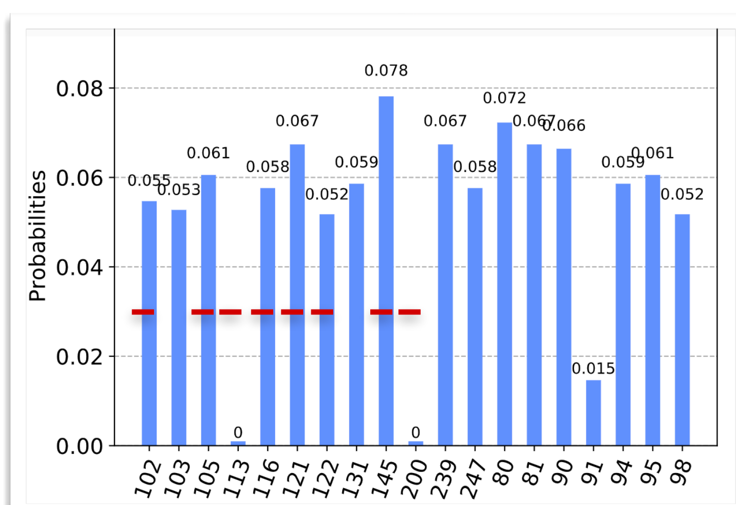
Preliminary implementation within QISKit

Accumulator Space for 8 tracks



Testing within a quantum simulator





vote counts

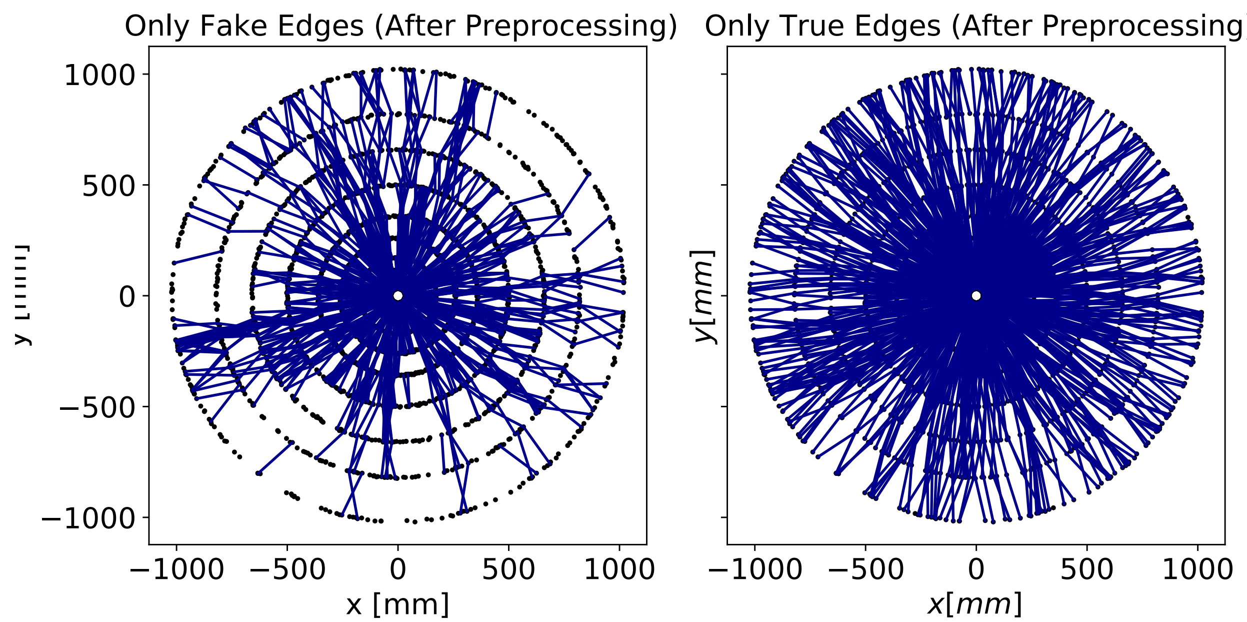
Local Maxima Detection using Grover-Long Algorithm

```
track_index

array([array([13, 19, 22, 28, 35, 48, 52]),
       array([ 2,  5, 16, 36, 40, 49]),
       array([23, 29, 30, 32, 43, 53, 54]),
       array([17, 18, 23, 30, 33, 39, 45, 50]),
       array([17, 18, 23, 29, 30, 33, 39, 50]),
       array([ 0,  9, 14, 34, 38, 42]), array([ 1, 11, 12, 20, 24, 27]),
       array([ 7,  8, 10, 37, 46, 57]), array([17, 23, 29, 30, 32, 54]),
       array([17, 29, 32, 43, 53, 54])], dtype=object)
```

Chen et al, arXiv:1908.07943

Slide Credit: A. Yadav



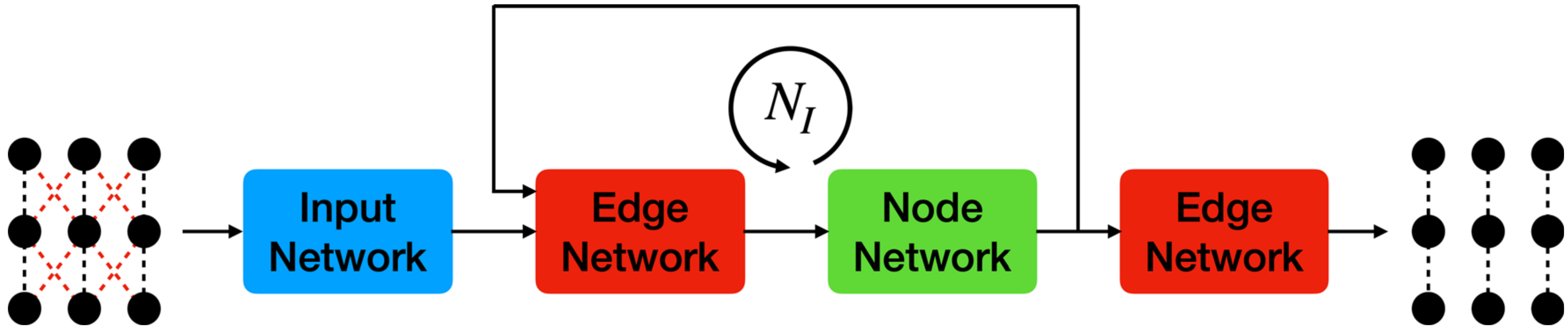
Algorithm 4: Quantum Graph Neural Networks (QGNN)

Cenk Tüysüz[1,2], Federico Carminati[3], Bilge Demirköz[1], Daniel Dobos[4,6], Fabio Fracas[3,7], Kristiane Novotny[4], Karolos Potamianos[4,5], Sofia Vallecorsa[3], Jean-Roch Vlimant[8]

[1] *Middle East Technical University, Ankara, Turkey*
[2] *STB Research, Ankara, Turkey*
[3] *CERN, Geneva, Switzerland*
[4] *gluoNNet, Geneva, Switzerland*
[5] *DESY, Hamburg, Germany*
[6] *Lancaster University, Lancaster, UK*
[7] *University of Padua, Padua, Italy*
[8] *California Institute of Technology, Pasadena, California, USA*

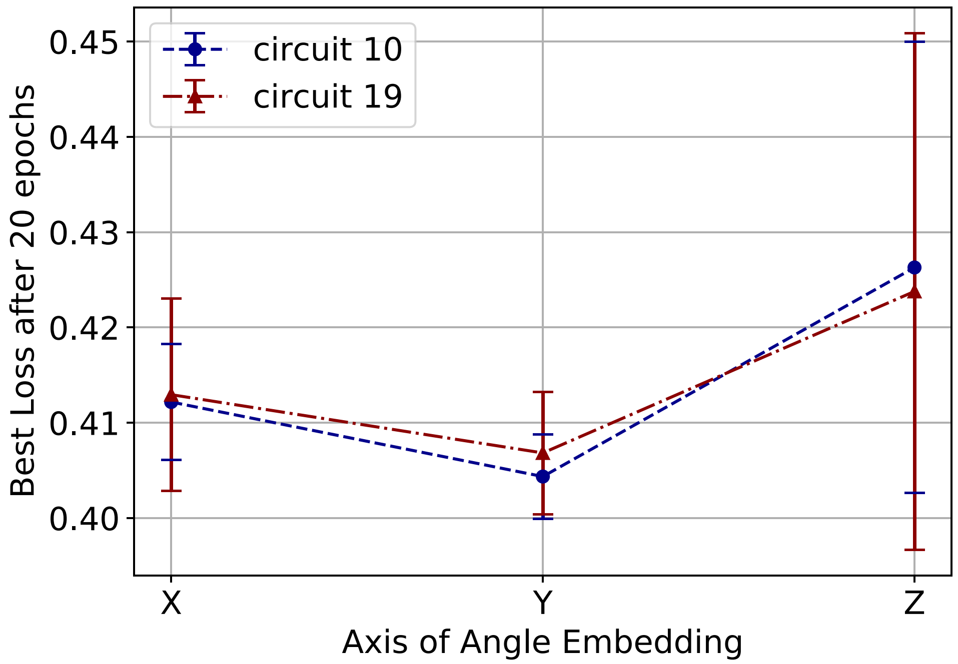
Quantum Graph Neural Networks

- GNNs for particle tracking are under development by a number of groups
- Recent studies of the application of **QGNNs** to particle tracking
  - Hybrid quantum-classical algorithm
  - Encode the hit coordinates as angles
  - Iteratively apply quantum edge and node networks to propagate information to all detector layers
  - Final application of the edge network classifies the segments

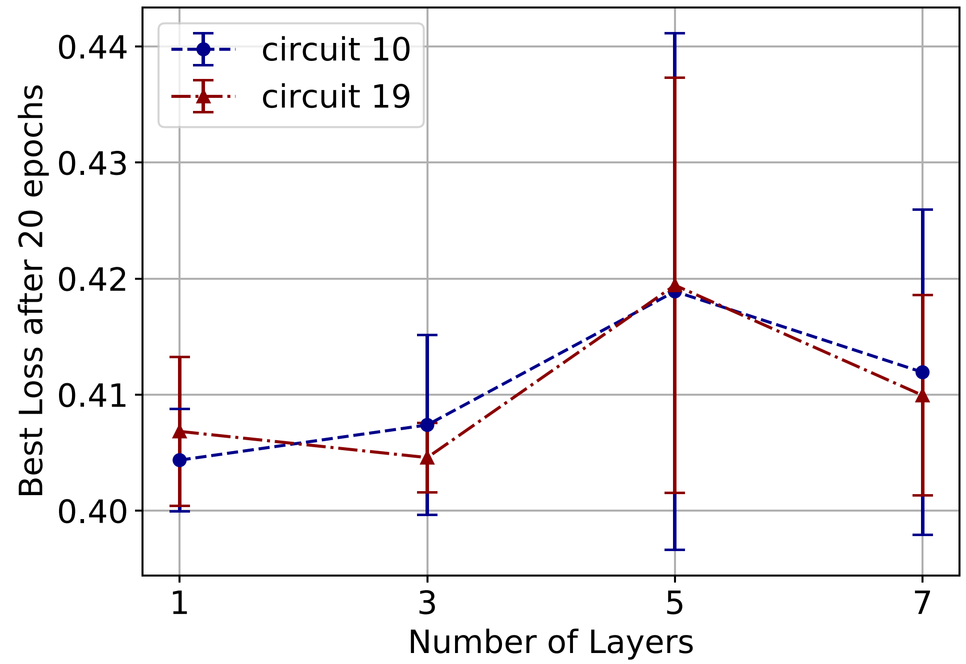


arXiv:2003.08126, arXiv:2007.06868.pdf, Tuysuz et al, 2021

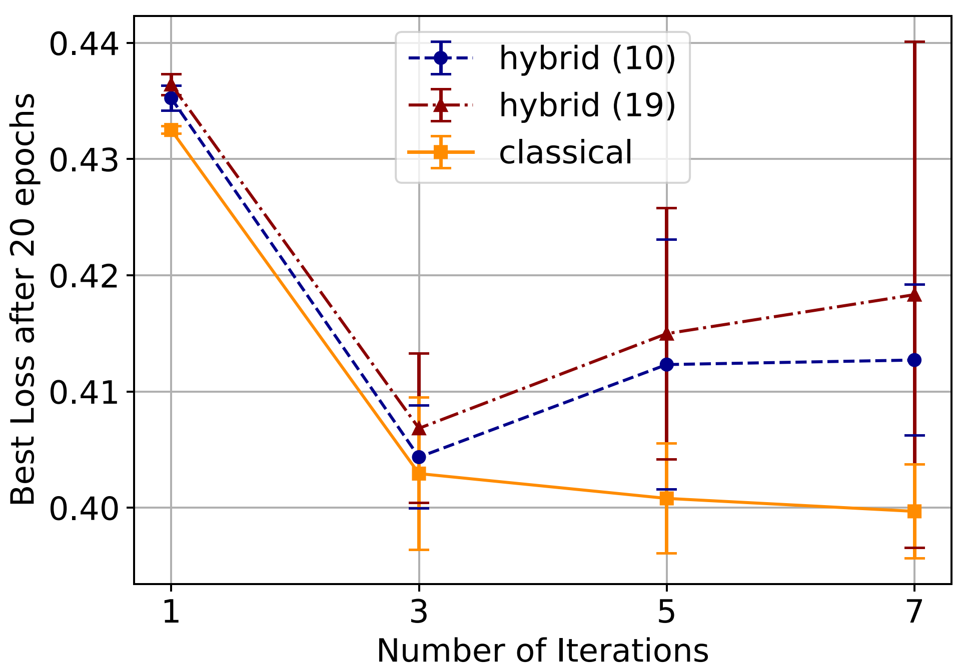
QGNN Results



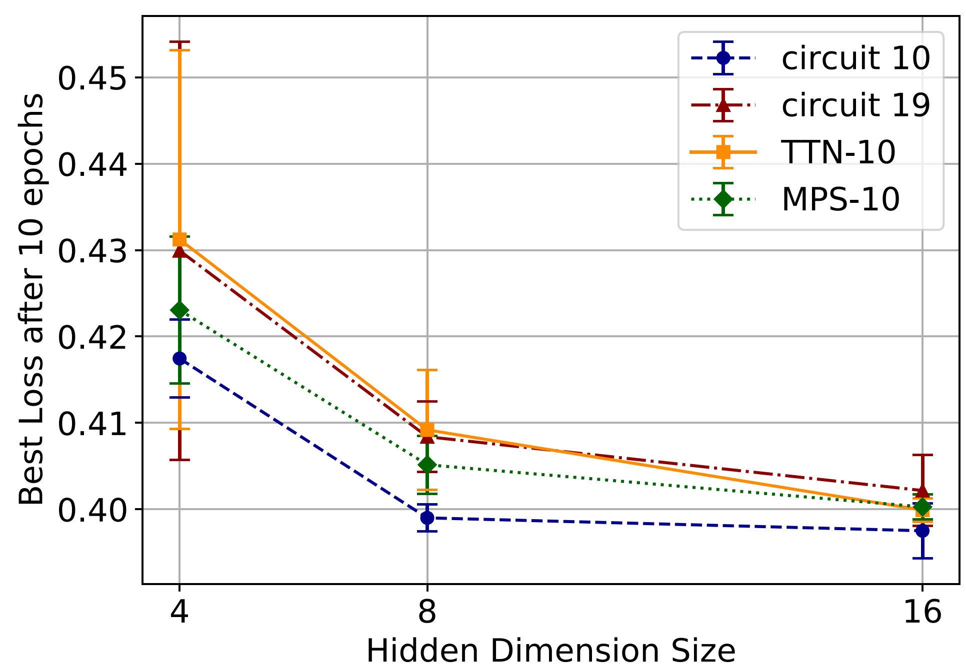
(a) Axis of angle embedding comparison.



(b) Number of layers (N_L) comparison.



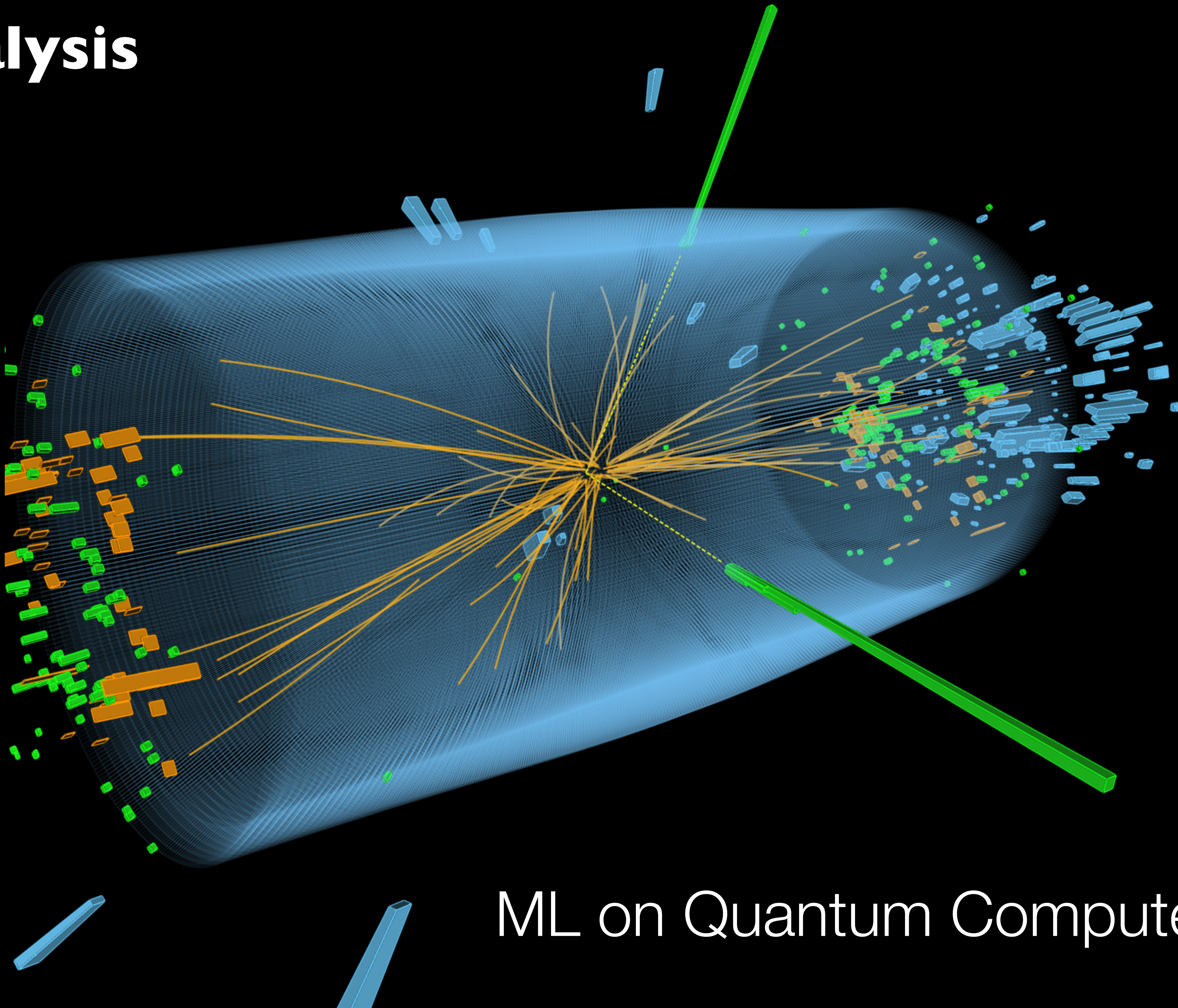
(c) Number of iterations (N_I) comparison.



(d) Hidden dimension size ($N_D = N_Q$) comparison.

arXiv:2003.08126, arXiv:2007.06868.pdf, Tuysuz et al, 2021

Analysis



ML on Quantum Computers

Quantum Machine Learning

- Recently rapid development in the field of **quantum machine learning**
- As quantum circuits are differentiable, train by minimizing a cost function
- Two general categories have been explored
  - **Variational** algorithms: classical optimizer to train quantum circuit
  - **Kernel** methods: identify key features, e.g. support vector machines
- In most cases, implemented as **classical-quantum hybrid** algorithms
- Machine learning is used **extensively** in HEP, natural to explore if such methods can be useful
  - Not particularly constrained by computing power, but care about obtaining ultimate performance
- However, HEP data has high dimensionality and uses large/complex machine learning models
  - Need to **simplify problems** to use current quantum computers

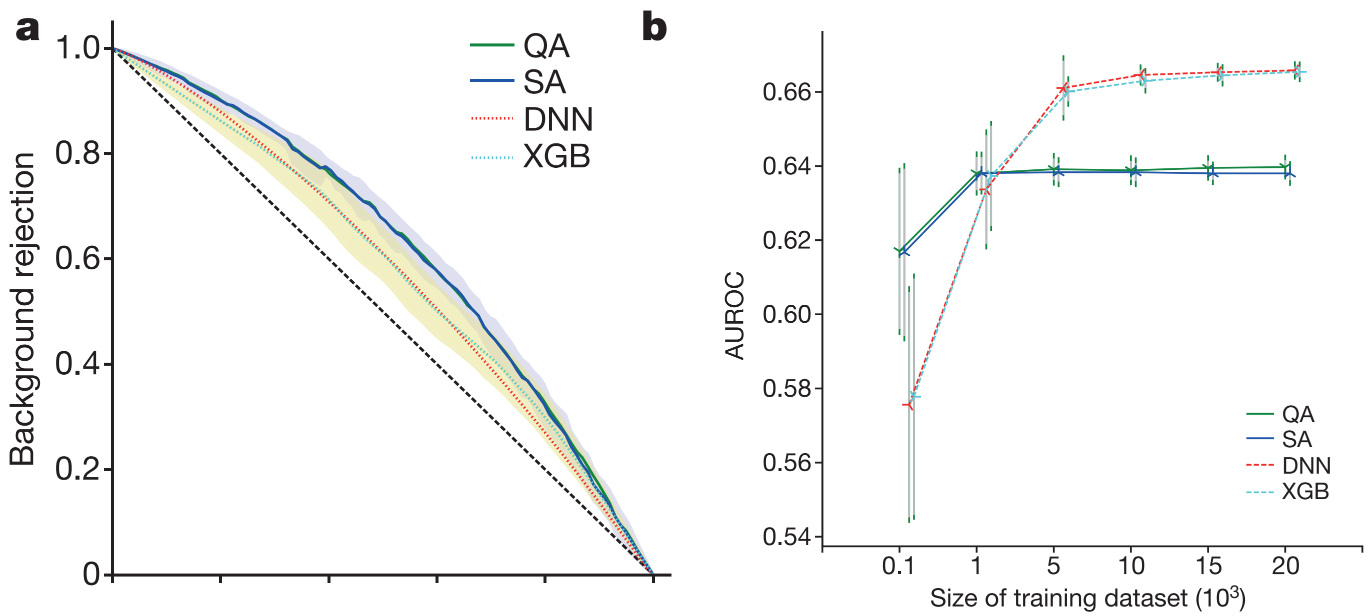
See Guan et al for a recent review

QML Examples

doi:10.1038/nature24047

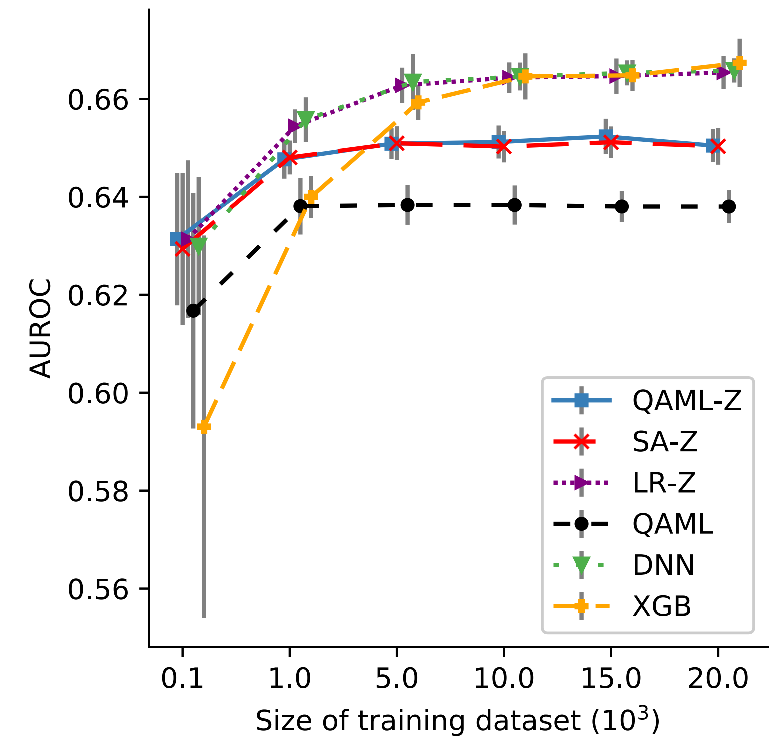
Solving a Higgs optimization problem with quantum annealing for machine learning

Alex Mott[1]†*, Joshua Job[2,3]*, Jean-Roch Vlimant[1], Daniel Lidar[3,4] & Maria Spiropulu[1]

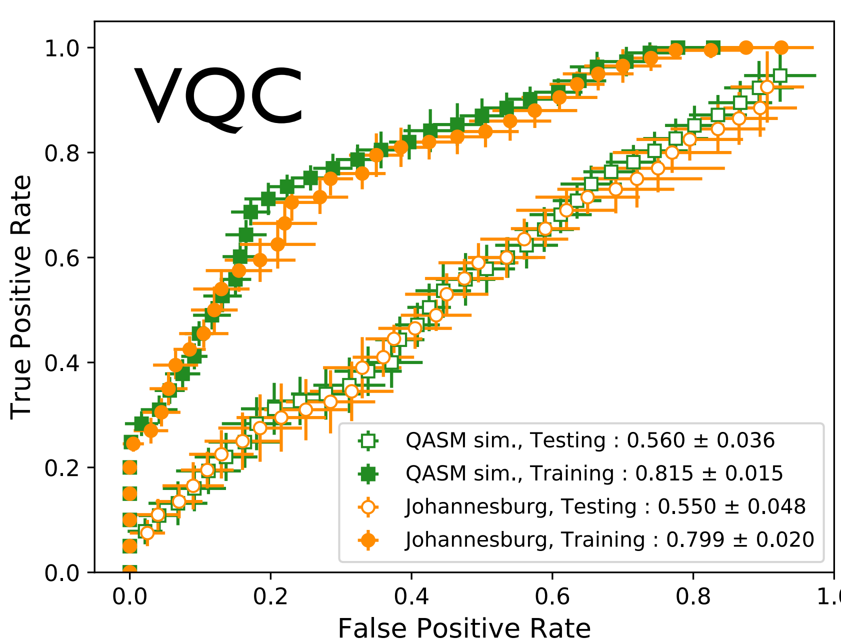


Mott, et al, doi:10.1038/nature24047

QAML with zooming

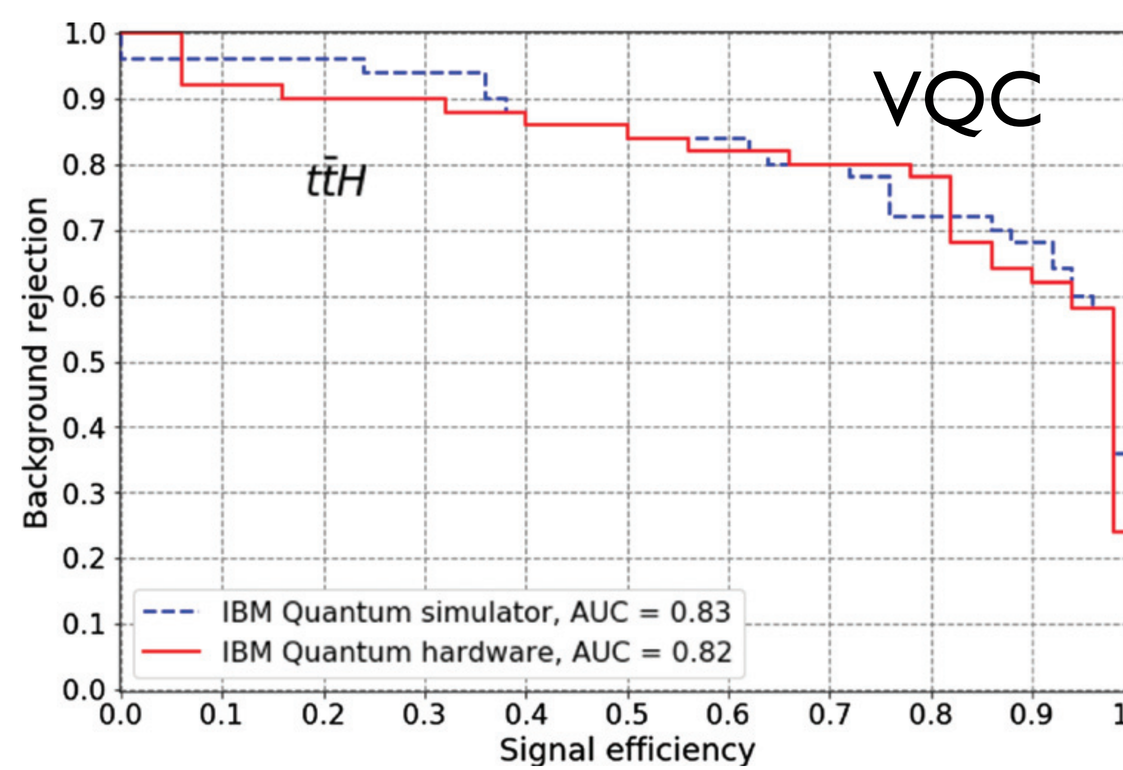


Zlokapa et al, arXiv: 1908.04480



VQC = Variational Quantum Classification

Terashi et al, arXiv:2002.09935.pdf



Wu et al, . Phys. G: Nucl. Part. Phys. 48 125003

Conclusion

- Quantum computing offers the exciting potential for the development of new algorithms which could allow us to obtain better **computational performance**, better **physics performance** or both
- Presented four different algorithms for pattern recognition on quantum computers and a teaser about quantum machine learning for analysis
  - Collectively provide **proof-of-concept** that quantum computers can be used for track reconstruction
- Current algorithms are **limited** in their capacity by the number of available **qubits** and their **fidelity**
  - Track reconstruction algorithms will require large amounts of data to be **transferred** to the quantum computers
- Thus, while such algorithms are promising, it is **too early** to conclude about how large a role quantum computers will play for track reconstruction at future high-energy physics experiments

Recent review: Gray and Terashi, 2022