Particle tracking with NISQ computers

Tim Schwägerl | Bari, 25.10.2022 | with Karl Jansen, Cigdem Issever and others

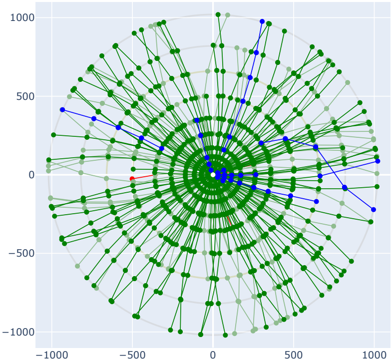


Figure: Hits and tracks in an ATLAS-like detector.

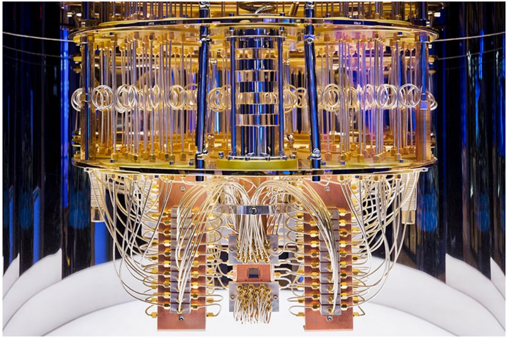


Figure: IBM quantum computer.

Overview

- Why do we need improved methods for particle tracking ?
- How could quantum computing be applied to the problem ?
- Proof of principle for small instances in simulation and on IBM quantum computers.

Reconstruction of charged particles

Why is it challenging ?

- Reconstruction time for currently used algorithms scales combinatorial with increasing proton-proton interactions per bunch-crossing (pile-up μ).
- Large values up to $\mu = 1000$ are expected for future collider experiments.
- New algorithms have to be developed to ensure high sensitivities of future experiments.

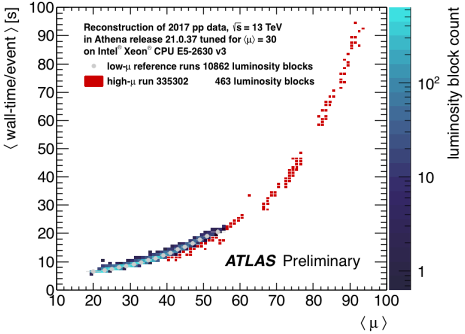


Figure: The reconstruction time per event of classical pattern recognition algorithms as a function of μ. ATLAS 2017.

Quantum computing

What is possible today ?

- Heuristic algorithms designed to run on noisy intermediate-scale quantum (NISQ) computers. Preskill 2018.
- Variational quantum eigensolver (VQE) approximating the ground state of given Hamiltonians. Peruzzo et al. 2014.
- Proposed to estimate the ground state energy of molecules. Can also be applied to combinatorial optimization problems.

VQE (2014)

- On a **quantum computer** the expectation value $\lambda_{\vec{\theta}} = \langle\psi(\vec{\theta})|H|\psi(\vec{\theta})\rangle$ is measured for a parameterized state $|\psi(\vec{\theta})\rangle$. This is an upper bound for the minimum eigenvalue $\lambda_{min} \leq \lambda_{\vec{\theta}}$.
- On a **classical computer** the parameters $\vec{\theta}$ are iteratively optimized.

Quantum computing

What will be possible in the near future ?

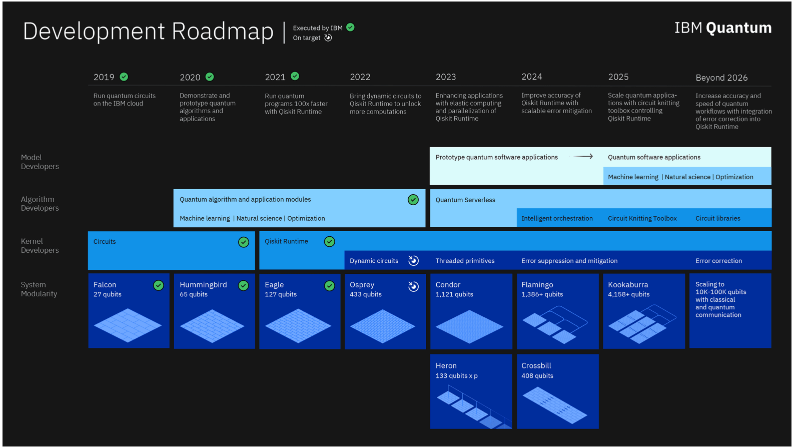


Figure: Anticipating the future of quantum-centric supercomputing. IBM 2022.

Quadratic unconstrained binary optimization (QUBO)

How can VQE be used for particle tracking ?

- Distinguish true triplets $T_i = 1$ from random combinations of three hits $T_i = 0$.
- Construct a Hamiltonian H such that the true triplets make up its ground state. Bapst et al. 2019.

$$H = \sum_i a_i T_i + \sum_i \sum_{j \neq i} b_{ij} T_i T_j \qquad (1)$$

- Linear terms a_i rate the quality of single triplets. Quadratic terms b_{ij} express the compatibility of triplets.

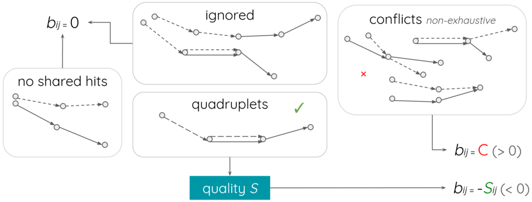


Figure: Triplets that form a valid quadruplet are assigned a beneficial negative weight. Bapst et al. 2019.

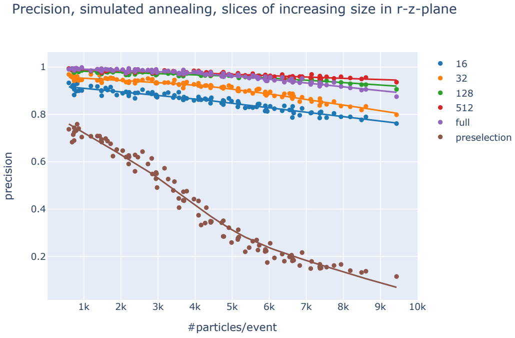
Using VQE to solve QUBO overview

Example for 5 triplets

- Construct triplet candidates T_i, compute coefficients a_i, b_{ij} to construct H.
- Perform VQE using e.g. the encoding $|\psi(\vec{\theta})\rangle = |T_4T_3T_2T_1T_0(\vec{\theta})\rangle$ of triplets in qubits.
- Assume that VQE converged to the state $|\psi\rangle = \alpha|00000\rangle + \beta|00001\rangle + \gamma|00011\rangle$ with $|00011\rangle$ being the ground state of H.
- Repeatedly preparing and measuring $|\psi\rangle$ yields results 00000, 00001 and 00011 with probability $|\alpha|^2$, $|\beta|^2$ and $|\gamma|^2$.
- If $|\gamma|^2$ is sufficiently large, the ground state can be identified (lowest energy) and the algorithm returns $T_0 = T_1 = 1$ and $T_2 = T_3 = T_4 = 0$.
- Apply post-processing to construct tracks from triplets.

Dividing the full QUBO into smaller slices

How can NISQ computers be used for particle tracking ?



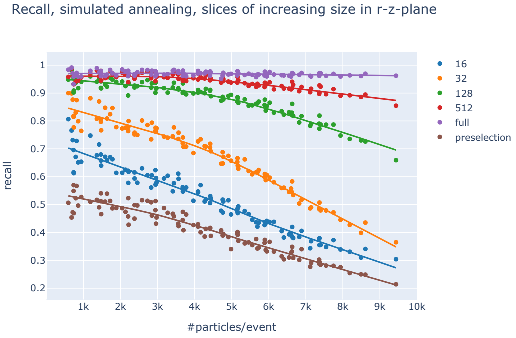
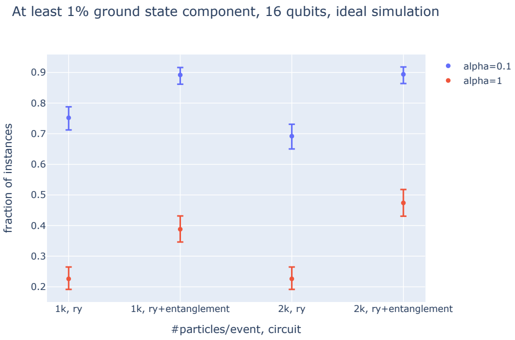


Figure: Precision and recall as a function of track density for QUBO slices of increasing size in the r-z-plane.

Performance of VQE for small QUBO slices

Mean and 95% confidence interval for 50 slices (5 for ibmq_kolkata) and 10 initial points.



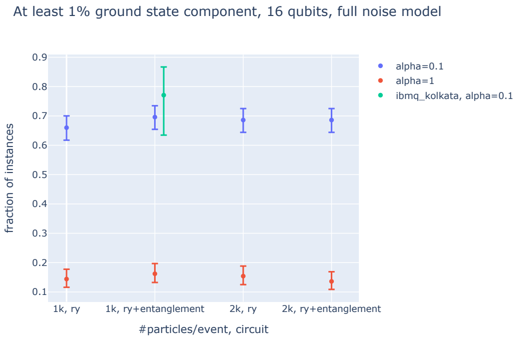


Figure: Fraction of instances with at least 1% ground state component in an ideal simulation, using a full noise model and on the quantum computer ibmq_kolkata.

Summary and open questions

Summary

- Particle tracking is a challenging problem asking for constant improvements.
- If VQE scales up to the size of near-term available hardware, reasonable values for precision and recall can be achieved.
- In principle VQE could be used to tackle the particle tracking problem.

Open questions

- Does entanglement benefit binary optimization problems ?
- How to overcome challenges in scaling-up VQE ?
- Will VQE be competitive to classical methods ?

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Thank you!

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Backup

Particle Tracking

The ATLAS inner detector (ID)

- Three different systems immersed in a magnetic field to measure direction, momentum and charge of particles.
- Pixel Detector: 92 million silicon pixels distributed over four layers.
- Semiconductor Tracker (SCT): 4 thousand silicon strips with 6 million readout channels.
- Transition Radiation Tracker (TRT): 300 thousand drift tubes.

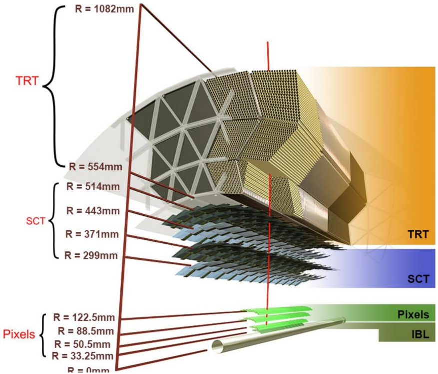


Figure: Layout of the ID around the LHC beam pipe. Pequenao 2008

Particle Tracking

ATLAS tracking algorithm overview

- Clusterization: Assemble clusters from raw measurements and assign space-points.
- Iterative combinatorial track finding: Form track seeds from sets of three space-points. Build track candidates from these triplets T_i.
- Ambiguity solving: Resolve overlaps between track candidates and reject low-quality tracks.
- TRT extension: Extend tracks into TRT and perform high-resolution fit.

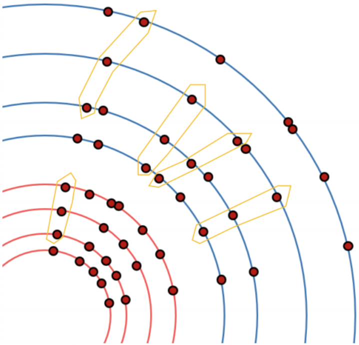


Figure: Track seeds in an ATLAS-like detector.

Dataset and selection

Focus on high p_T tracks ($p_T \geq 1GeV$). Bapst et al. 2019.

- Hard QCD interaction generating a $t\bar{t}$-pair plus 200 soft QCD interactions.
- A triplet is created iff:

$$\text{\#holes } H_i \leq 1$$
$$\text{curvature } |(q/p_T)_i| \leq 8 * 10^{-4}$$
$$\text{angle between doublets } \delta\Theta_i \leq 0.1$$

- A quadruplet (T_i, T_j) is created iff:

$$|\delta((q/p_T)_i, (q/p_T)_j)| \leq 1 * 10^{-4}$$
$$S(T_i, T_j) > 0.2$$

- $a_i = 0.5(1 - e^{1-\frac{|d_0|}{1.0}}) + 0.2(1 - e^{1-\frac{|z_0|}{0.5}})$
- $S(T_i, T_j) = \frac{1-\frac{1}{2}(|\delta(q/p_{T_i}, q/p_{T_j})| + max(\delta\Theta_i, \delta\Theta_j))}{(1+H_i+H_j)^2}$
- $b_{ij} = \begin{cases} -S(T_i, T_j), & \text{if } (T_i, T_j) \text{ is quadruplet,} \\ 1 & \text{if } (T_i, T_j) \text{ is conflict,} \\ 0 & \text{otherwise.} \end{cases}$

Details on VQE

How to introduce entanglement ?

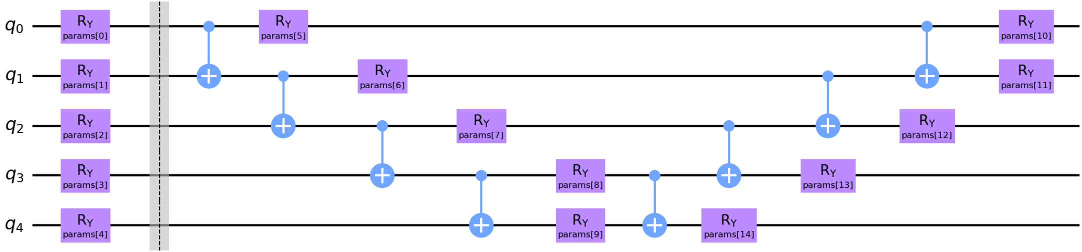


Figure: Circuit based on the Layer VQE approach. Liu et al. 2022. First, the initial rotation layer is optimized. Before reaching convergence, an additional layer with rz- and cnot-gates is added. The initial rotation angles of the additional are set to zero to not disturb the previously reached state. Then, all parameters are optimized until convergence.

Details on VQE

Improving VQE for combinatorial optimization using CVaR. Barkoutsos et al. 2020.

- Optimizing $\lambda_{\vec{\theta}} = \langle \psi(\vec{\theta}) | H | \psi(\vec{\theta}) \rangle$ does not necessarily find states $|\psi(\vec{\theta})\rangle$ with a large ground state component.
- In practice, $\lambda_{\vec{\theta}}$ is approximated using K measurements $\lambda_{\vec{\theta},k}$:

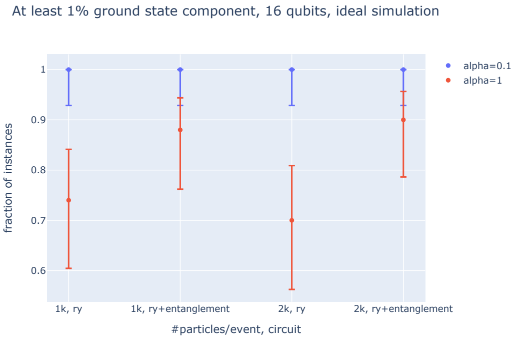
$$\lambda_{\vec{\theta}} \approx \frac{1}{K} \sum_{k=1}^{K} \lambda_{\vec{\theta},k} \tag{2}$$

- CVaR optimization considers the fraction α of measurements with lowest energy:

$$\lambda_{\vec{\theta},CVaR} \approx \frac{1}{\alpha K} \sum_{k=0}^{\alpha K} \lambda_{\vec{\theta},k} \tag{3}$$

Performance of VQE for small QUBO slices

Mean over 50 slices (5 for ibmq_kolkata). Lowest energy result of 10 initial points.



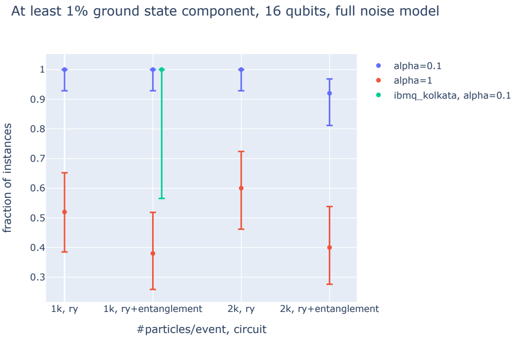


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Figure: Fraction of instances with at least 1% ground state component.