ACAT 2019

D-Wave The Quantum Computing Company™

# Charged Particle Tracking as a QUBO Problem Solved with Quantum Annealing-inspired Optimization

ACAT, Saas-Fee, March 10-15 2019

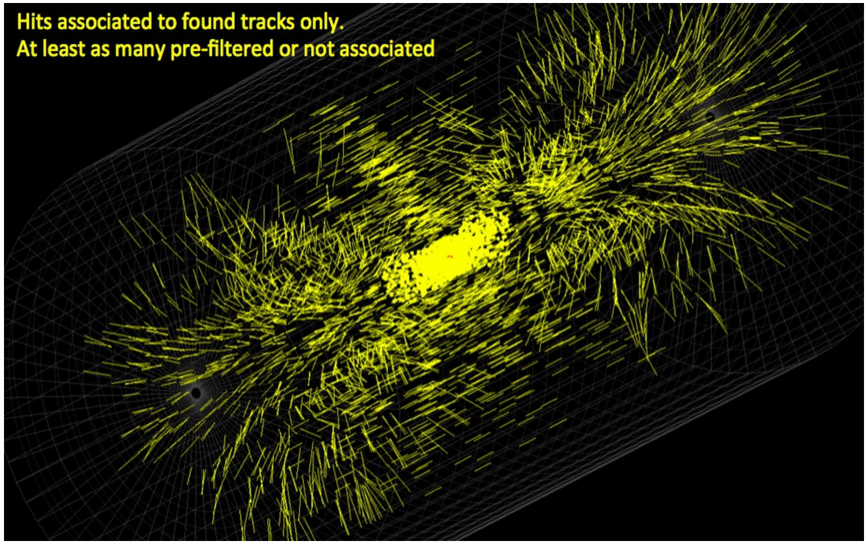

Jean-Roch Vlimant on behalf of the QMLQCF project team
Special credits to
Abhishek Anand and Alexander Zlokapa


# Outline

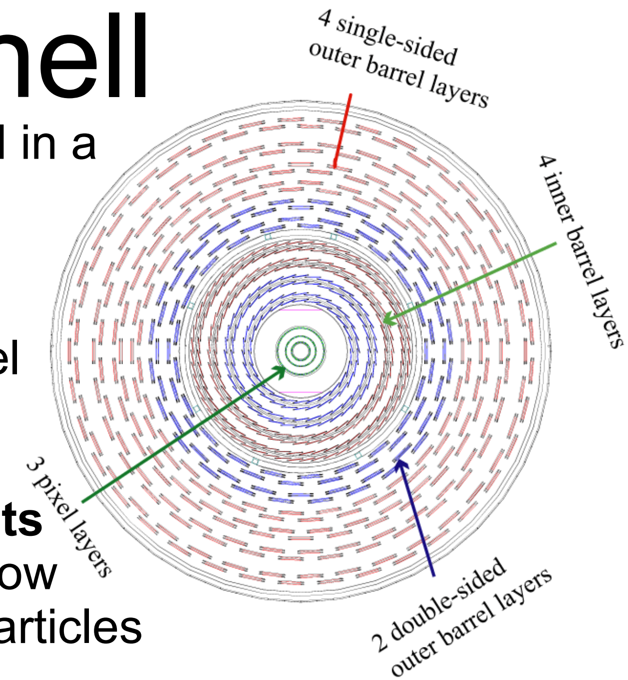
- Forewords on charged particle tracking and dataset
- Introduction to D-Wave and quantum annealing
- Hopfield Network and segment classification as a QUBO problem
- Results and outlooks

# The Challenge of Charged Particle Tracking at the HL-LHC

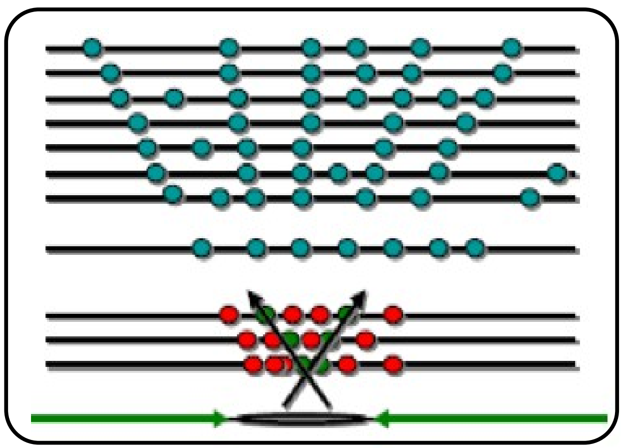
# Tracking in a Nutshell



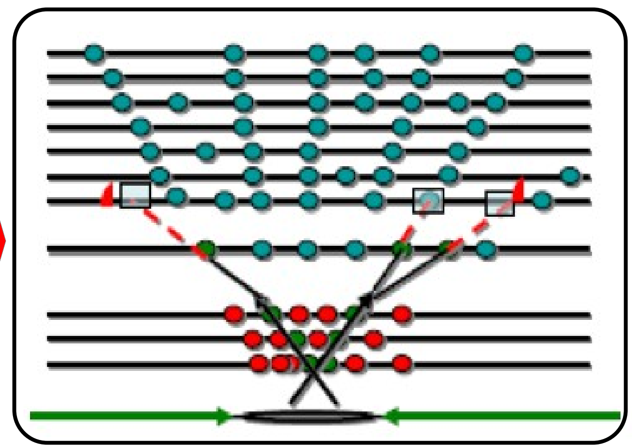

- Particle trajectory bended in a solenoid magnetic field
- Curvature is a proxy to momentum
- Particle ionize silicon pixel and strip throughout several concentric layers
- **Thousands of sparse hits**
- Lots of hit pollution from low momentum, secondary particles

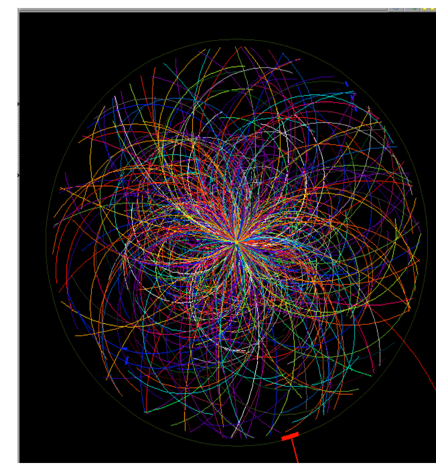



Seeding



Kalman Filter

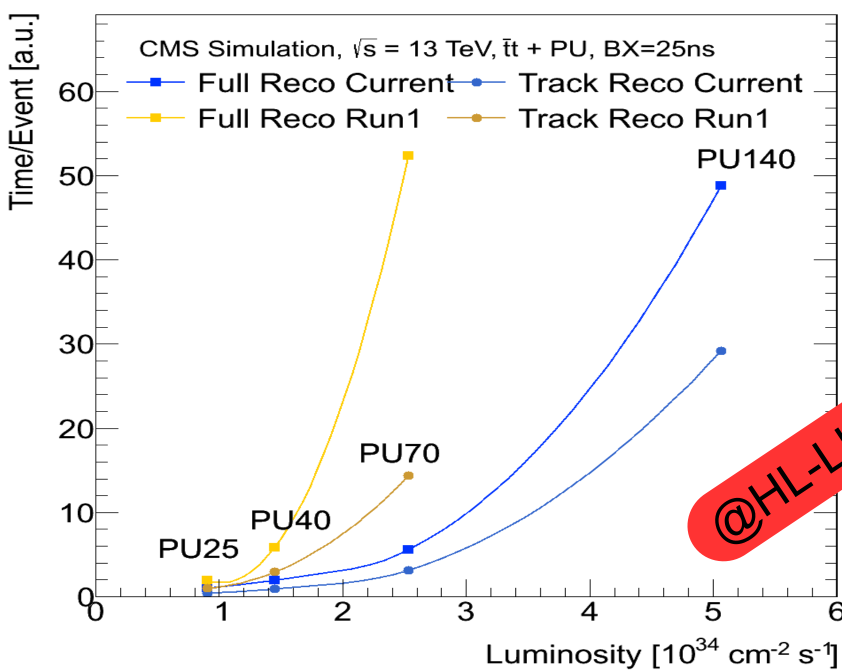


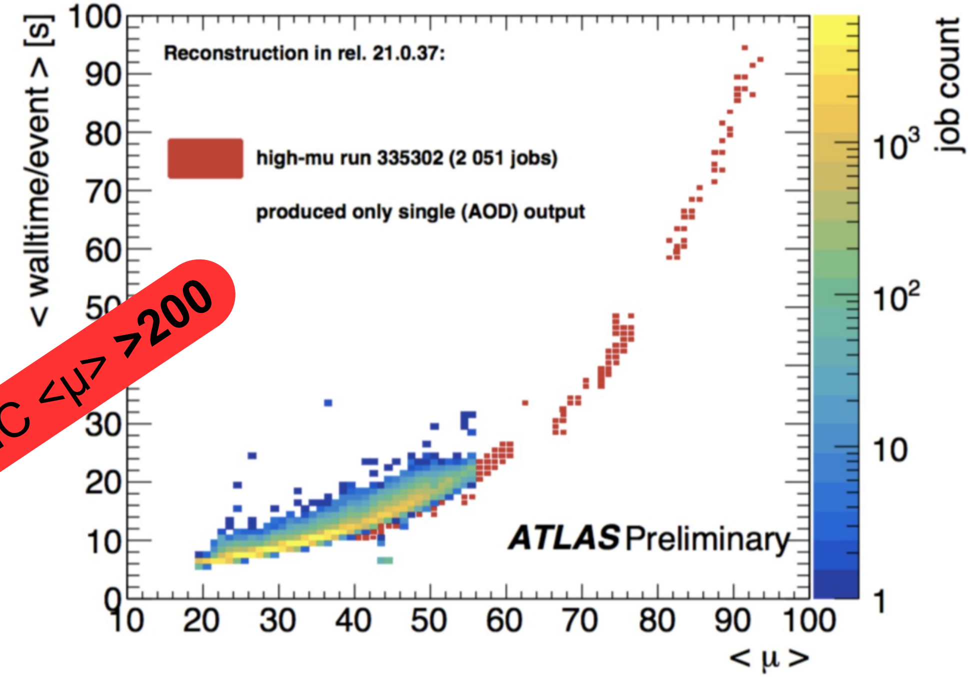


- **Explosion of hit combinatorics** in both seeding and stepping pattern recognition
- **Highly time consuming task** in extracting physics content from LHC data

# Cost of Tracking

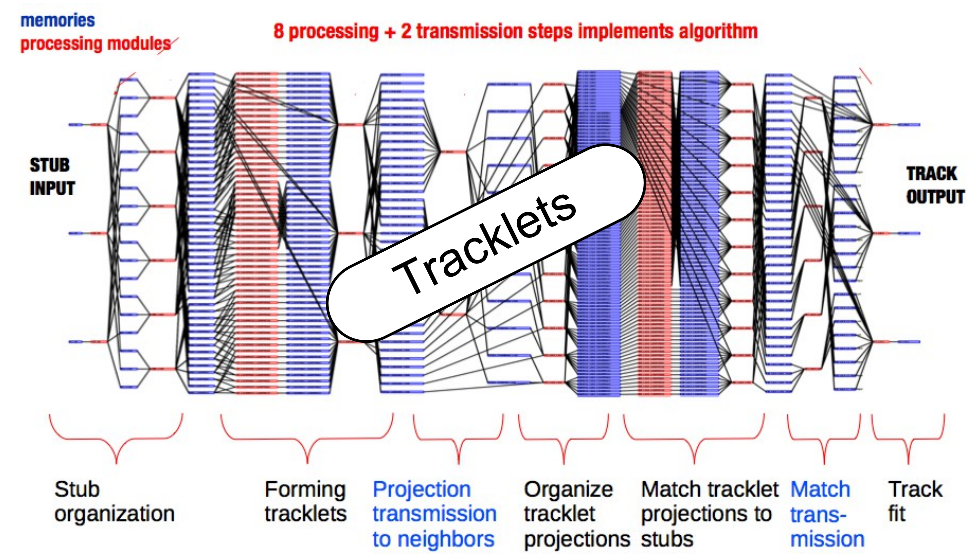
- CPU time consumption in HL-LHC era **surpasses computing budget**
  - ➔ Need for **faster algorithms**
- Charged particle track reconstruction is one of the most **CPU consuming task** in event reconstruction
  - ➔ Optimizations **mostly saturated**
- Large fraction of CPU required in the HLT. **Cannot perform tracking inclusively**
  - ➔ **Approximation** allowed in the trigger

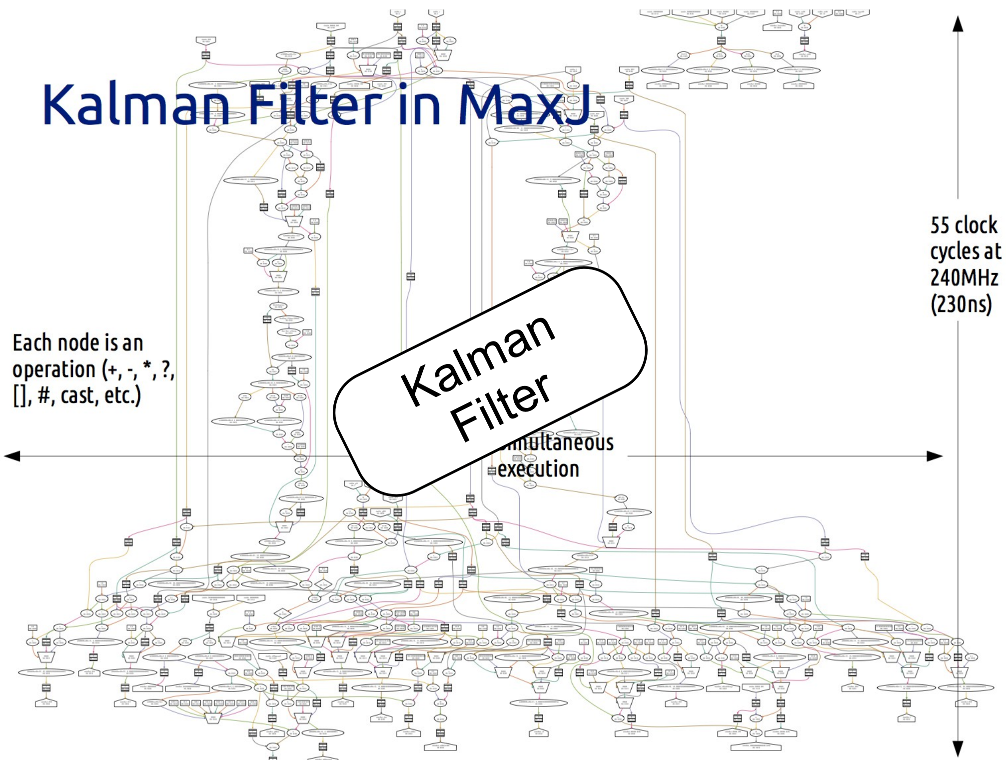


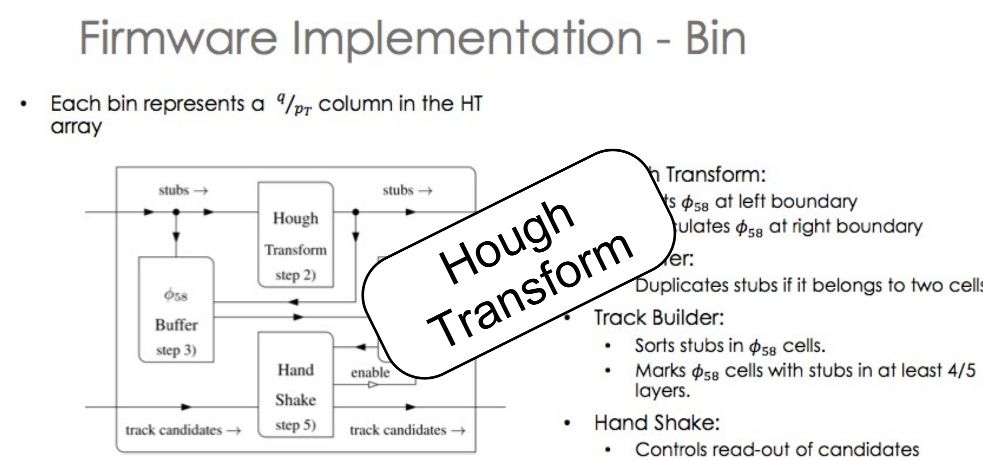



# Fast Hardware Tracking

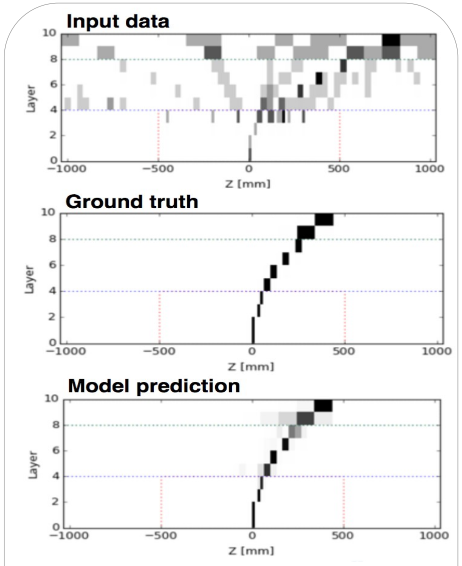
- Track trigger implementation for Trigger upgrades development on-going
- Several approaches investigated
- **Dedicated hardware is the key** to fast computation.
- **Not applicable for offline** processing unless through adopting heterogeneous computing.



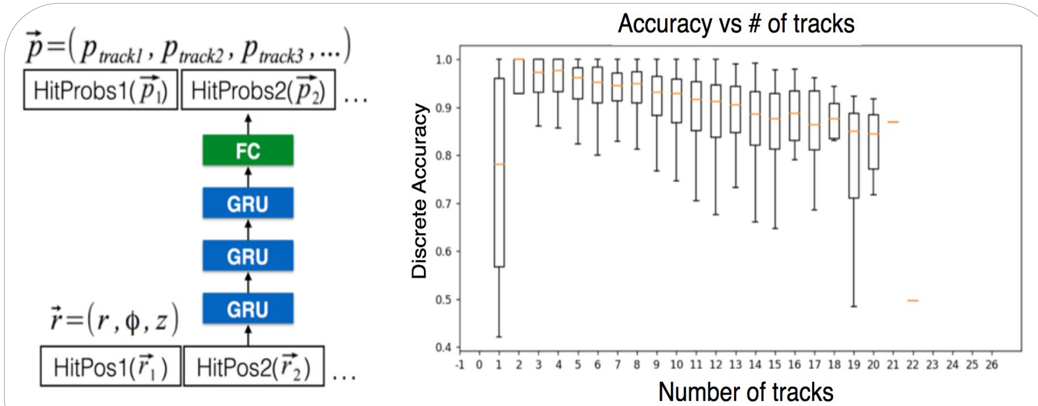



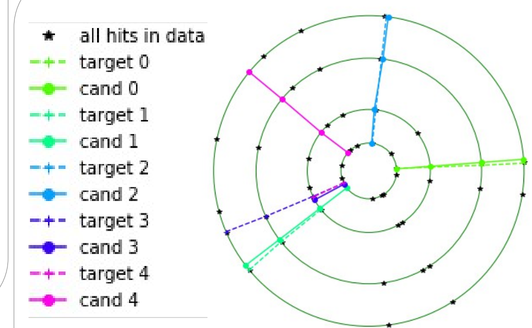
# Deep Learning Approaches




Track following with RNN




End-to-end hit assignment

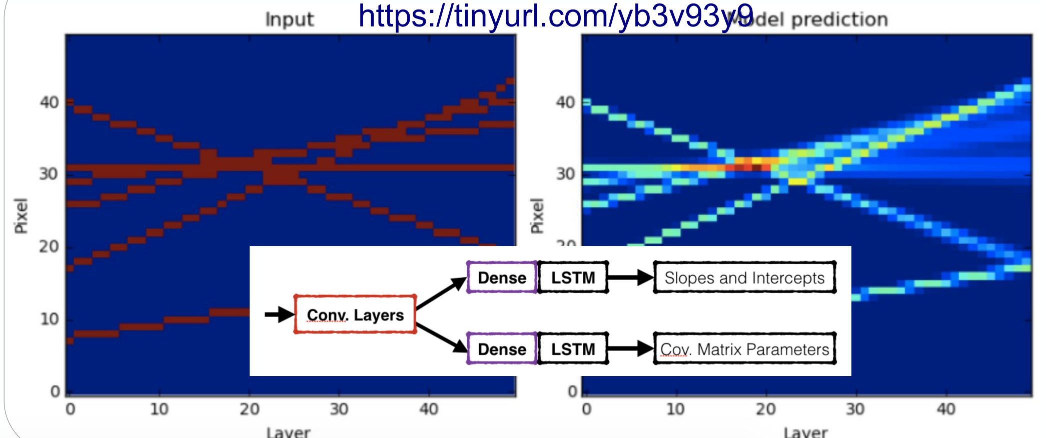


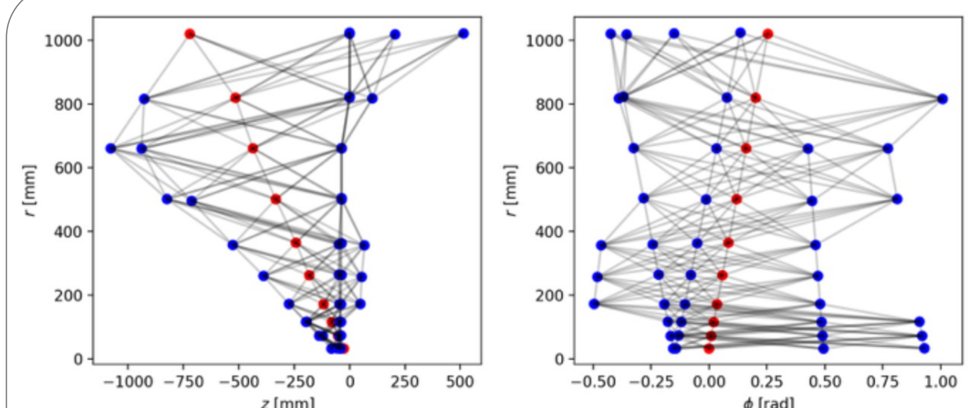

Seq-to-seq track finding

https://heptrkx.github.io/

https://indico.cern.ch/event/587955/contributions/2937540/

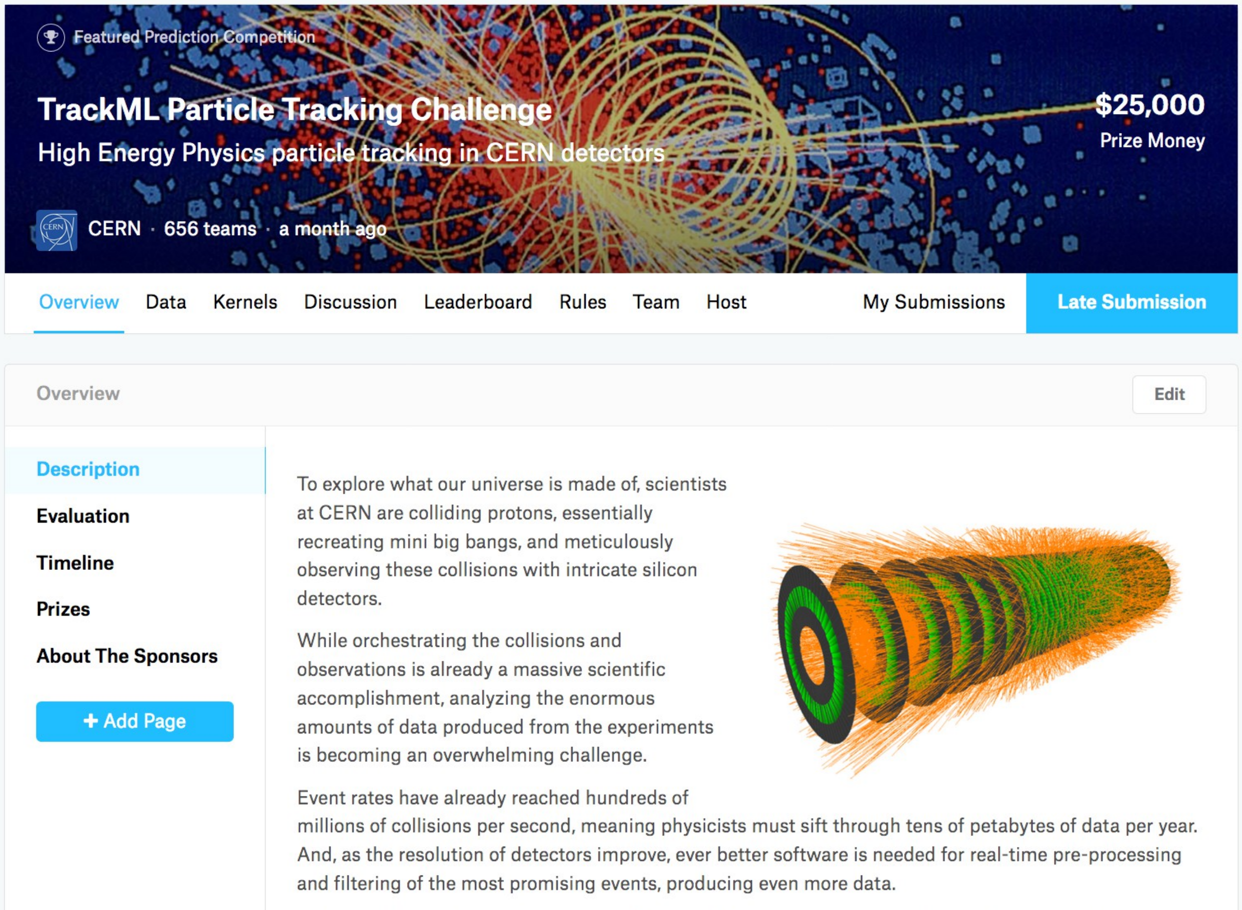
https://tinyurl.com/yb3v93y9




https://indico.cern.ch/event/587955/contributions/2937570/

# Charged Particle Tracking Dataset




- This work uses the public dataset of the TrackML Particle Tracking Challenge (Kaggle, codalab).
- Simulating the dense environment expected for HL-HLC. Average of 200 proton-proton interaction per bunch crossing.

TrackML sponsors

https://www.kaggle.com/c/trackml-particle-identification
https://competitions.codalab.org/competitions/20112

# Motivation

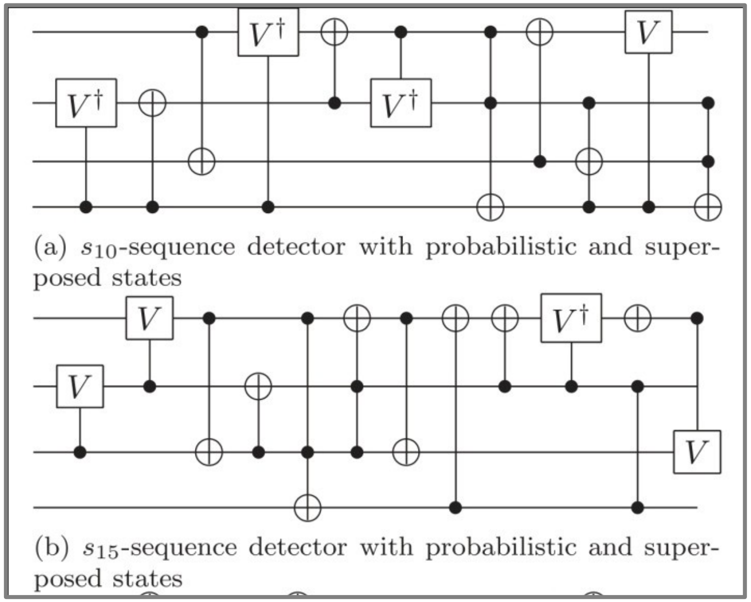
- Classical charged particle tracking algorithms suffer from combinatorial explosion

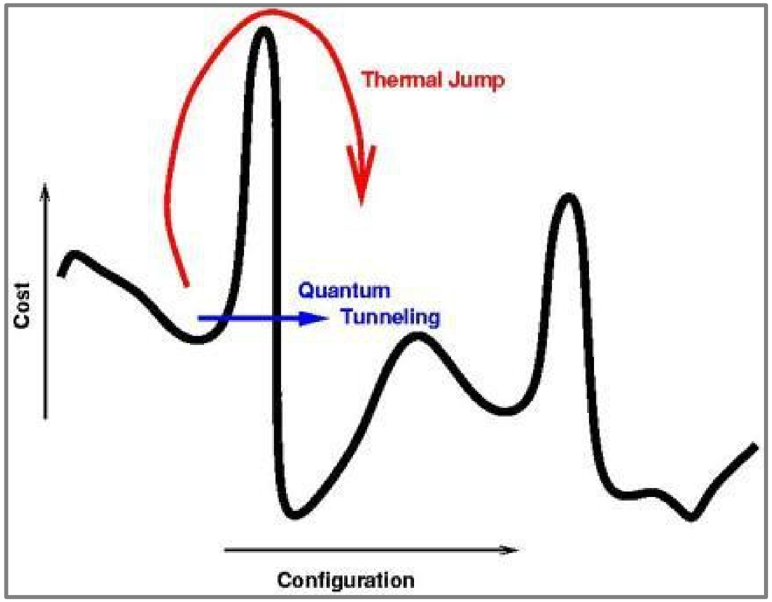
- Embrace the combinatorics considering all possible branches of track candidates, and solve the complex optimization problem with quantum annealing

# The D-Wave Computing System

# D-Wave 2X™

# qubit and qubit




<u>Quantum Circuits</u>

Series of quantum gates operating on a set of quantum states.

<u>Quantum Annealing</u>

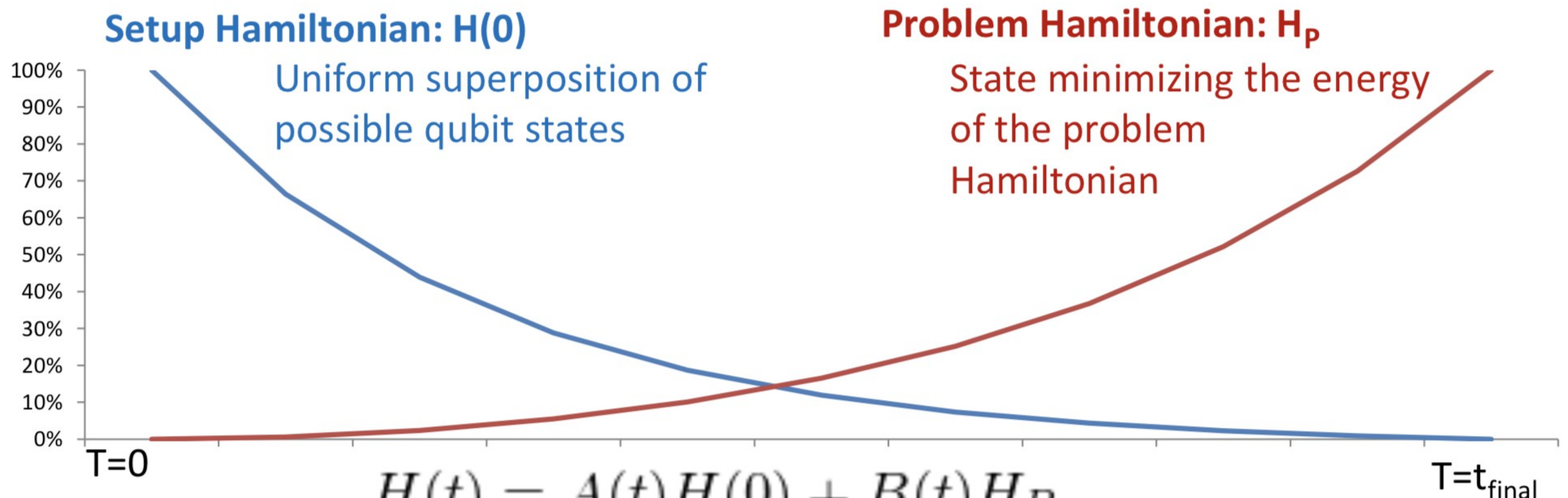
Evolution of a quantum system to a low T Gibbs state

**That's D-Wave !**

# Quantum Annealing

# Adiabatic Quantum Annealing

- System setup with trivial hamiltonian H(0) and ground state
- Evolve adiabatically the hamiltonian towards the desired Hamiltonian $H_p$
- **Adiabatic theorem** : with a slow evolution of the system, the state stays in the ground state.




$$H(t) = A(t)H(0) + B(t)H_P$$

https://arxiv.org/abs/quant-ph/0001106
https://arxiv.org/abs/quant-ph/0104129

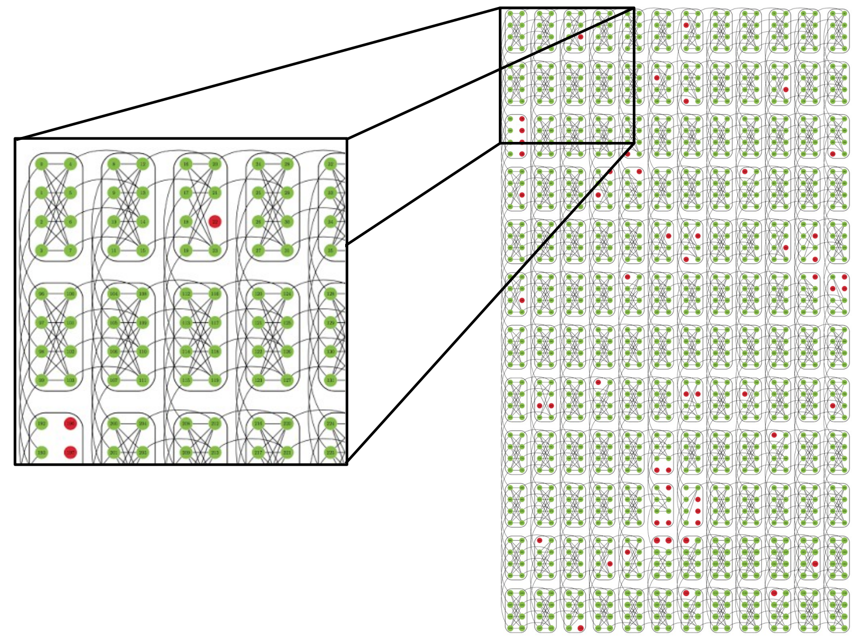
# Space of Hamiltonian

Runs over **all** quBit pairs

$$H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

External magnetic field

Interactions



Chimera graph embedding

Runs over **adjacent** quBits

$$H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

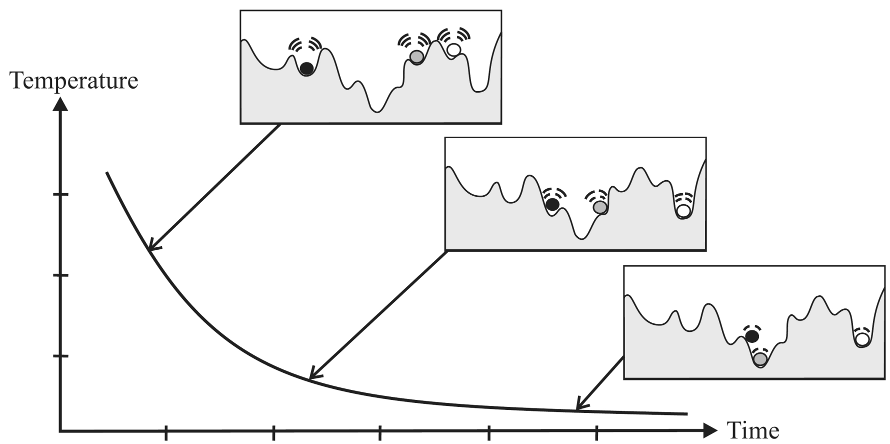
External magnetic field

Interactions

- ~1000 qubits on chimera graph can only encode ~40 qubits full Ising Hamiltonian
- Quadratic Unconstrained Binary Optimization (QUBO) can be mapped to an Ising Hamiltonian with change of variable {0,1}↔{-1,1}

# Ising Model Heuristic Solution

- Monte-Carlo based method to find ground state of energy functions
- Random walk across phase space
  - ➔ accepting descent
  - ➔ accepting ascent with probability $e^{-\Delta E/kT}$
- Decrease T with time




Applied to the QUBO problem, and finds the **ground state**. SA in the legends.

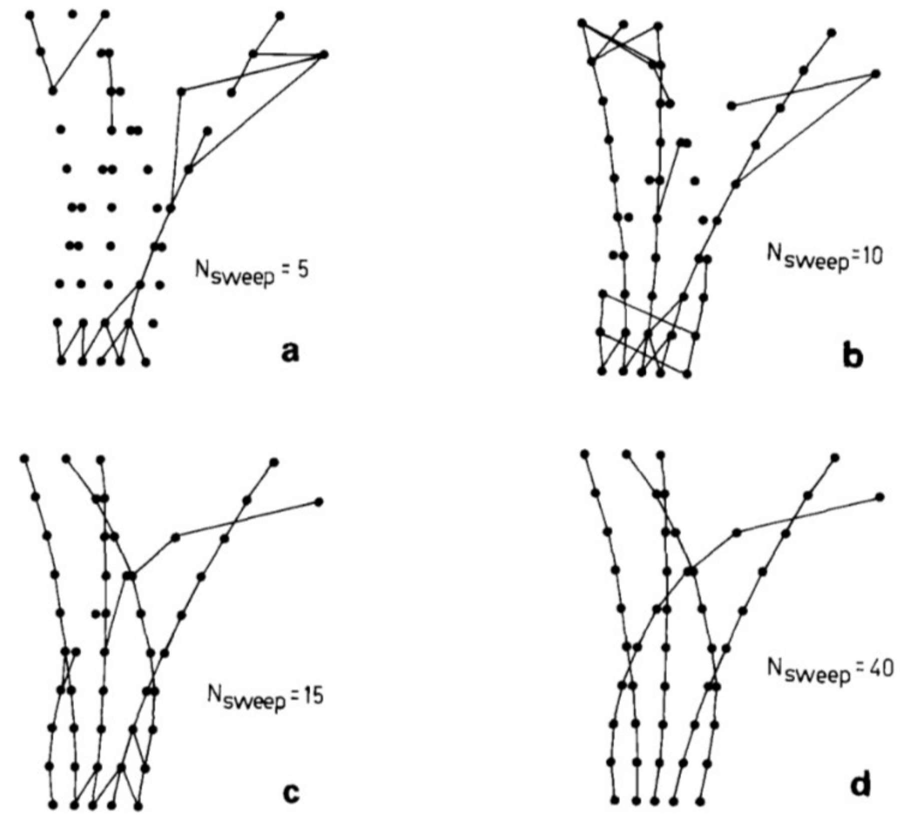
# Charged Particle Tracking using Adiabatic Quantum Annealing

See also H. Gray et al.
https://indico.cern.ch/event/708041/contributions/3308730/

# Hopfield Network Approach

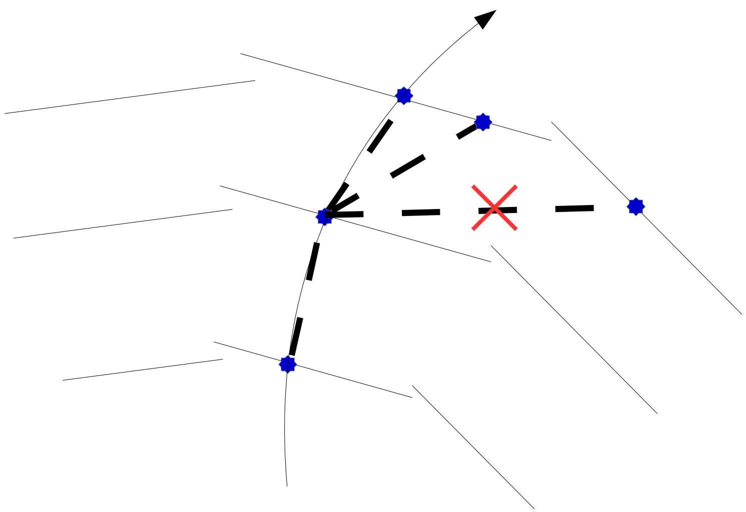
- Developed by John Hopfield in 1982
- fully-connected, single-layer NN; **complete graph**
- vertices: $n$ binary units, $\{s_n\} \in \{0,1\}^n$
- edges: symmetric weight matrix, $w \in \mathbb{R}^n \times \mathbb{R}^n$
- energy associated with each network configuration (assignment of units):

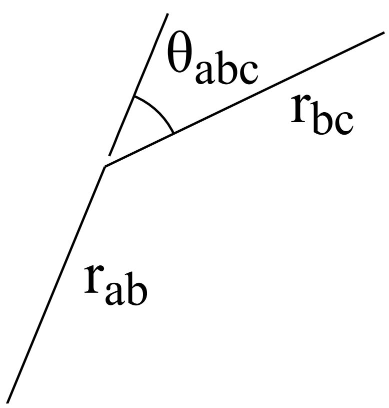
$$E = \boxed{-\frac{1}{2}\sum_{i,j} w_{ij} s_i s_j}$$ **QUBO!**




[Peterson, 1989]

# Framing the Problem






- **Segment ≡ pair of hits** on consecutive layers of the detector
- Assign a **boolean to each segment** representing whether the segment is within a track or not

- Limits the number of hits/segments
  - ➔ Separating the hits in **16 sector in φ**
  - ➔ pre-filtering the segments on Δφ and Δz to reduce the number of spurious bad segments

- Segment opening in r-phi-z plane in which helical segments are aligned
- Azimuthal angle in cartesian coordinate in which high pT tracks segments are straight

# Segment QUBO

**Helix Term**
Segments along an helix

**High pT Term**
Aligned pair of segments

**Beam spot Term**
Segment pointing at the origin

$$\sum_{a,b,c}\left(\frac{\cos^{\lambda}\theta_{abc}+\rho\cos^{\lambda}\phi_{abc}}{r_{ab}+r_{bc}}+\eta\left(z_c-r_c\frac{z_c-z_a}{r_c-r_a}\right)^{\zeta}\right)s_{ab}s_{bc}$$

$$+\alpha\left(\sum_{a,b\neq c}s_{ab}s_{ac}+\sum_{a\neq b,c}s_{ac}s_{bc}\right)+\sum_{a,b}\left(\beta+\gamma P(s_{ab})\right)s_{ab}$$

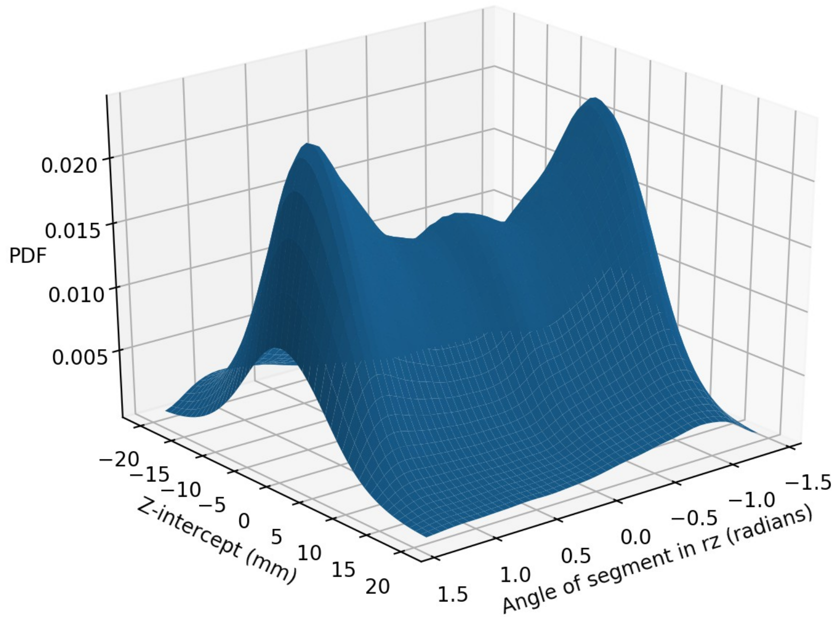
**Bifurcation Term**
No shared hits on valid segment

**Inhibition Term**
Reduced number of segments

**GP Term**
Use the quality of segment

# Resolving Sub-Group

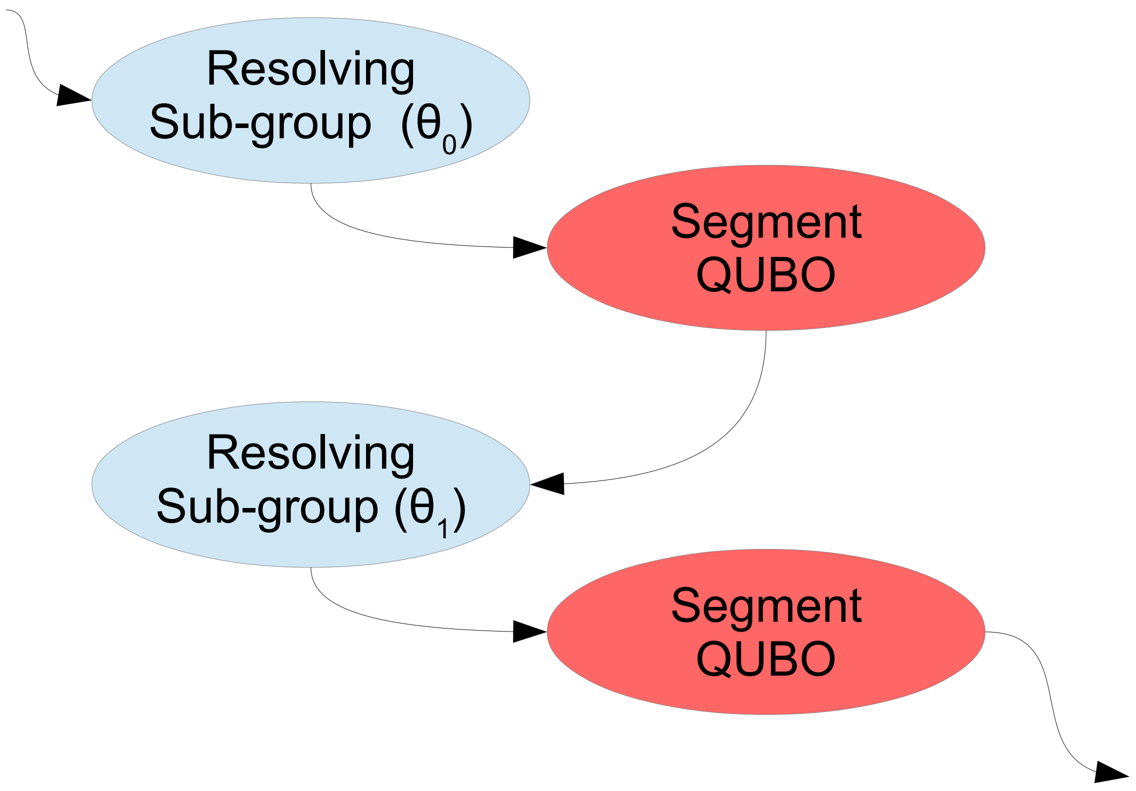
- Full all-to-all QUBO problem cannot fit on dWave. Aim at identifying **sub-groups of segments that can fit on the hardware**




- Train a gaussian kernel density estimator on true single segment
- Aiming at reducing the number of false segments, retaining

- Force segment off based on $\cos\theta_{abc}$
  - $\cos\theta_{abc} = 0$ if $\theta_{abc} > \theta_0$
- 5 best neighbors
- Solvable in polynomial time

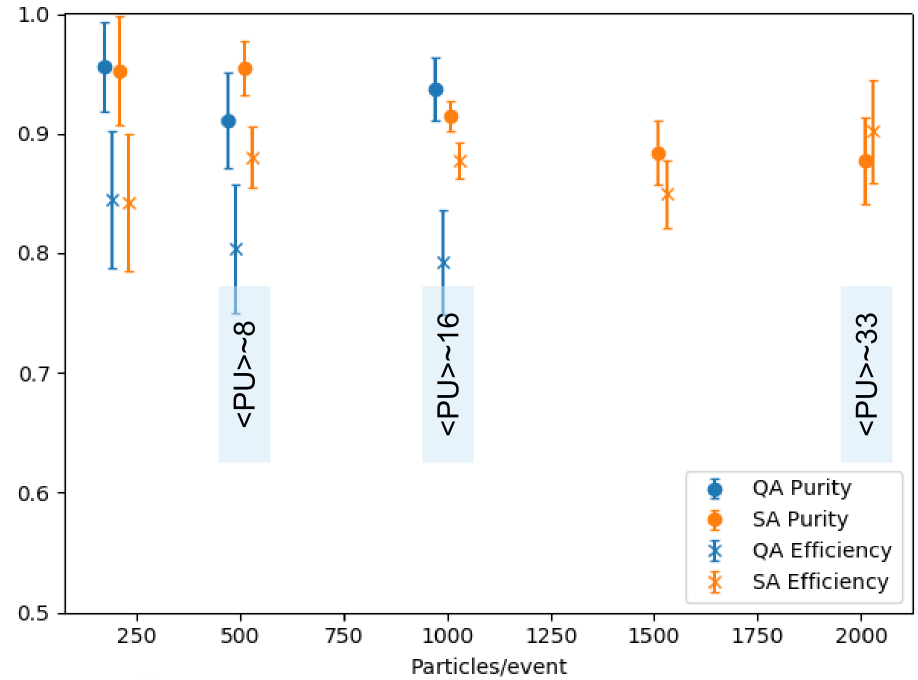
# QA-Tracking Workflow

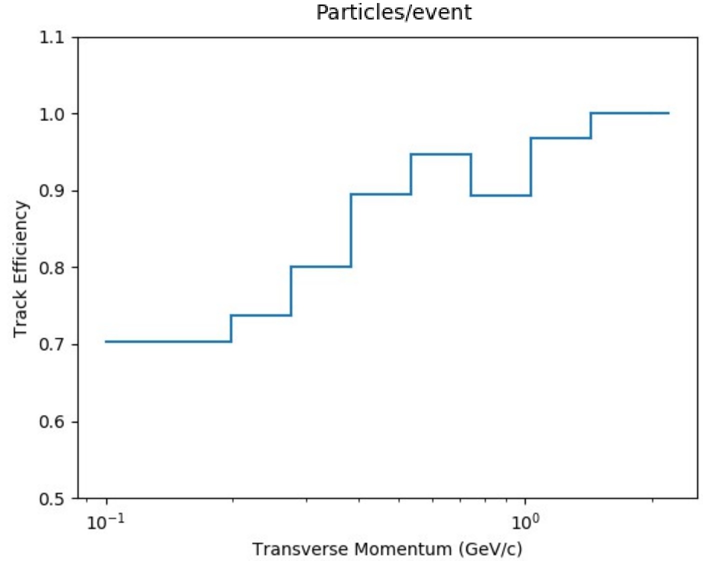


# Performance

- Simulated annealing and Quantum annealing are in perfect agreement at 200 tracks
- Simulated annealing solves the exact problem at all multiplicity
- Limitation on number of qubits prevents from solving events beyond 200 tracks on Dwave ; solving a contrive problem
- Purity and Efficiency are measured with respect to true tracks with at least three hits

➢ Promising tracking efficiency for the algorithm up to 2000 tracks per event



# Conclusion

- QMLQCF Scouting for applications of quantum annealing (among others) in HEP
- Charged particle tracking interpreted as a segment classification can be expressed in a QUBO problem
- Experimentation on dWave imposes some stringent algorithmic restrictions
- Limited hardware size limits the complexity of the problem that can be solved

# Acknowledgments

This project is supported in part by the United States Department of Energy, Office of High Energy Physics Research Technology Computational HEP and Fermi Research Alliance, LLC under Contract No. DE-AC02-07CH11359. The project is also supported in part under ARO grant number W911NF-12-1-0523 and NSF grant number INSPIRE-1551064. The work is supported in part by the AT&T Foundry Innovation Centers through INQNET, a program for accelerating quantum technologies. We wish to thank the Advanced Scientific Computing Research program of the DOE for the opportunity to first present and discuss this work at the ASCR workshop on Quantum Computing for Science (2015). Award Number: DE-SC0019227, Quantum Machine Learning and Quantum Computation Frameworks for HEP (QMLQCF), California Institute of Technology, Pasadena, CA

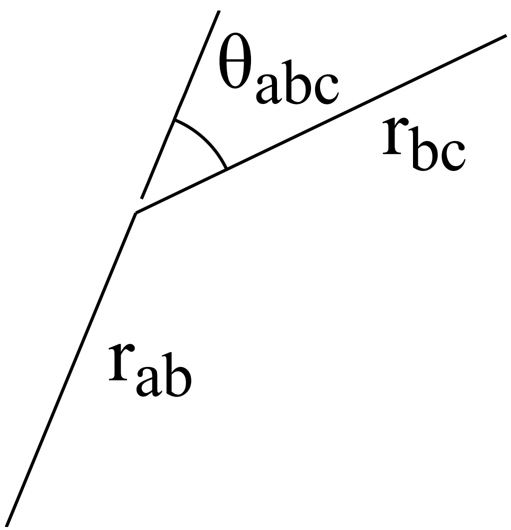
Part of this work was conducted at "iBanks", the AI GPU cluster at Caltech. We acknowledge NVIDIA, SuperMicro and the Kavli Foundation for their support of "iBanks".

# Problem Parameters Optimization

- Parameters of the hamiltonian are tuned using bayesian optimization, modeling the figure of merit with gaussian processes.
- Accuracy (# of properly labeled / # of segments) use as f.o.m
- Global inhibition model : $\alpha$=3.E$^{-3}$, $\beta$=2.63E$^{-8}$, $\lambda$=7
- Threshold model : $\alpha$=5.E$^{-3}$, $\beta$=1.E$^{-6}$, $\lambda$=7

# Edge Affinity

- Helical bias: tracks are straight in cylindrical coordinates
- Momentum bias: high-PT tracks are straight in rectangular coordinates
- Short-edge bias: long tracks of short edge segments




Helical bias (cylindrical angle)

Momentum bias (rectangular angle)

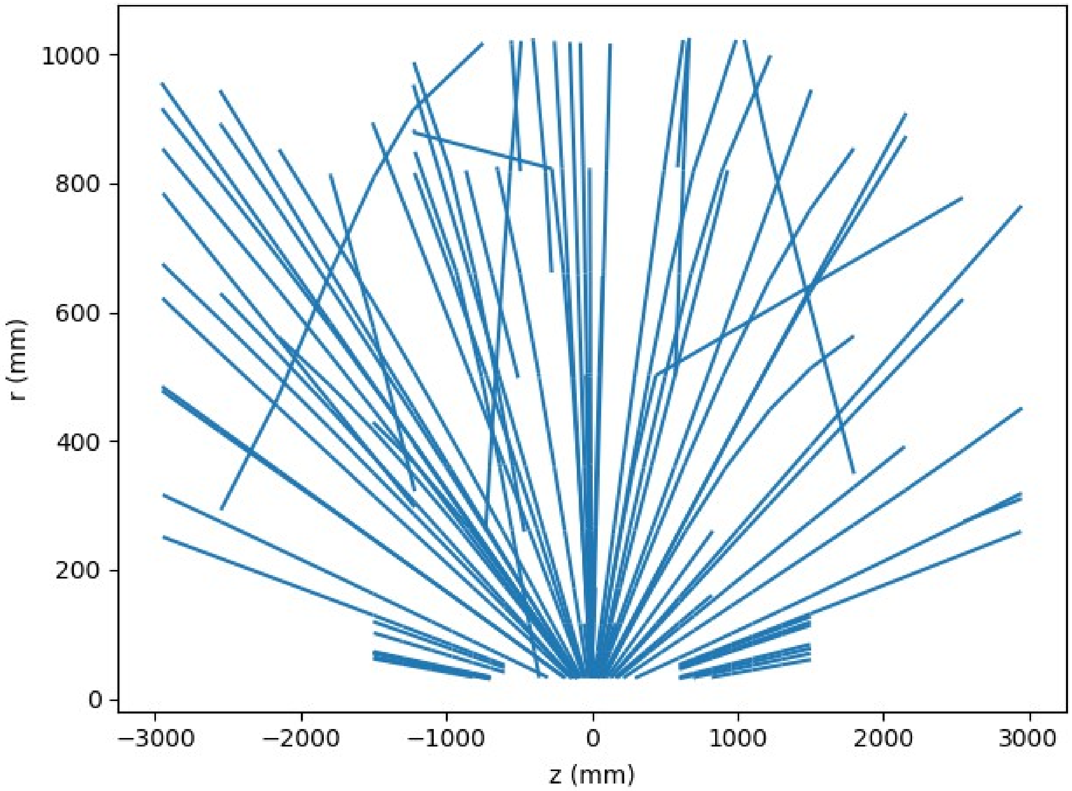
$$\sum_{a,b,c} \frac{\cos^{\lambda}\theta_{ab} + \rho\cos^{\lambda}\phi_{ab}}{r_{ab} + r_{bc}} s_{ab} s_{bc}$$

Short-edge bias

Ising variables (1 or 0)

# Cross-Term Penalties

- Beam spot penalty: penalize tracks that originate further from the origin



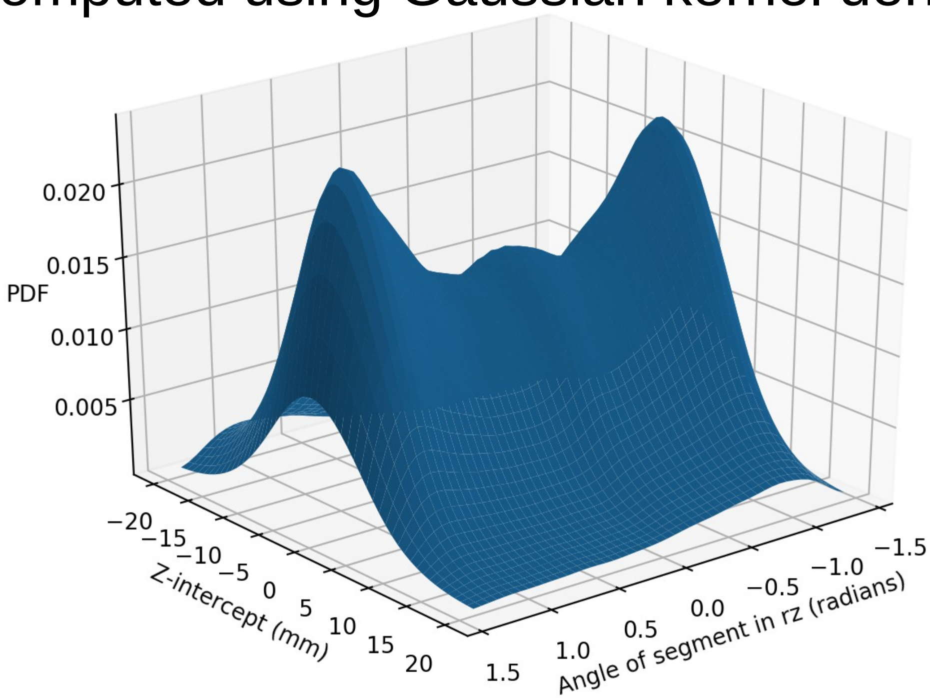

Z-intercept penalty

$$\sum_{a,b,c} \eta \left( z_c - \frac{z_c - z_a}{r_c - r_a} r_c \right)^{\zeta} s_{ab} s_{bc}$$

Ising variables (1 or 0)

# Single-Edge Bias

- Global inhibition: limits total number of edges turned on
- Prior probability: Bayesian prior based on edge position in *rz*-plane
  - Computed using Gaussian kernel density estimation




Global inhibition

Bayesian prior

$$\sum_{a,b} [\beta + \gamma P(s_{ab})] s_{ab}$$

Ising variable (1 or 0)

# Extra Material

# References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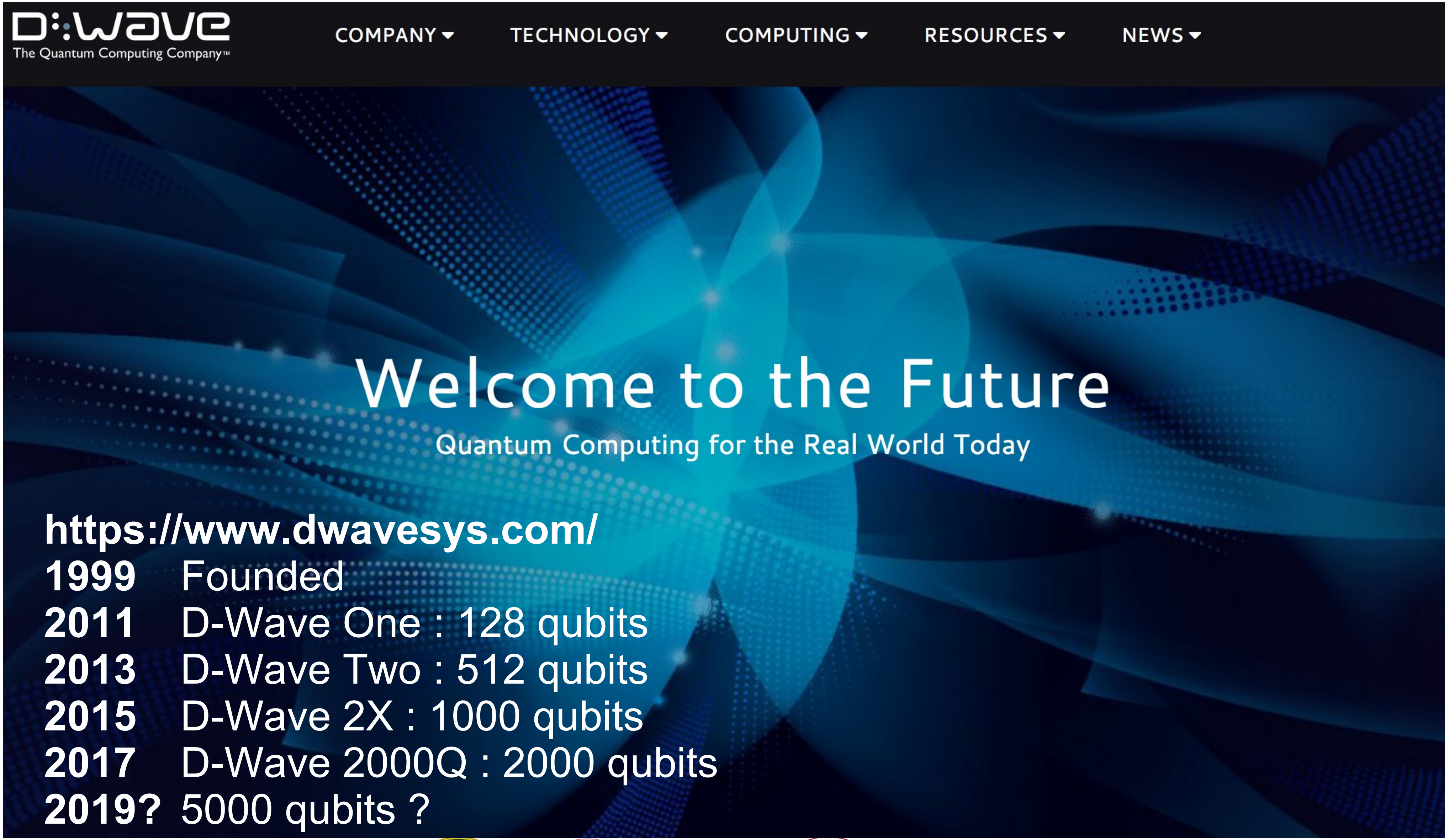
# The D-Wave Company




**https://www.dwavesys.com/**

**1999** Founded
**2011** D-Wave One : 128 qubits
**2013** D-Wave Two : 512 qubits
**2015** D-Wave 2X : 1000 qubits
**2017** D-Wave 2000Q : 2000 qubits
**2019?** 5000 qubits ?

# D-Wave Hamiltonian And Chimera Graph

# D-Wave Hamiltonian

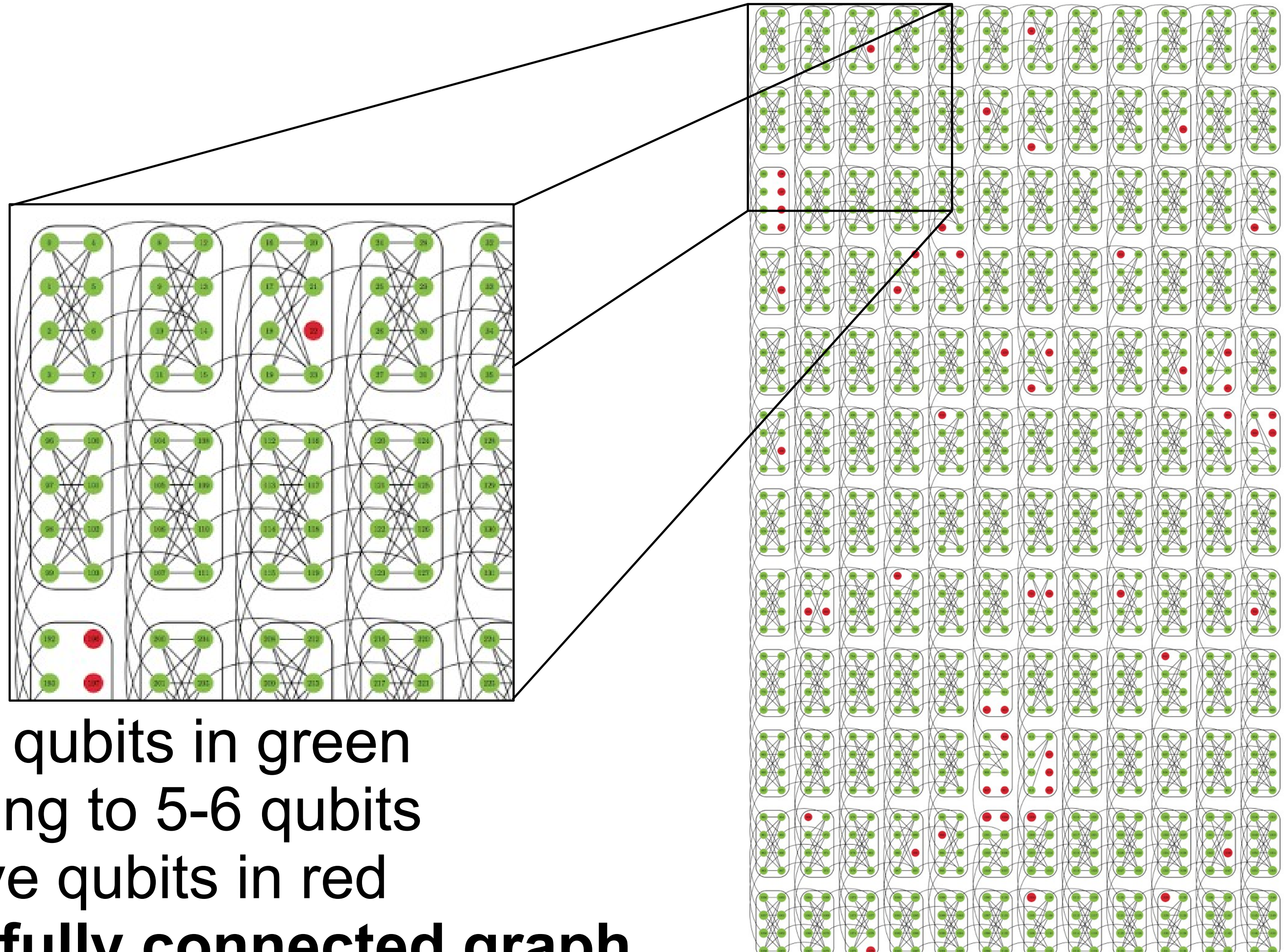
Runs over **adjacent** quBits

$$H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

External magnetic field

Interactions

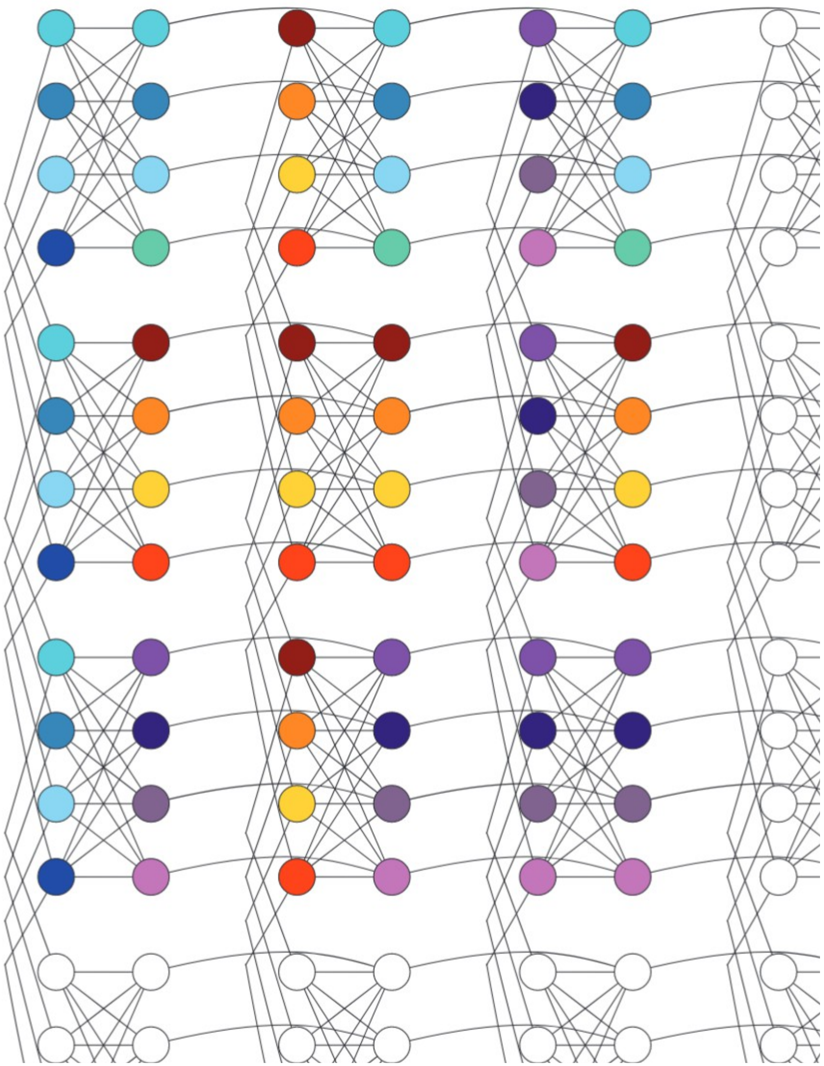
# D-Wave qubit Adjacency



Active qubits in green
Coupling to 5-6 qubits
Inactive qubits in red
**Not a fully connected graph**

# Model Embedding

# Full Ising Model



- Create chains of spins through the chimera graph
- Split local fields across all qubits in the chain
- Tightly couple ($J_F$=6)

- Non-unique embedding. Heuristic approach.

- Suppressing spin flip within chain as error correction.
- Use majority vote

→ Approximately full Ising Model with ~<40 spins

https://arxiv.org/abs/1210.8395

# Ising Hamiltonian

Runs over **all** quBit pairs

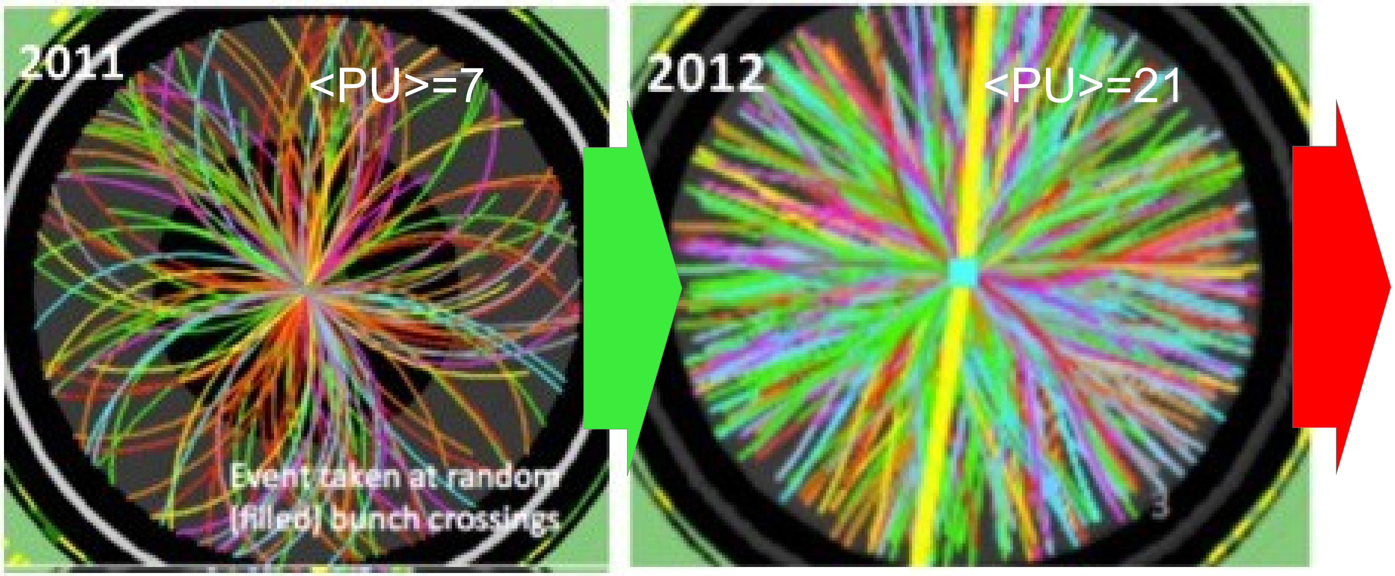
$$H_{\text{Ising}} = \sum_i h_i \sigma_i^z + \sum_{ij} J_{ij} \sigma_i^z \sigma_j^z$$

External magnetic field

Interactions

# High Luminosity LHC
# The Challenge

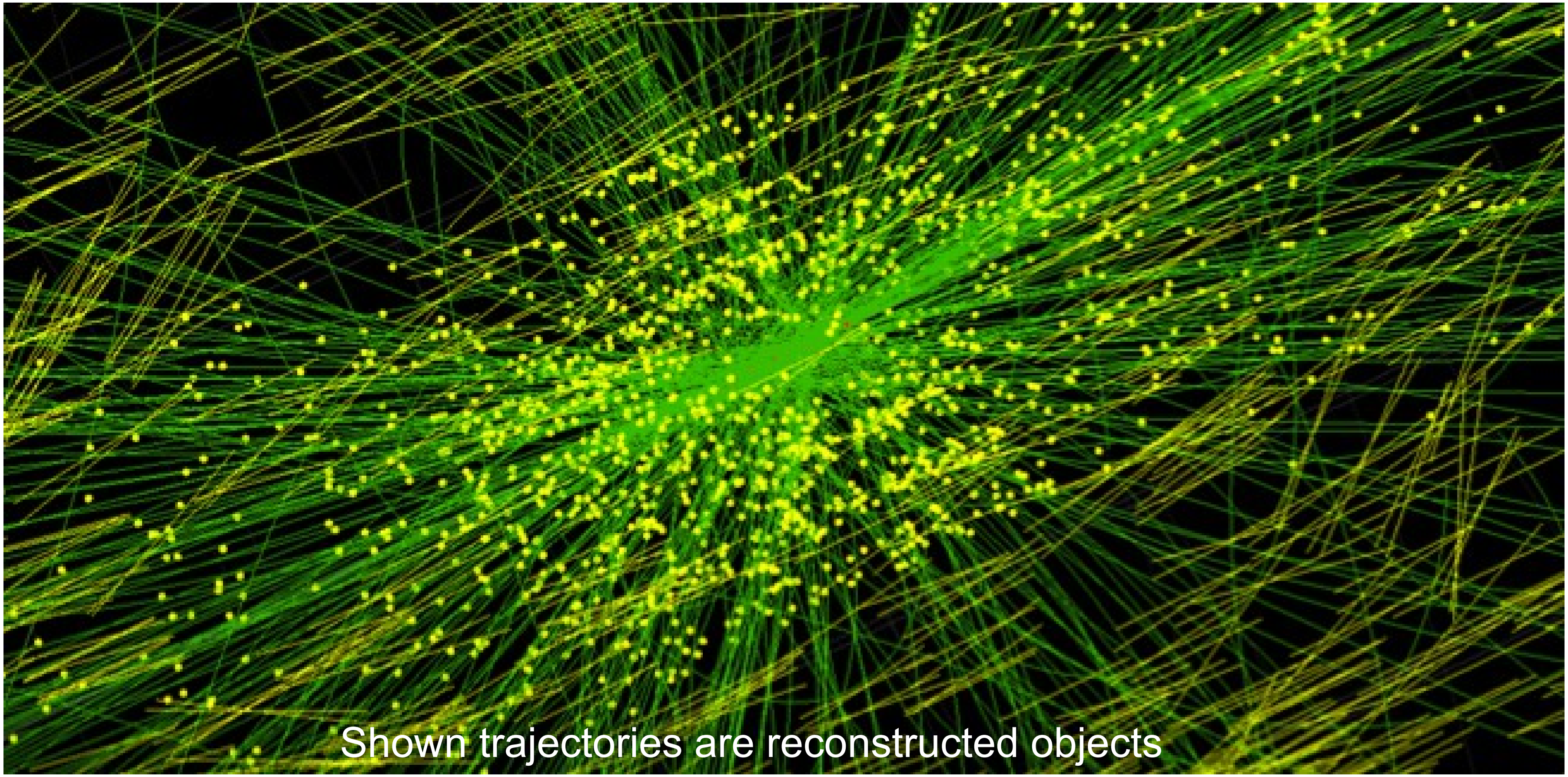
# HL-LHC Challenge




**<PU>=140-200**
**10x more hits**
**Circa 2025**

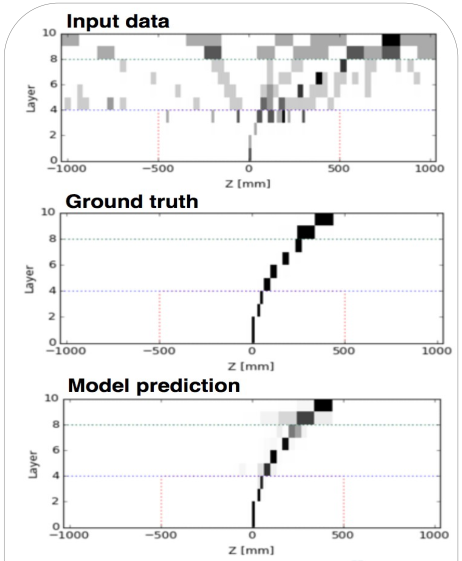
- CPU time extrapolation into HL-LHC era far **surpasses growth in computing budget**
- **Need for faster algorithms**
- Approximation allowed in the trigger

# Complexity and Ambiguity

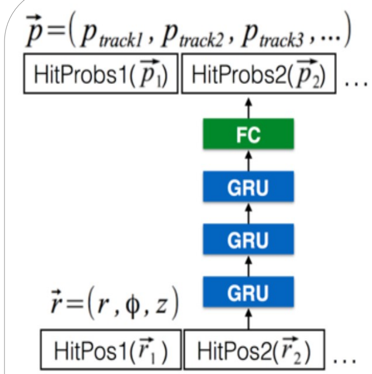


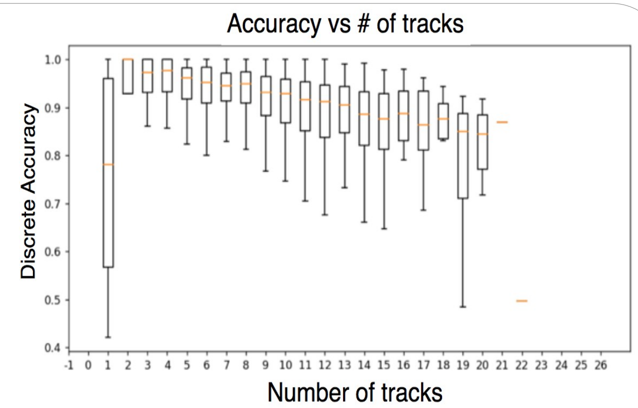

The future holds **much more hits**

# HEP.TrkX Approaches

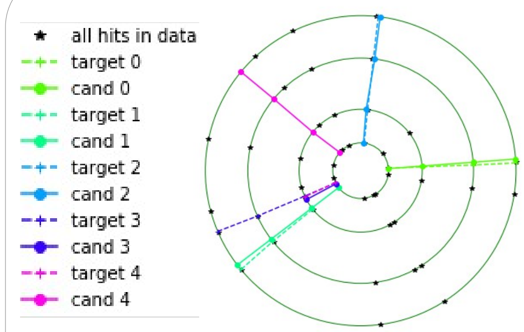



Track following with RNN



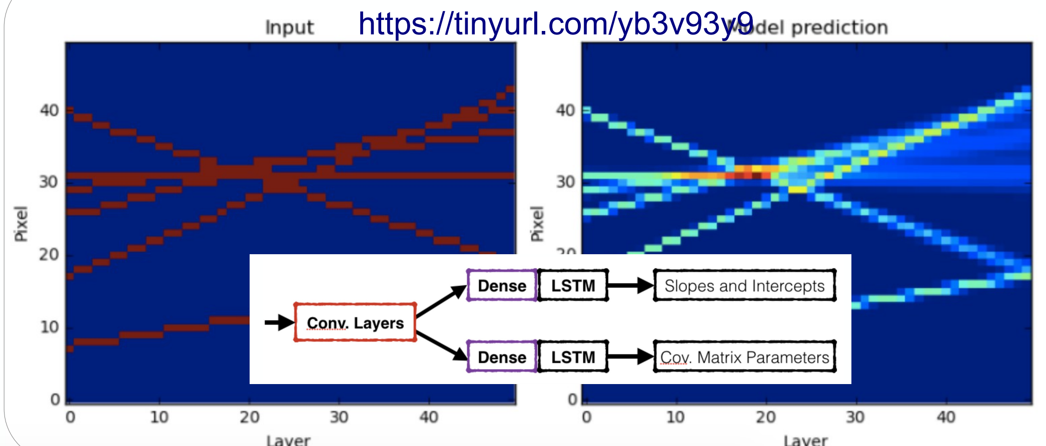

End-to-end hit assignment

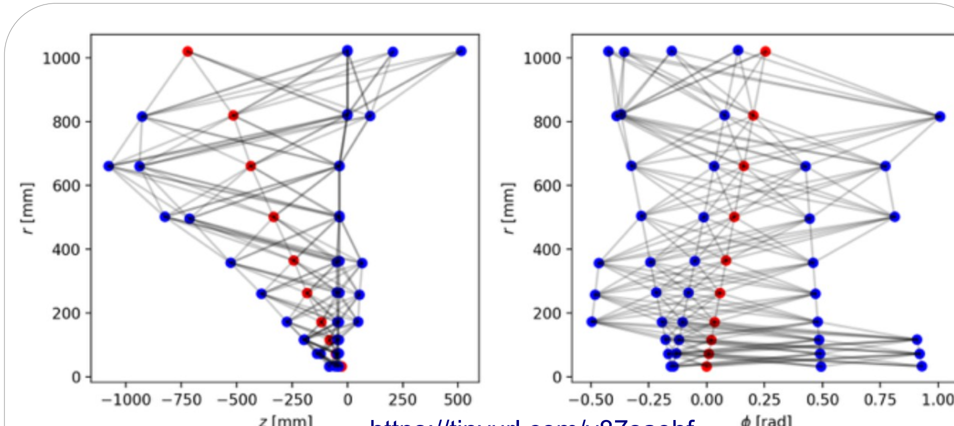



Seq-to-seq track finding

https://heptrkx.github.io/

https://tinyurl.com/yb3v93y9




https://tinyurl.com/y87saehf

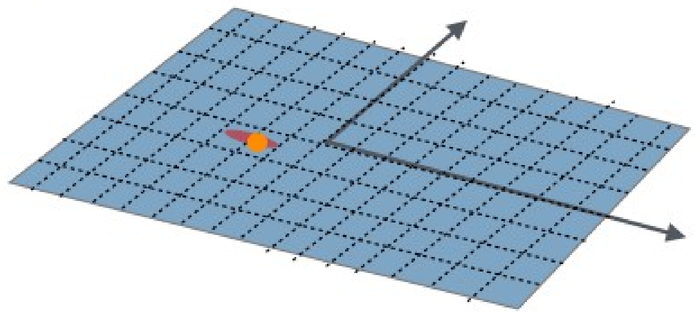
# Tracking **Not** In a Nutshell

Several Times

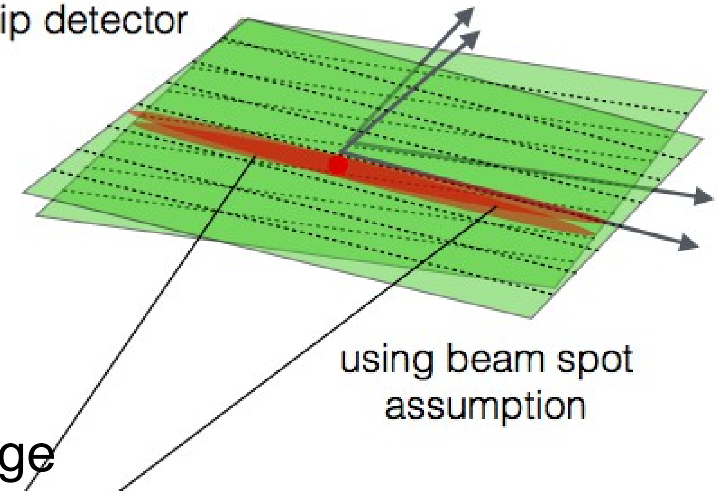
- **Hits preparation**
- **Seeding**
- **Pattern recognition**
- **Track fitting**
- **Track cleaning**

# Hit Preparation

pixel detector

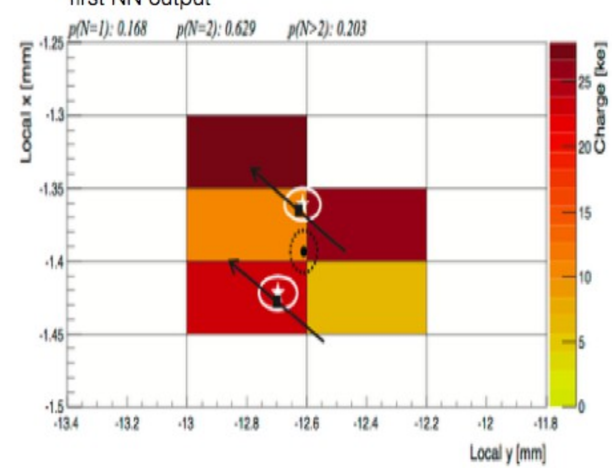


strip detector



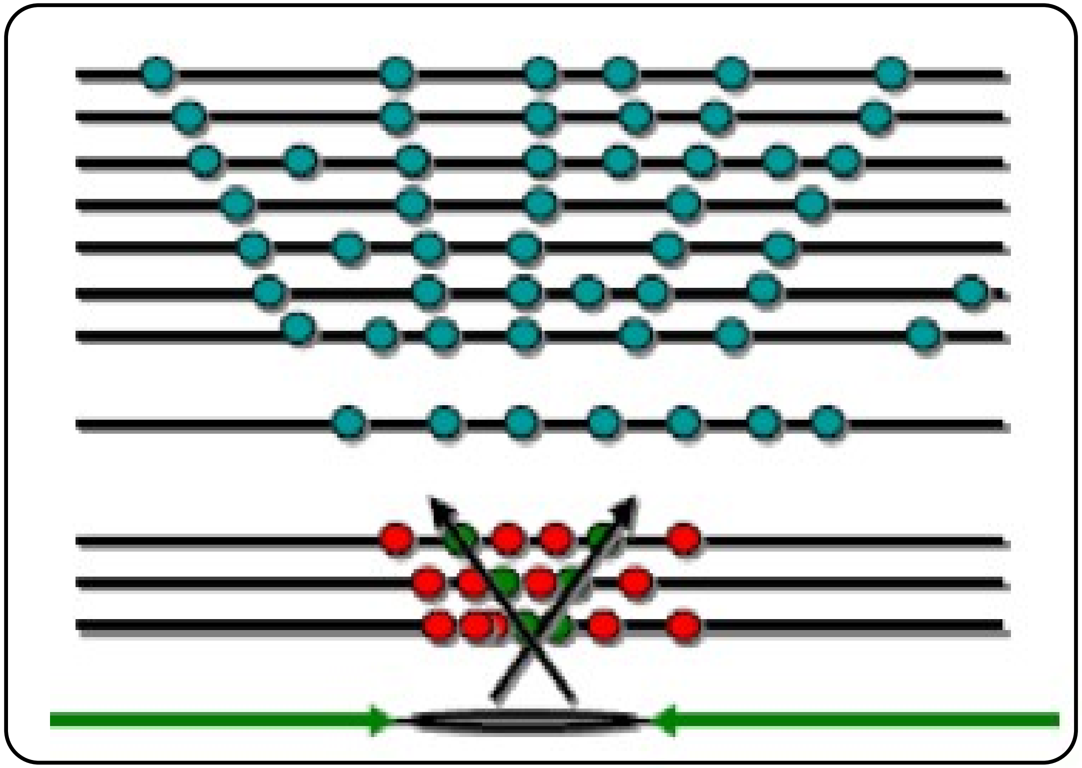
using beam spot assumption

- Calculate the hit position from barycenter of charge deposits
- Use of neural net classifier to split cluster in ATLAS
- Access to trajectory local parameter from cluster shape
- Remove hits from previous tracking iterations
- HL-LHC design include double layers giving more constraints on the local trajectory parameters



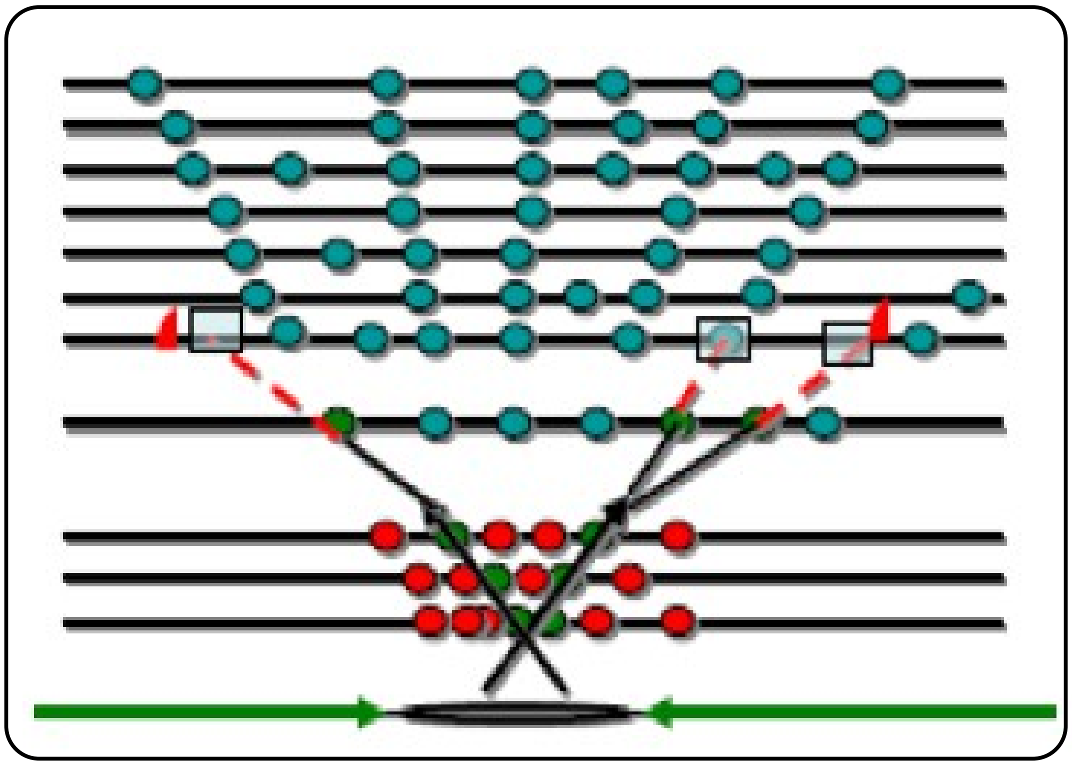

Example of cluster split

# Seeding



- Combinatorics of 2 or 3 hits with tight/loose constraints to the beam spot or vertex
- Seed cleaning/purity plays in an important in reducing the CPU requirements of sub-sequent steps
  - ➔ Consider pixel cluster shape and charge to remove incompatible seeds
- Initial track parameters from helix fit

# Pattern Recognition



- Use of the Kalman filter formalism with weight matrix
- Identify possible next layers from geometrical considerations
- Combinatorics with compatibles hits, retain N best candidates
- No smoothing procedure
- Resilient to missing modules
- Hits are mostly belonging to one track and one track only
- Hit sharing can happen in dense events, in the innermost part
- Lots of hits from low momentum particles

# Kalman Filter

$$K_k = C_{k|k-1} H_k^{\top} (V_k + H_k C_{k|k-1} H_k^{\top})^{-1}$$

$$p_{k|k} = p_{k|k-1} + K_k \, (m_k - H_k p_{k|k-1})$$

$$C_{k|k-1} = (I - K_k H_k) C_{k|k-1}$$

$H_k$ is the projection matrix

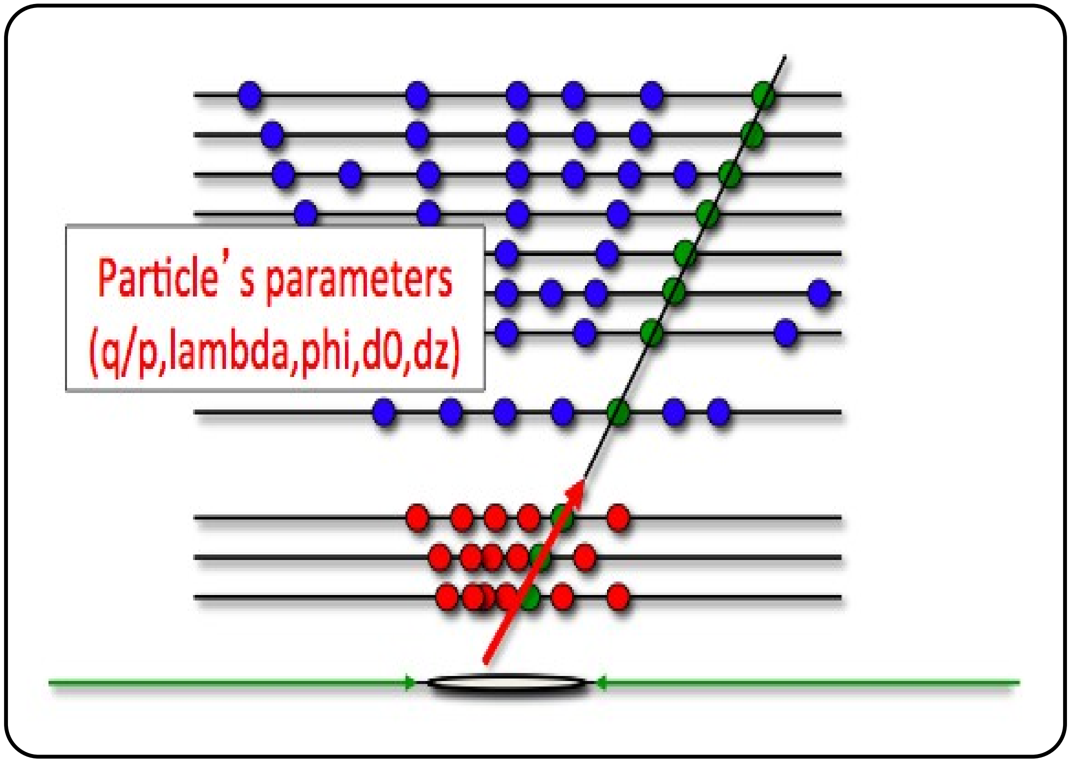
$V_k$ is the hit covariance matrix

$p_{i|j}$ is the trajectory state at i given j

$C_{i|j}$ is the trajectory state covariance matrix at i given j

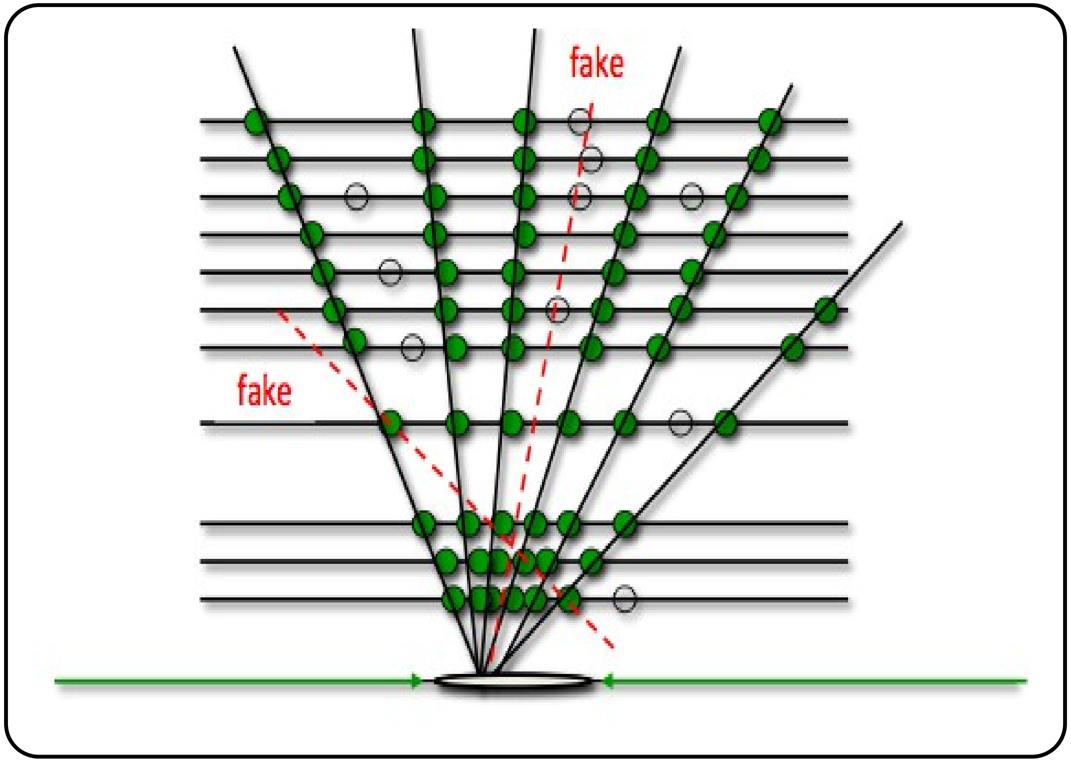
- Trajectory state propagation done either
  - ✓ Analytical (helix, fastest)
  - ✓ Stepping helix (fast)
  - ✓ Runge-Kutta (slow)
- Material effect added to trajectory state covariance
- Projection matrix of local helix parameters onto module surface
  - → Trivial expression due to local helix parametrisation
- Hits covariance matrix for pixel and stereo hits properly formed
  - ✗ Issue with strip hits and longitudinal error being non gaussian (square)

# Track Fitting




- Use of the Kalman filter formalism with weight matrix
- Use of smoothing procedure to identify outliers
- Field non uniformity are taken into account
- Detector alignment taken into account

# Cleaning, Selection



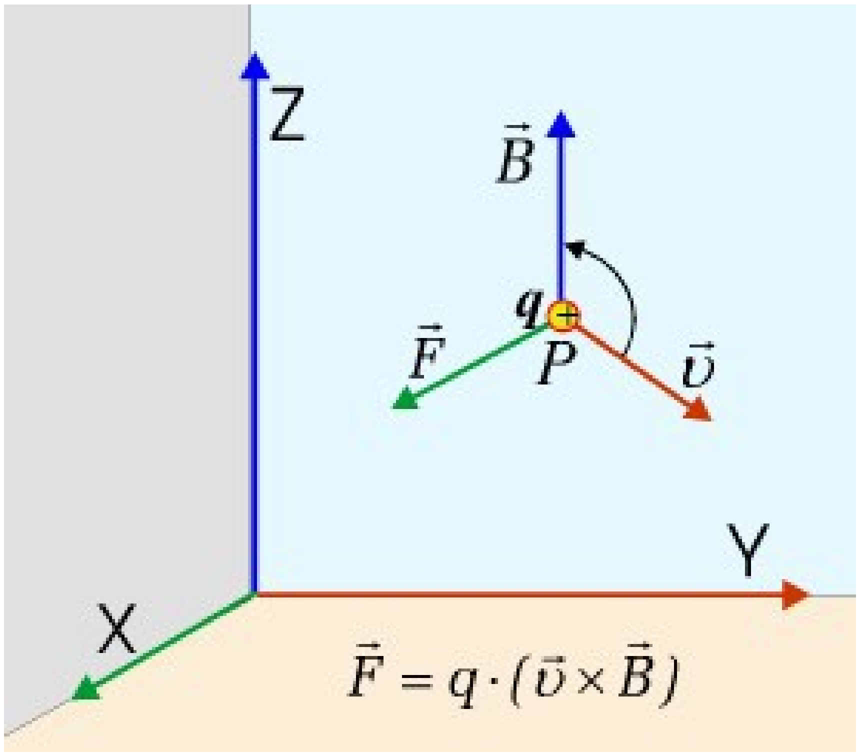

- Track quality estimated using ranking or classification method
  - ➔Use of MVA
- Hits from high quality tracks are remove for the next iterations where applicable

# A Charged Particle Journey

*First order effect : electromagnetic elastic interaction of the charge particle with nuclei (heavy and multiply charged) and electrons (light and single charged)*

*Second order effect : inelastic interaction with nuclei.*

# Magnetic Field

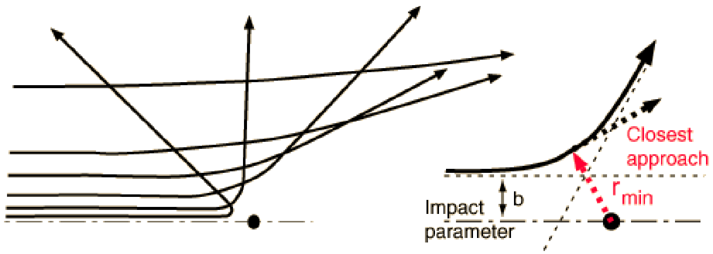



- Magnetic fieldB  acts on charged particles in motion : Lorentz Force
- The solution in uniform magnetic field is an helix along the field : 5 parameters
- Helix radius proportional to the component of momentum perpendicular to B
- Separate particles in dense environment

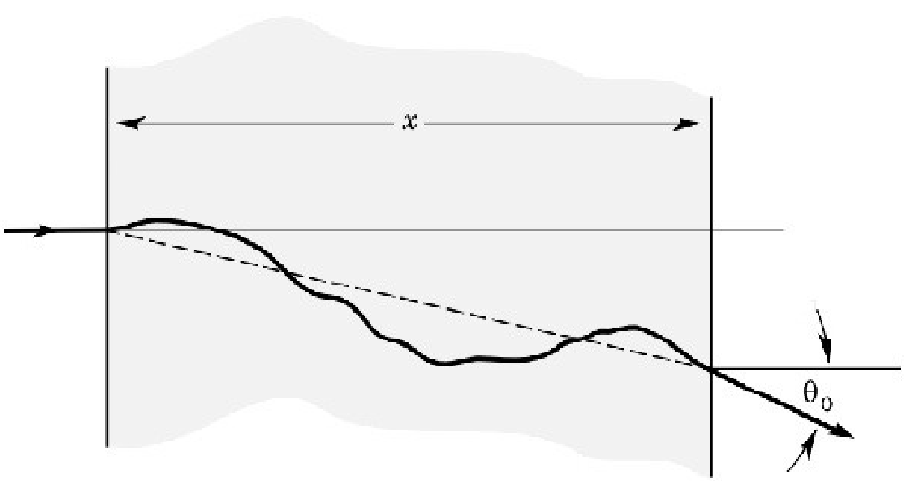
→ Bending induces radiation : bremsstrahlung

→ The magnetic field has to be known to a good precision for accurate tracking of particle

# Multiple Scattering




- **Deflection on nuclei** (effect from electron are negligible)
- Addition of scattering processes
- Gaussian approximation valid for substantial material traversed

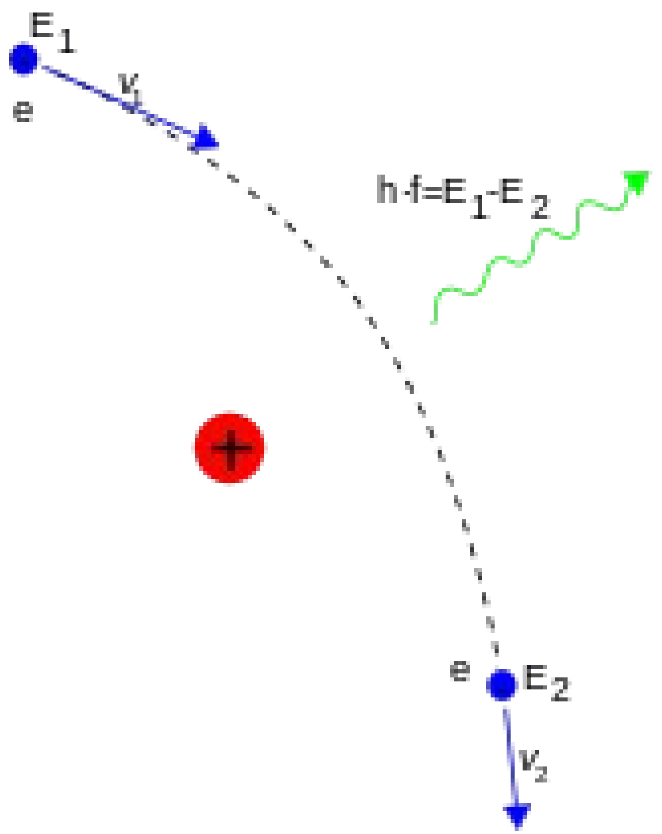



**Gaussian Approximation**

$$\theta^2 = \left(\frac{13.6MeV}{\beta cp}\right)^2 * \frac{x}{X_0}$$

β -particle velocity
ρ – material density
P - particle momenta

# Bremsstrahlung




- Electromagnetic radiation of charged particles under acceleration due to nuclei charge
- Significant at low mass or high energy
- Discontinuity in energy loss spectrum due to photon emission and track curvature

➔ Can be observed as kink in the trajectory or presence of collinear energetic photons

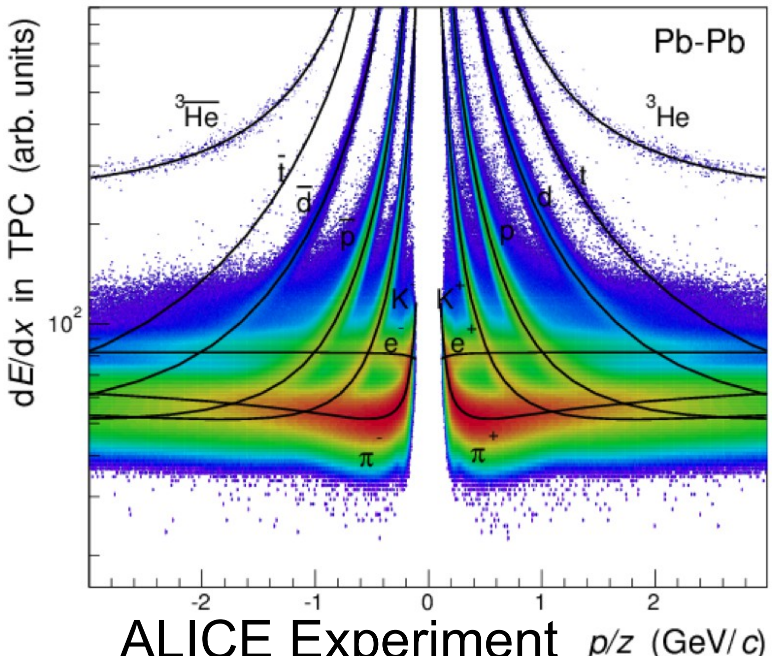
# Energy Loss

- Momentum transfer to electrons when traversing material (effect of nuclei is negligible

- Energy loss at low momentum depends on mass : can be used as mass spectrometer

$$dE/dx = k_1 \frac{Z}{A}\frac{1}{\beta^2}\rho\left(\ln\left(\frac{2m_e c^2\beta^2}{I(1-\beta^2)}\right)-\beta^2-\frac{\delta}{2}\right)$$

β -particle velocity
ρ – material density
Z - atomic number of absorber
A – mass number of absorber
I – mean excitation energy
δ – density effect correction factor – material dependent and β dependent




ALICE Experiment

# Summary on Material Effects

- Collective effects can be estimated statistically and taken into account in how they modify the trajectory

- Bremstrahlung and nuclear interactions significantly distort trajectories