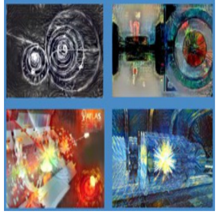


Graph Networks in High Energy Physics

Fifth Machine Learning in High Energy Physics Summer School
1-10 July 2019

Jean-Roch Vlimant, jvlimant@caltech.edu

Outline

I. Physics at the LHC

II. The case for Machine Learning

III. Collider Data Representation

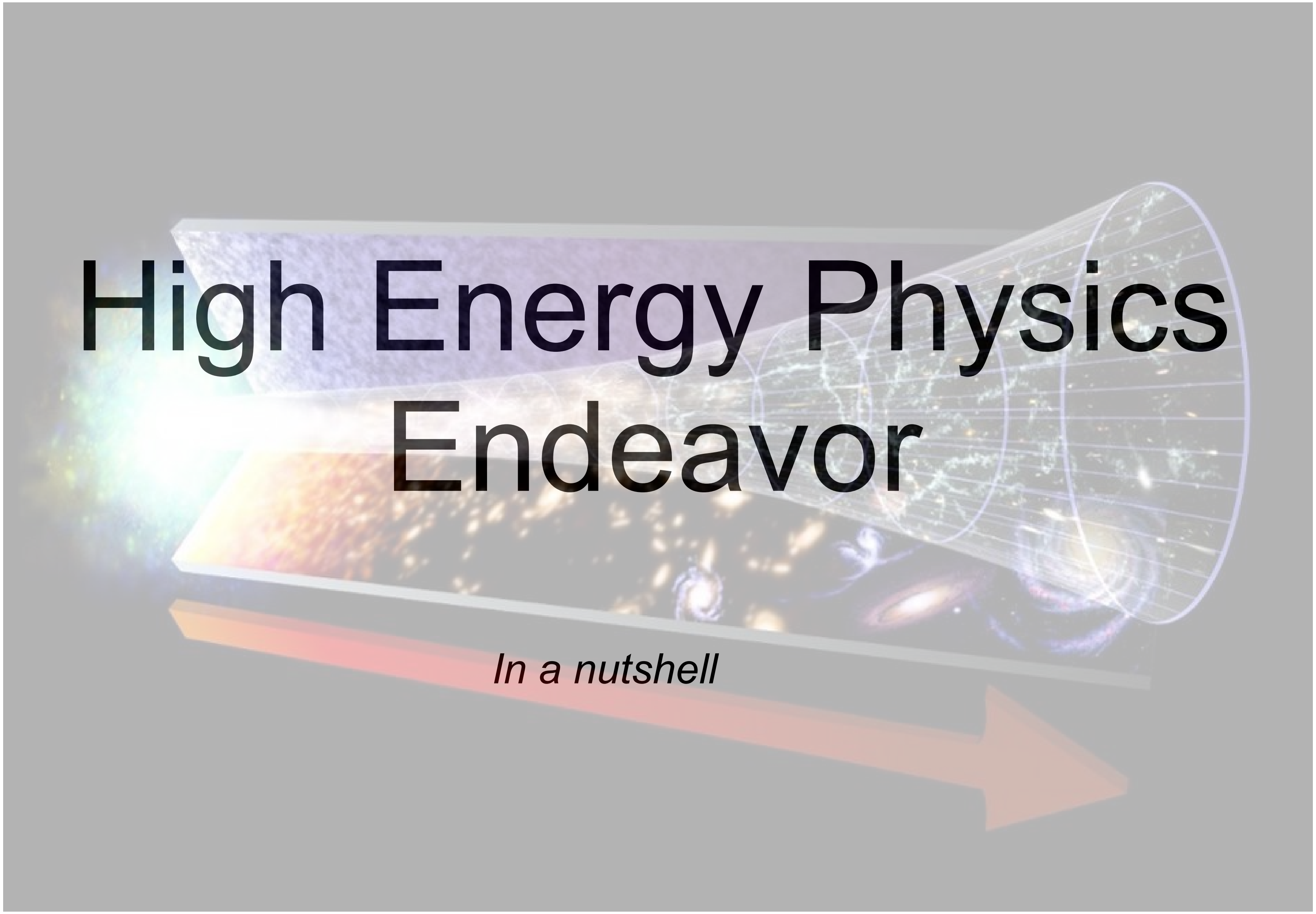
IV. Graph Networks & applications

Covering the following

- *Tracking with GNN*
- *Learning irregular geometry with Distance-weighted GNN*
- *Pile-Up mitigation with GGCNN*
- *Jet identification with Interaction network*

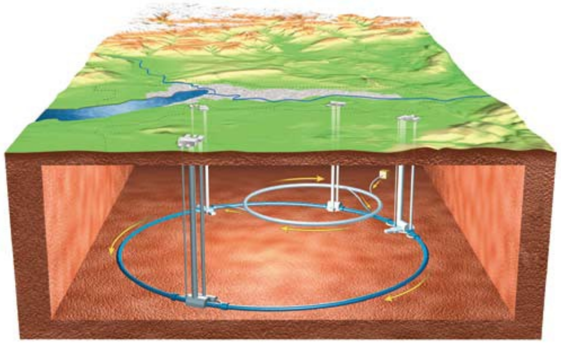
Relevant work not covered: icecube, MPJet, CloudJet, stopGNN, showerGAN

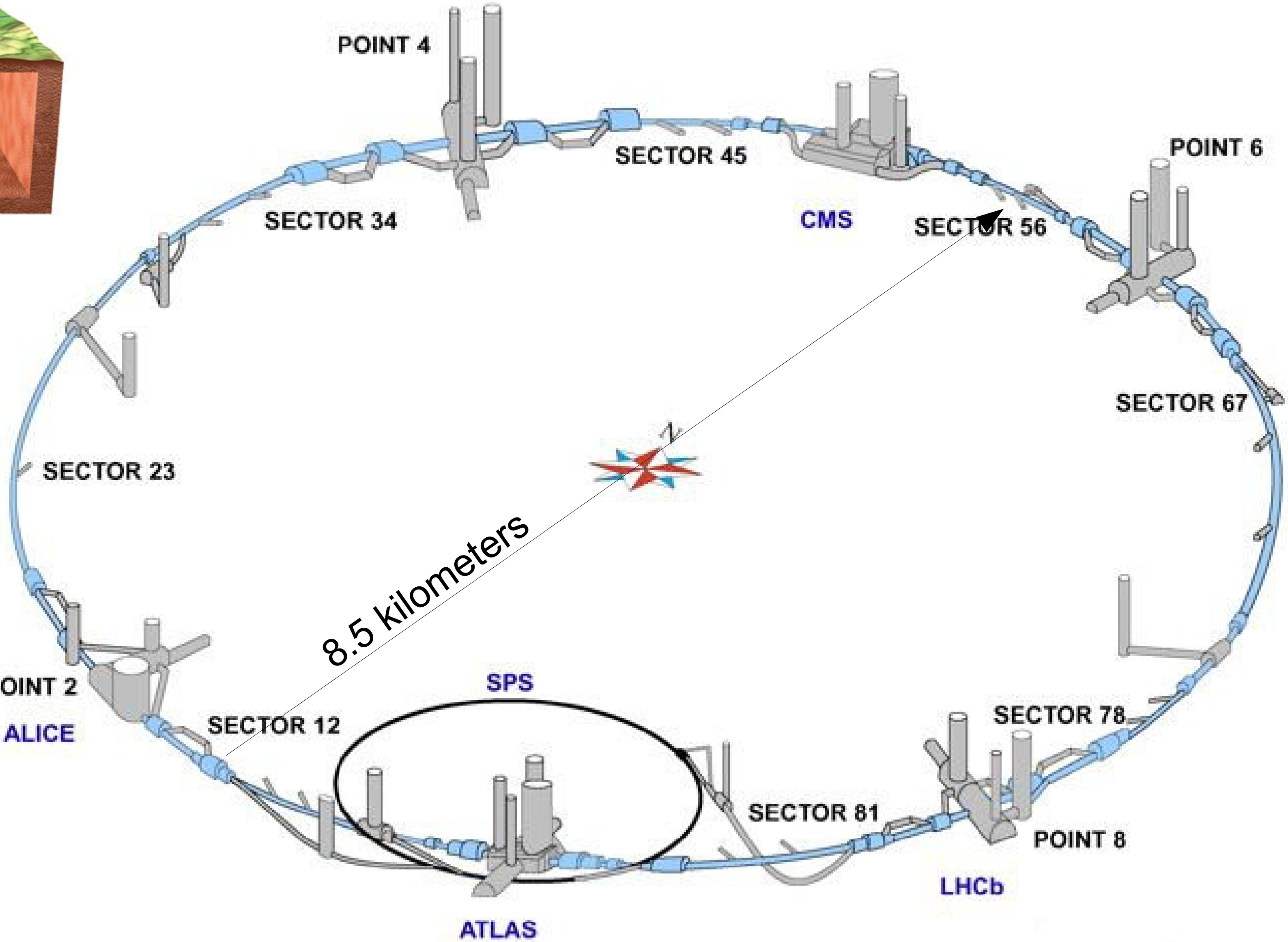
High Energy Physics Endeavor



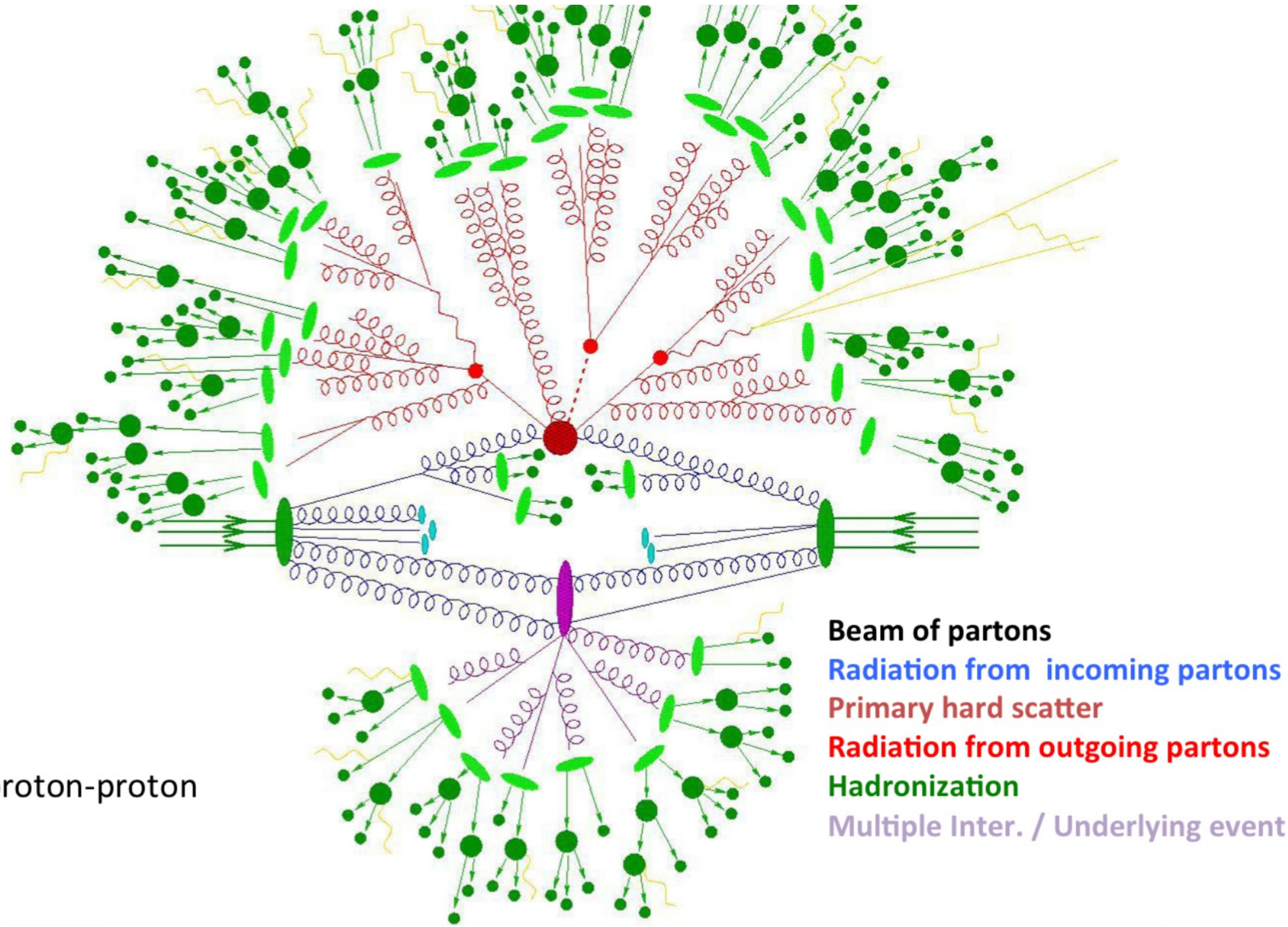
In a nutshell

The Large Hadron Collider





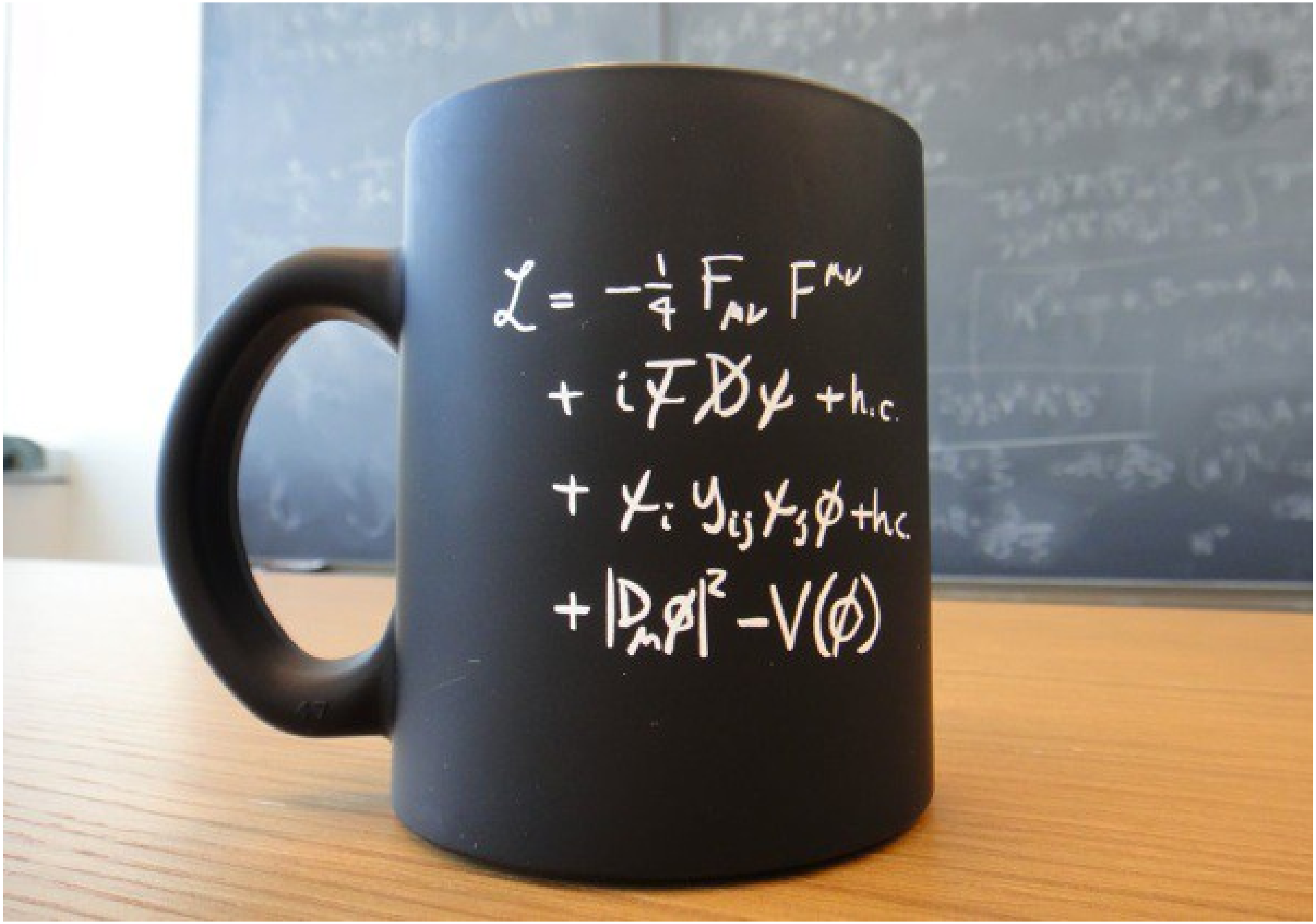
Colliding Hadrons



Typical proton-proton collision

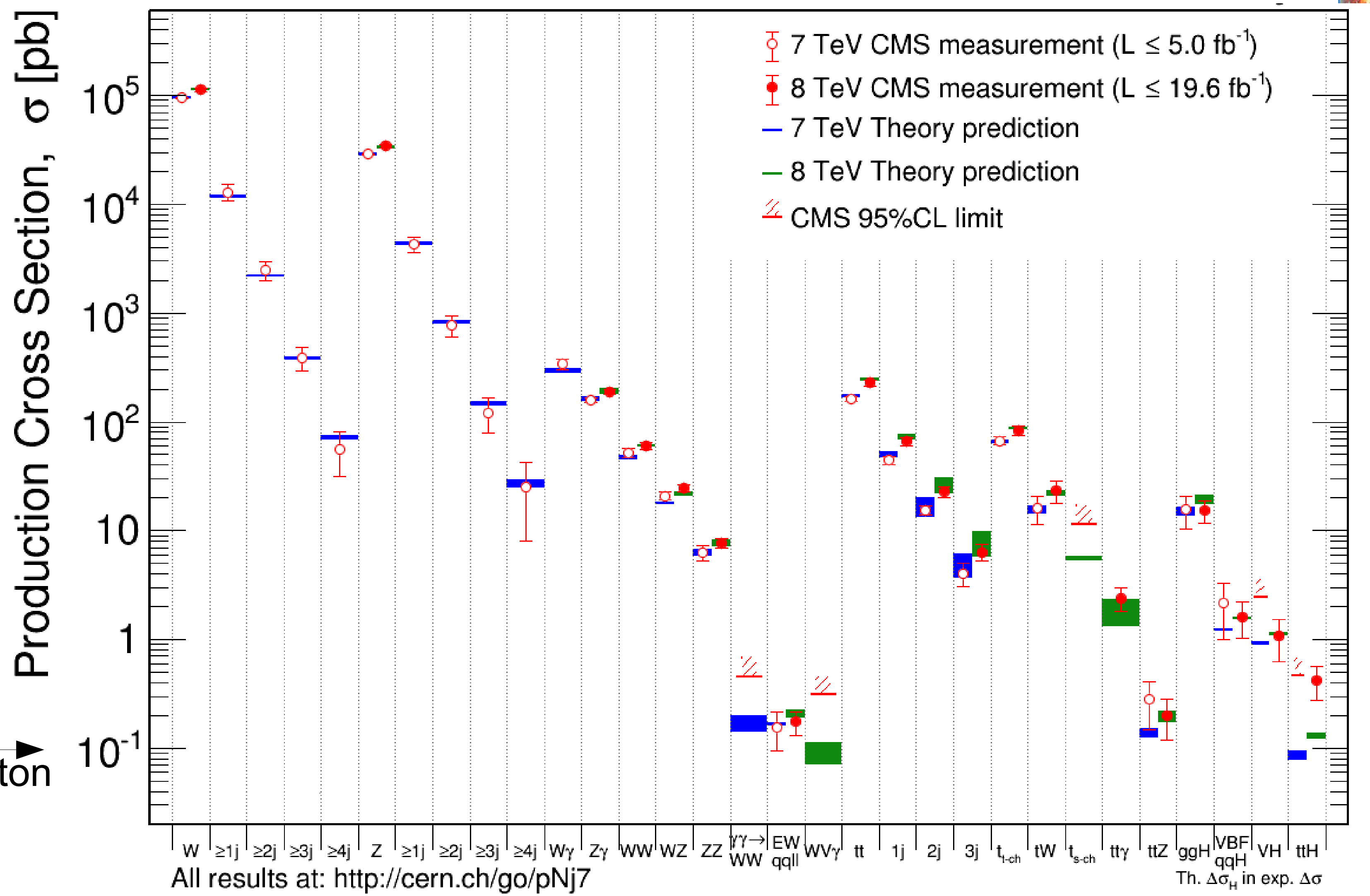
Probing fundamental laws of physics as large spectrum of particles (known and unknown) can be produced

The Standard Model



Well demonstrated effective model
We can predict most of the observations
We can use a large amount of simulation

Size Of The Challenge

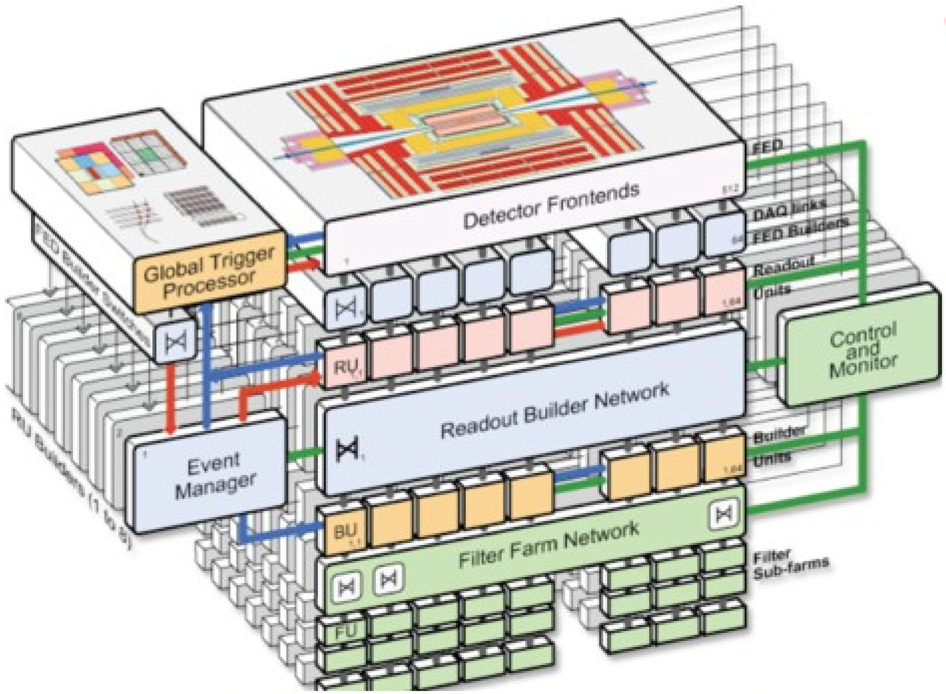


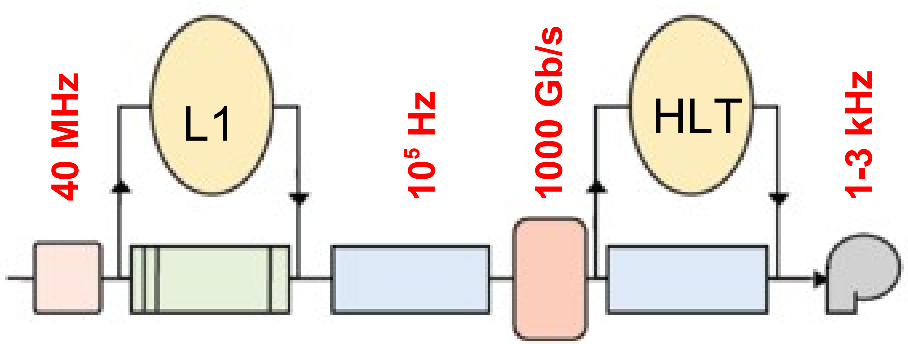
1 event every 500.000 proton collision

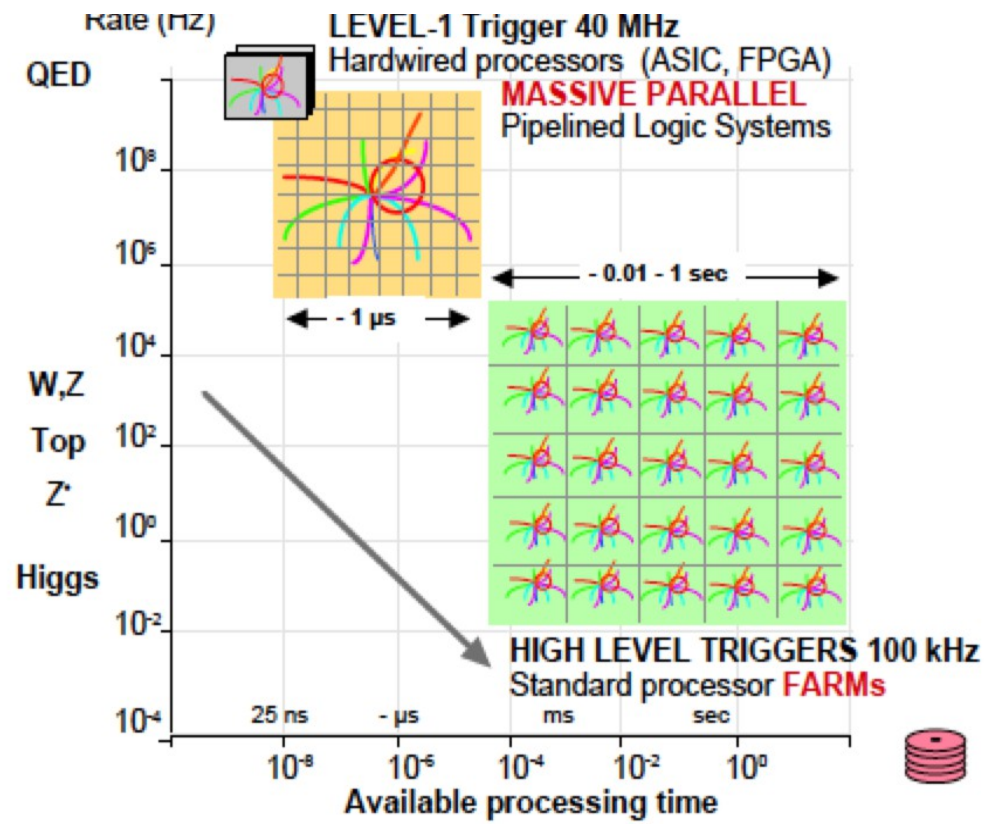
Low probability of producing exotic and interesting signals.
Observe rare events from a large amount of data.

Event Filtering

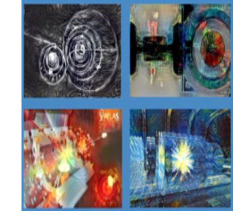
Tr





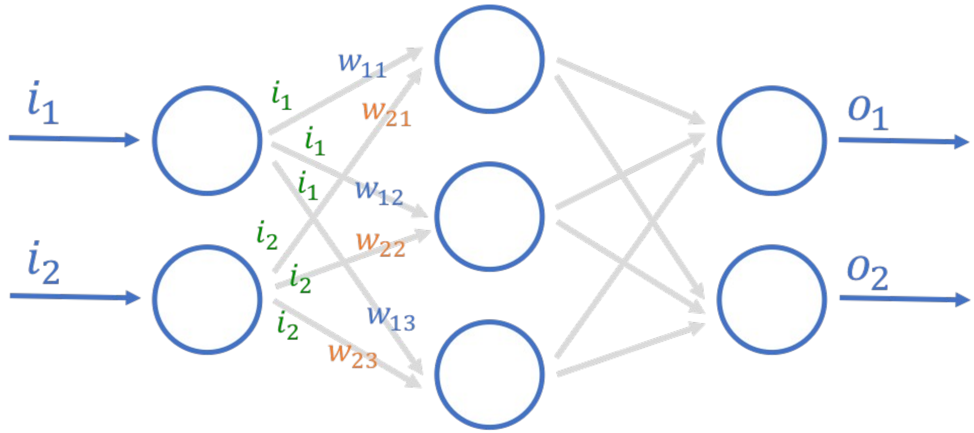


Ultra fast decision to keep the relevant data.
In hardware and software.



The Case for Machine Learning

Operation Vectorisation

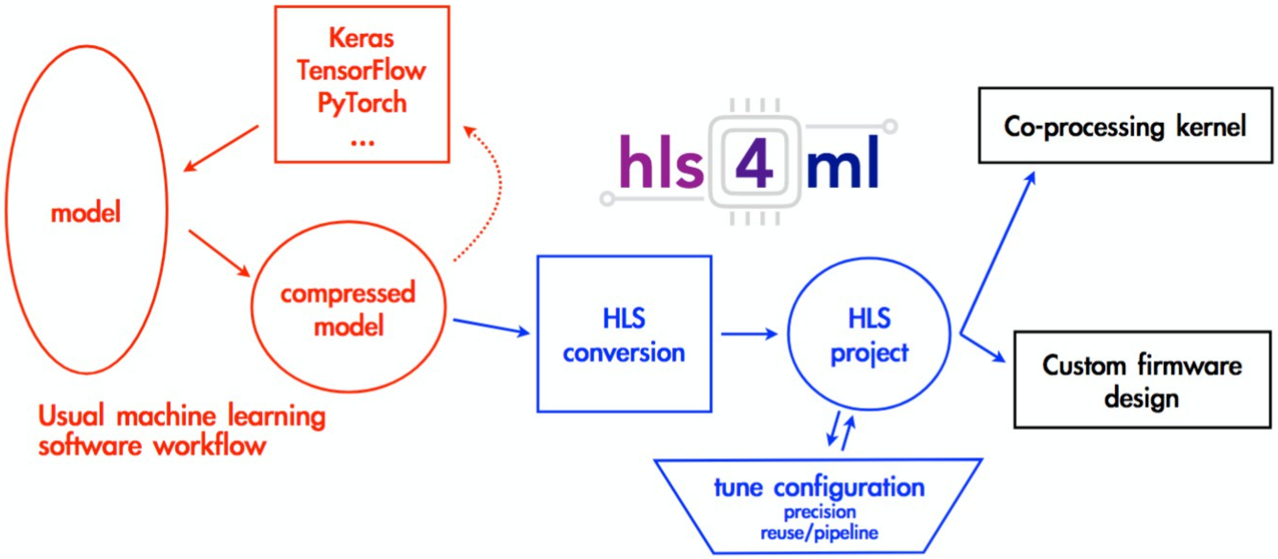


ANN ≡ matrix operations ≡ parallelizable

$$\begin{bmatrix} w_{11} & w_{21} \\ w_{12} & w_{22} \\ w_{13} & w_{23} \end{bmatrix} \cdot \begin{bmatrix} i_1 \\ i_2 \end{bmatrix} = \begin{bmatrix} (w_{11} \times i_1) + (w_{21} \times i_2) \\ (w_{12} \times i_1) + (w_{22} \times i_2) \\ (w_{13} \times i_1) + (w_{23} \times i_2) \end{bmatrix}$$

Computation of prediction from artificial neural network model can be **vectorized to a large extend.**

Hyper-Fast Prediction



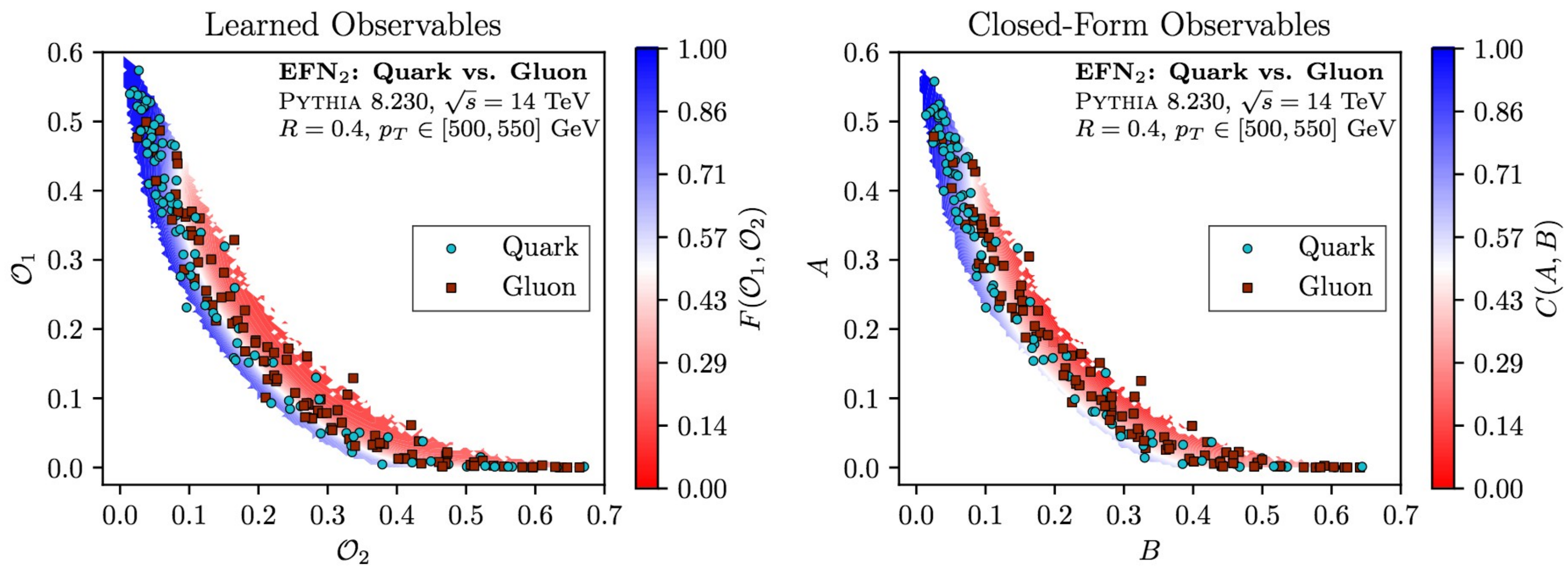
Synthesis FPGA firmware
from trained ANN

https://hls-fpga-machine-learning.github.io/hls4ml/

J. Duarte et al.https://arxiv.org/abs/1804.06913

Prediction from artificial neural network model can be **done on FPGA**, GPU, TPU, ...

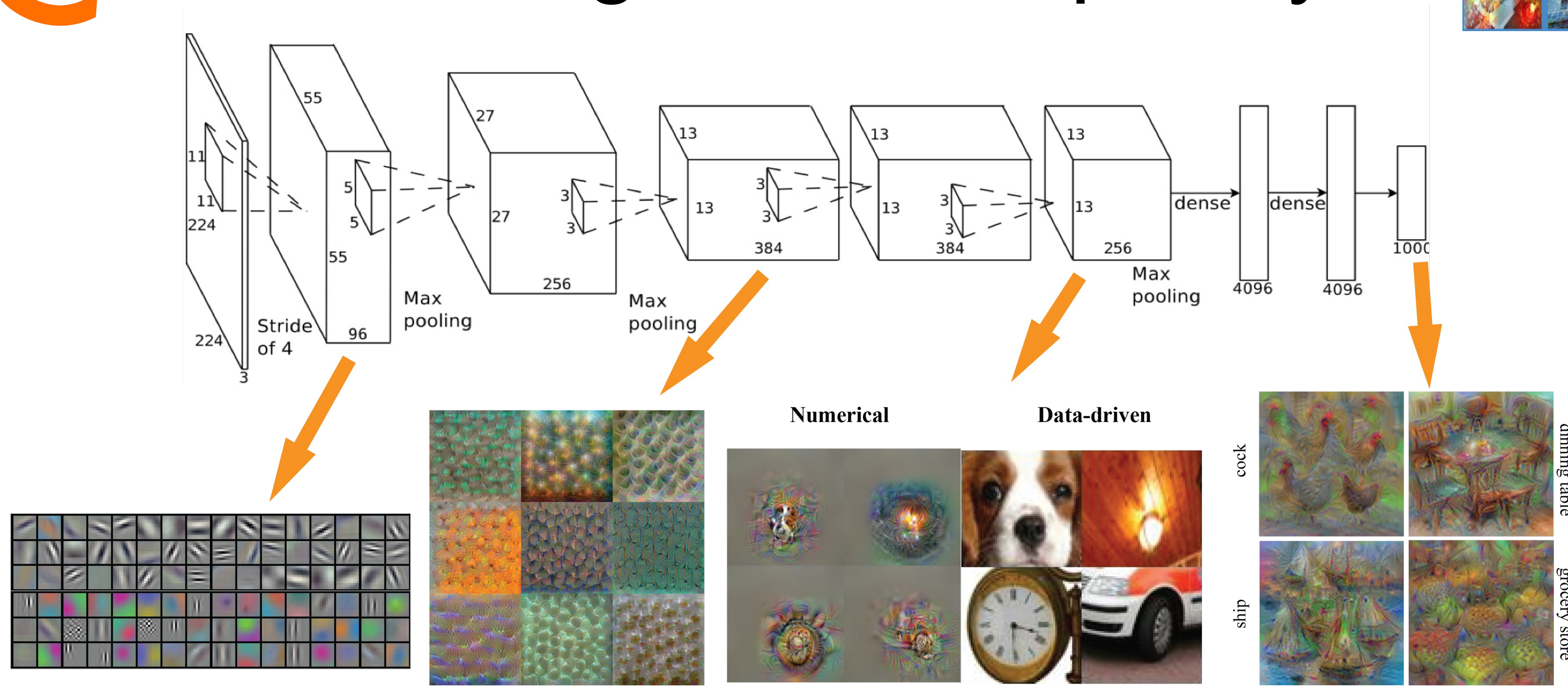
Physics Knowledge



P. Komiske, E. Metodiev, J. Thaler, https://arxiv.org/abs/1810.05165

Machine Learning can **help understand Physics**.
We can make **better models with Physics**.

Learning from Complexity



Conv 1: Edge+Blob | Conv 3: Texture | Conv 5: Object Parts | Fc8: Object Classes

“Simple” machine learning model can **extract information from complex dataset.**

More classical algorithm counter part may take **years of development.**

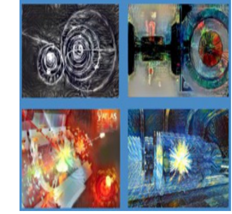
<u>Take home message :</u>

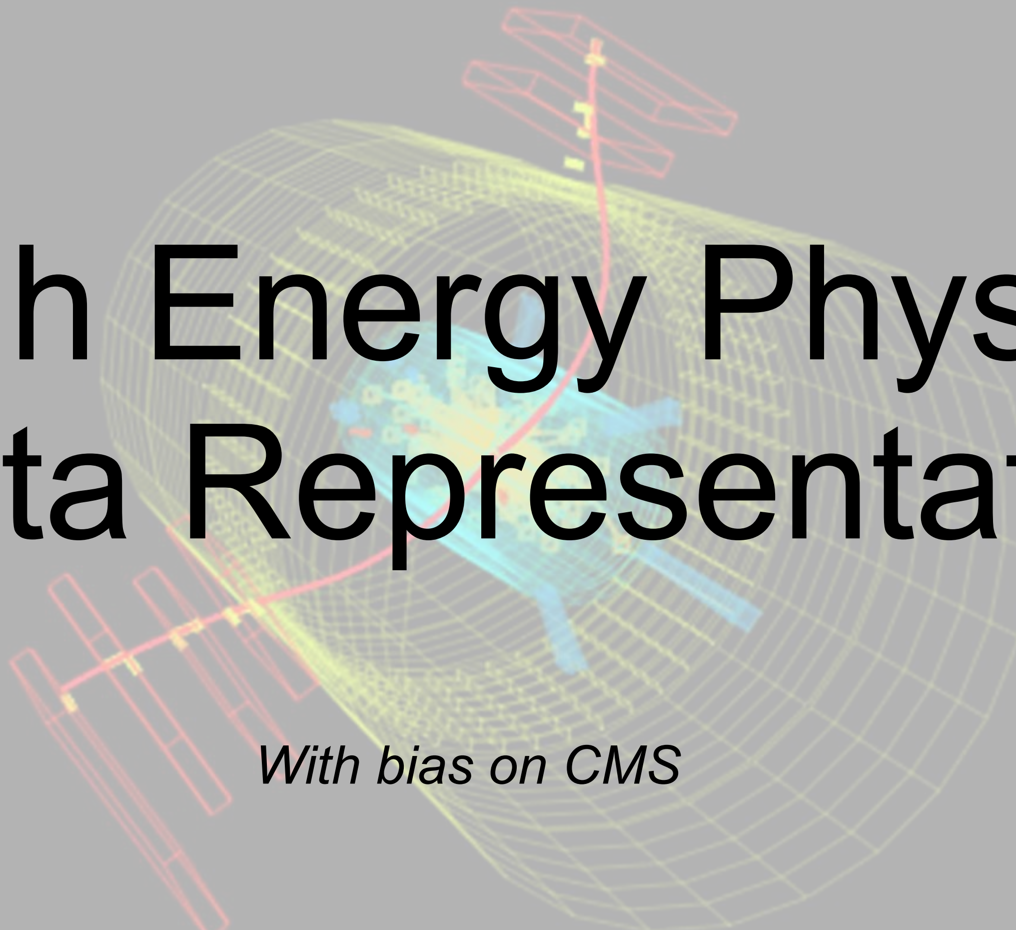
Measure rare and exotic processes from orders of magnitude larger backgrounds.

The Standard Model predicts with precision what to expect from many processes.

Reconstruct, identify and reject large amount of event within resource constraints.

Machine learning is a path forward in a resource constrained environment.

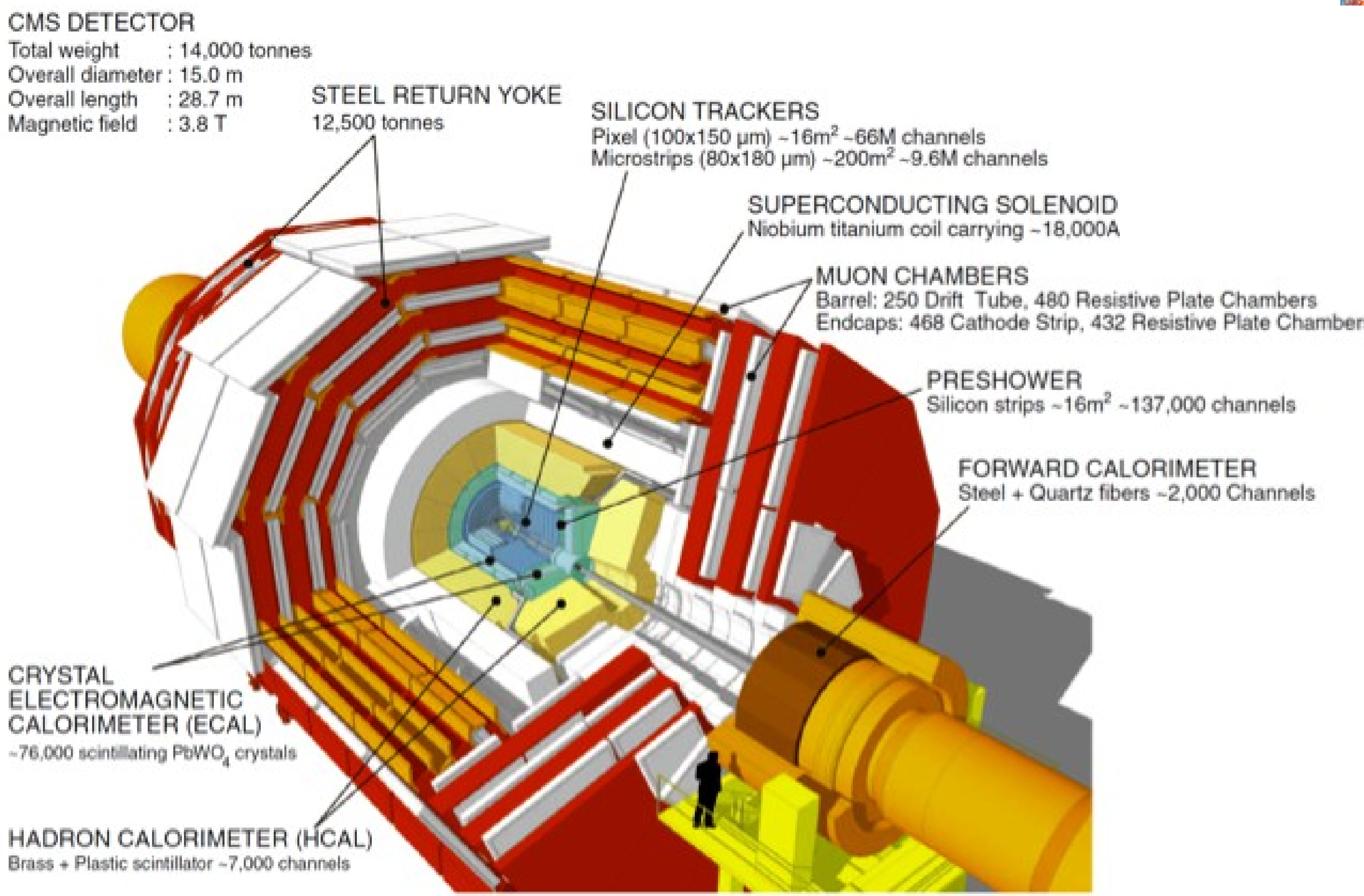




High Energy Physics Data Representation

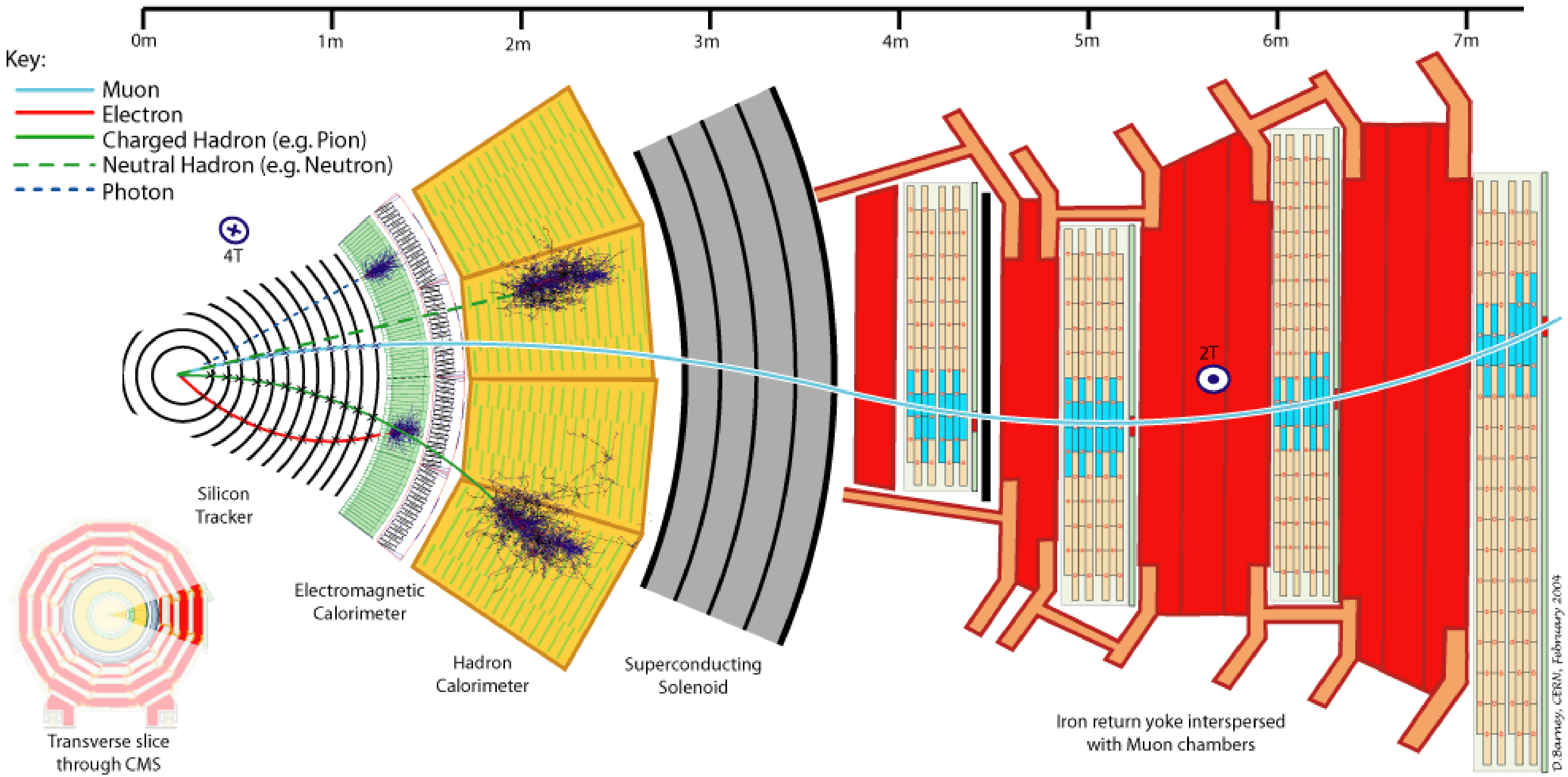
With bias on CMS

CMS Detector



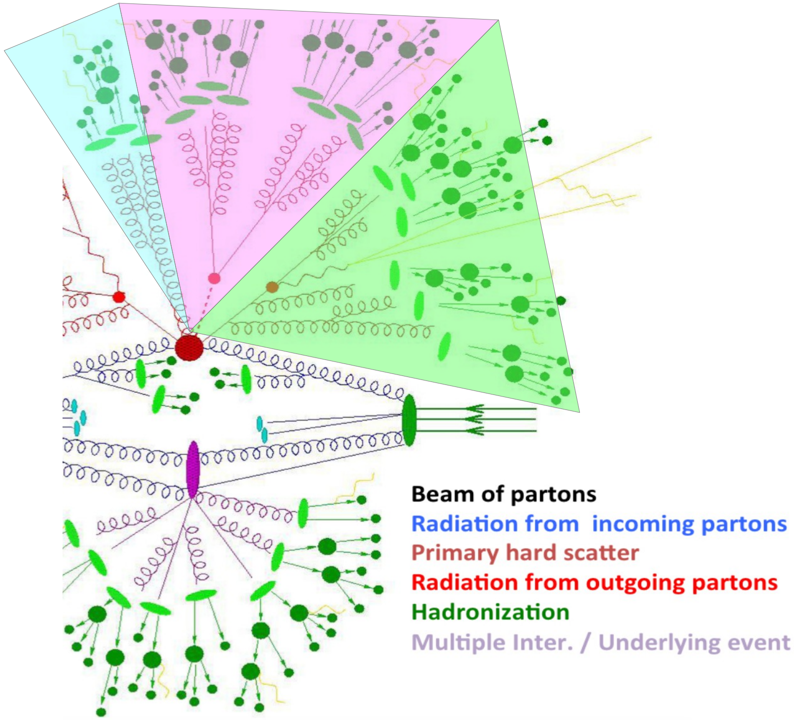
Heterogenous detector, with complex geometry.
About 100M channels in the read-out.

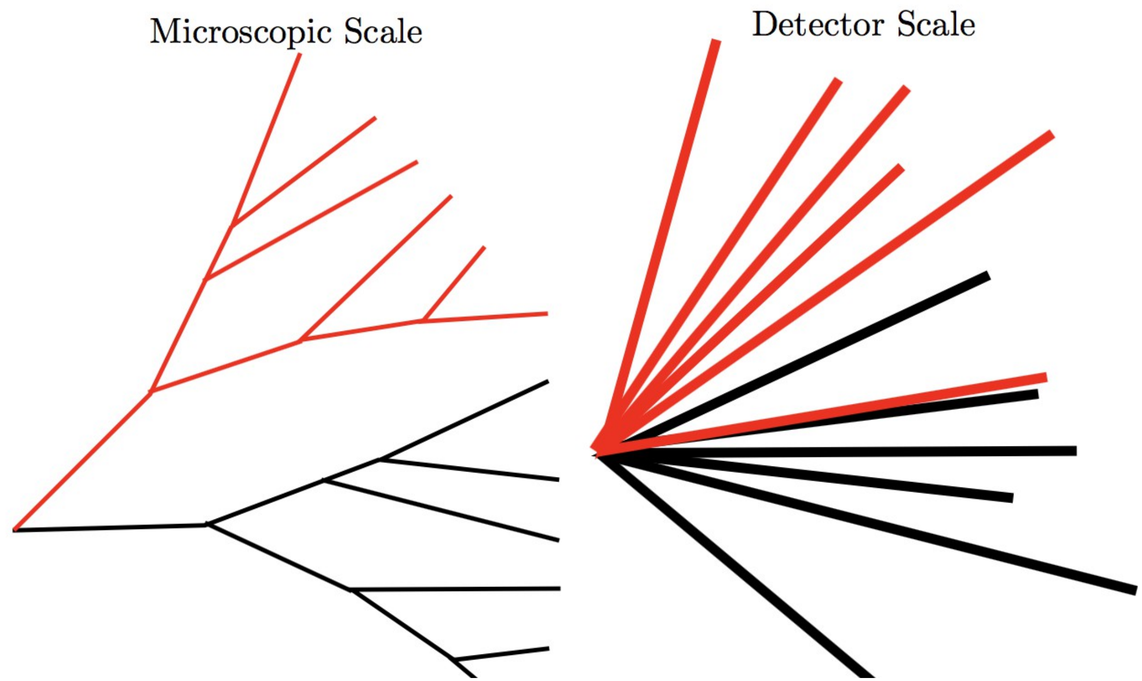
A Journey Through Matter



Particles leave hints of their passage in sub-detectors.
Specific (but overlapping) pattern for each particle type.

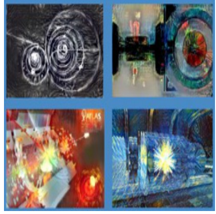
What is a Jet





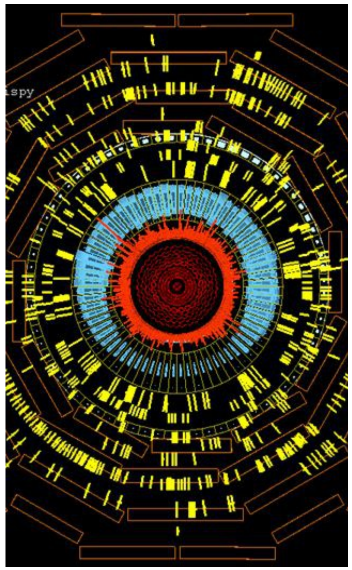
Quark&gluons hadronize as they propagate.
Any particle decaying in quark/gluons will result in a “jet” of particles in the direction of the original particle.
Ambiguities on the original particle gets worse in boosted systems.

From RAW to High Level data

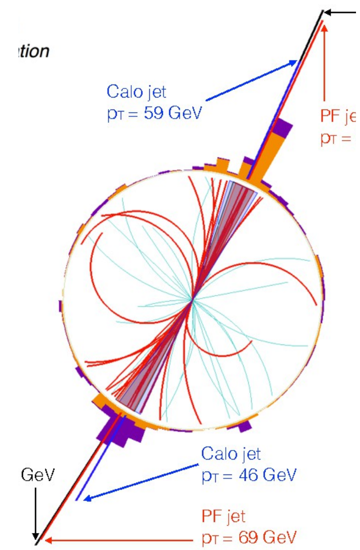


Detector Data

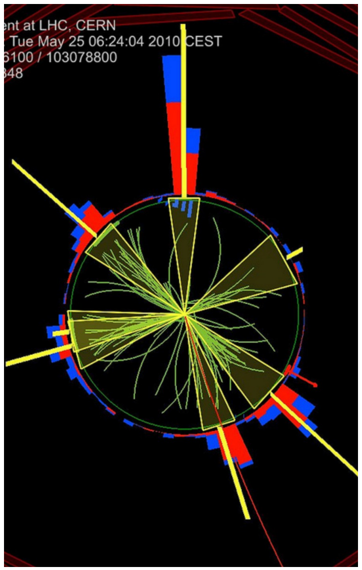
Local reconstruction



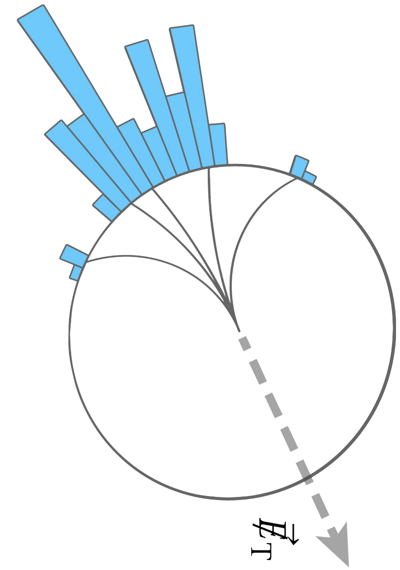
Particle representation



Jet Clustering



High level features



Event Processing

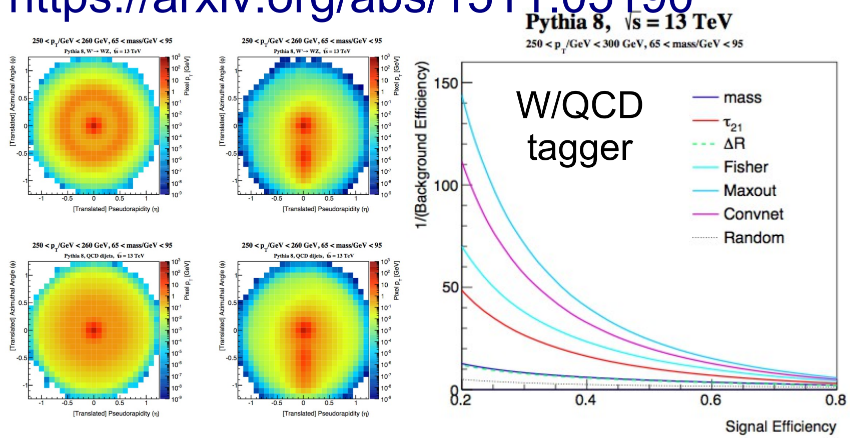
Dimensionality reduction

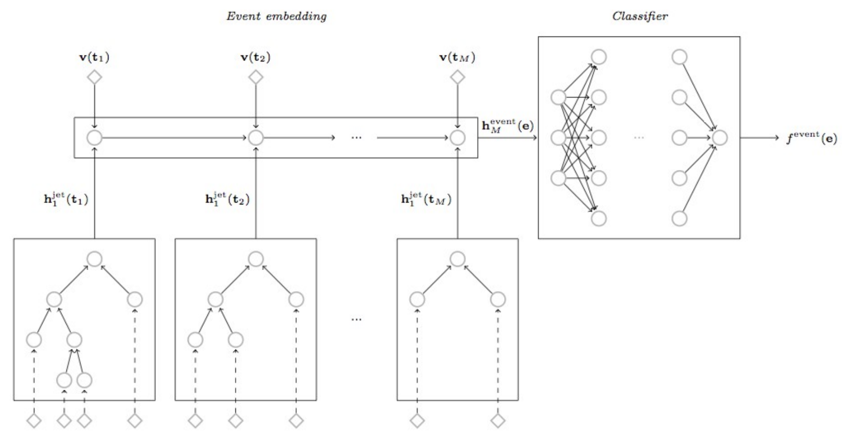
Globalization of information

The reconstruction of an event goes from the digital signal of the individual sub-detector to a sequence of particles, jets, and high-level features

Images and Sequences

Jet Imaging
https://arxiv.org/abs/1511.05190

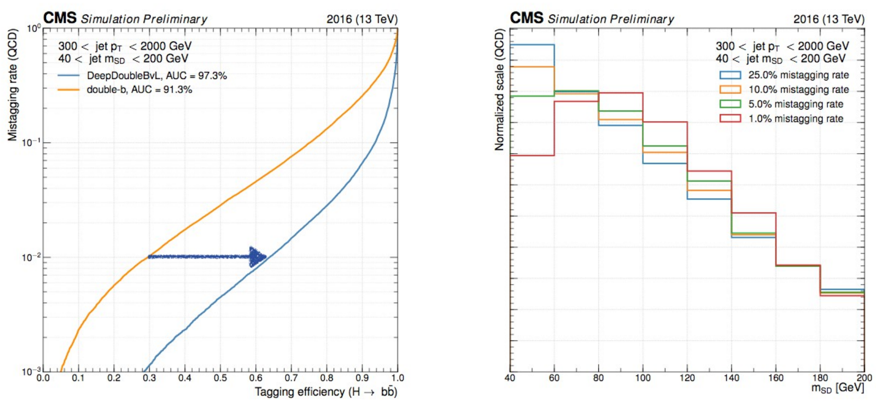




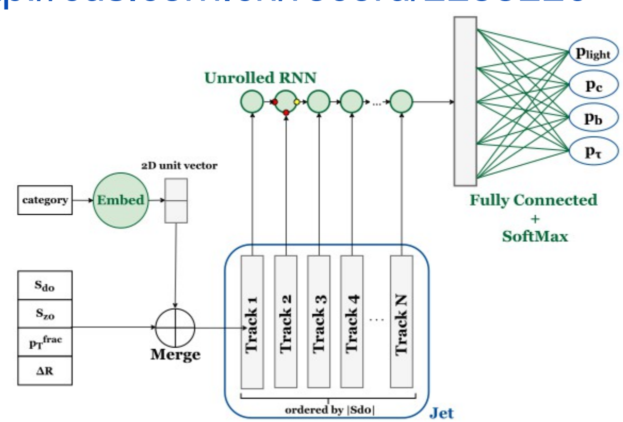
QCD-Aware Recursive Neural Networks for Jet Physics.
https://arxiv.org/abs/1702.00748

DP-2018/033 DEEP DOUBLE-B TAGGER

- Large performance gain over BDT
- Default algorithm still "learns" the mass ⇒ mass sculpting



B-Jet with Recurrent Neural Networks
http://cds.cern.ch/record/2255226



Possible loss of information with image representation.
Choice on ordering with sequence representation.

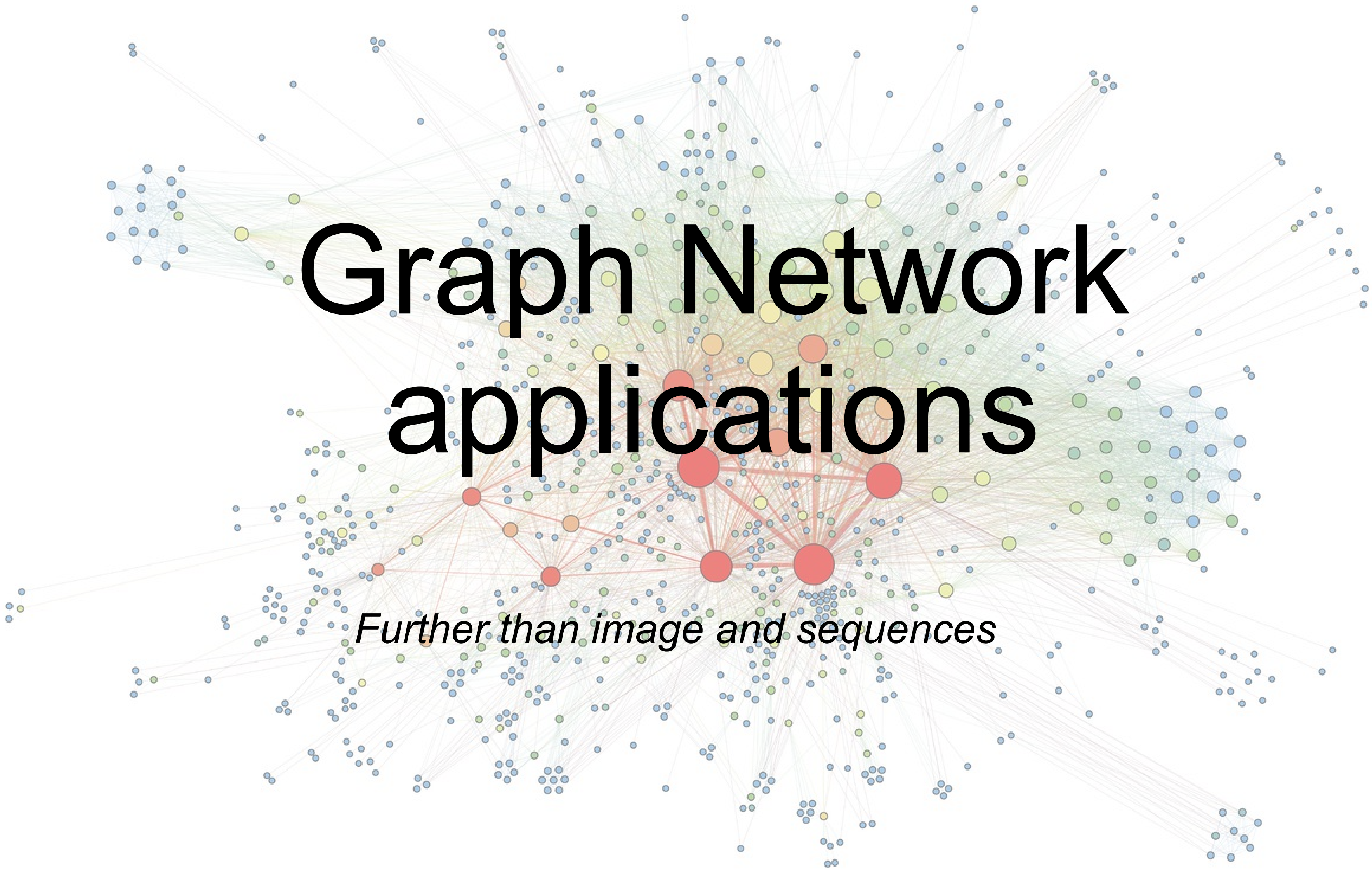
<u>Take home message :</u>

An event is a snapshot of the hints left by thousands to tens of thousands of particles.

Particle identification is mostly a pattern recognition task.

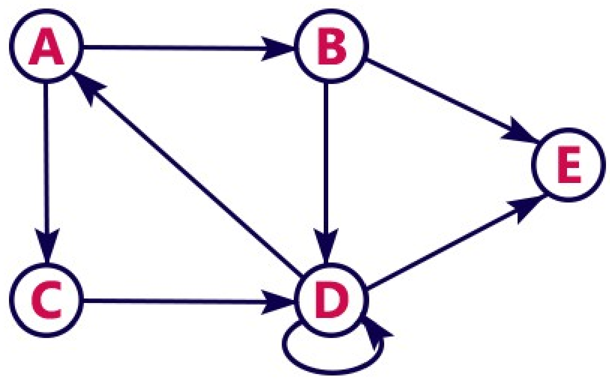
Graph-like data representation seems natural at many level.

Graph Network applications



Further than image and sequences

Forewords on Graph



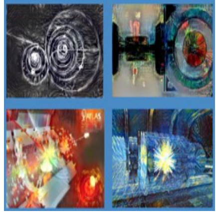
$$\begin{array}{c c} & \begin{array}{ccccc} A & B & C & D & E \end{array} \\ \begin{array}{c} A \\ B \\ C \\ D \\ E \end{array} & \begin{bmatrix} 0 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \end{array}$$

http://btechsmartclass.com/data_structures/graph-representations.html

A graph is composed of

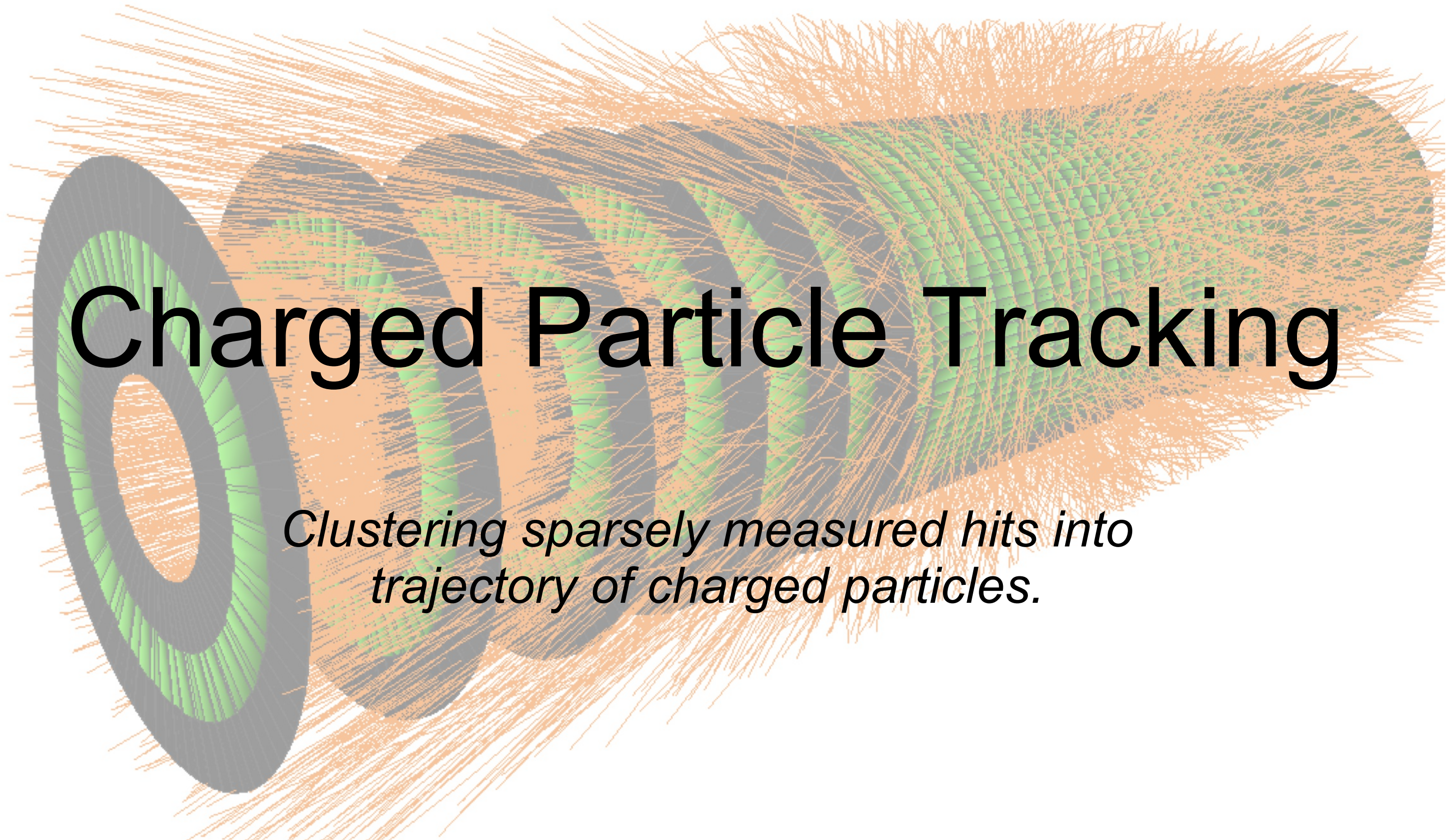
- **Nodes** that can be represented as a vector.
- **Edges** that can be represented with the adjacency matrix.

→ Flowing of information using matrix operations.
→ With machine learning on graphs, edges and nodes might acquire internal representations.



Overview

- **Charged particle tracking**
  Connecting the sparse hits left by particles along trajectory
- **Calorimeter reconstruction**
  Assemble pattern of energy depositions
- **Pile-up mitigation**
  Reducing the impact of concurrent proton-proton interactions
- **Jet Identification**
  Unveil the origin of collimated spray of particles



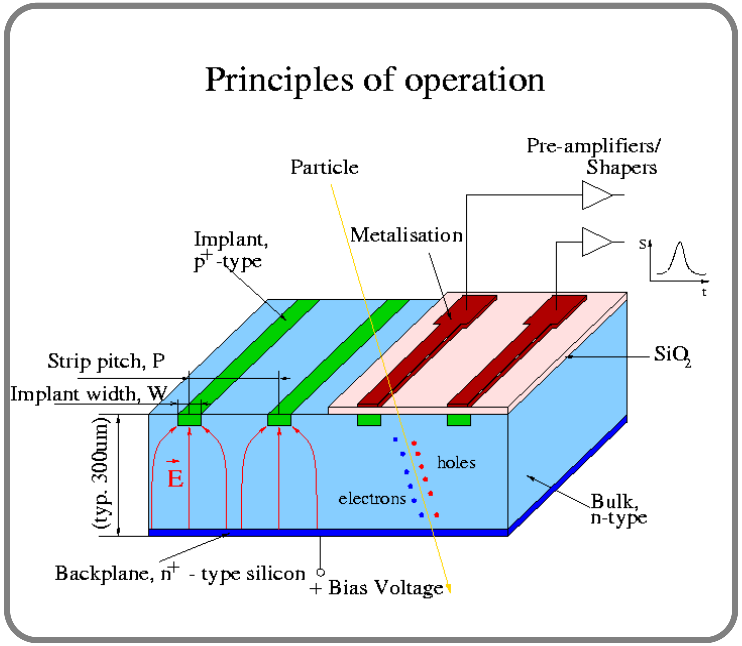
Charged Particle Tracking

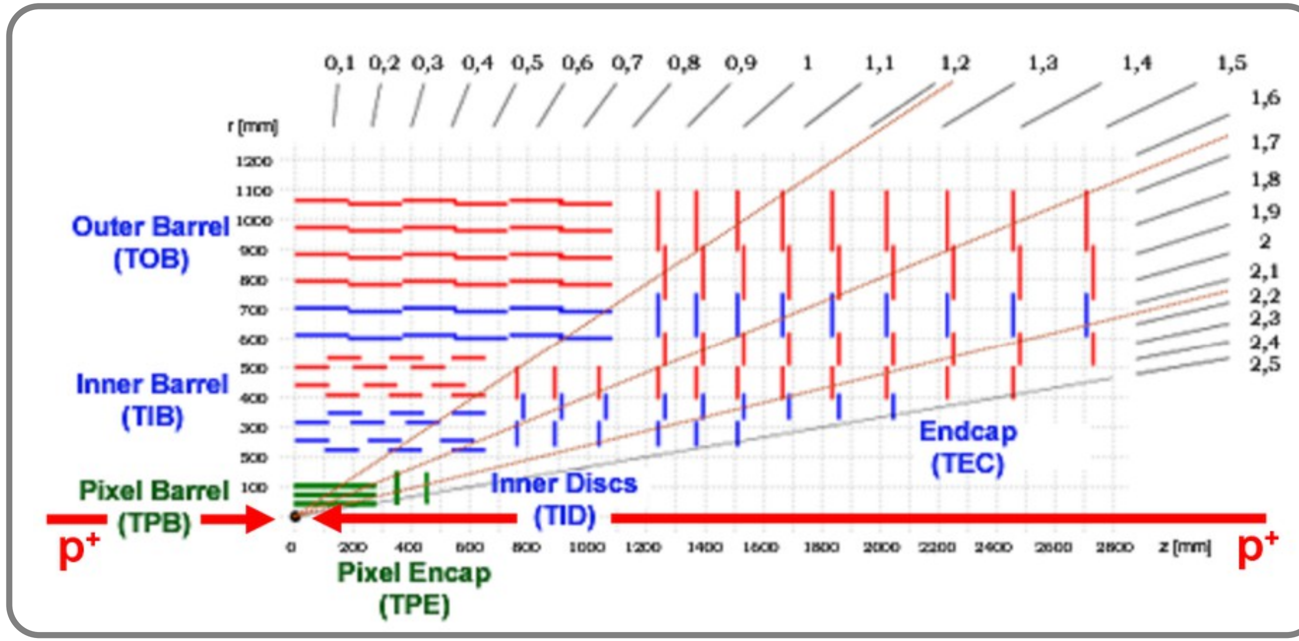
Clustering sparsely measured hits into trajectory of charged particles.

With Steven Farrell, Paolo Calafiura, Mayur Mudigonda, Prabhat, Dustin Anderson, Stephan Zheng, Josh Bendavid, Maria Spiropulu, Giuseppe Cerati, Lindsey Gray, Jim Kowalkowski, Panagiotis Spentzouris, Aristeidis Tsaris, Xiangyang Yu

https://arxiv.org/abs/1810.06111

Tracker – 101

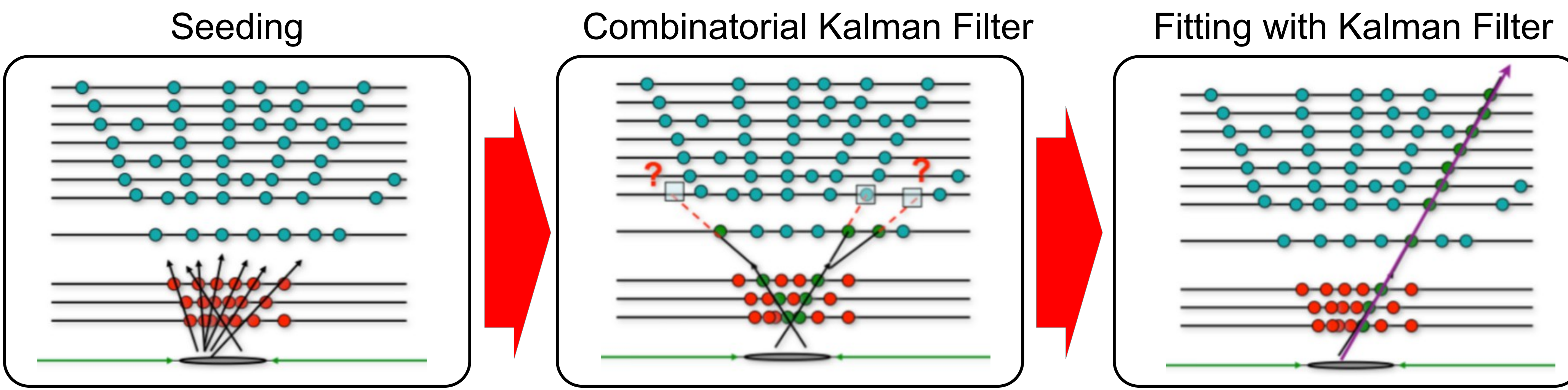




- Ionizing particle leaves a signal in silicon detector
- Sensitive cells with different shape
  - squares : pixel
  - rectangle : strips
- Organized in hermetic layers of modules

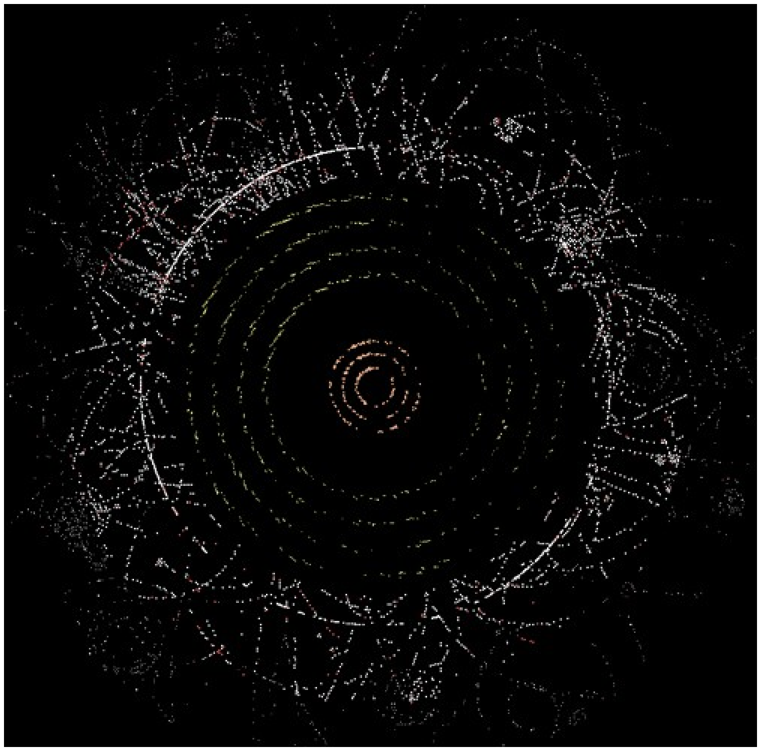
Particle Tracking – 101

- Particle trajectory bended in a solenoidal magnetic field
  - Curvature is a proxy to momentum
- **Thousands of sparse hits**
- Hits pollution from low momentum, secondary particles

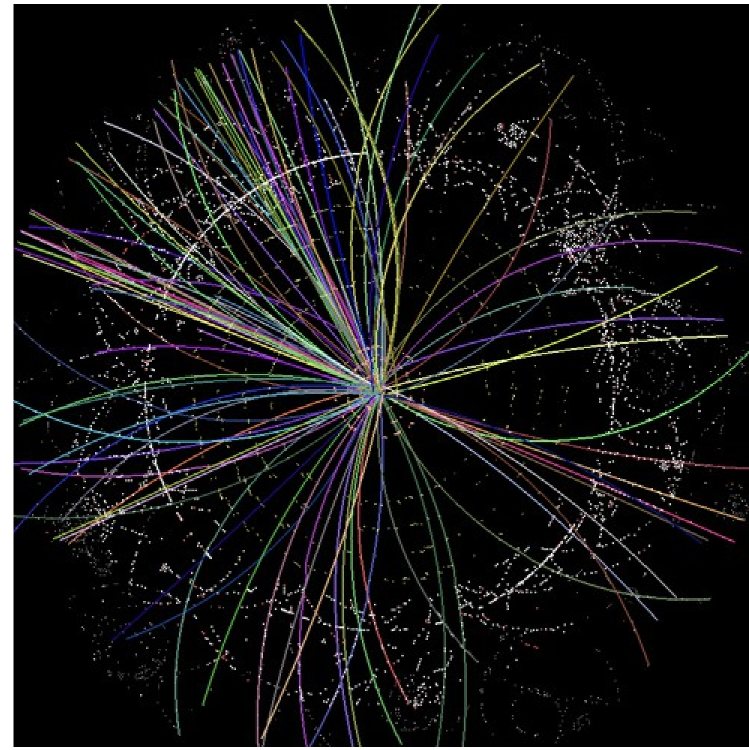


- **Explosion of hit combinatorics** in both seeding and stepping pattern recognition
- **Highly computing consuming task** in extracting physics content from LHC data

Name of the Game



From hits ...



... to trajectory & parameters

Other ML Solutions

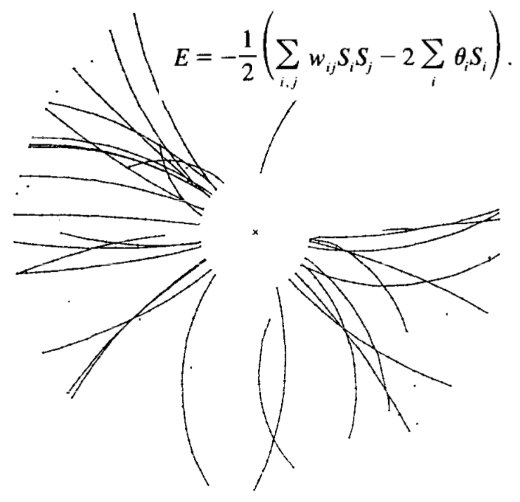
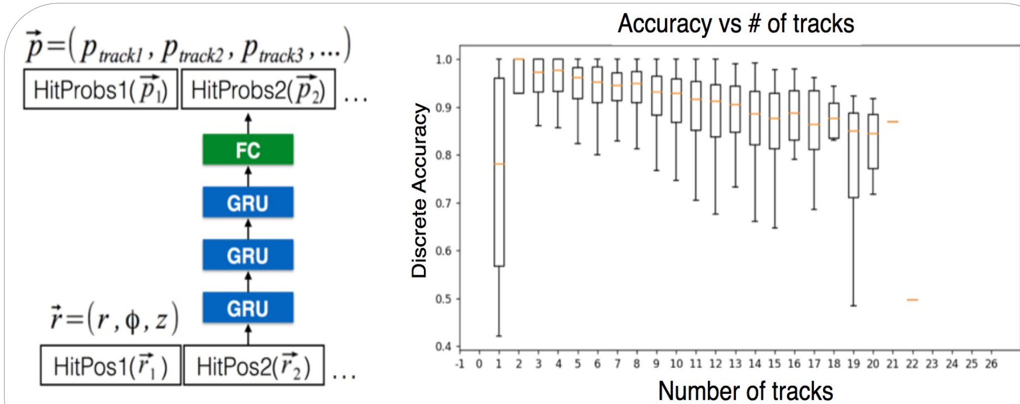
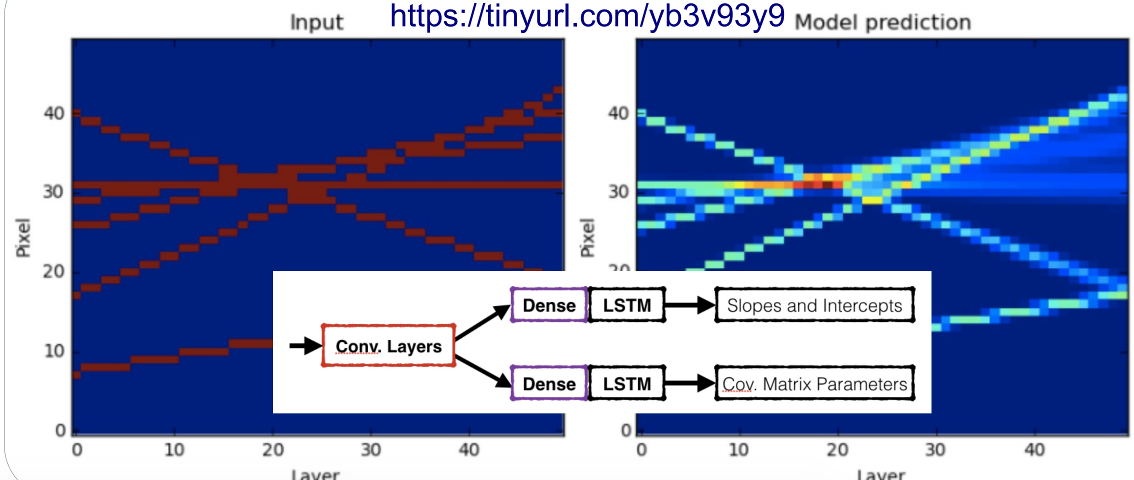


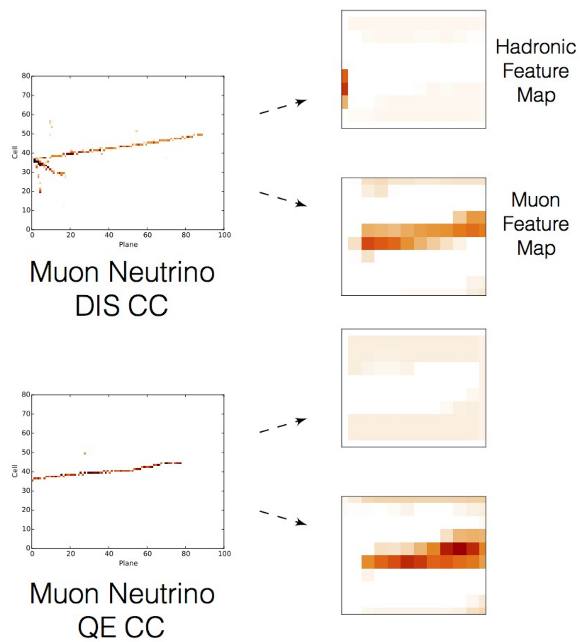
Fig. 4. Tracks in the ALEPH TPC reconstructed with a Hopfield net [13]. https://tinyurl.com/y9swquw6



End-to-end hit assignment

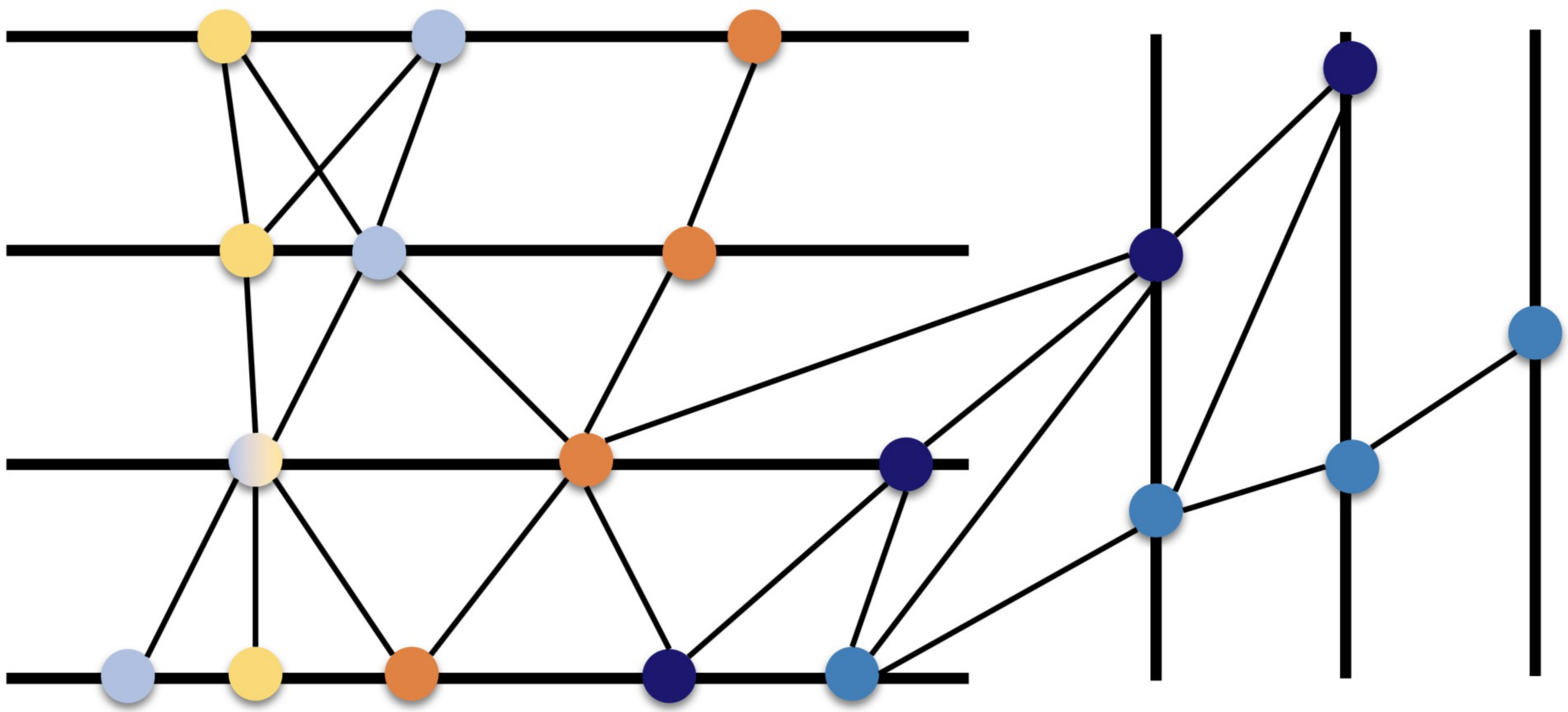
https://tinyurl.com/yb3v93y9





https://arxiv.org/abs/1604.01444

Tracker Hit Graph

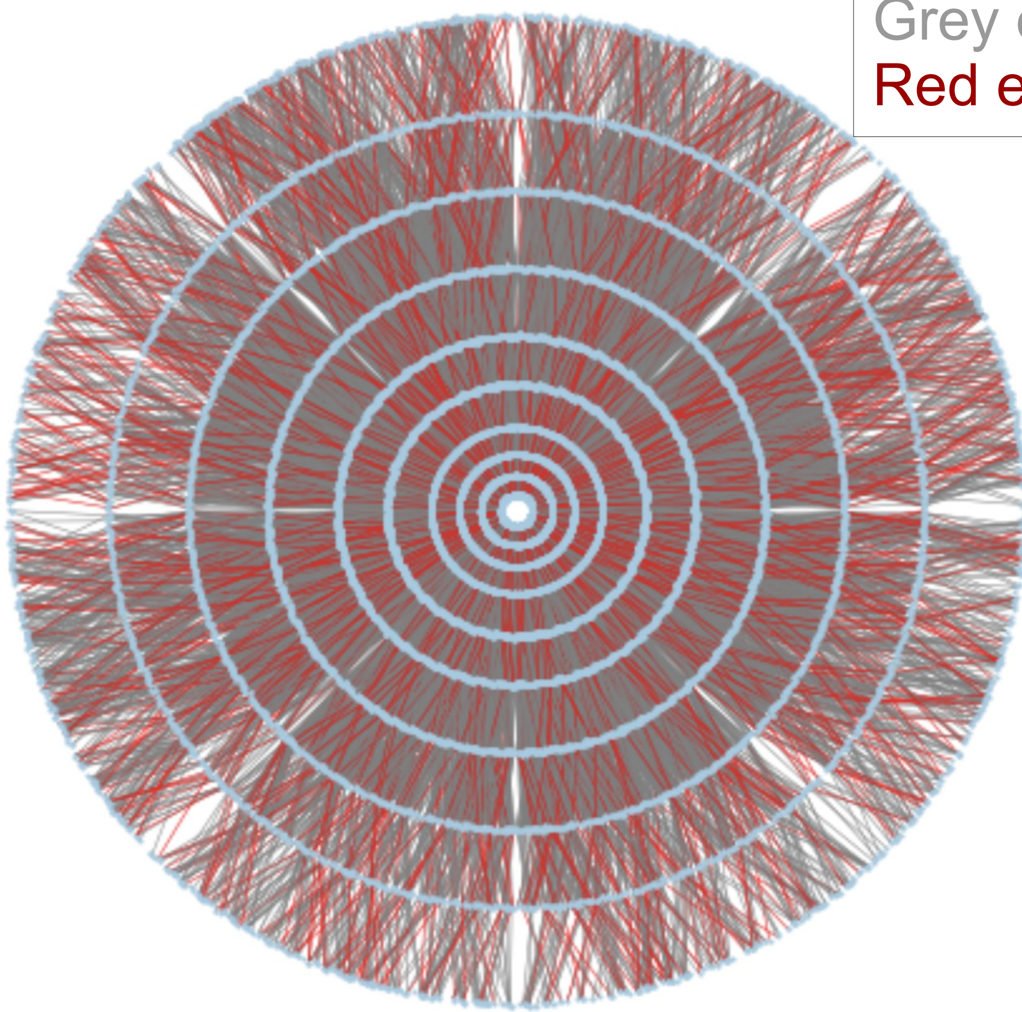


Graph construction

- One tracker hit ≡ one node
- Sparse edges constructed from geometrical consideration

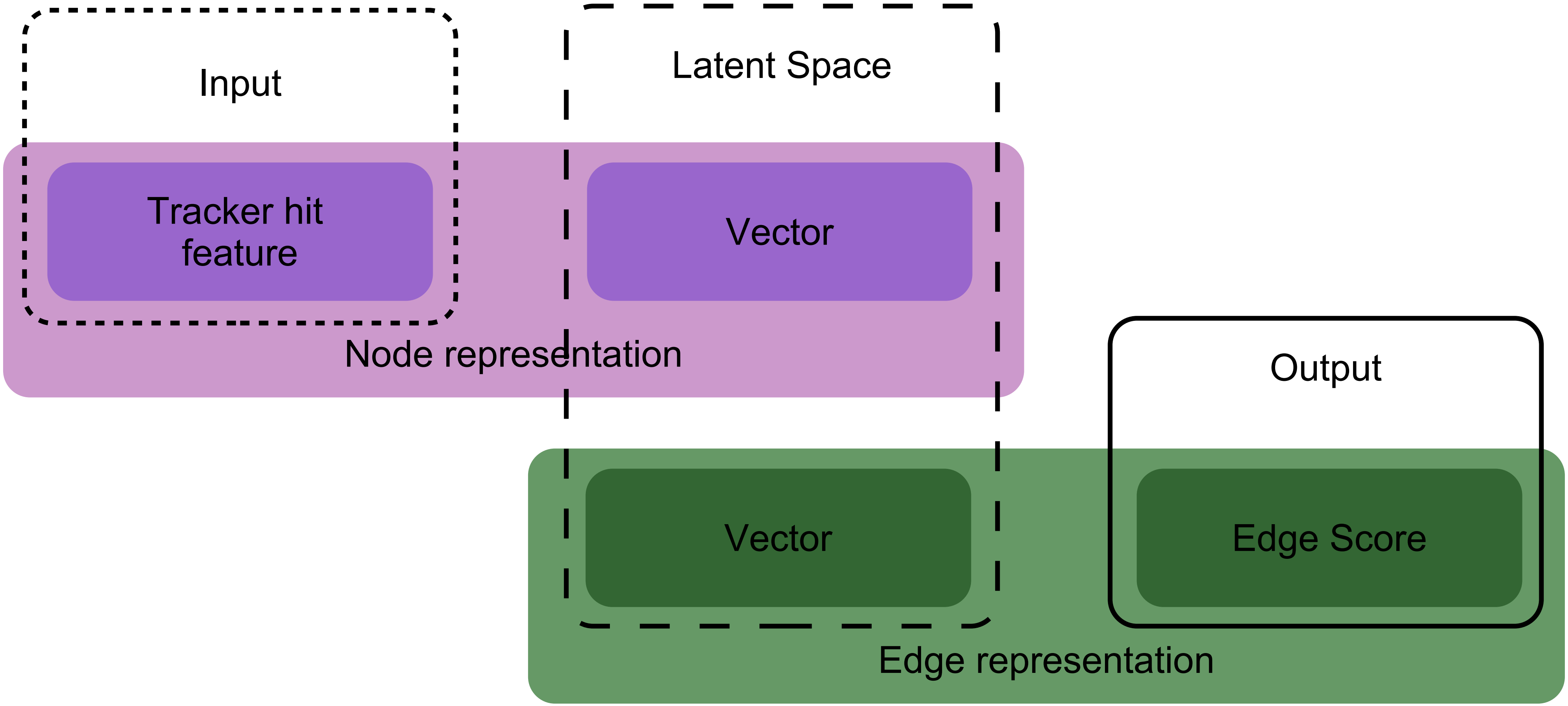
➔ Edge classification ≡ reconstructing the trajectory of particles

Edge Classification



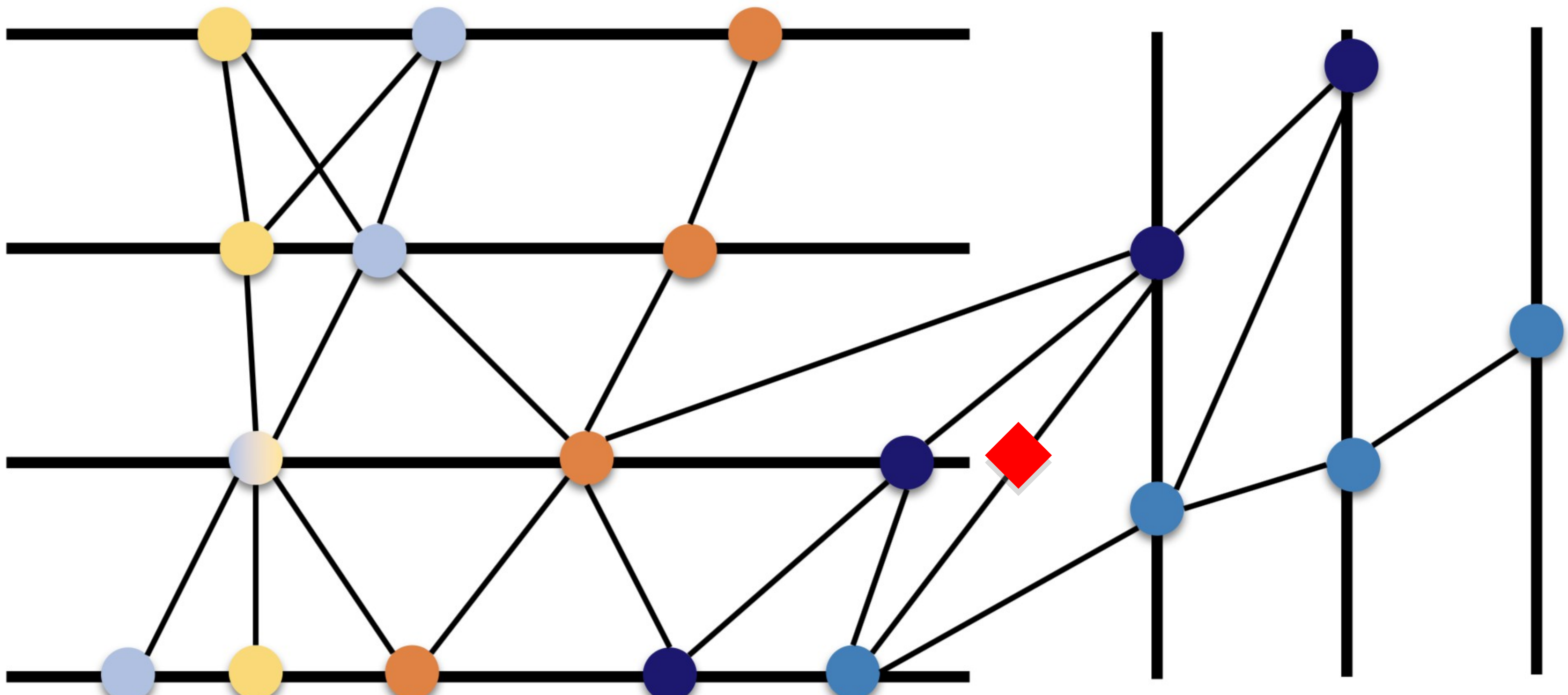
Grey edge: fake
Red edge : true

Node & Edge Representations



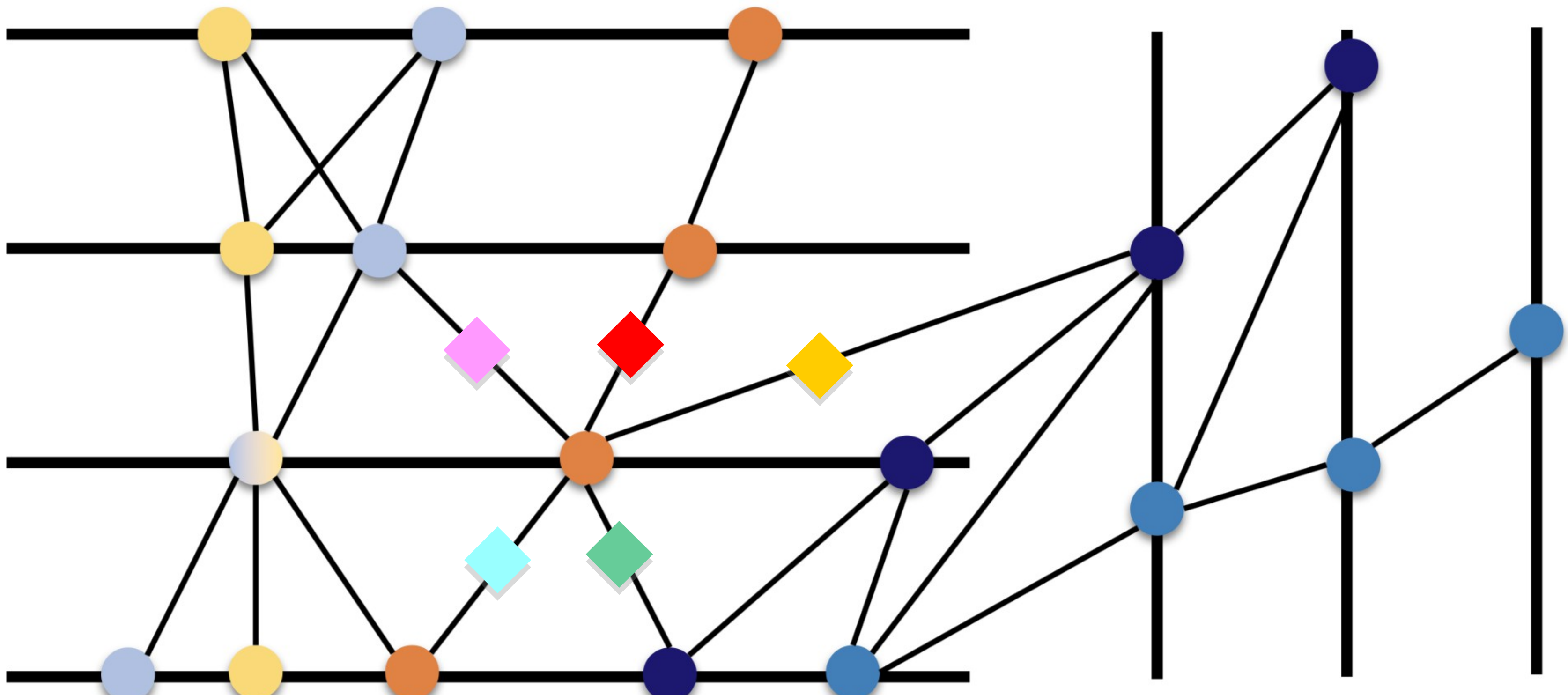
Edge representation is not the edge score.
Final edge score extracted from the latent edge representation.

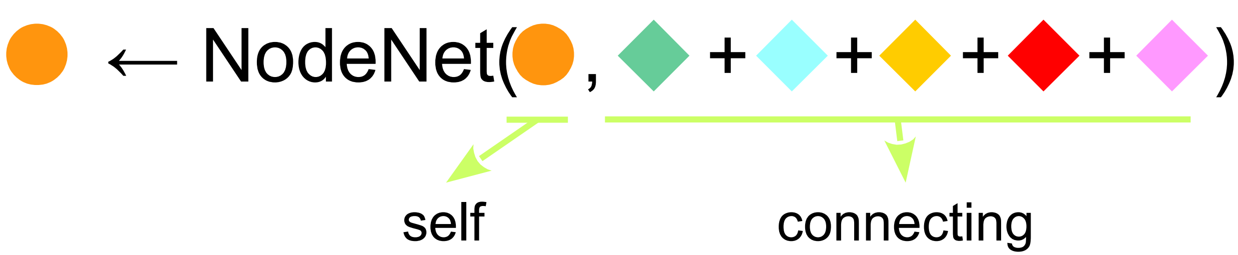
Edge Network



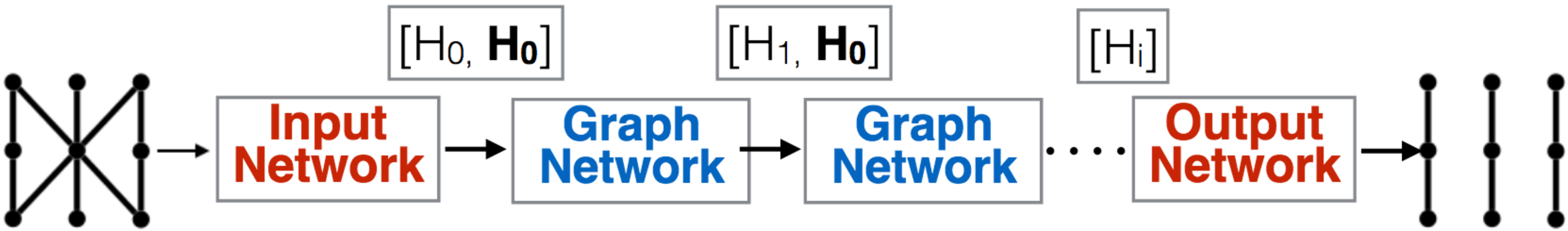
◆ ← EdgeNet(●,●)

Node Network





Message Passing Model

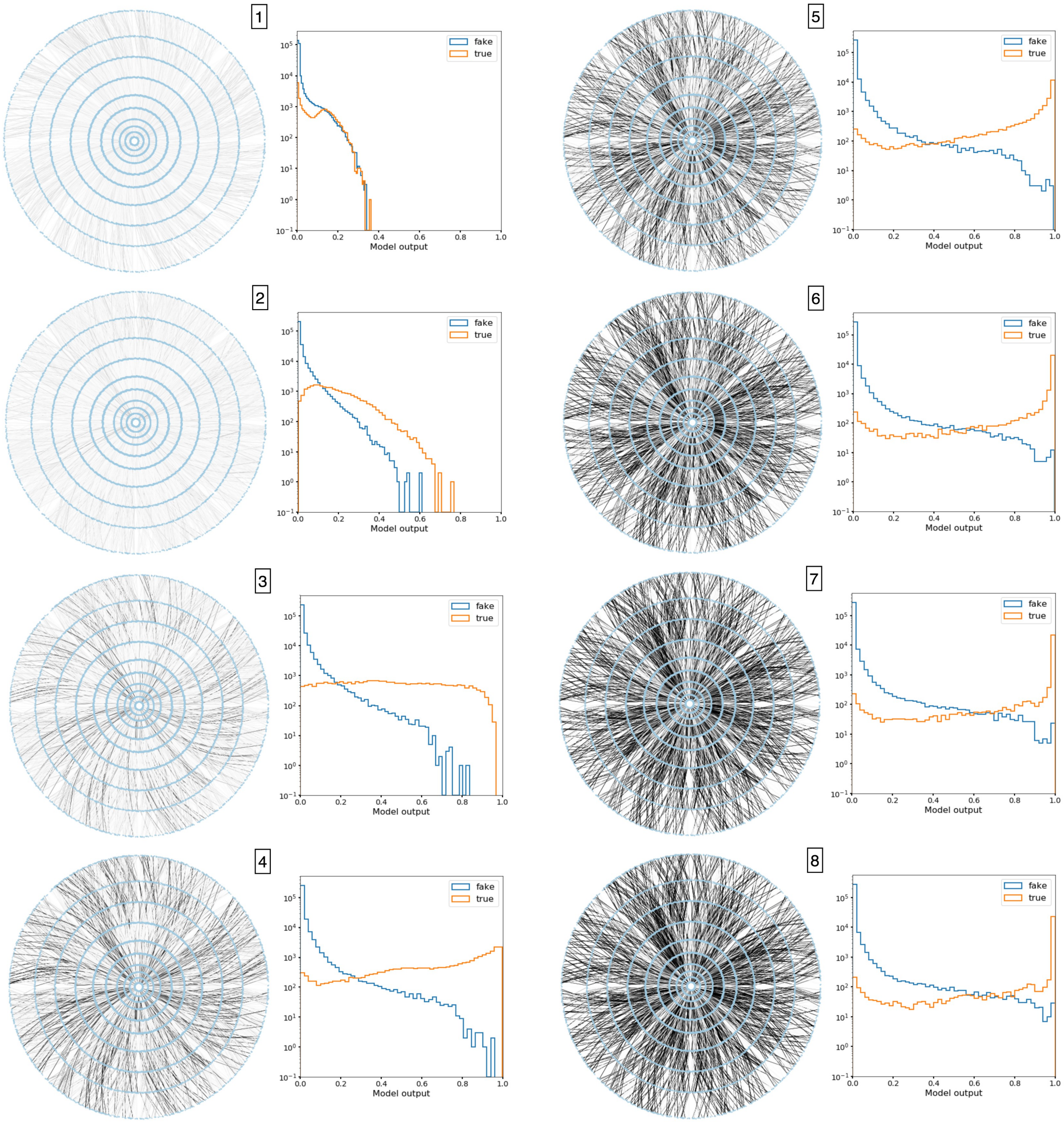


- Graph is sparsely connected from consecutive layers
- Edge representation computed from features at the ends
- Node representation computed from the sum over all connected edges

→ Correlates hits information through multiple (8) iterations of (Graph Network)

→ Uses https://github.com/deepmind/graph_nets TF library

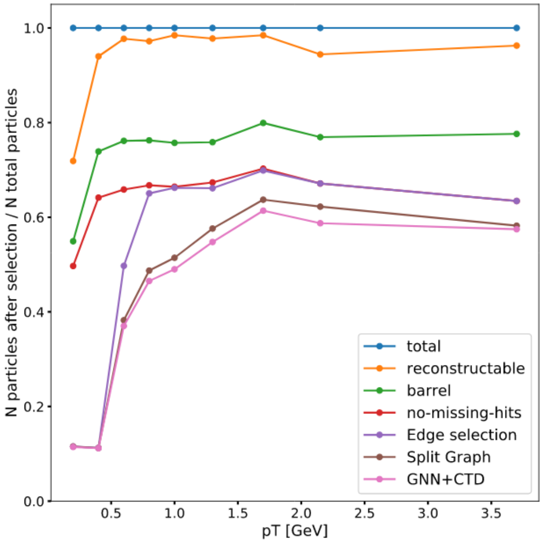
Information Flow



- Checking edge score after each step of graph network.
- Effective output of the model is in step 8.
- Full track hit assignment learned in last stages of the model.
- Tracklets learned in intermediate stages.

Performance

one-event	N-particles	ratio w.r.t Total	ratio w.r.t Reconstructable	relative ratio
Total	11170	100%		100%
Reconstructable	9635	86%	100%	86%
Barrel	7492	67%	78%	78%
No-missing hits	6600	59%	69%	88%
Edge selection	3114	28%	32%	**47%**
Split graph	2668	24%	28%	**86%**
GNN	2590	23%	27%	**97%**



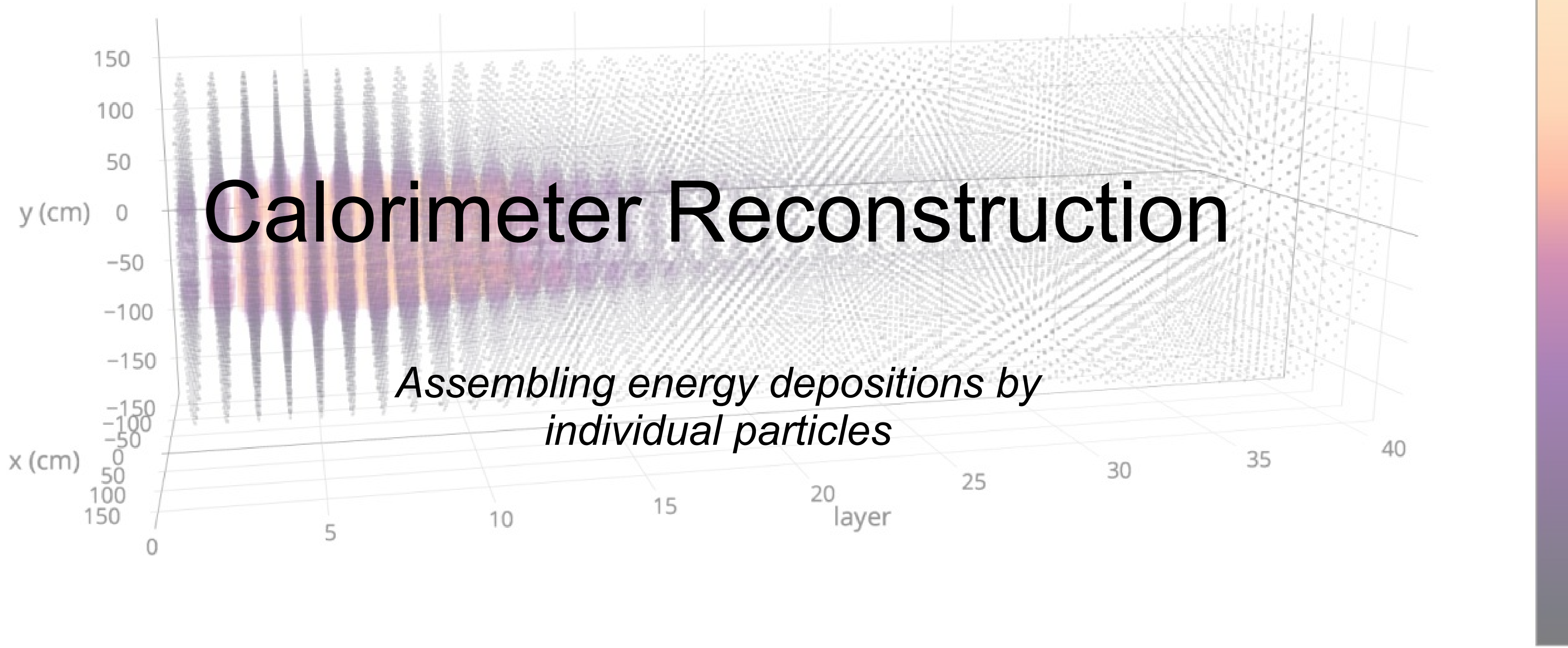
- Tracks formed with a simple algorithms that traverse the hit graph over high-score edges.

→ Promising performance, once passed acceptance cut for training purpose

Remarks

- *The construction of the graph can limit the type of tracks that can be found.*
- *Over-connectivity produces highly unbalanced classes (many more fake edges than true).*
- *Computation graph can become cumbersome if the sparsity is not taken into account.*
- *What have we done with the Physics knowledge of particle dynamic ?*
- *Promising results but no solution yet ; stay tune for results from Exa.trkX.*

https://github.com/HEPTrkX/heptrkx-gnn-tracking
https://github.com/xju2/heptrkx-gnn-tracking

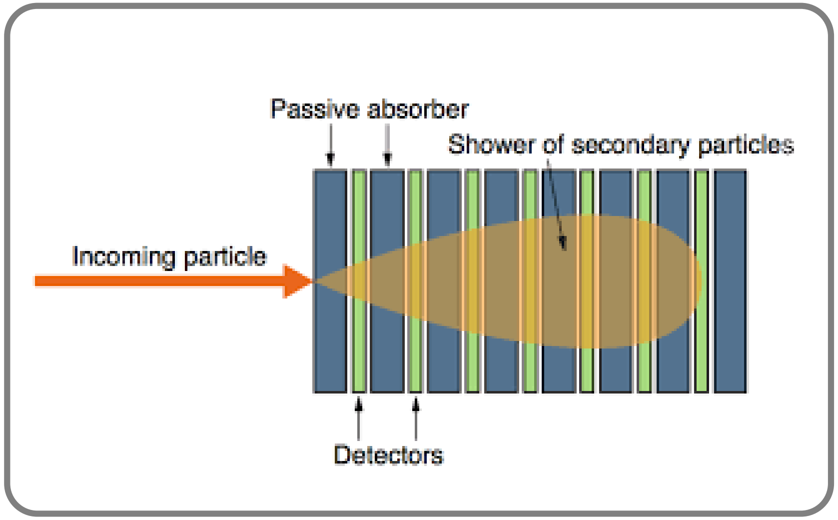


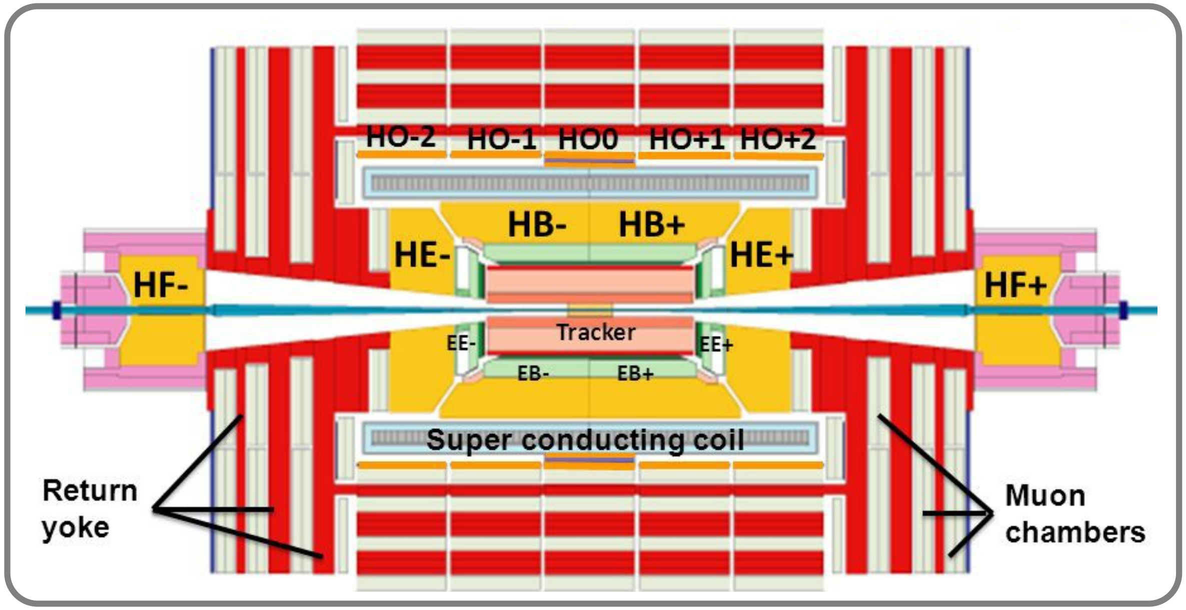
Calorimeter Reconstruction

Assembling energy depositions by individual particles

***by** Shah Rukh Qasim, Jan Kieseler, Yutaro Liyama, Maurizio Pierini*
https://arxiv.org/abs/1902.07987

Calorimetry – 101

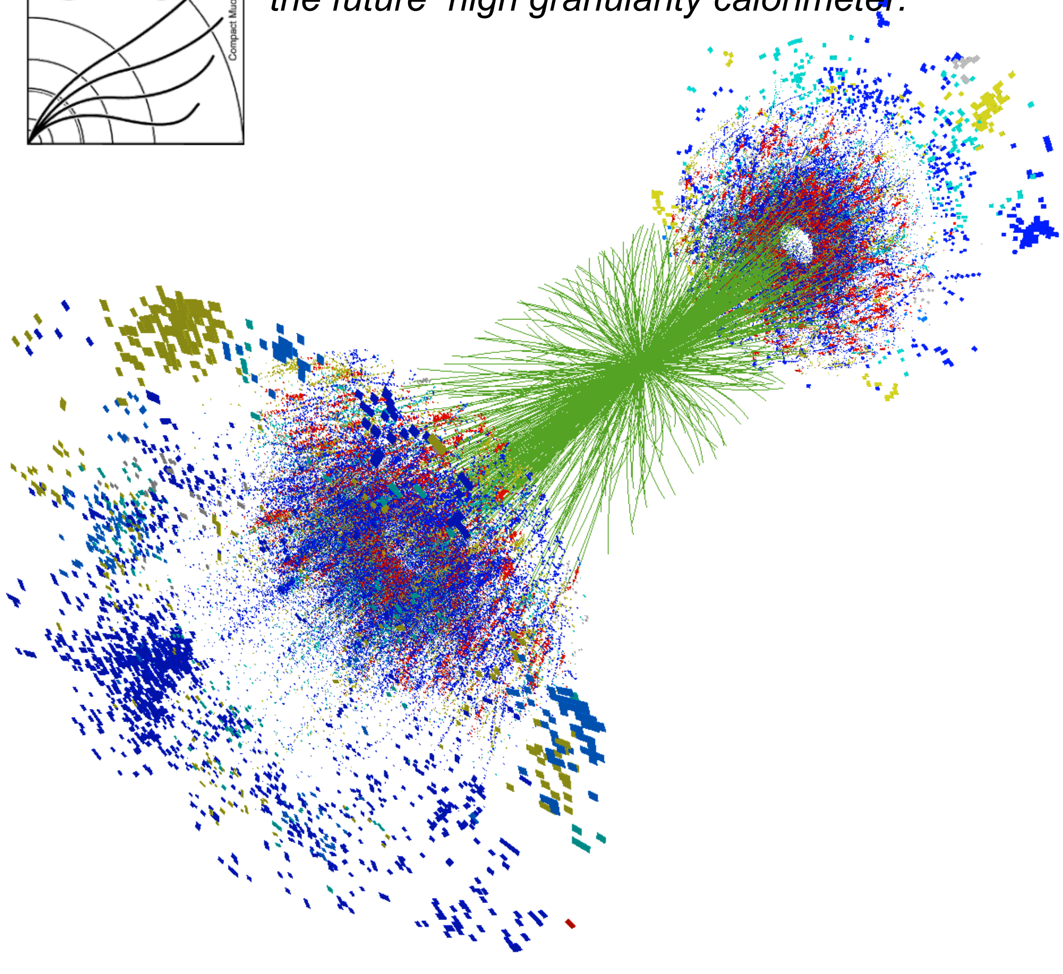




- Induced particle shower through material
- Destructive/stopping interaction with matter
- Sensitive cells measure properties of secondary particles
- Multiple technology available for sensitive material
- Assembled to hermetically cover most of all particles

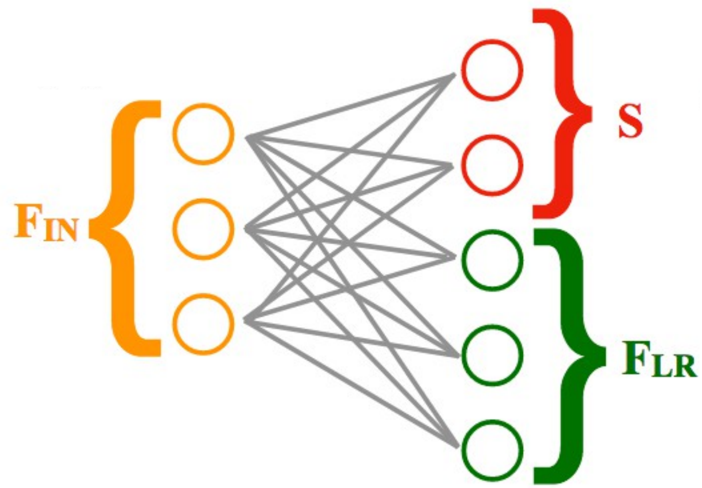
Name of The Game

Ground truth color coded event display of the future high granularity calorimeter.



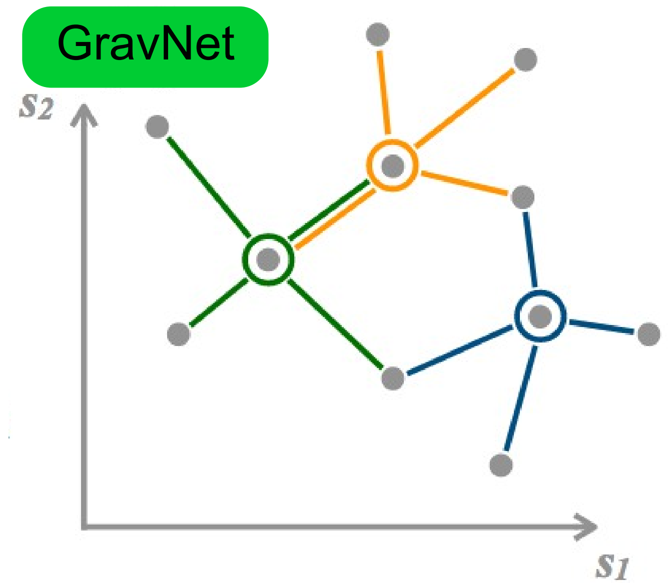
Associate each energy deposition from the secondary particles to their primary particle

Feature Encoding



The calorimeter cell features are transformed into a **locations/distances** interpreted in some abstract space and an **internal representation**, using a fully connected network.

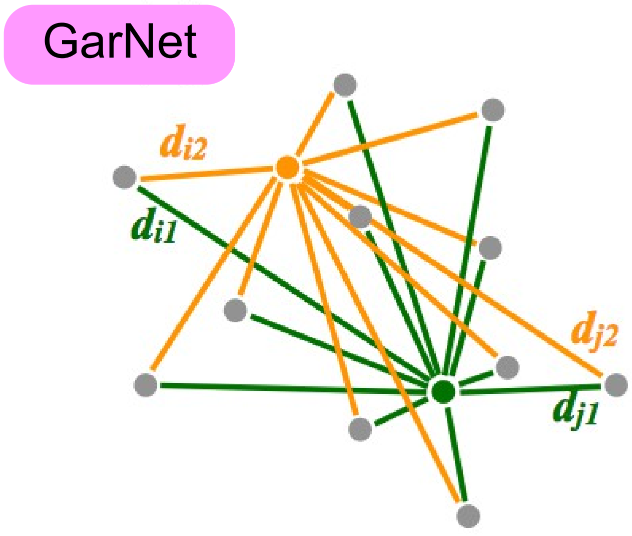
Abstract Space – GravNet



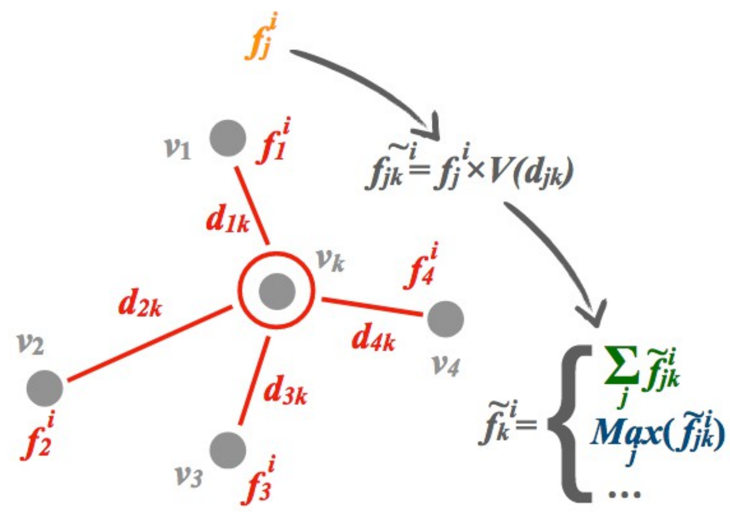
GravNet: graph defined from N nearest neighbours using **S** as location in abstract space.

Abstract Space – GarNet

GarNet: graph defined with extra nodes using **S** as distance to attractors in abstract space.

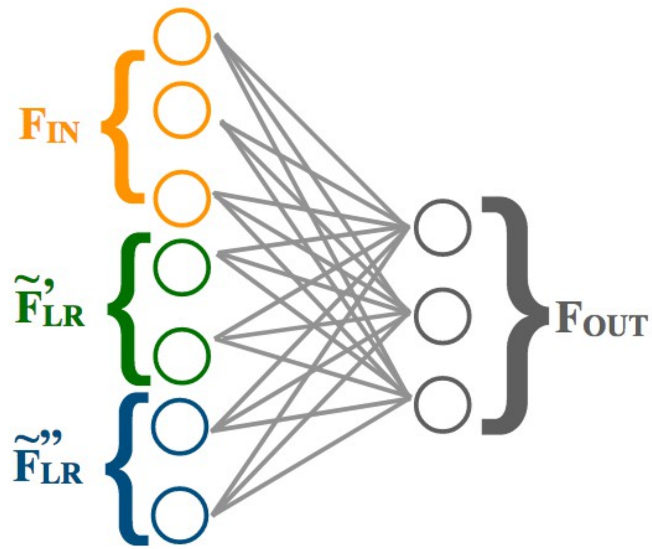


Internal Representation



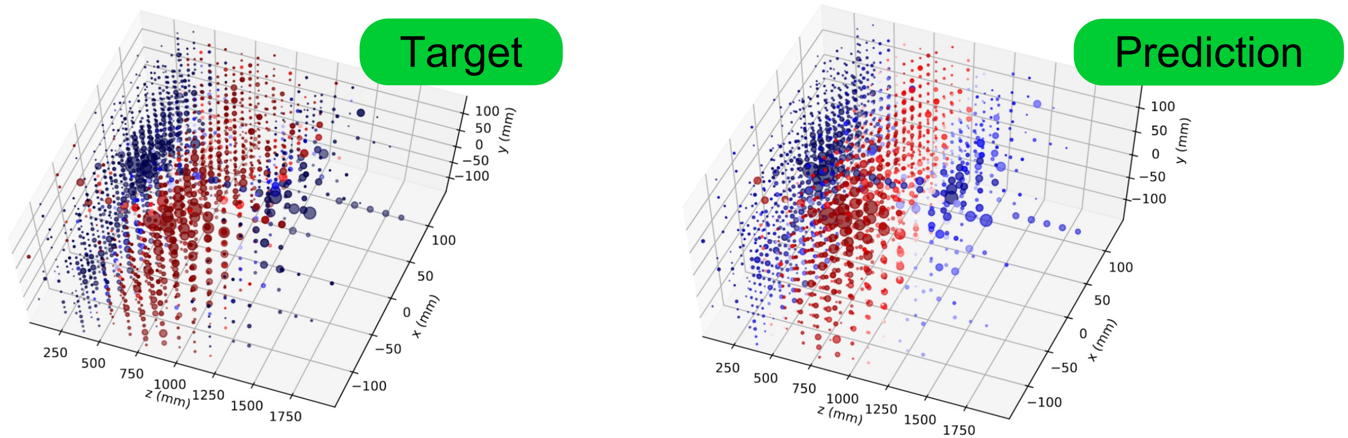
The internal representation are weighted using a potential of the distances through each edge (**V(d$_{jk}$)**), and new representation is calculated from **the mean** or **the max**.

Feature Extraction



Prediction are extracted per calorimeter cell, from **initial features** and gathered **internal representations**, using a fully connected network.

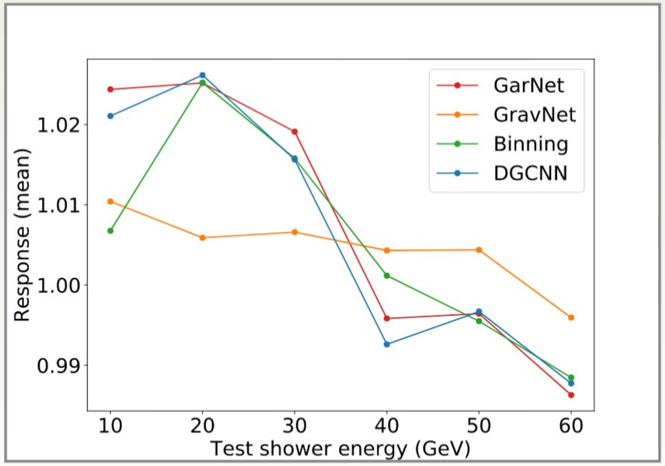
Performance

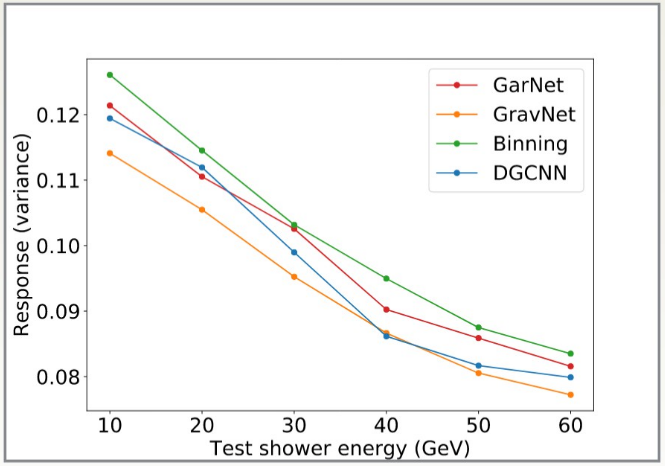


Overlapping showers from two charged pions.

- Focus on the overlap region, only (20-80 % overlap)
- Define energy response

$$R_k = \frac{\sum_i E_i p_{ik}}{\sum_i E_i t_{ik}}$$





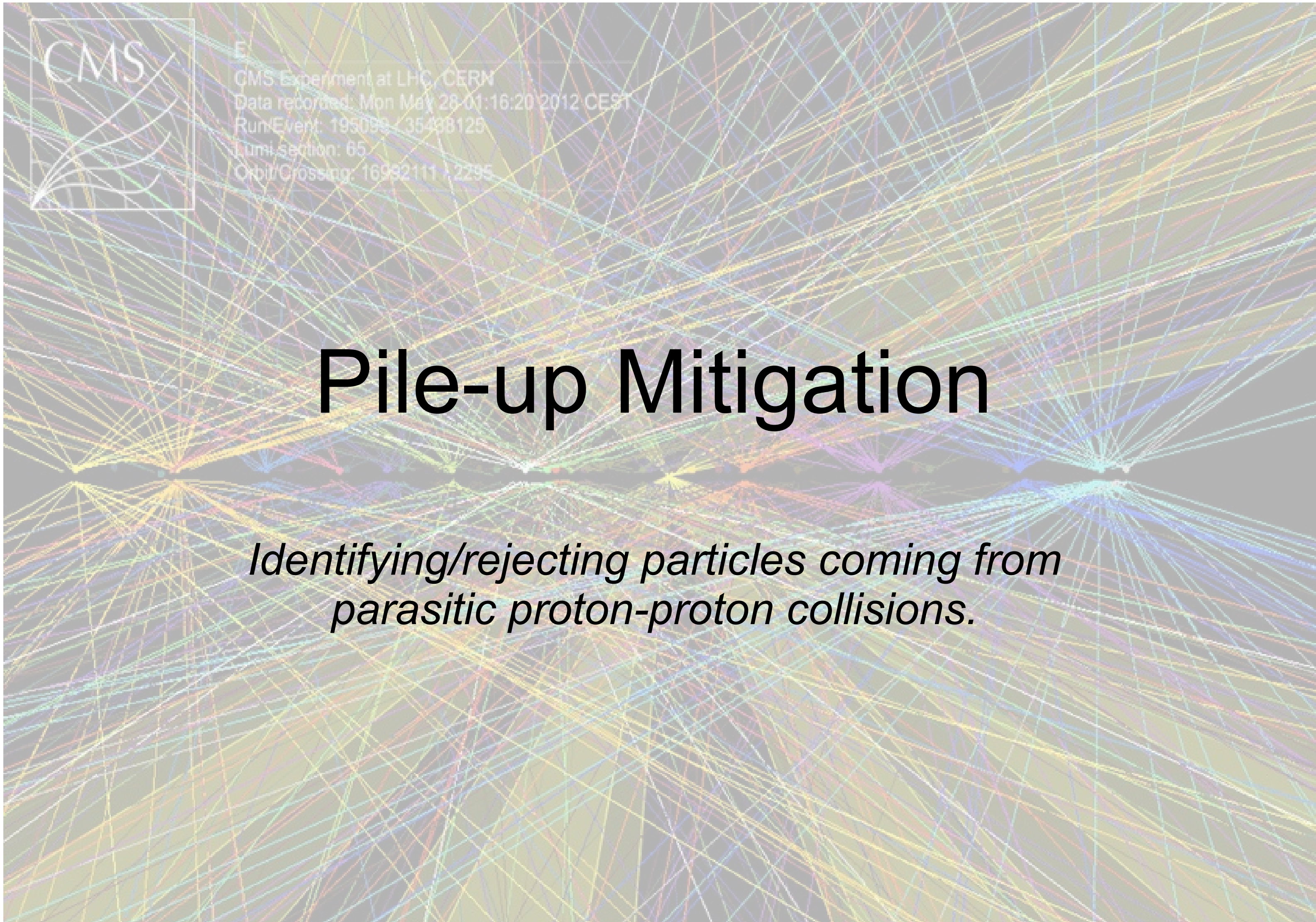
- The graph network based approaches outperform the CNN approach
- The GravNet model outperforms all approaches

Slide J.Kieseler

Remarks

- *Graph representation seems to be appropriate for calorimeter with complex geometry.*
- *Graph connections may be dynamic (k-nn) as long as the computation graph remains differentiable.*
- *Node representation interpreted in abstract space to match the needs.*
- *People are also working on “Edge classification” models*
- *What have we done with the Physics knowledge of particle shower dynamic ?*

https://github.com/jkiesele/caloGraphNN

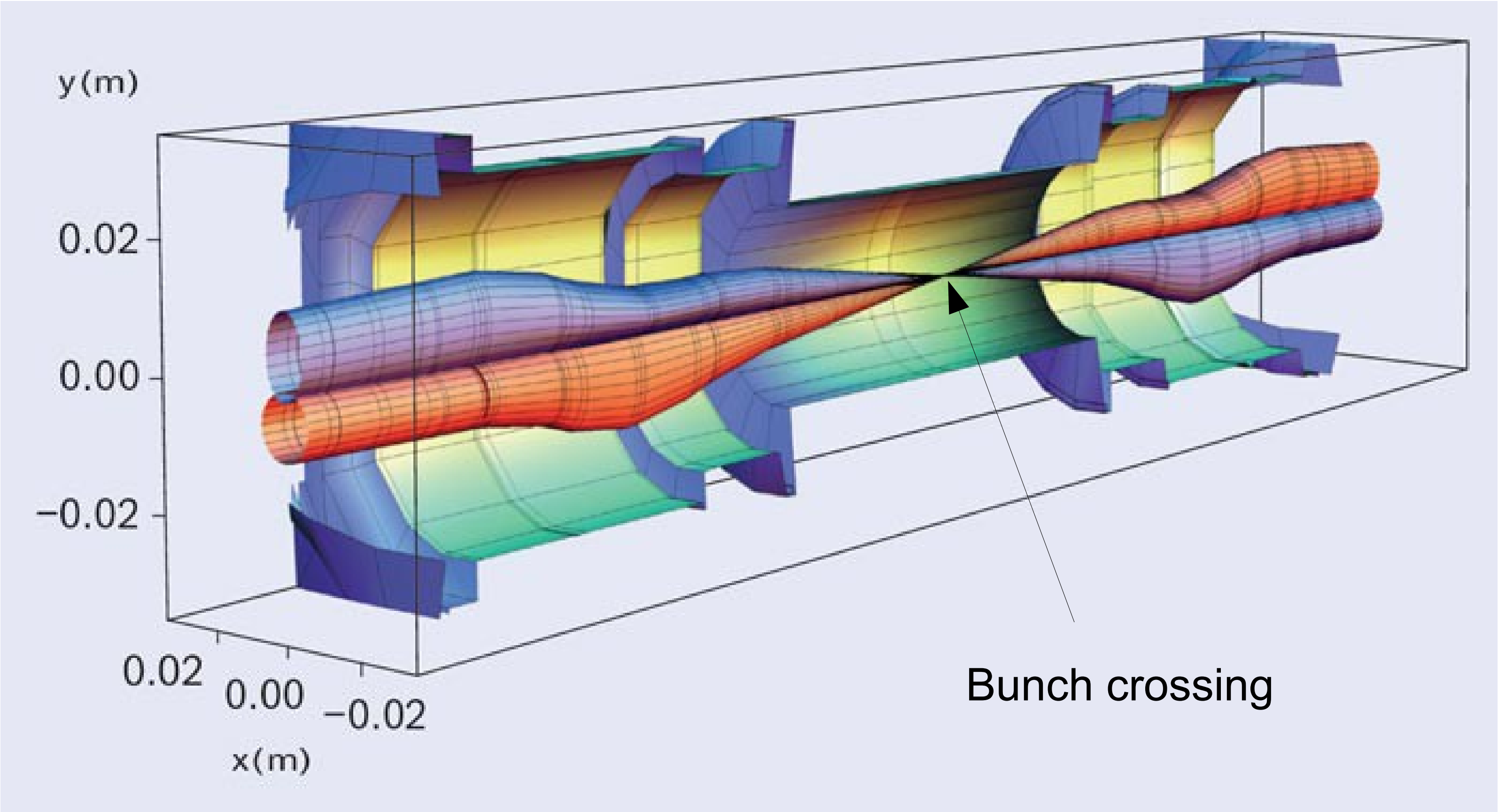


Pile-up Mitigation

Identifying/rejecting particles coming from parasitic proton-proton collisions.

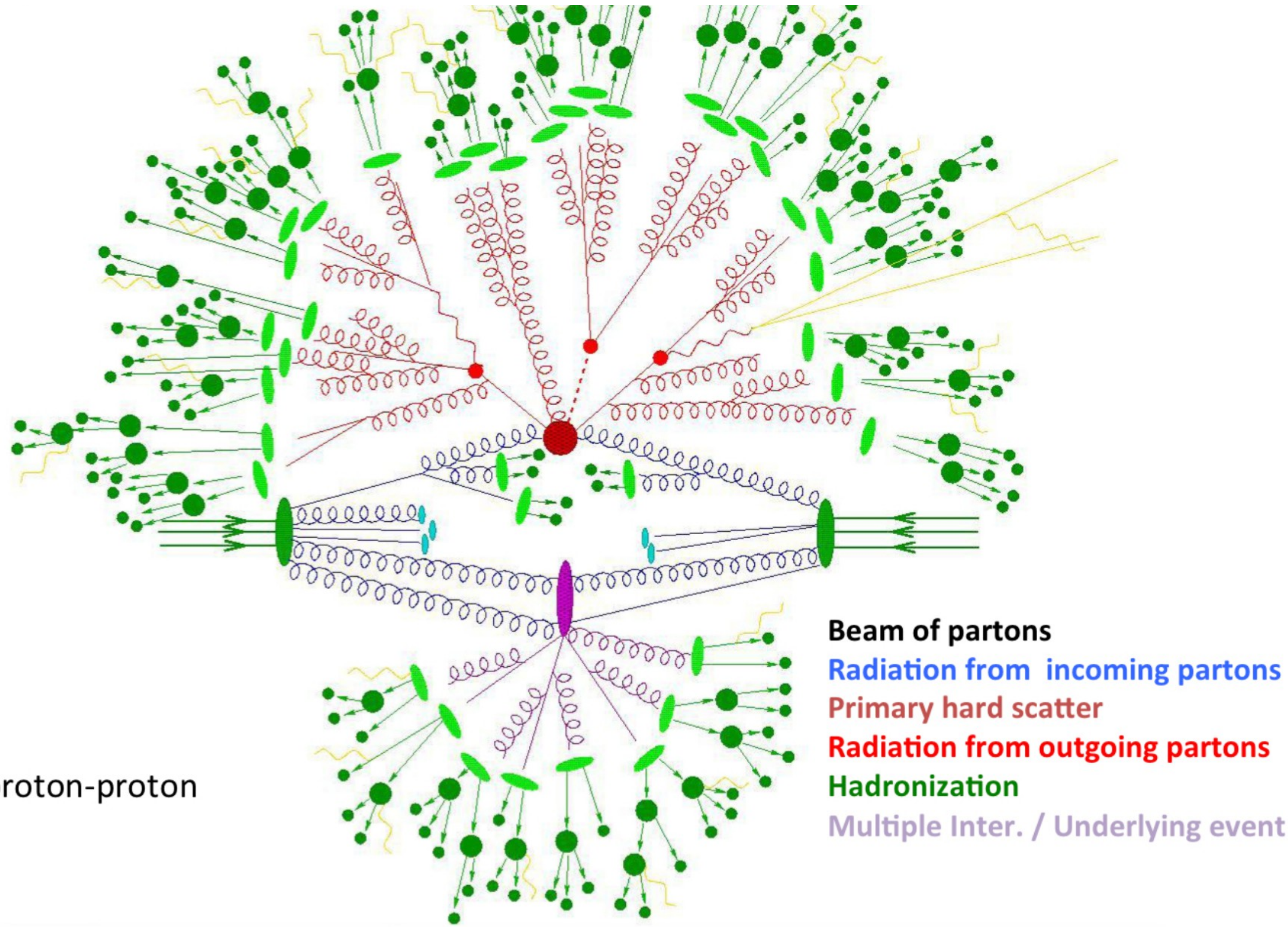
With Jesus Arjona Martinez, Olmo Cerri, Maurizio Pierini, Maria Spiropulu
https://arxiv.org/abs/1810.07988

Bean Crossing – 101



- Rate of interactions can be driven up
  - Bunch crossing every 25 ns (40MHz)
  - Density of protons per bunch
- Concurrent interactions is the simplest route for increased rate of interactions

Pileup – 101

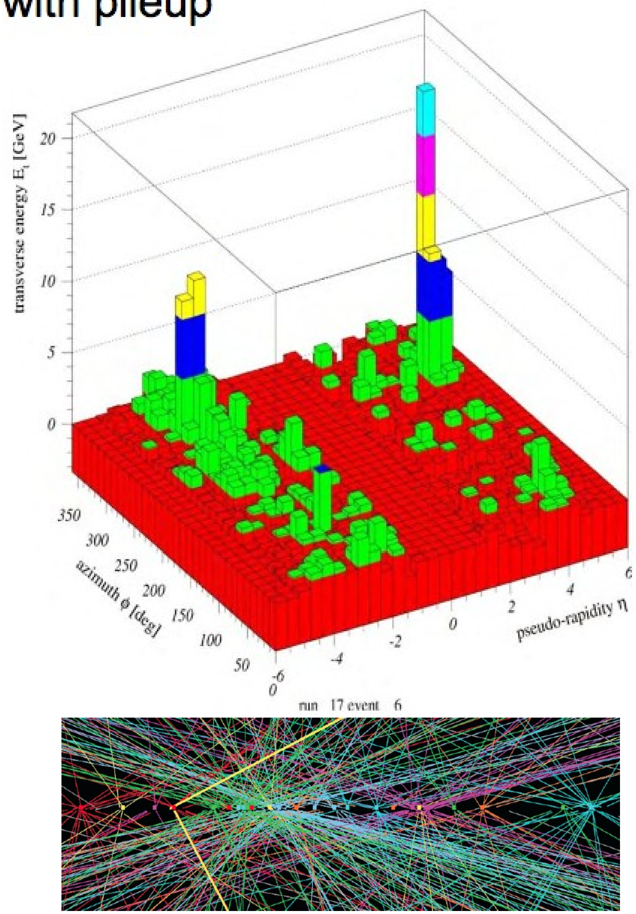


Typical proton-proton collision

Bunch crossing every 25 ns / 40MHz ≡ one event.
Multiple collisions per bunch (pile-up) for increased probability.
200 averaged pileup in the horizon 2025.

Name of the Game

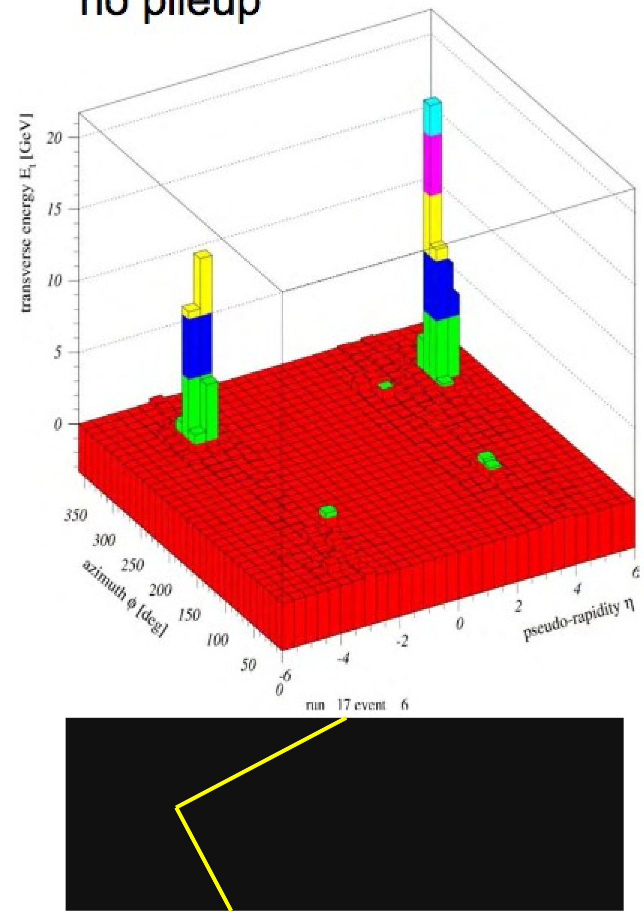
with pileup



Neutral hadron?

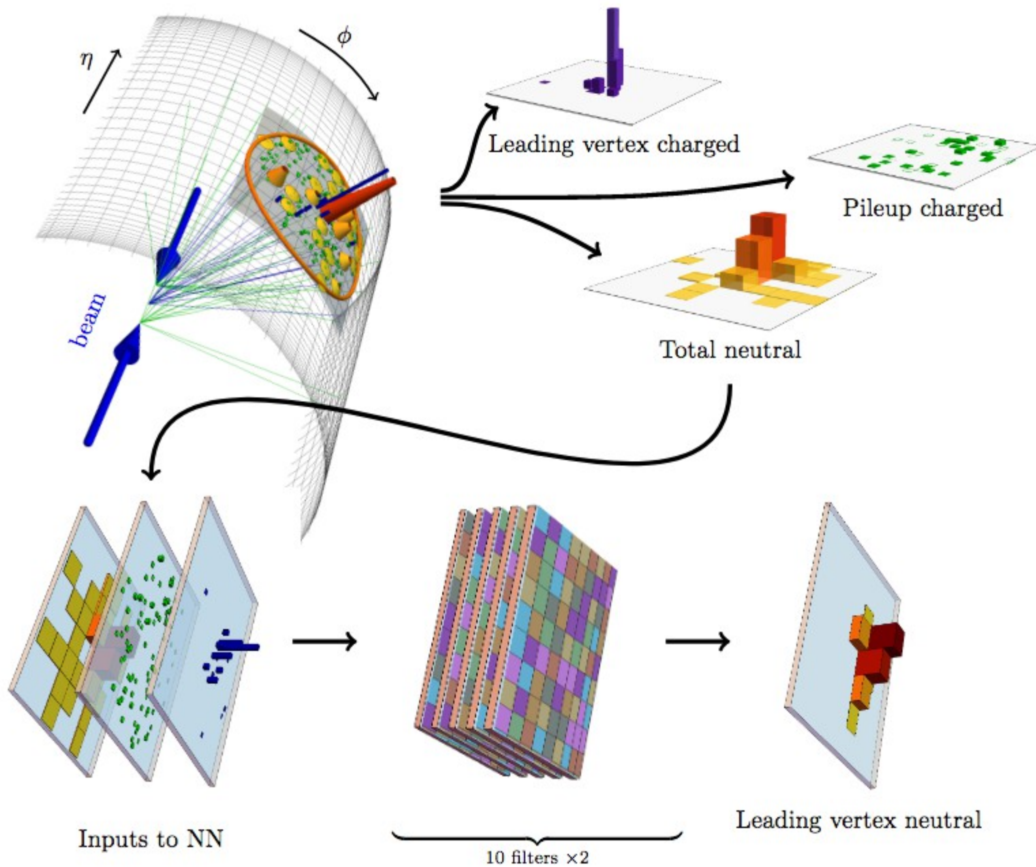
Charged hadron removed using track/vertex

no pileup



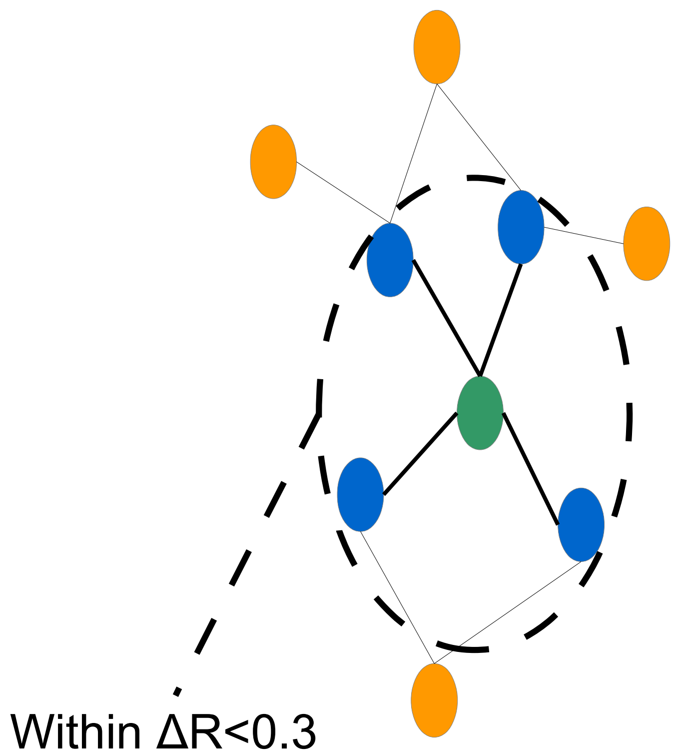
Identify & remove the contribution of **neutral particles** coming from parasitic interactions.

Other ML Solutions



PUMML
https://arxiv.org/abs/1707.08600

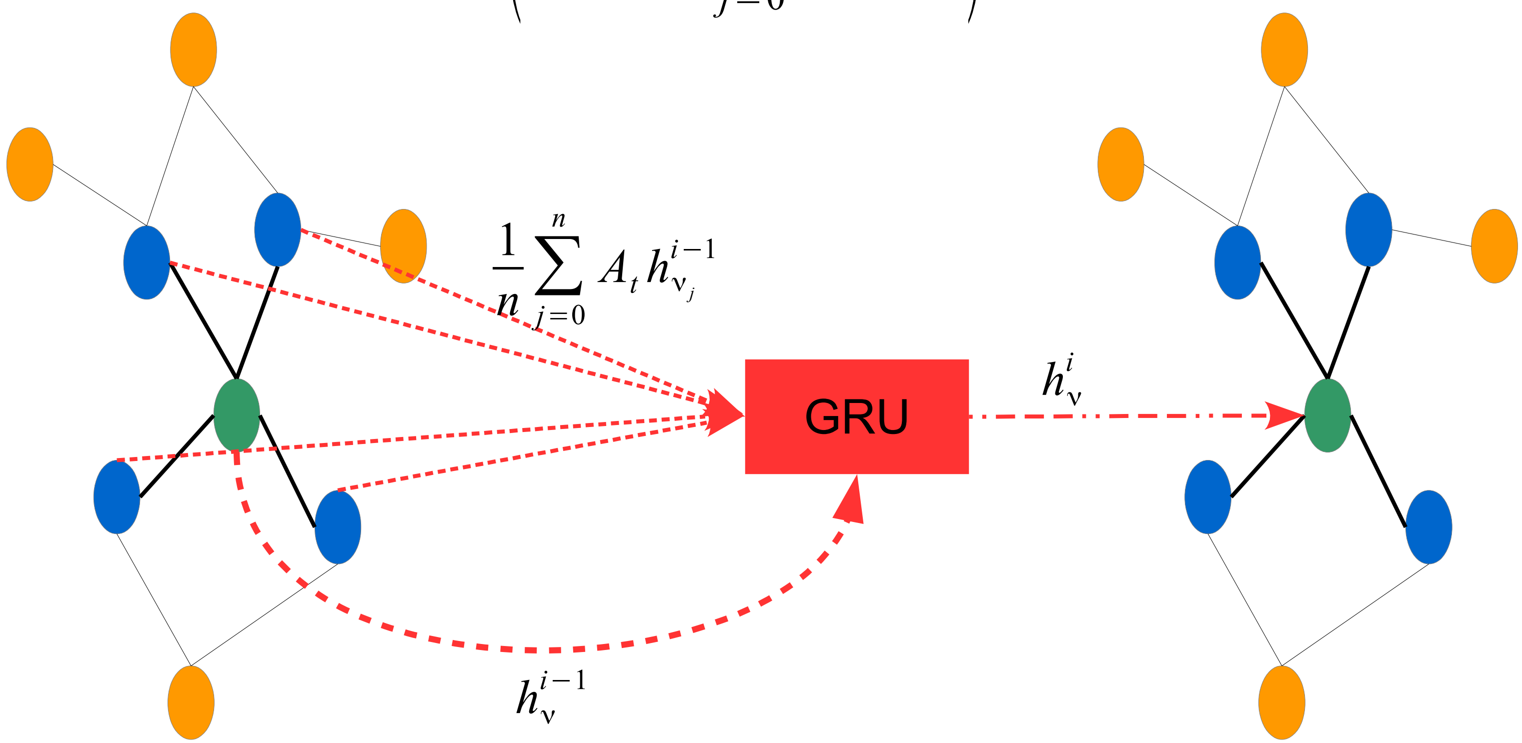
Graph Construction



Graph constructed with **one particle** per node.
Edges of graph connecting **geometrically close particles**.
per-particle and global features assigned to nodes.

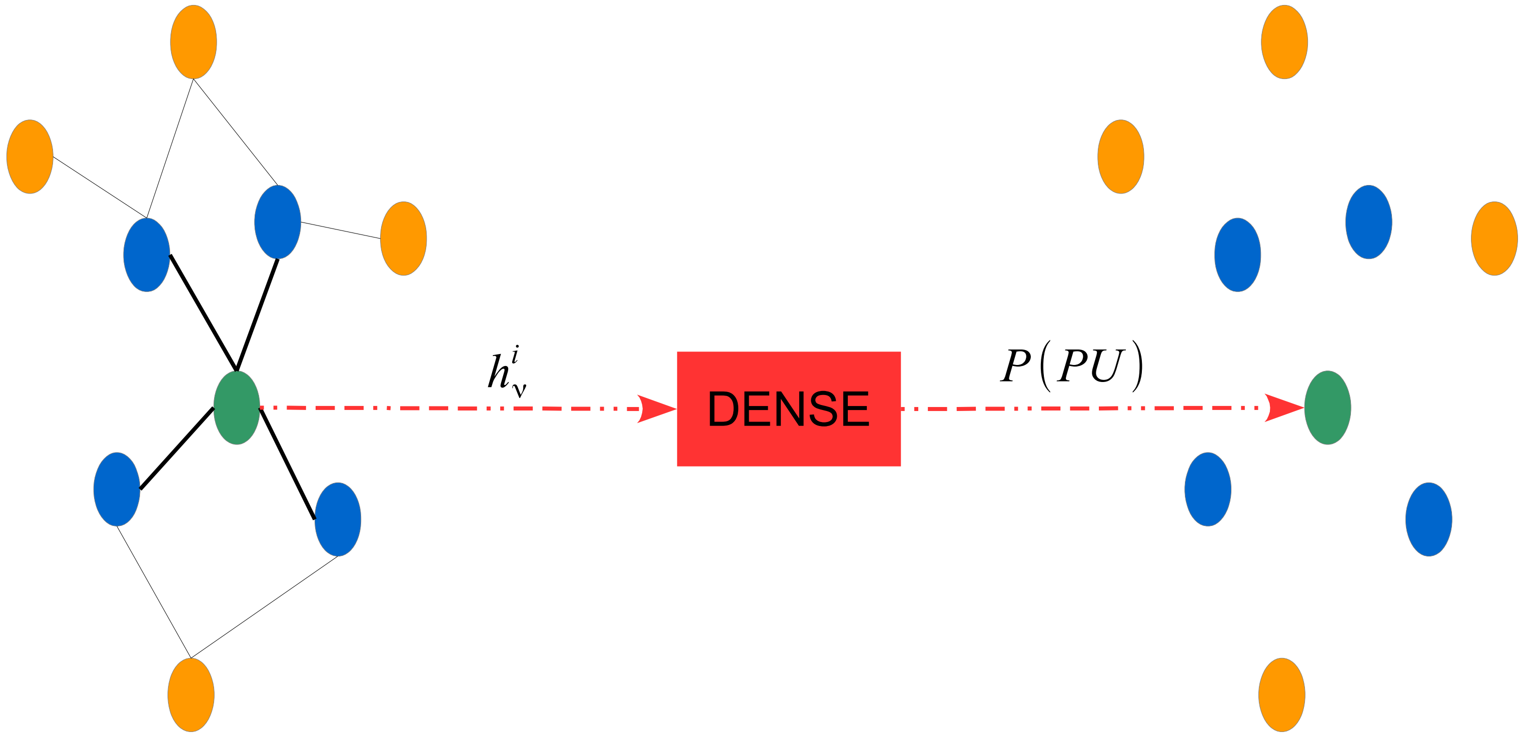
Updating Rule

$$GRU\left(h_{\nu}^{i-1}, \frac{1}{n}\sum_{j=0}^{n} A_t h_{\nu_j}^{i-1}\right) \rightarrow h_{\nu}^{i}$$



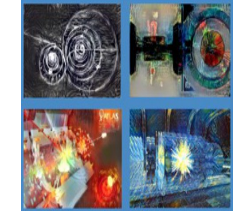
Hidden/internal representation of the each node/particle updated with gated recurrent unit (GRU) models

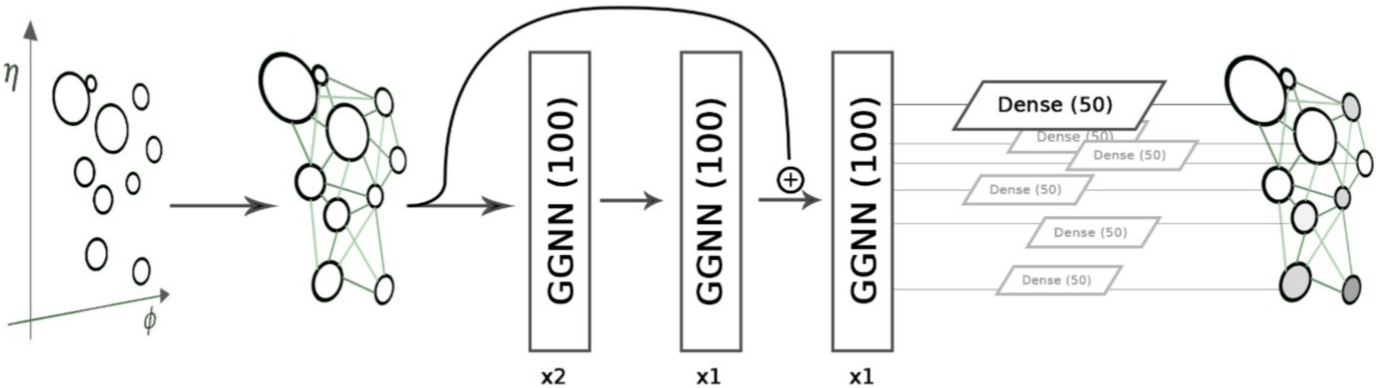
Pile-up Classifier

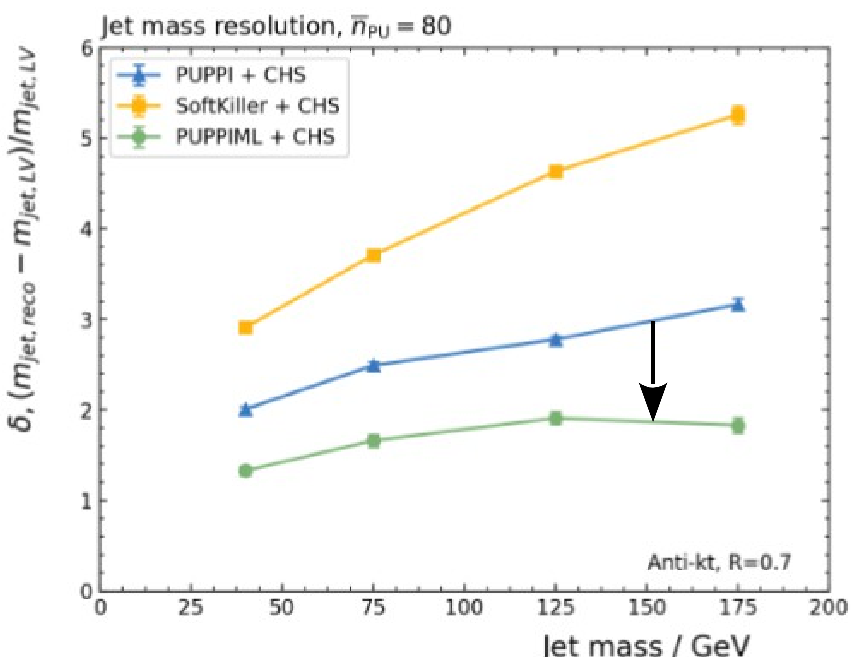


Binary classification extracted from the hidden/internal representation of the each node

Model Performance

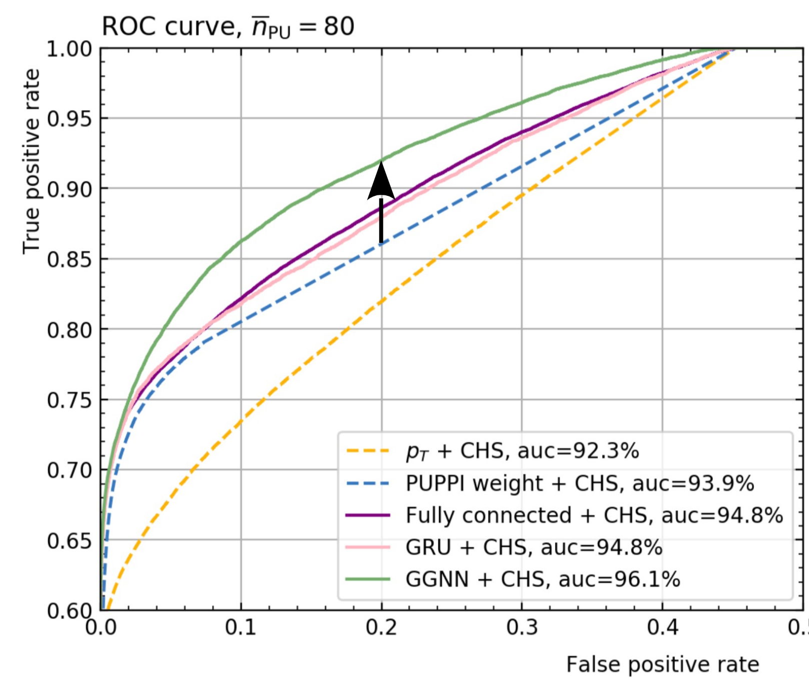






Improved energy resolution over state of the art pile-up removal methods.

Better rejection of underlying parasitic collisions.

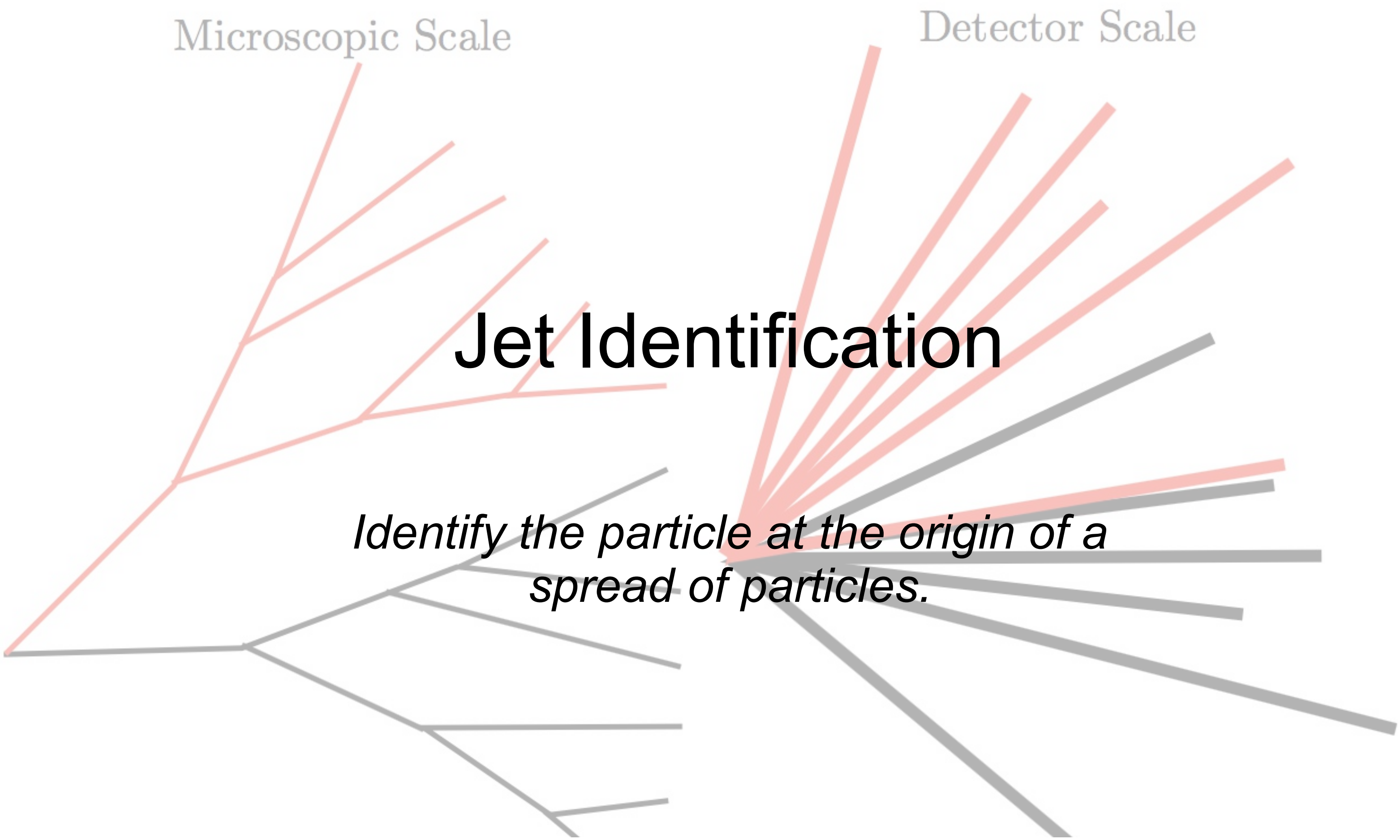


Remarks

- *Handling of global features in addition to per-particle features. In early stage, could be injected at later stage.*
- *Possibility to setup as a one-sided denoising algorithm.*
- *Can this be trained on data?*

https://github.com/jarjonam/PUPPI_ML
will turn public “soon”

Jet Identification

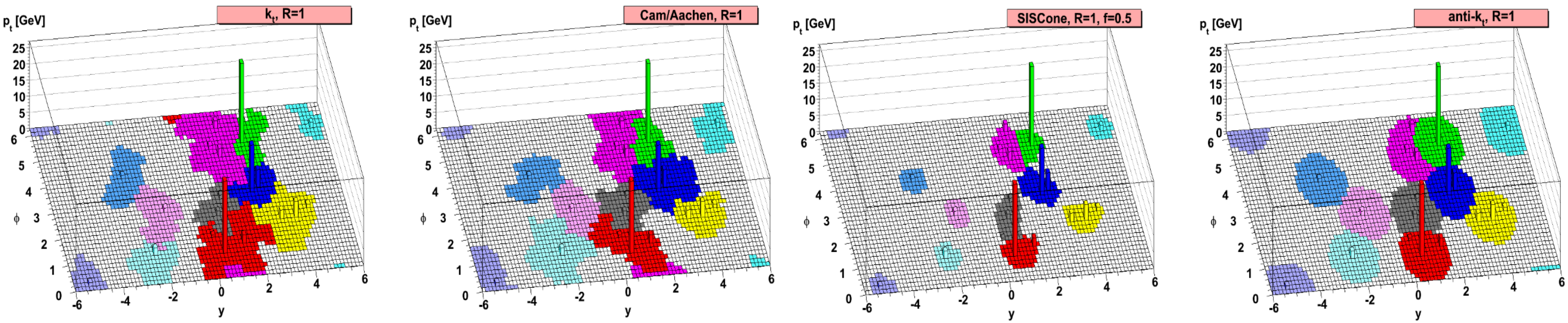


Identify the particle at the origin of a spread of particles.

With Eric A. Moreno, A. Periwal, Olmo Cerri, Javier M. Duarte, Harvey B. Newman, Thong Q. Nguyen, Maurizio Pierini, Maria Spiropulu

Jet Reconstruction – 101

Clustering of particles/objects based on a distance metric.
Physics content/properties depends on the metric.

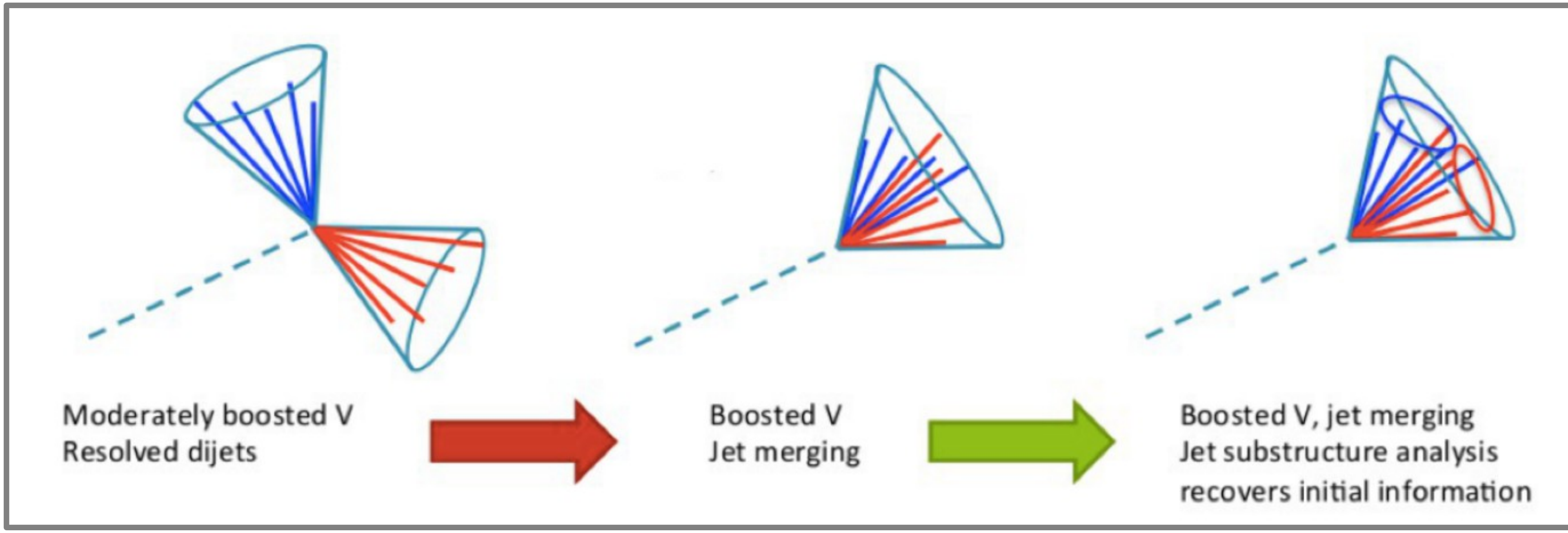


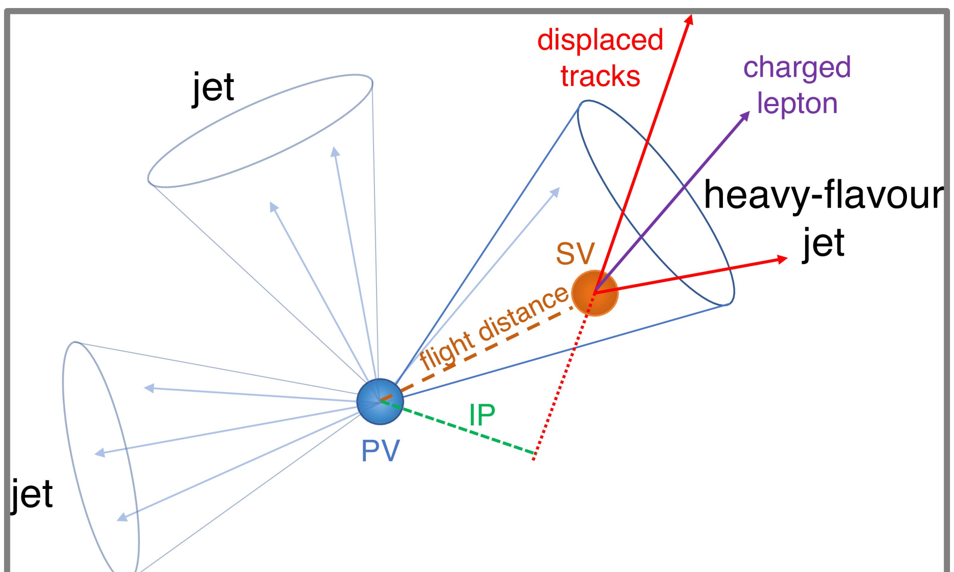
Three members of a family of algorithms:

$$d_{ij} = \min(k_{ti}^{2p}, k_{tj}^{2p}) \frac{\Delta y^2 + \Delta\phi^2}{R^2} \qquad \begin{cases} p=1 & k_t \\ p=0 & \text{Cam/Aachen} \\ p=-1 & \text{anti-}k_t \end{cases}$$

Fastjet algorithm
https://arxiv.org/abs/1111.6097

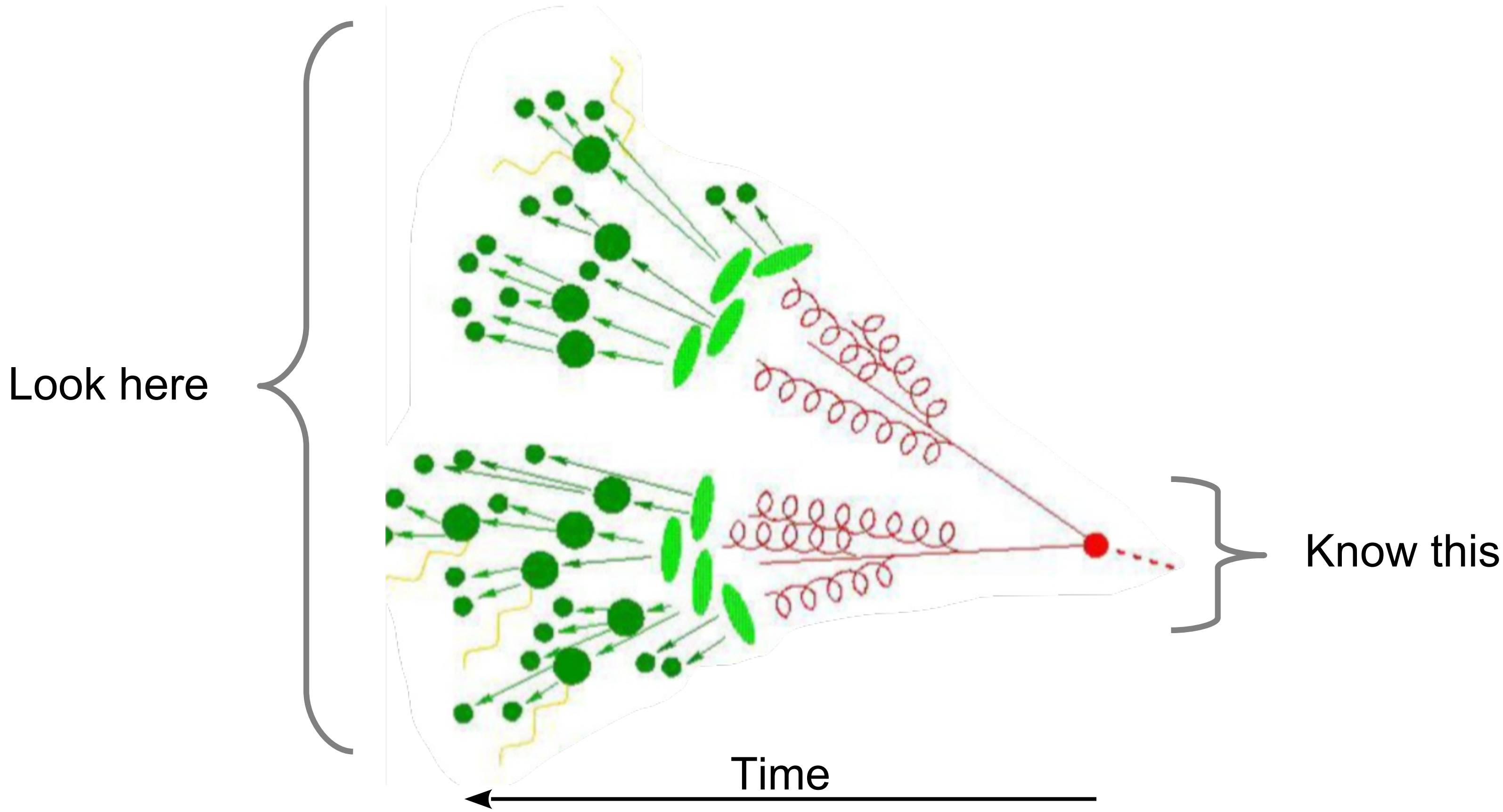
Jet Tagging – 101





- Secondary vertex is used to probe late decay of constituents
- Jet substructure derived from particle constituents used in boosted topologies

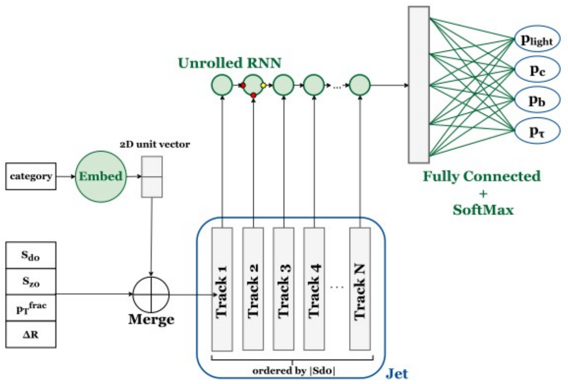
Name of the Game

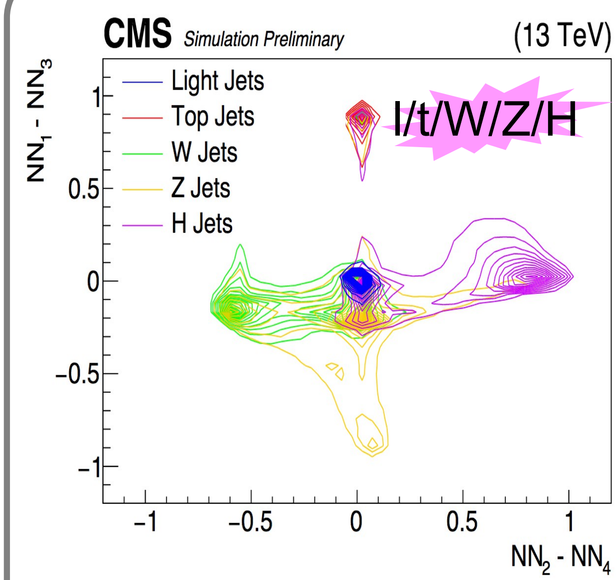


Tell the characteristics of the particle at the origin of a bundle of secondary particles, looking at constituents and characteristics.

Other ML Solutions

B-Jet with RNN
http://cds.cern.ch/record/2255226

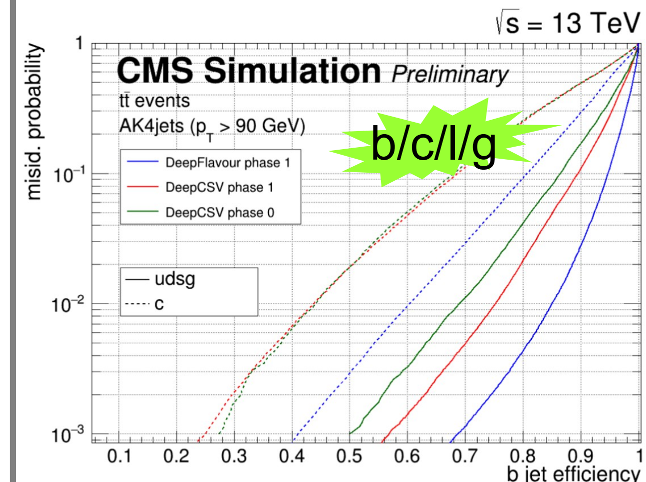




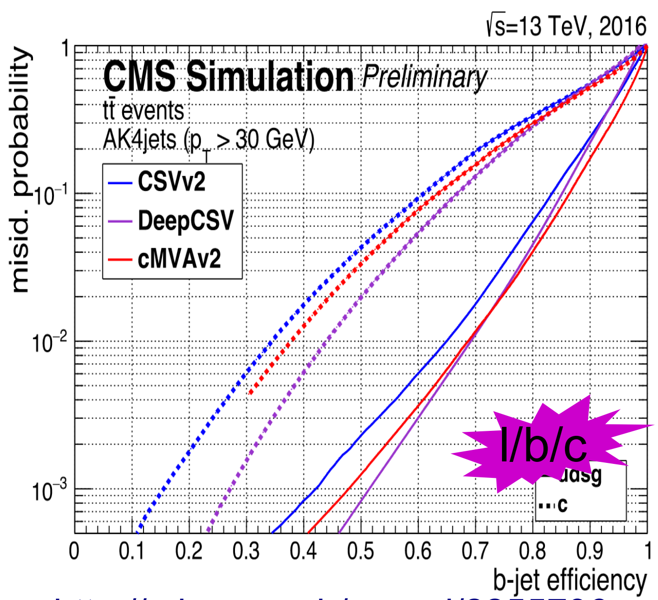
https://cds.cern.ch/record/2275226/

Jet-level features computed in hypothesized rest frame in dense multi-class neural net.

Jet-level, vertex-level and particle-level features in Conv1D/LSTM/FC multi-class neural net.



https://cds.cern.ch/record/2627468

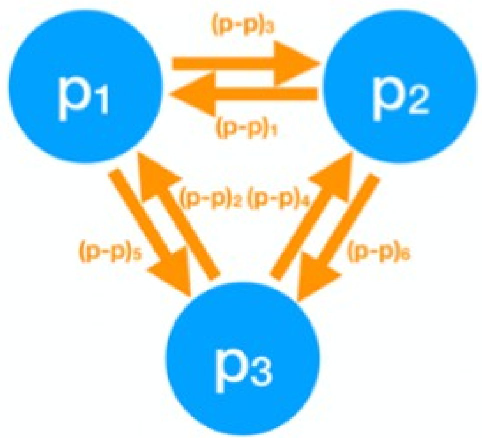


http://cds.cern.ch/record/2255736

Combining jet-level, vertex-level and track-level features in FC NN.

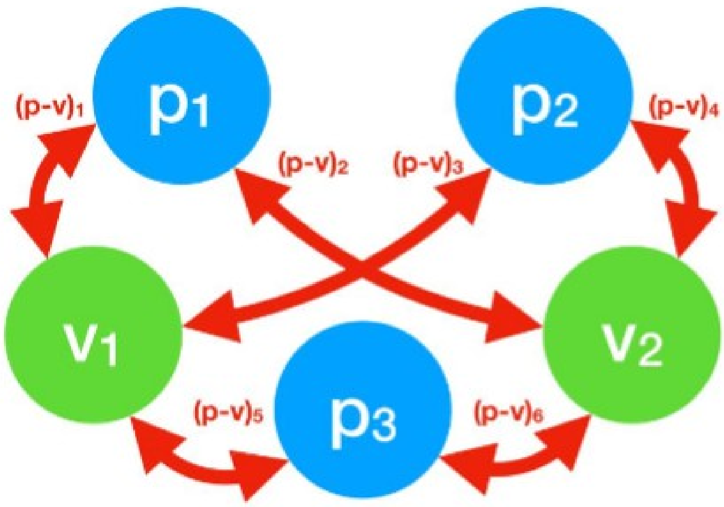
For more, see
https://arxiv.org/abs/1709.04464
https://indico.cern.ch/event/745718/

Particle Interaction



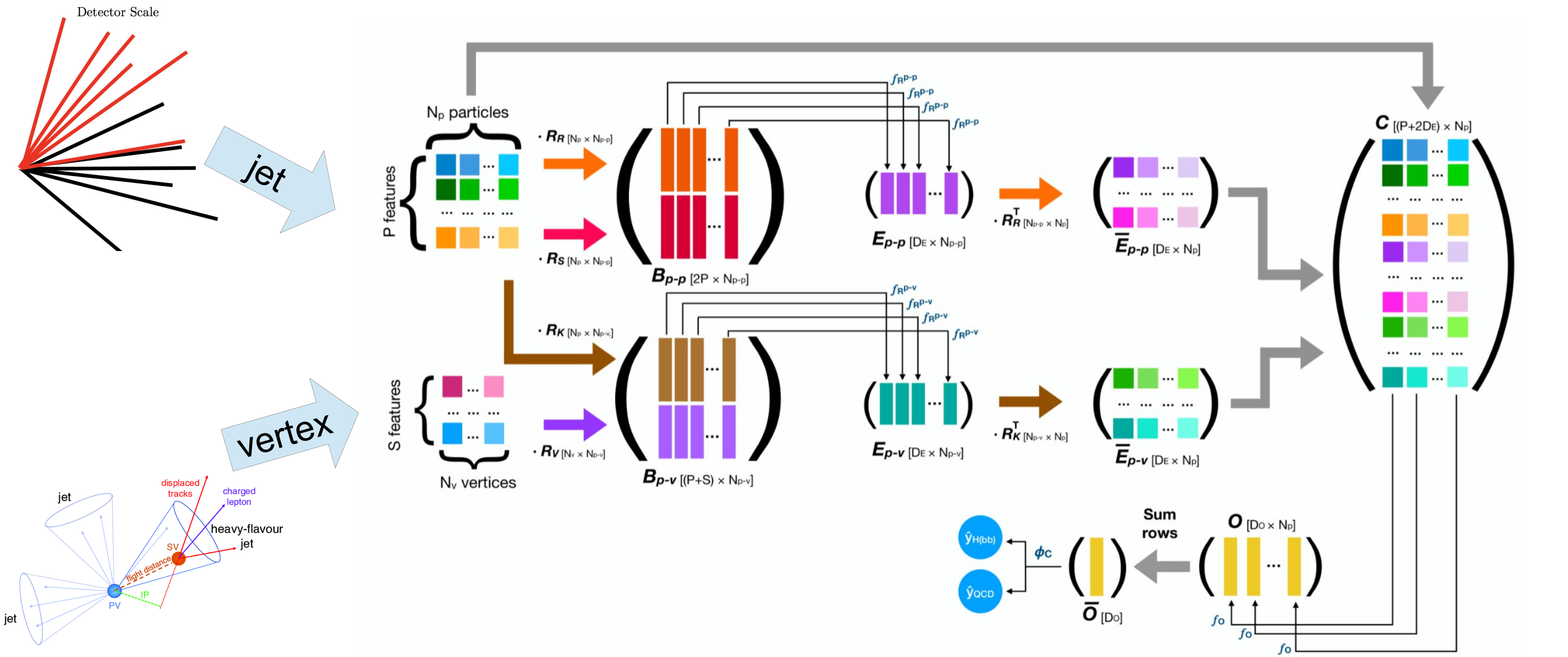
Learning interaction between particles with an all-to-all connected graph.

Particle/Vertex Interaction



Learning interaction between
charged particles and vertex with
all-to-all connected graph.

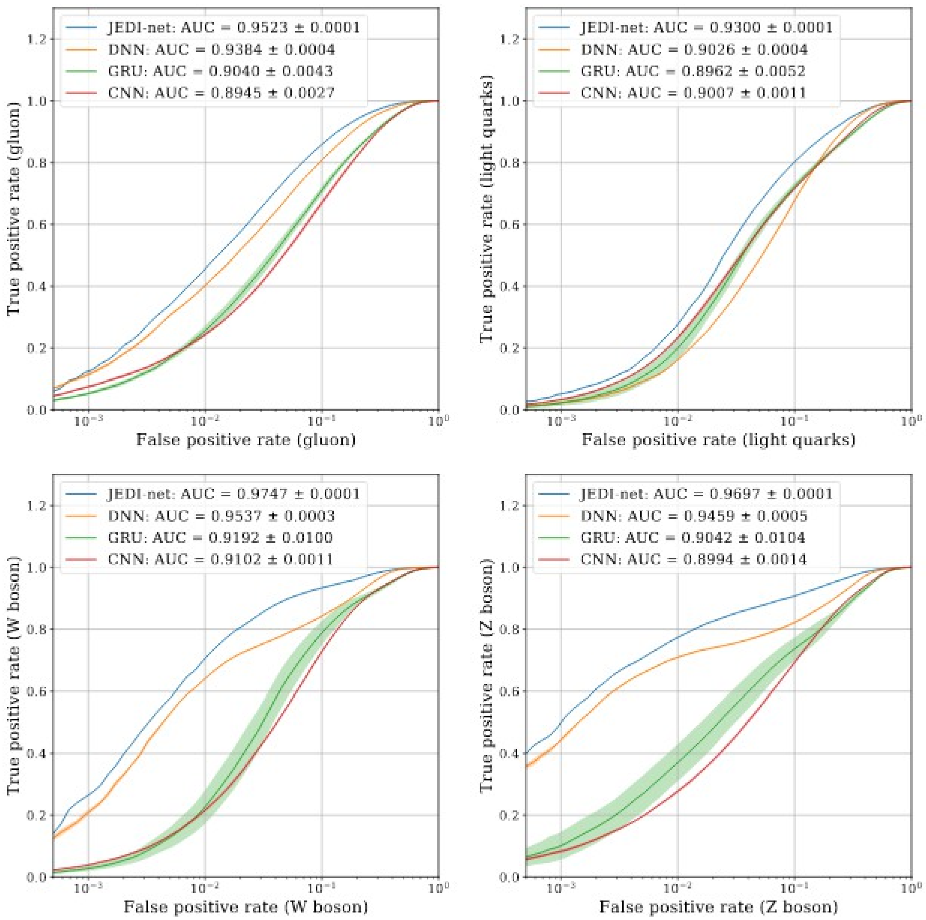
Jet-id with Graph Network



All particles of a jet, and vertex added on an all-to-all message passing graph network.
Graph-level classification (binary or multi-class)

Classification Performance

Out-perform other deep learning methods for jet multi-class categorization



Remarks

- *Single step of graph network thanks to all-to-all connectivity*
- *Extraction of a graph-level feature can be done in multiple ways.*
- *De-correlation with learning the mass done with adversarial, DDT, ...*
- *What have we done with the Physics knowledge of jet metrics ?*

https://github.com/eric-moreno/IN

Summary and Outlooks

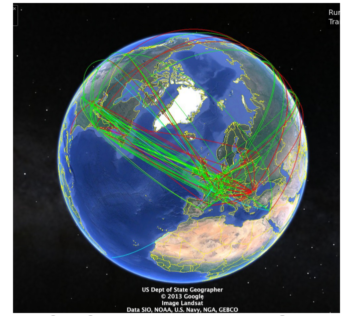
- Graphs are a very natural data representation in HEP.
  - Deep learning on graph helps on several HEP tasks.
    - Multiple ways of doing deep machine learning on a graph.
      - Further application of graph network to HEP to come.

Get in touch !

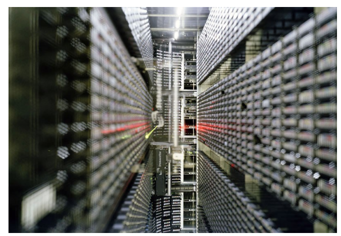
jvlimant@caltech.edu

Extra Material

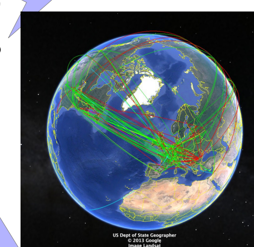
Analysis Pipeline



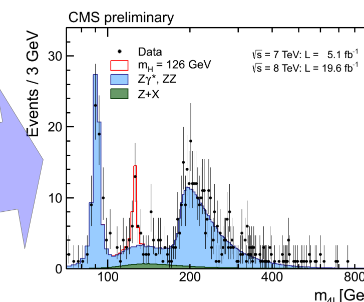
LHC Computing Grid
200k cores pledge to
CMS over ~100 sites



CERN Tier-0/Tier-1
Tape Storage
200PB total

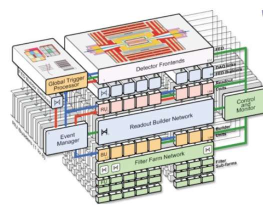


LHC Grid
Remote Access
to 100PB of data

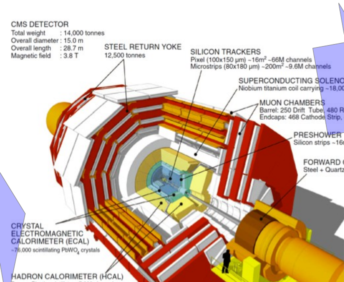


Rare Signal
Measurement
~1 out of 10^6

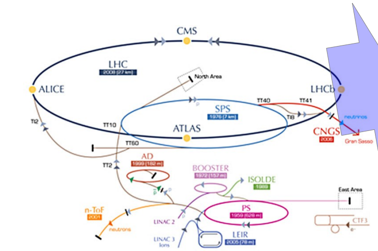
CERN Tier-0
Computing Center
20k cores dedicated



CMS L1 & High-
Level Triggers
50k cores, 1kHz



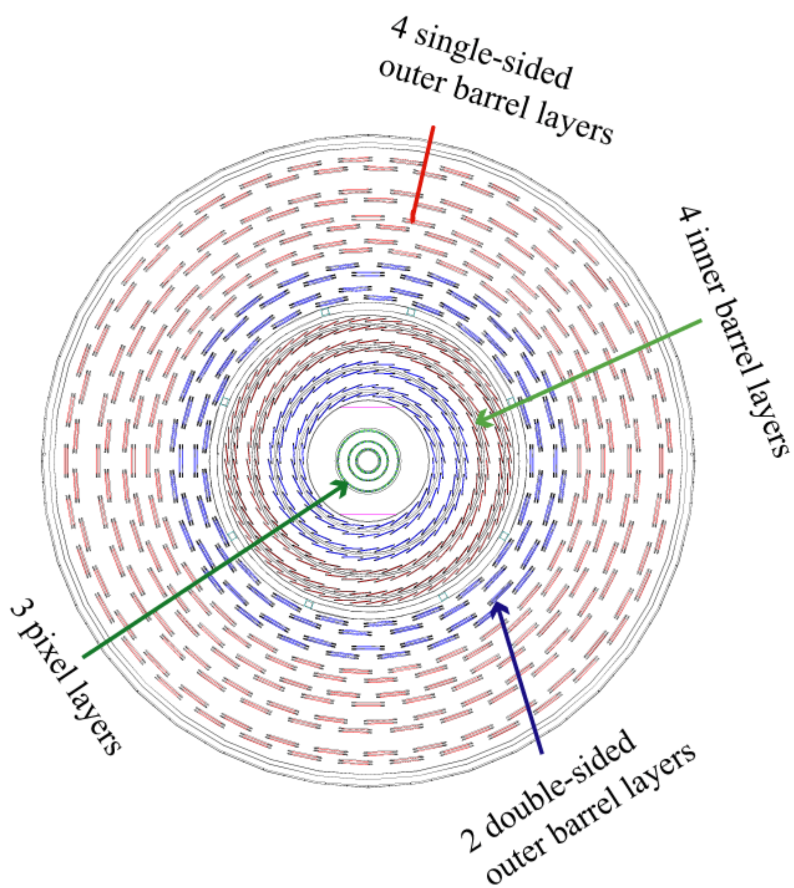
CMS Detector
1PB/s

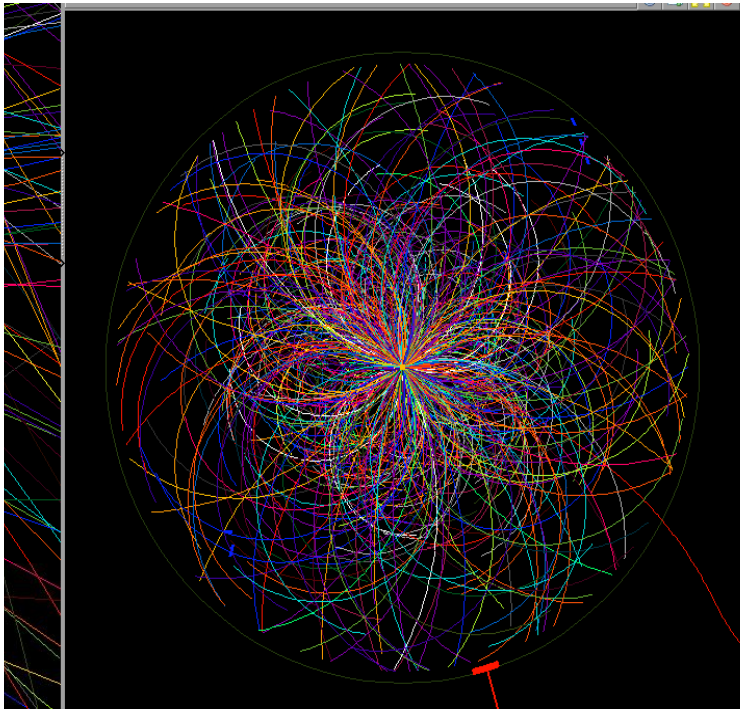


Large Hadron Collider
40 MHz of collision

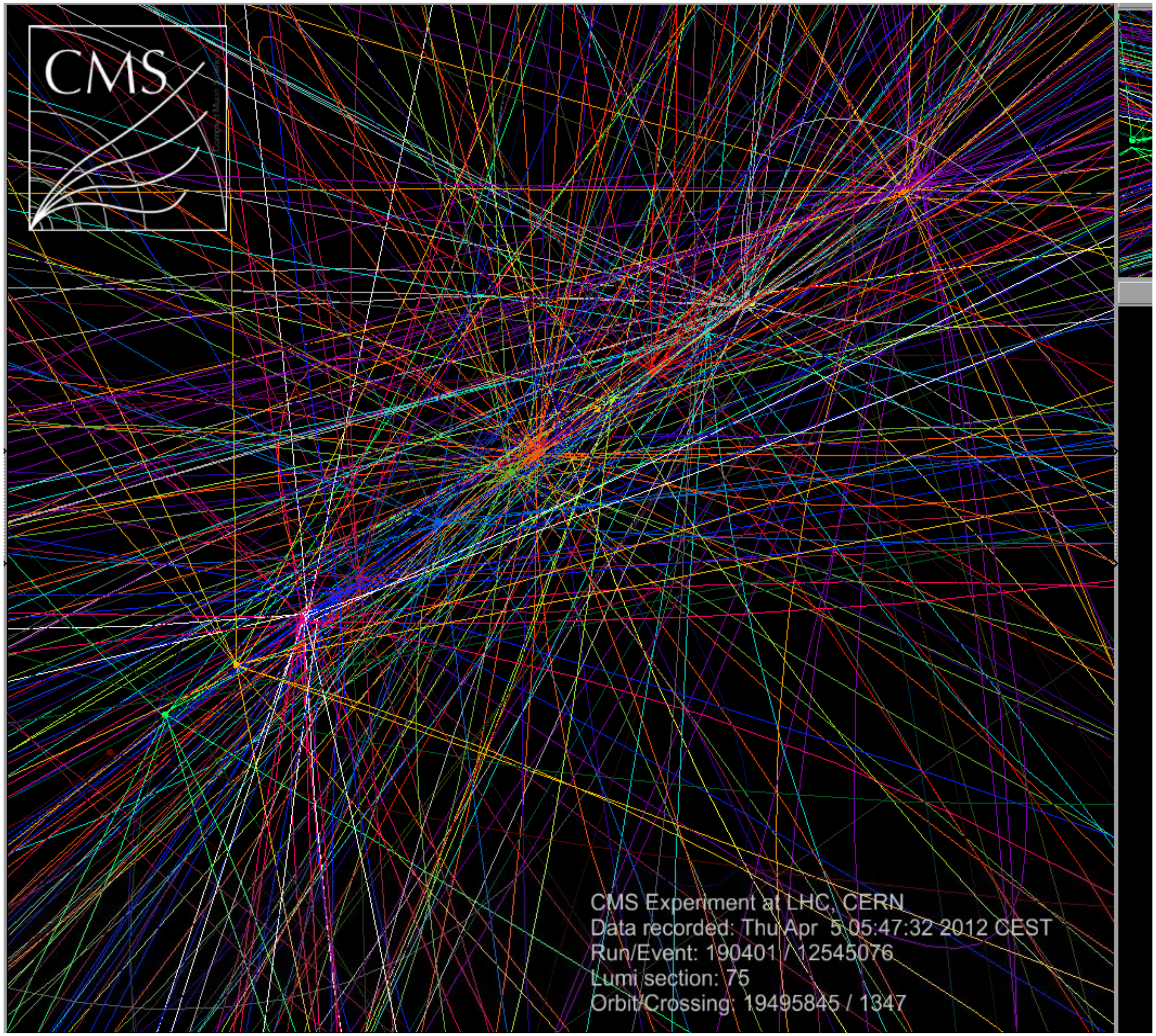
Tracks Pattern Recognition

- From sparse 2D/3D points reconstruct the path of a charged particle
- Iterative process using combinatorics, Kalman Fitting and Filtering
- Most CPU intensive part of the event reconstruction (~10s /event)
- Computation time scales ~quadratically with number of interactions
- Any fraction of patterns that can identified faster will make a difference



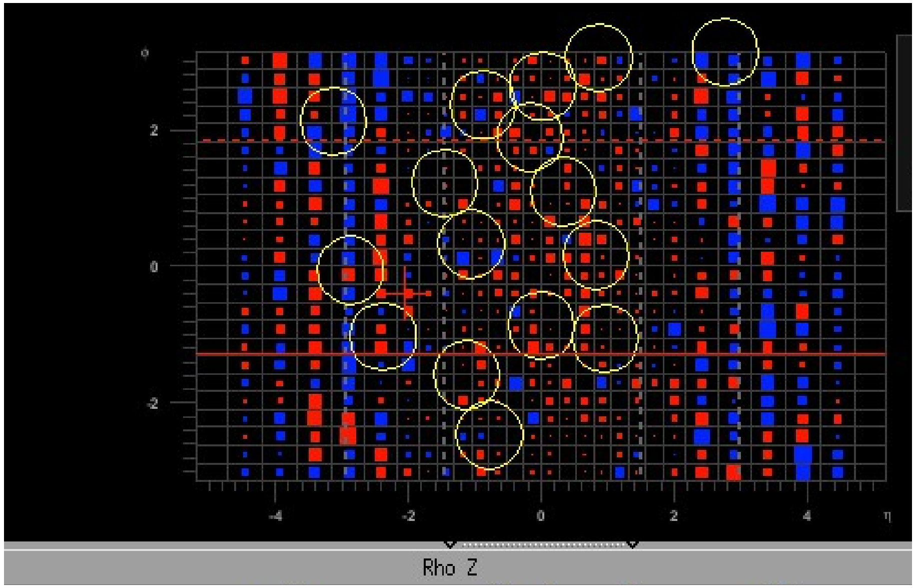


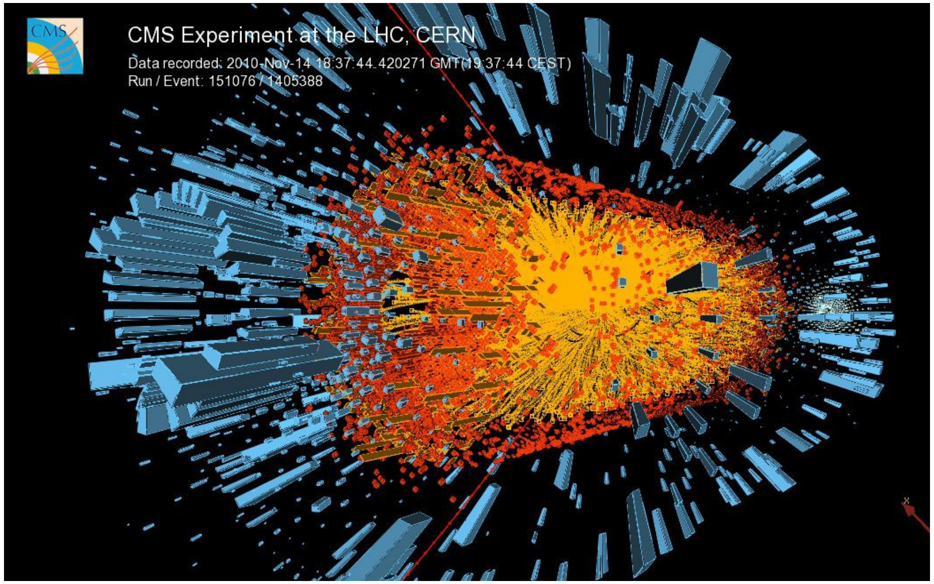
Vertex Identification



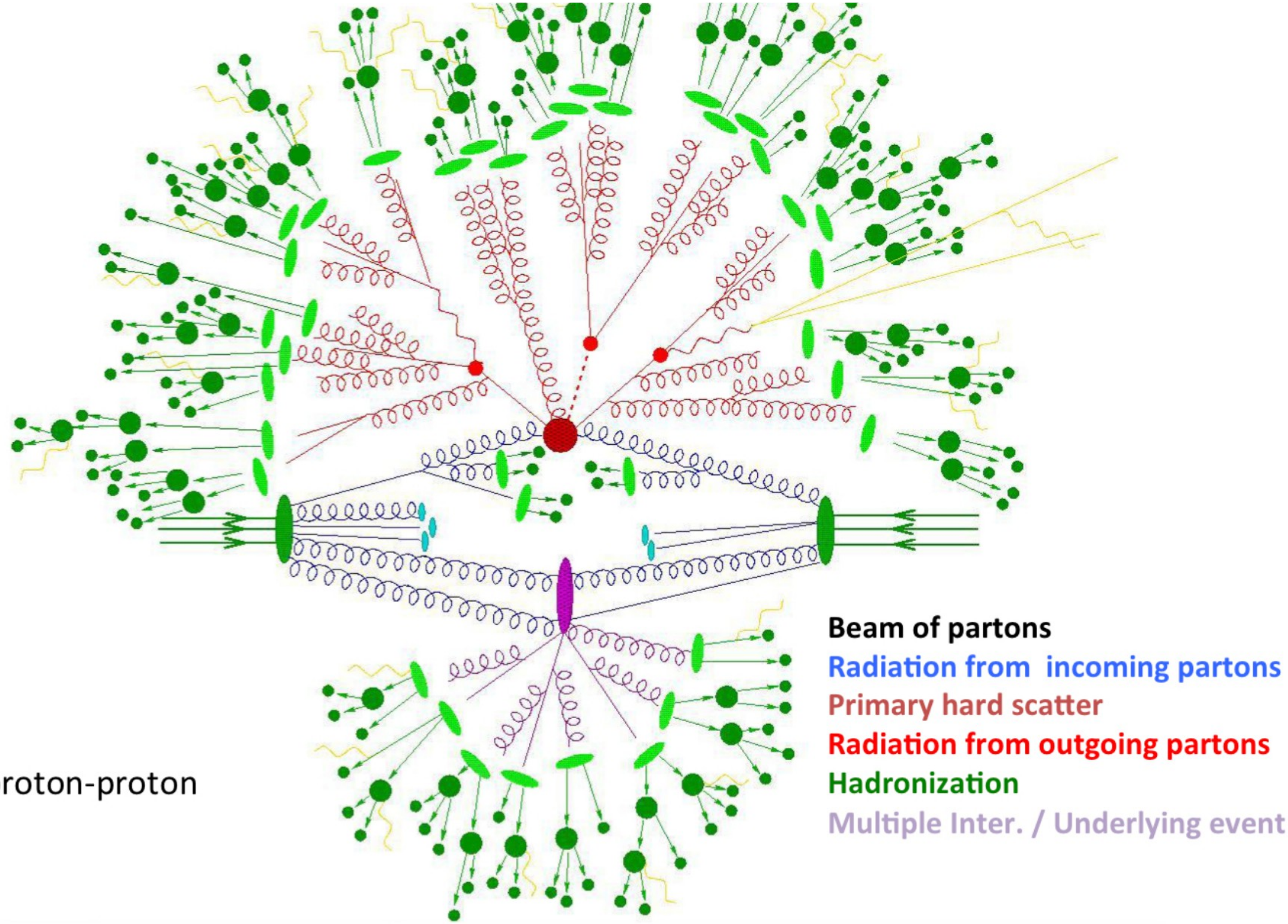
Energy Pattern Recognition

- Particles emitted from the interaction point are stopped in calorimeters (except for muons, neutrinos, …)
- Pattern of energy deposition is somehow characteristic
- Classical, physics driven methods have been used to recollect the total energy and identify the particle
- Efficient classifiers are being used on derived features
- Room for improvement in deriving the low level features
- How to deal with so many overlapping collisions





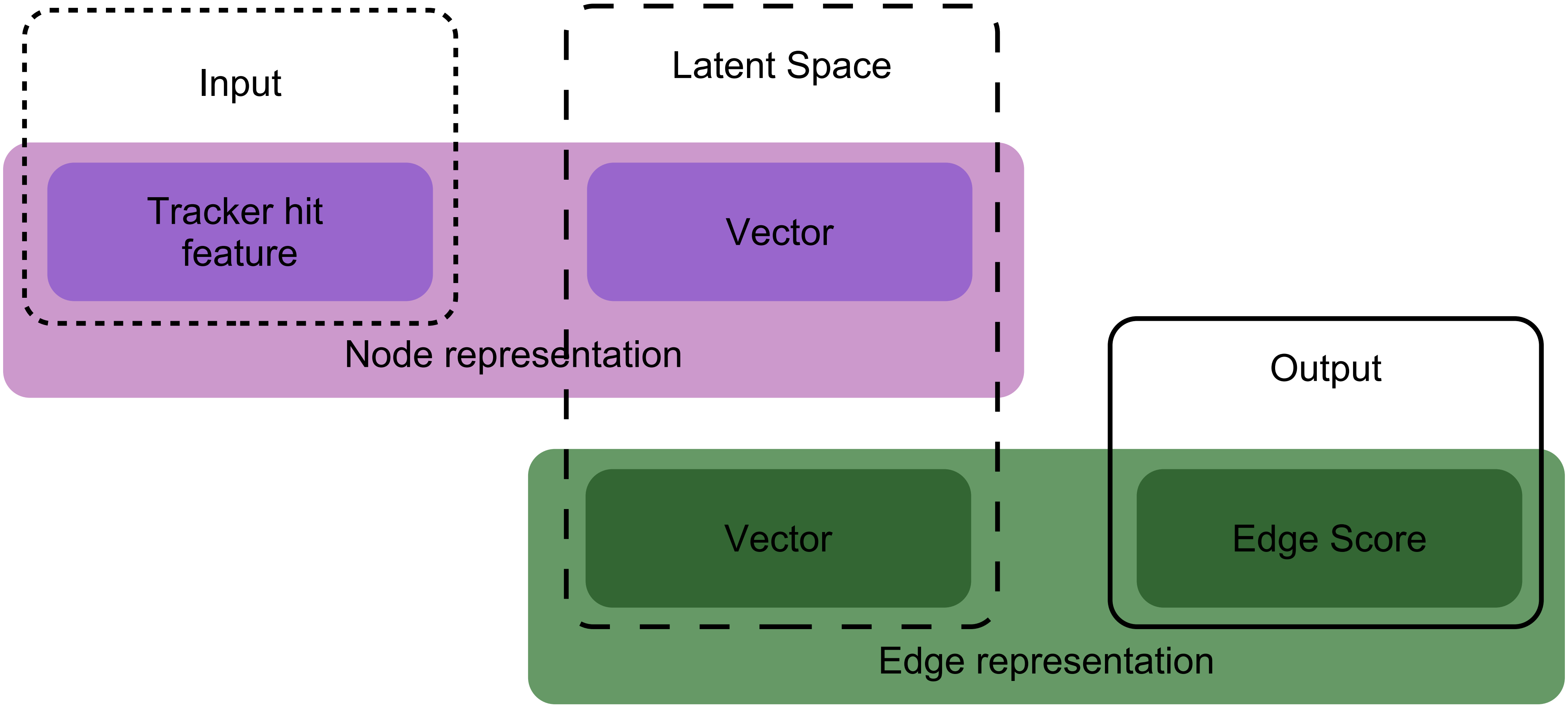
What is an Event



Typical proton-proton collision

Add 40 such on top of each other.
Up to 200 such overlay in the horizon 2025
One event every 25 ns / 40MHz

Node & Edge Representations



Multiple ways to pass the information from nodes to edges and edges to nodes (attention, message passing, ...)

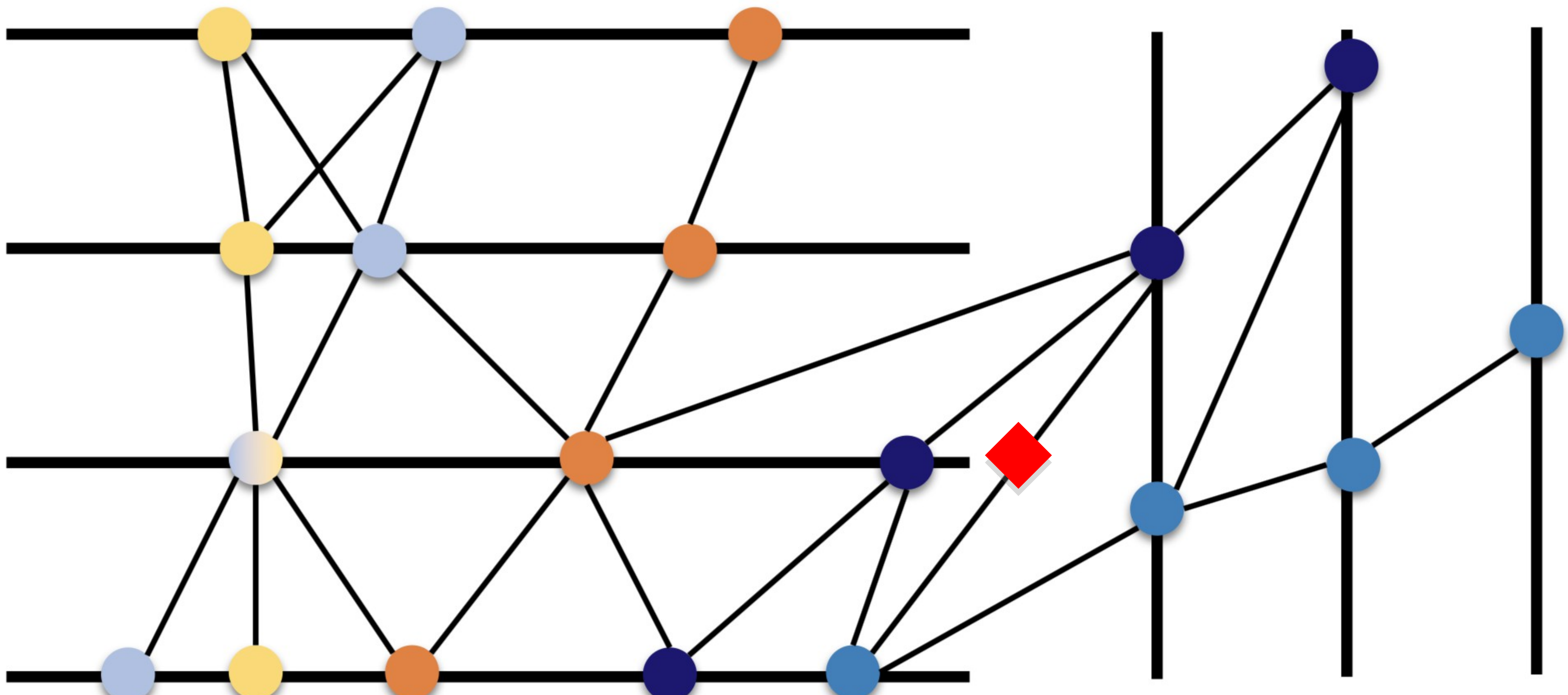
Neural Networks

- **Input Network**
  - ➢ Transforms from hit features (r,φ , z) to the node latent representation (N for 8 to 128)
  - ⬩ Dense : 3→...→N

- **Edge Network**
  - ➢ Predicts an edge weight from the node latent representation at both ends
  - ⬩ Dense : N+N→...→1

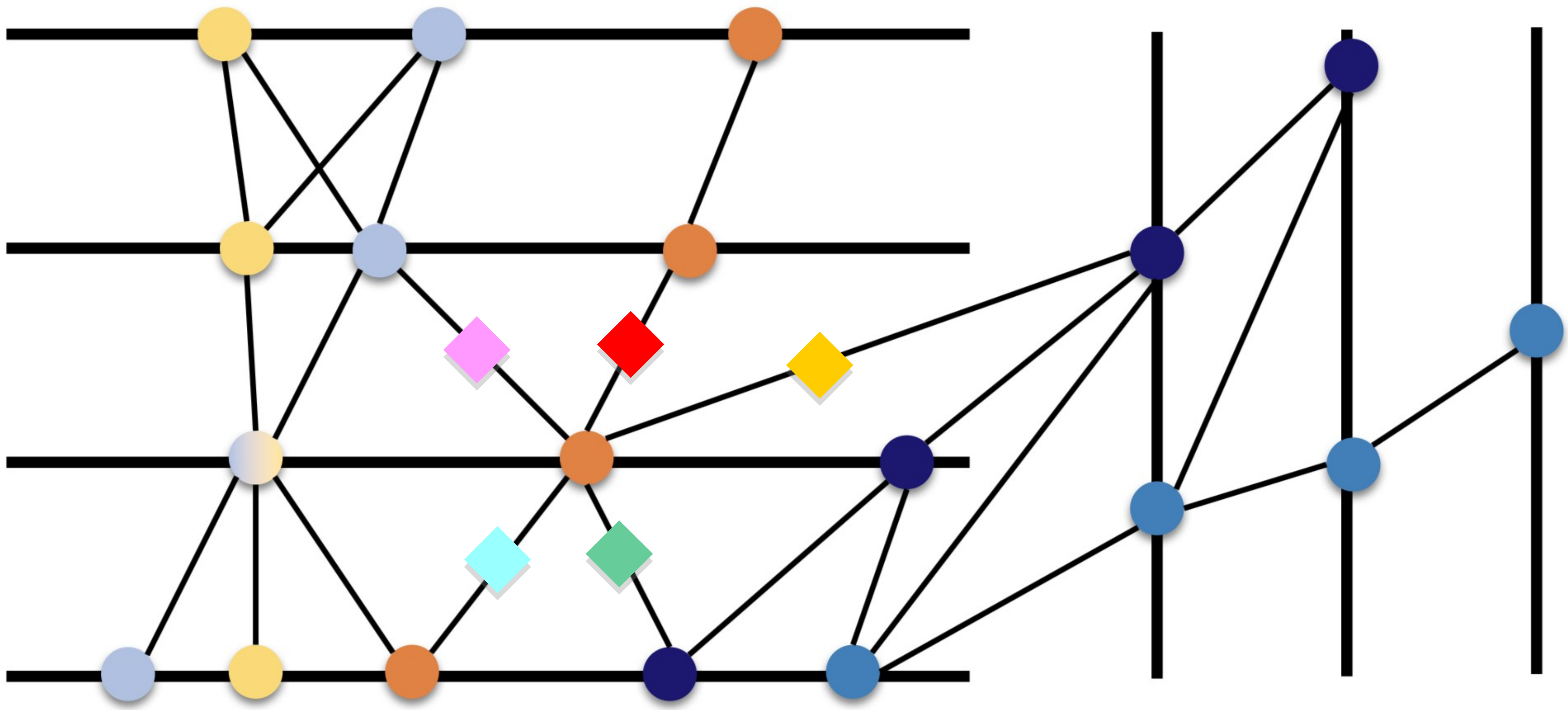
- **Node Network**
  - ➢ Predicts a node latent representation from the current node representation, weighted sum of node latent representation from incoming edge, and weighted sum
  - ⬩ Dense : N+N+N→...→N

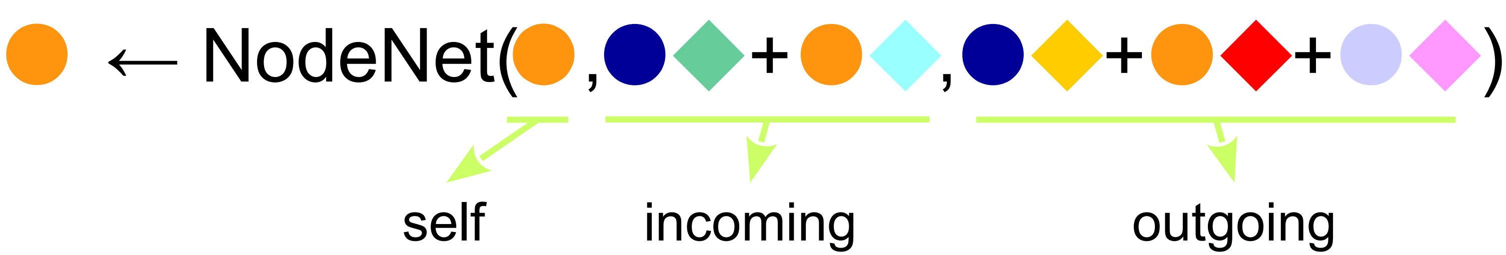
Edge Network



◆ ← EdgeNet(●,●)

Node Network



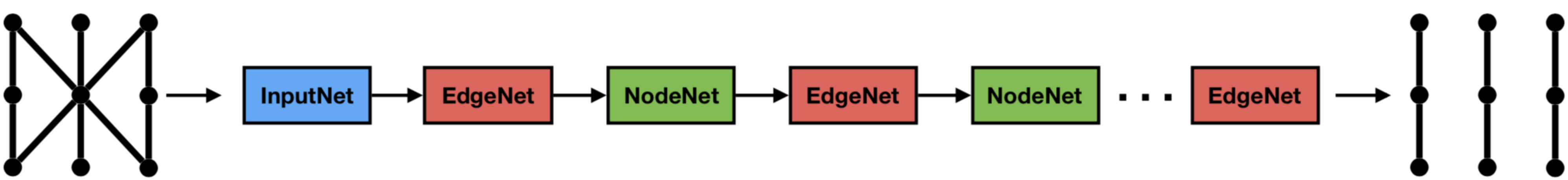


Information Flow

- Graph is sparsely connected from layer to layer
- InputNet + EdgeNet + NodeNet only correlates hits information on triplet of layers
  - The information from the outer hits and inner hits are not combined

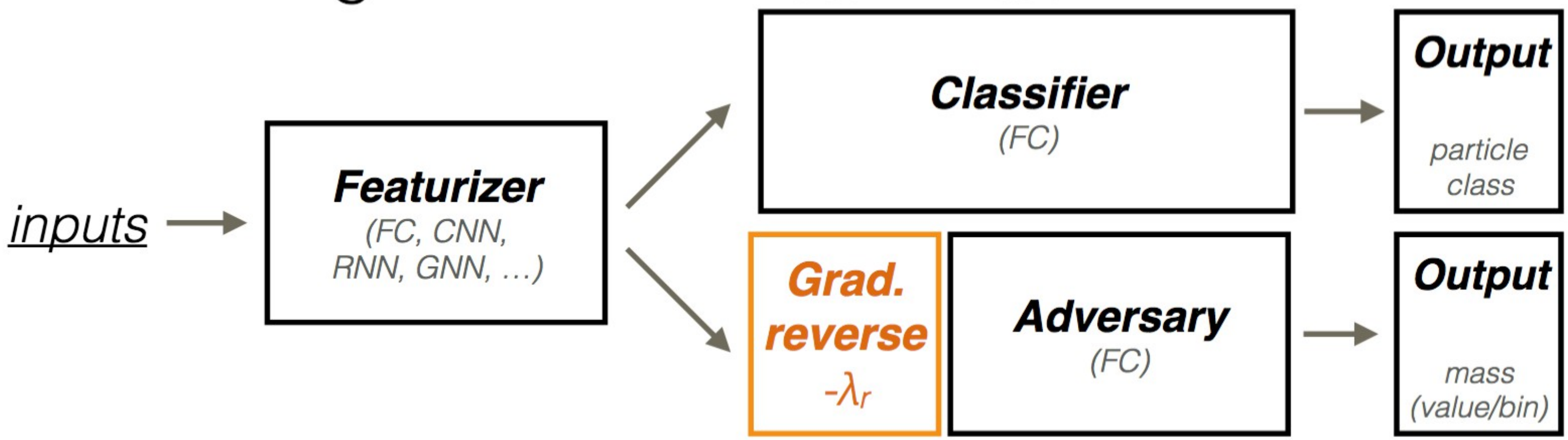
→ Correlates hits information through multiple (7) iterations of (EdgeNet+NodeNet)

→ Implemented in Torch https://github.com/HEPTrkX/heptrkx-gnn-tracking

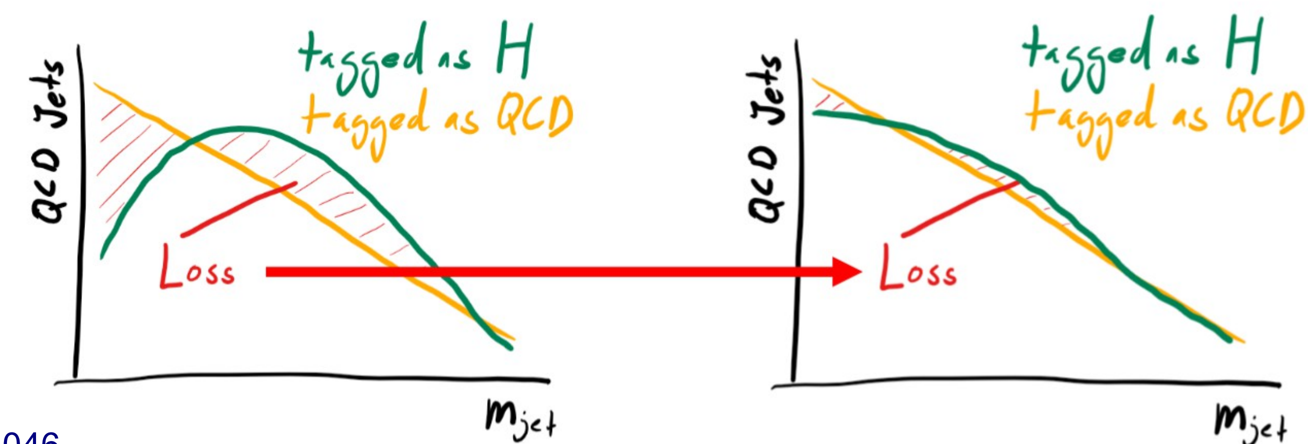


Mass Decorrelation

Adversarial training $L = L_{\text{disc}} + \lambda L_{\text{adv}}$



Dedicated "penalty term" $L = L_{\text{disc}} + \lambda D_{\text{KL}}$



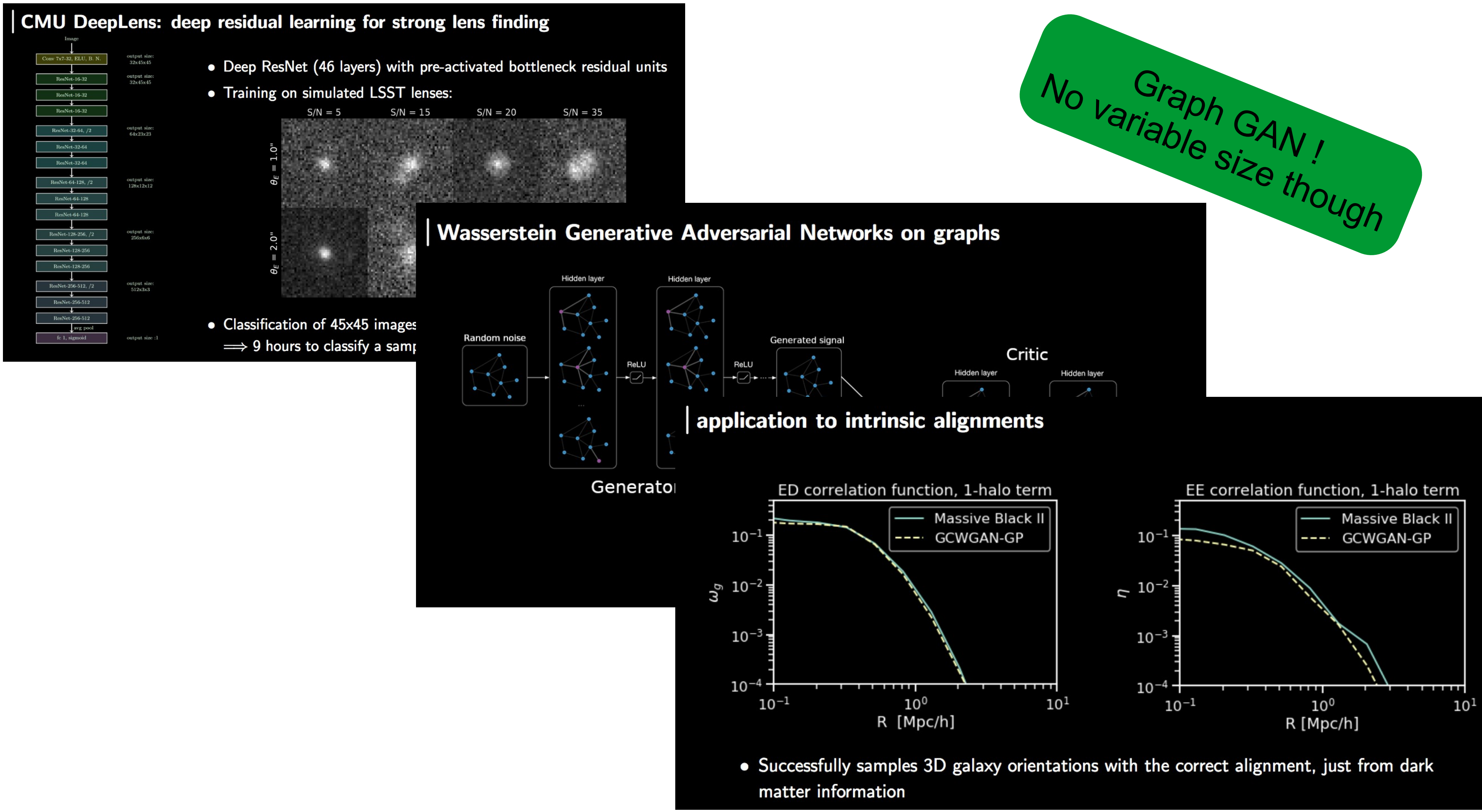
https://arxiv.org/abs/1611.01046
https://arxiv.org/abs/1409.7495
https://arxiv.org/abs/1603.00027

Slide J. Duarte

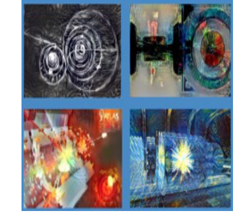
Decorrelates the model output from targeted quantities.

Deep Cosmology

Graph GAN !
No variable size though



F. Lanusse, Machine learning in cosmology
https://indico.cern.ch/event/708041/contributions/3308836/

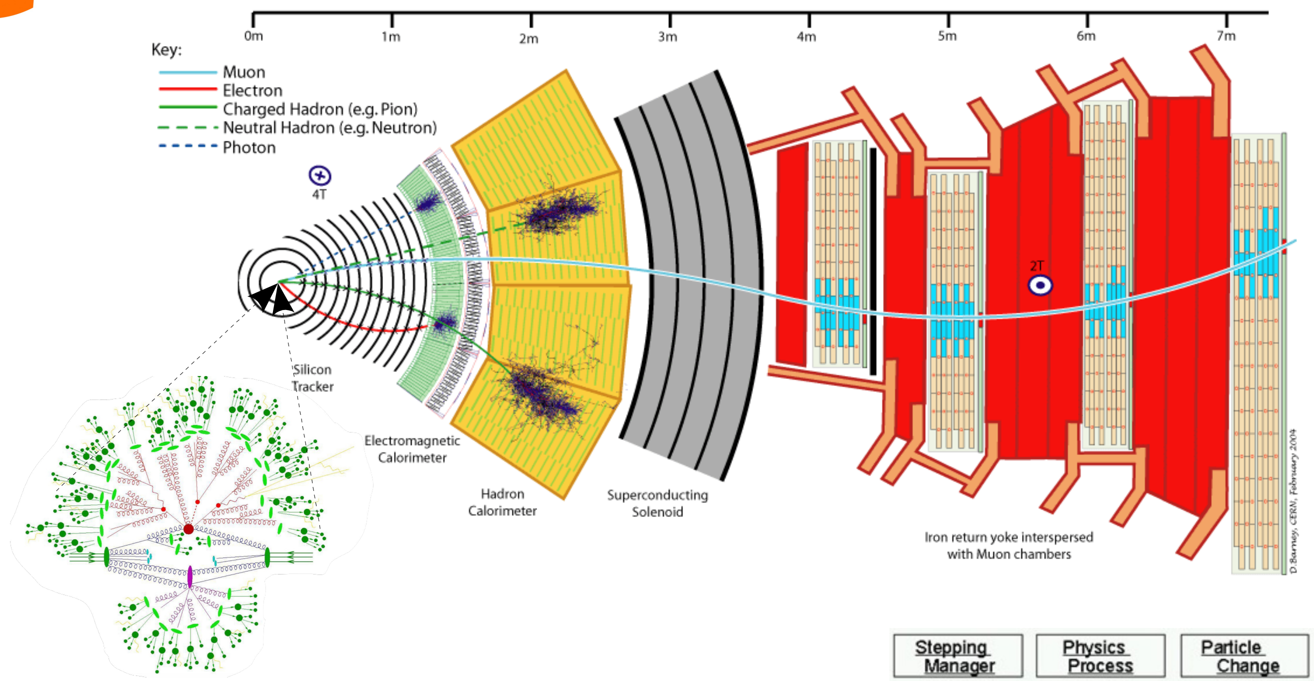


Shower Simulation

Simulating production of cascade of particles interacting with material

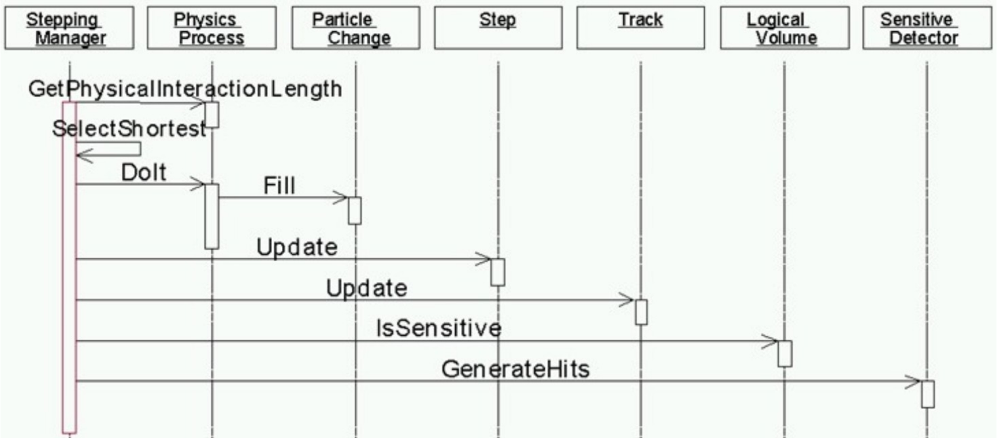
***by** Vladislav Belavin, Andrey Ustyuzhanin*

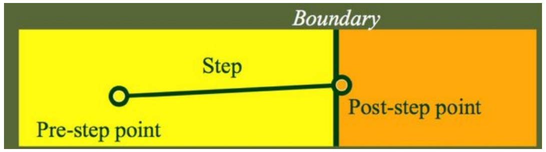
Geant4 – 101



- Generator simulates the beam interaction and initial particles.

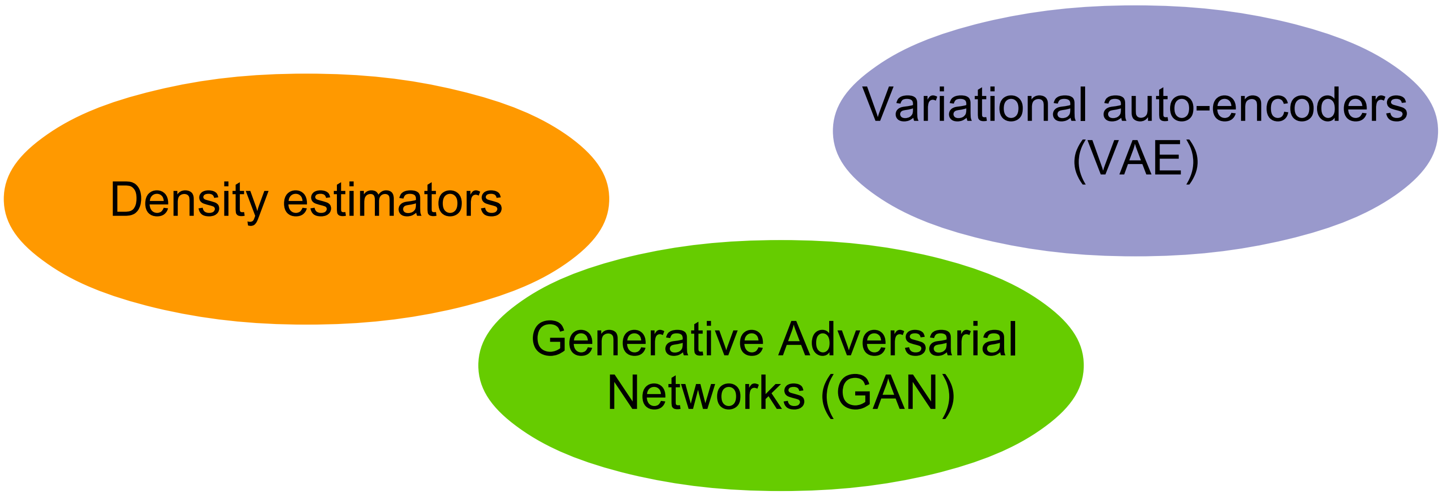
- Geant4 steps the particles through a detailed model of material and stochastically simulates energy depositions





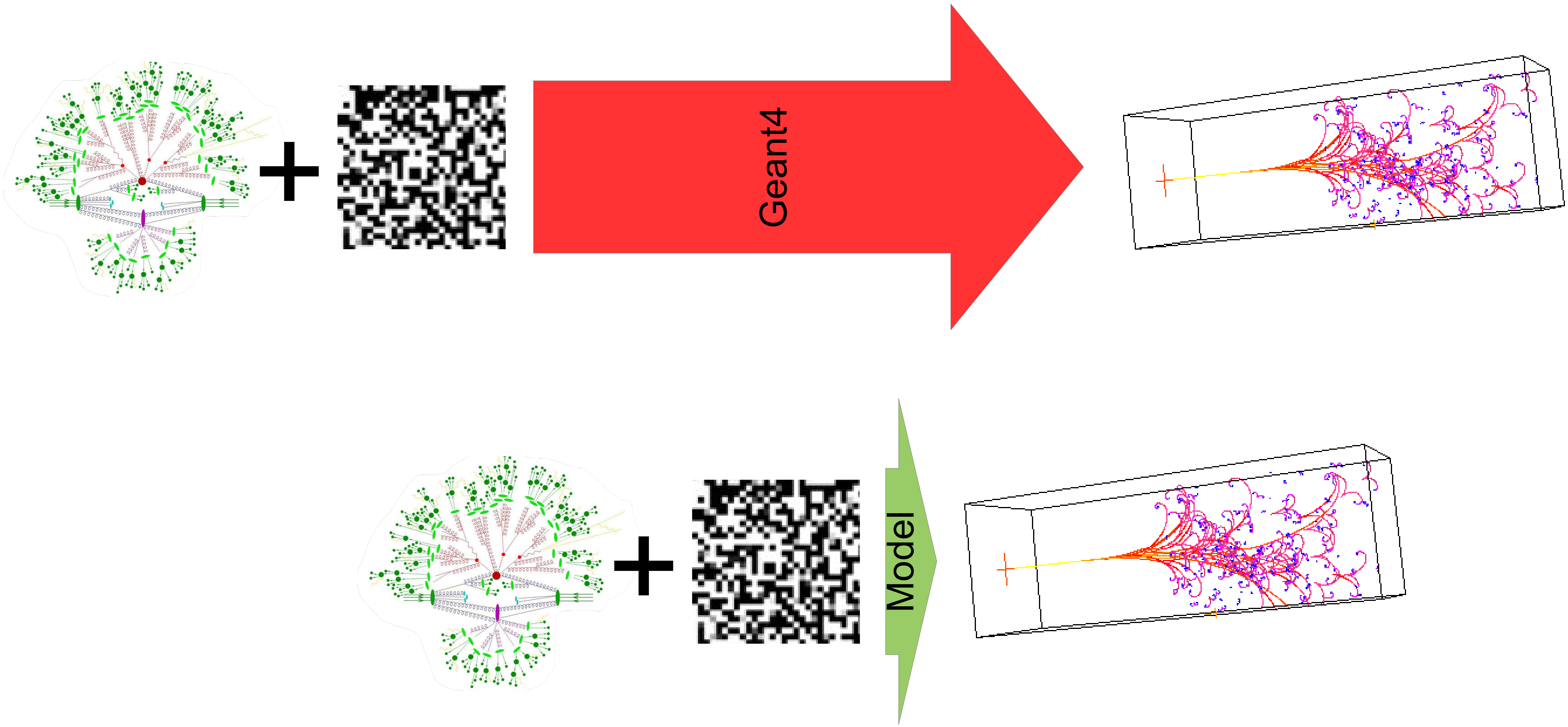
https://geant4.web.cern.ch/

Generative Model – 101



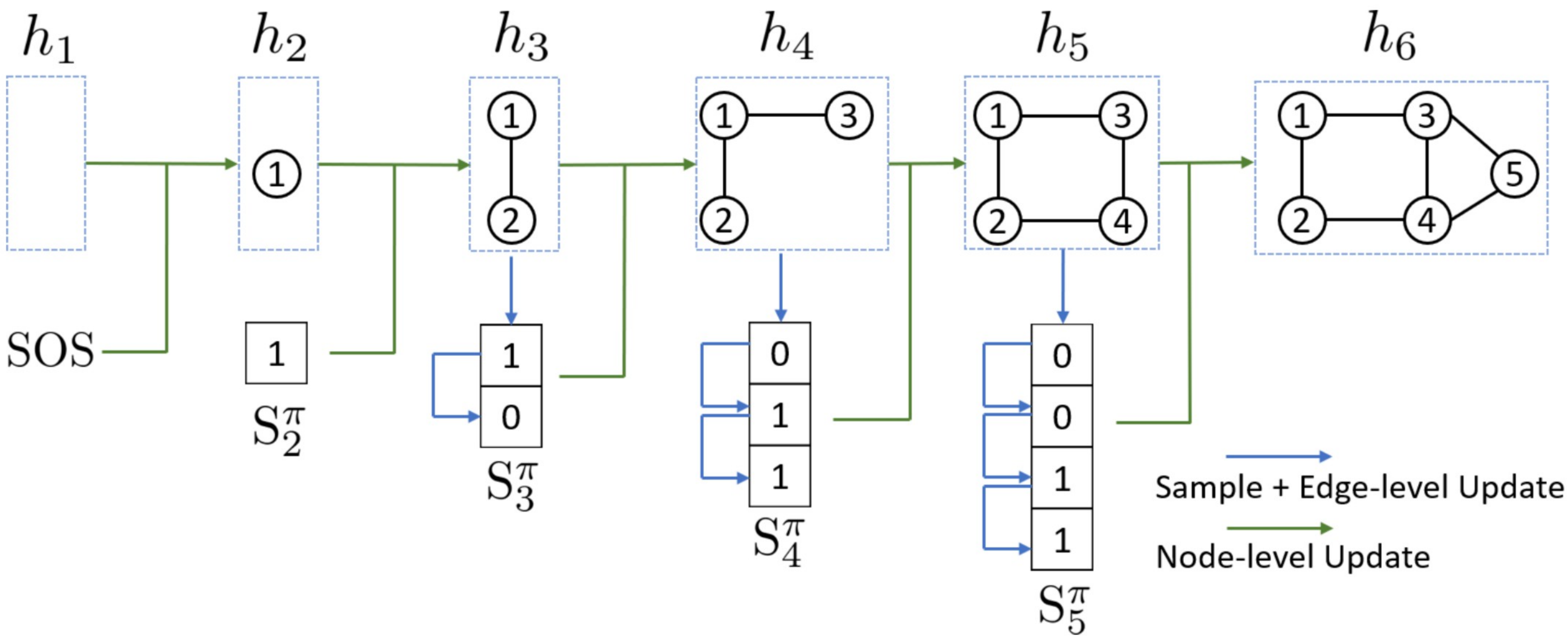
- Unsupervised machine learning (in the sense that there is no "truth labels").
- Being able to generate new samples as if coming from the original dataset.
- Surrogate fast generator of slow full simulator

Name of The Game



Produce samples similar to those of the full model, with high fidelity and much faster.

Graph Generator

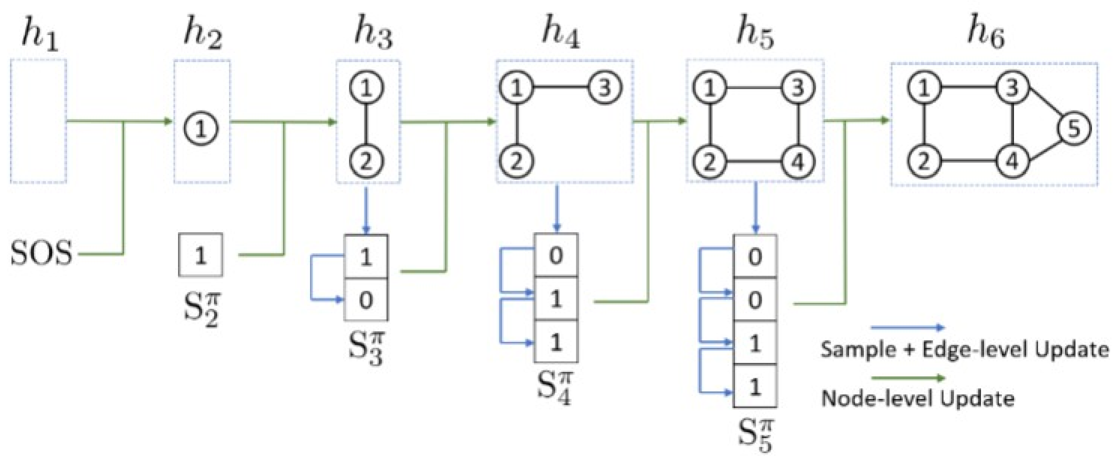


- Two recurrent models producing nodes and edges

https://arxiv.org/abs/1802.08773

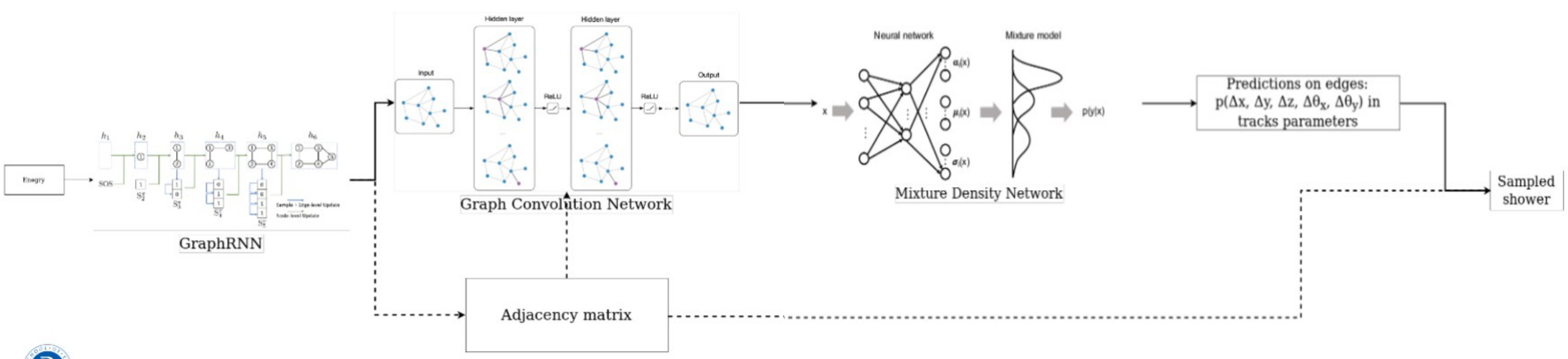
GraphRNN

- Graph-level RNN: generates sequence of nodes;
- Edge-level RNN: generates sequence of edges for each node.



https://arxiv.org/abs/1802.08773

Final architecture



https://indico.cern.ch/event/708041/contributions/3269731/