[ Detector of TrackML challenge ]

# High Energy Physics

## In the era of machine learning & data science

A. Salzburger (CERN)

@SaltyBurger

# Why listen to me ?

2001

**2003**

study of physics

***diploma thesis***

*Fast Simulation of Muons in the ATLAS Inner Detector and Muon System*

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*Simulate performance of different future detectors candidates for ATLAS*

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*Neural network based cluster splitting*

***Architect of Integrated Simulation Framework***

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**2013 - present**

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***Upgrade Software Coordinator***

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*Including Machine Learning R&D for track Reconstruction*

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  Focus on **exemplary** applications in HEP and only little on techniques

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  Focus on **exemplary** applications in HEP and only little on techniques
- For a long time of my career I had nothing to do with ML
  At least I thought so, until I found out differently
- ML terminology is appearing more and more in task assignments and research projects
  And I am still trying to make sense where it makes sense

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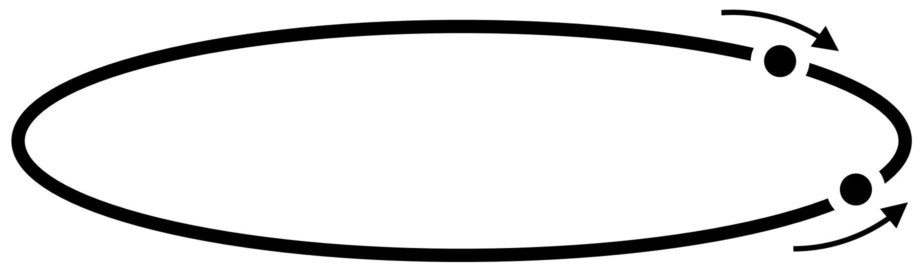
# HEP landscape in a nutshell*

COLLIDER



e.g. LHC

$\sqrt{s} =$ 14 TeV

$f_{coll} =$ 40 MHz

Image: CERN

*collider centric view

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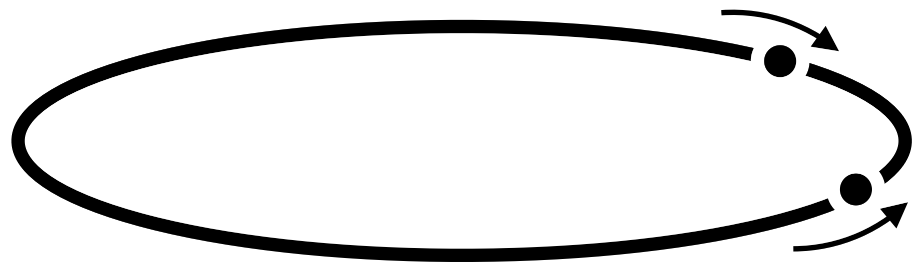

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$\sqrt{s} = $ 14 TeV

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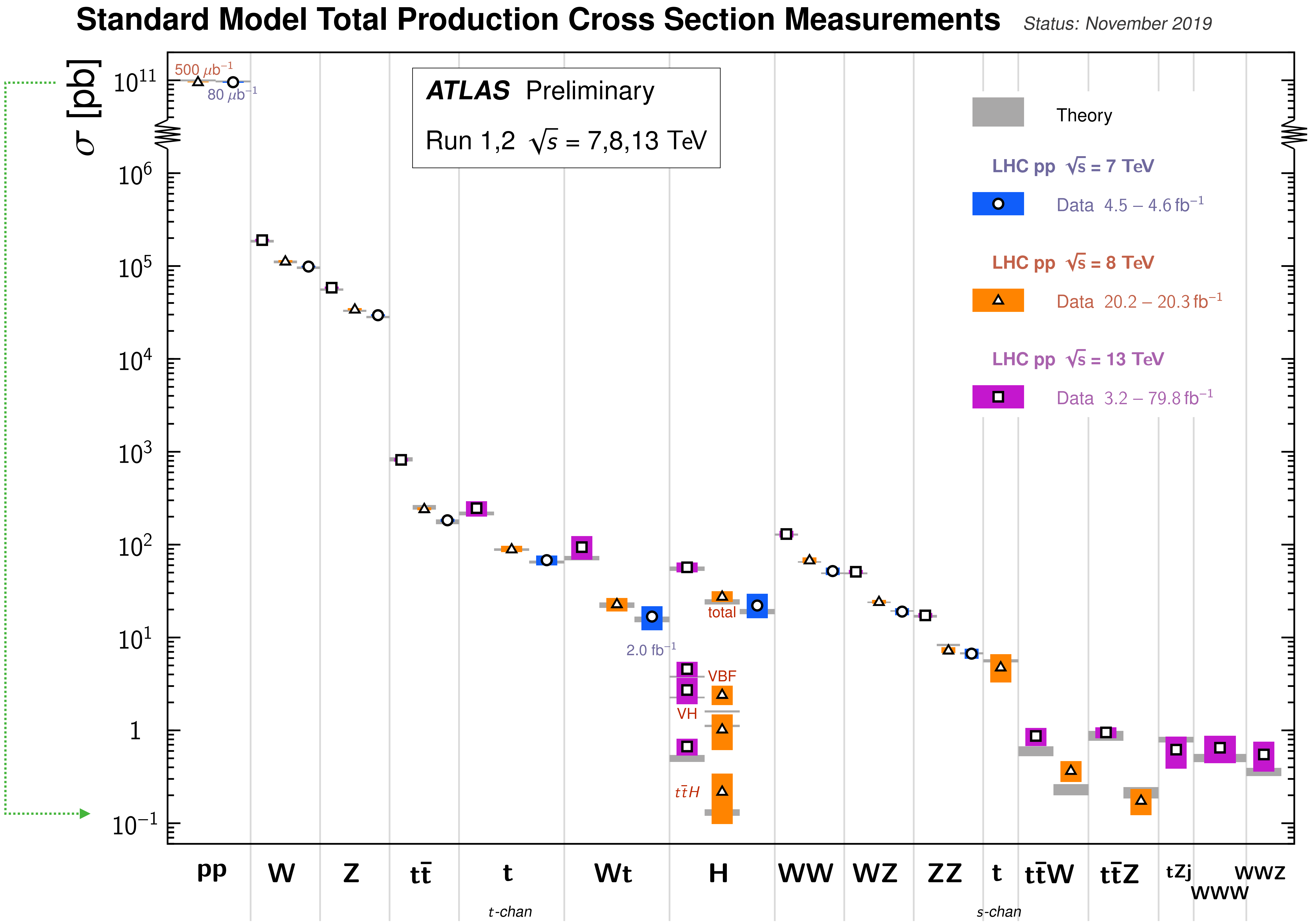
$10^{12}$



[ SM cross section summary, ATLAS ]

*collider centric view

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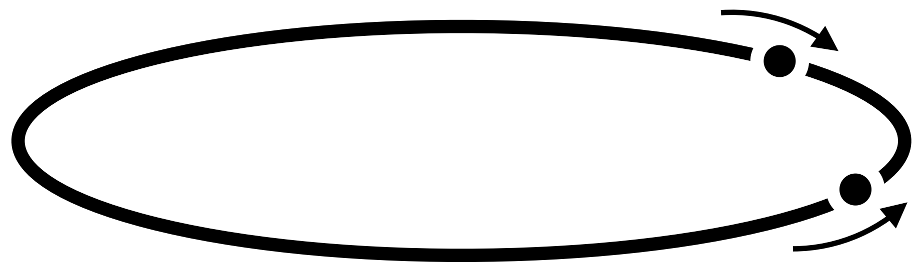
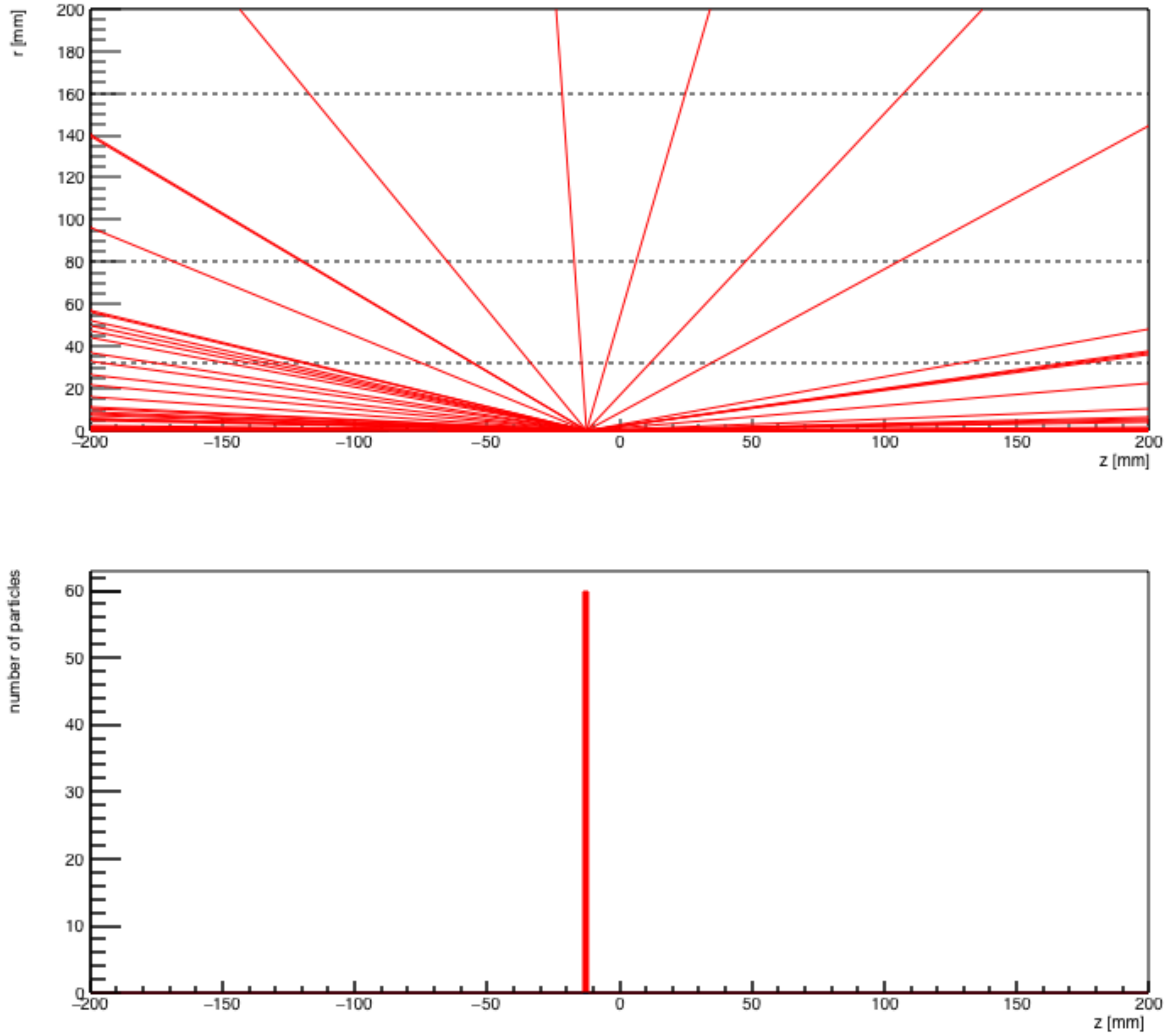


e.g. LHC

$\sqrt{s} =$ 14 TeV

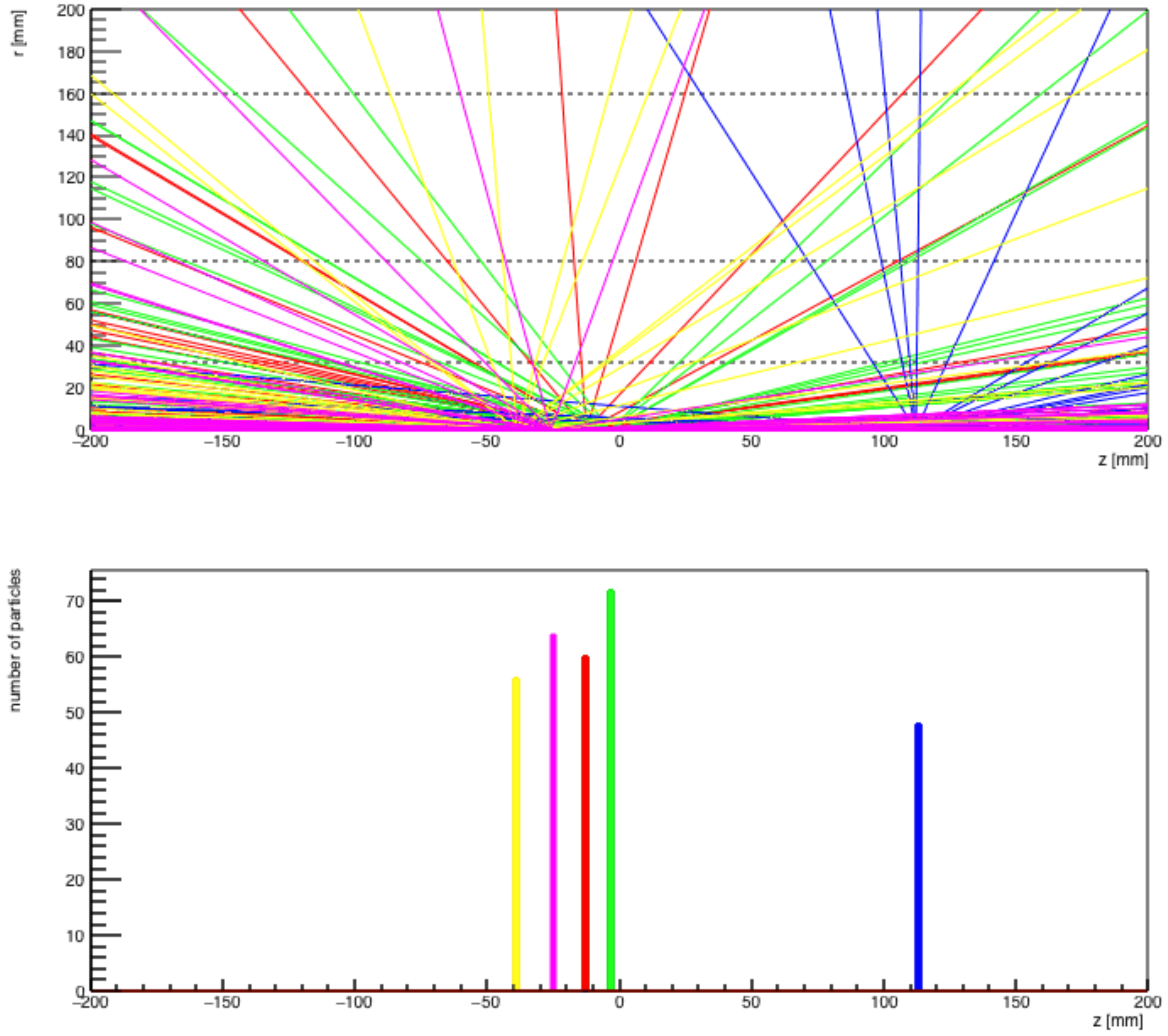
$f_{coll} =$ 40 MHz

$< \mu > \approx$ 200



$< \mu > = 1$

START-UP OF LHC (2009)
1 single P-P collision



$< \mu > = 5$

EARLY RUN-1 OF LHC (2010)
5 instantaneous P-P collision

*collider centric view

# HEP landscape in a nutshell*

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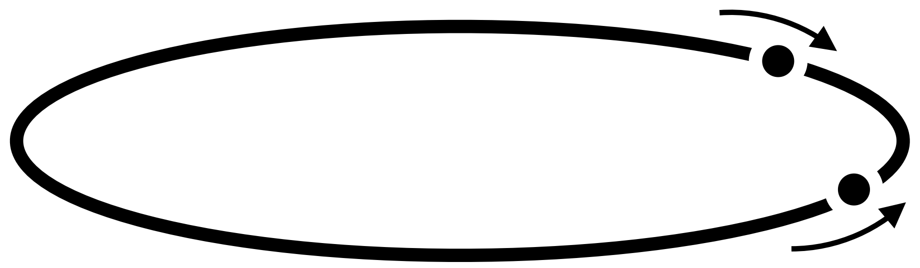
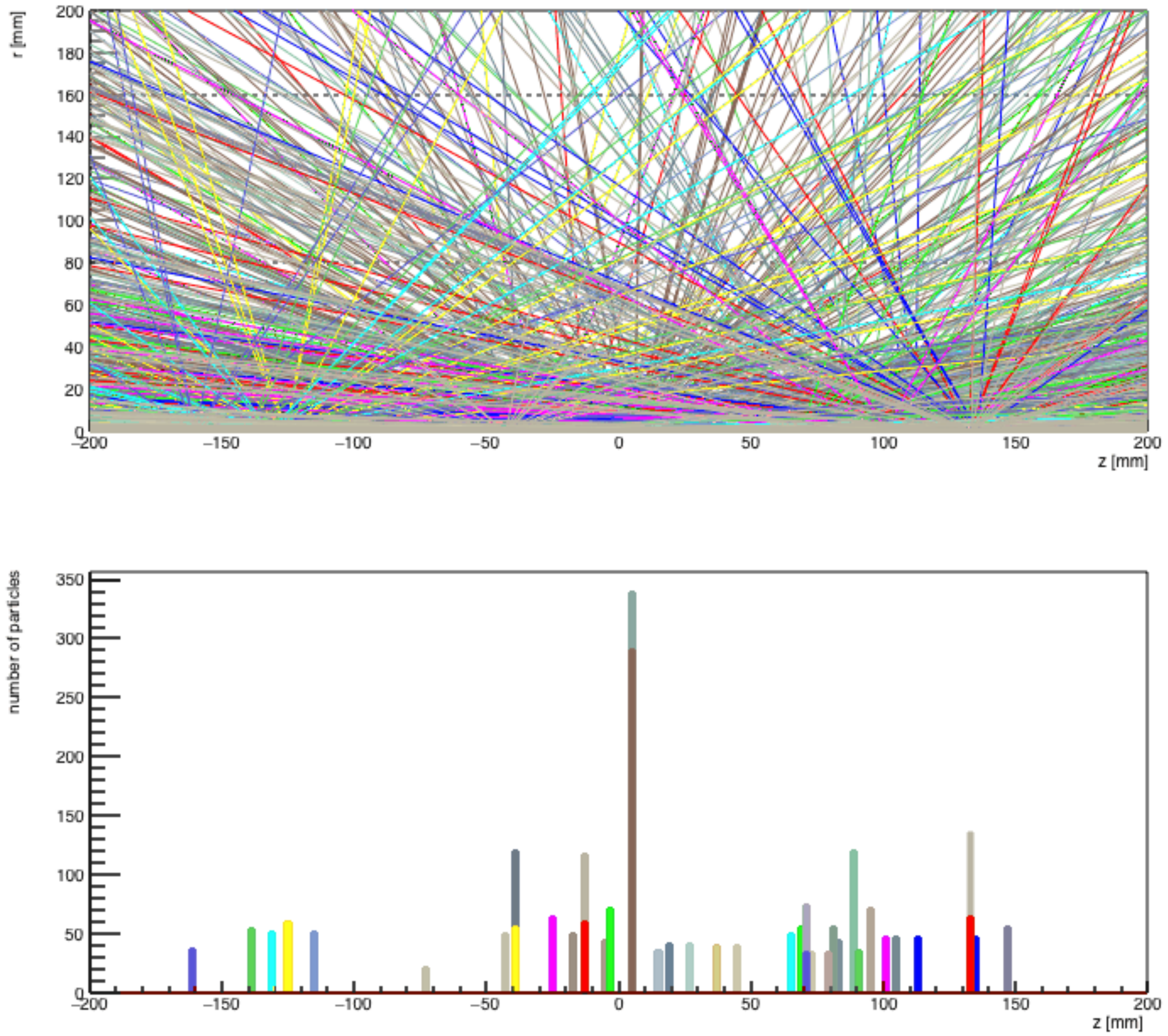


e.g. LHC

$\sqrt{s} = 14$ TeV

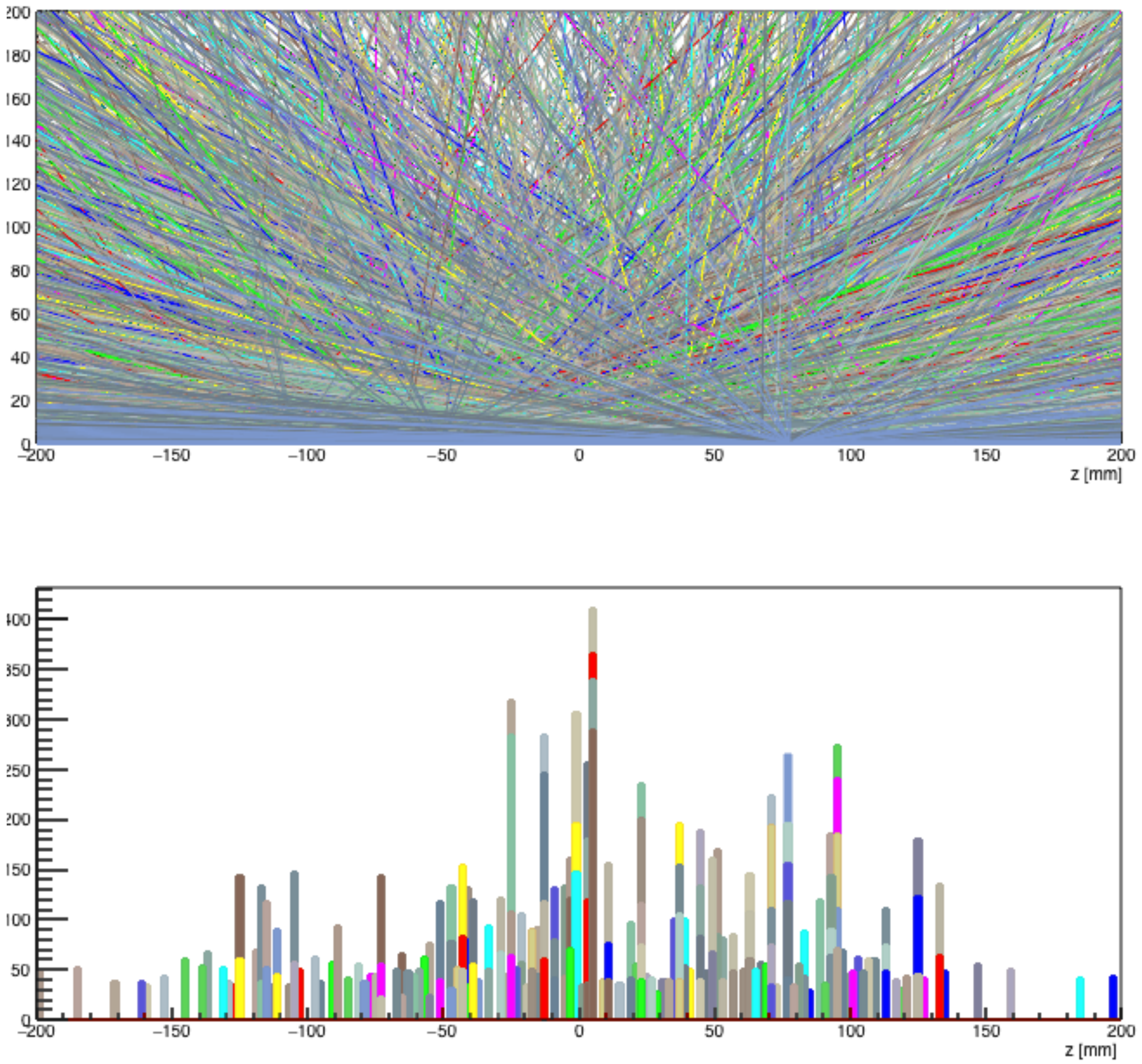
$f_{coll} = 40$ MHz

$< \mu > \approx 200$



$< \mu > = 40$

RUN1/2
~40 instantaneous P-P collision



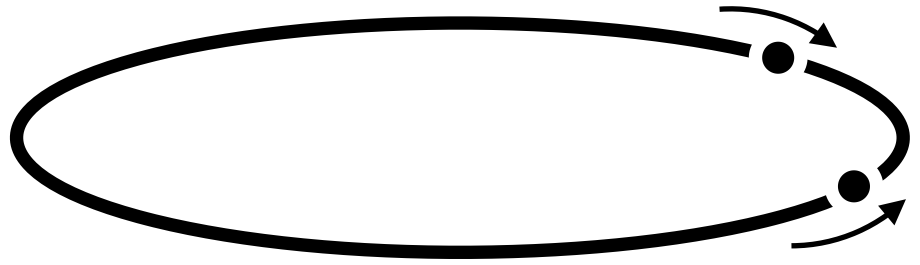
$< \mu > = 200$

HL-LHC (exp. 2027)
~200 instantaneous P-P collision

*collider centric view

# HEP landscape in a nutshell*

COLLIDER



e.g. CMS

R = 7.5 m

L = 21 m

W = 14 kT

~$10^8$ readout channels

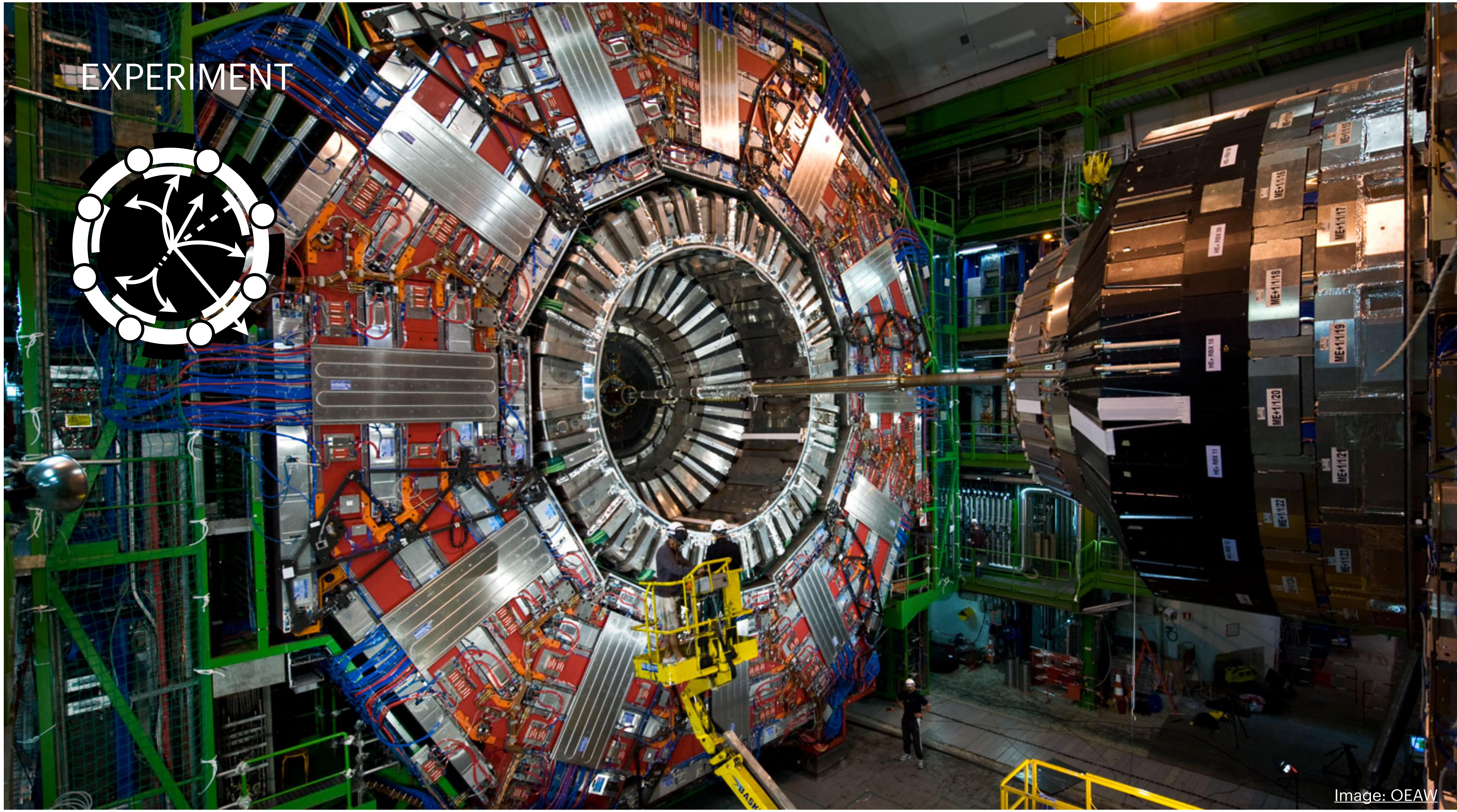


Image: OEAW

*collider centric view

# HEP landscape in a nutshell*

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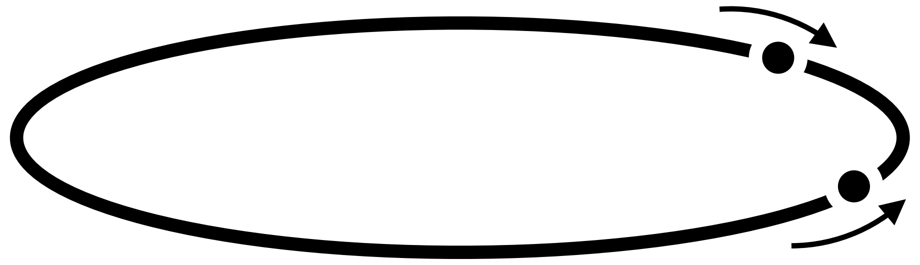
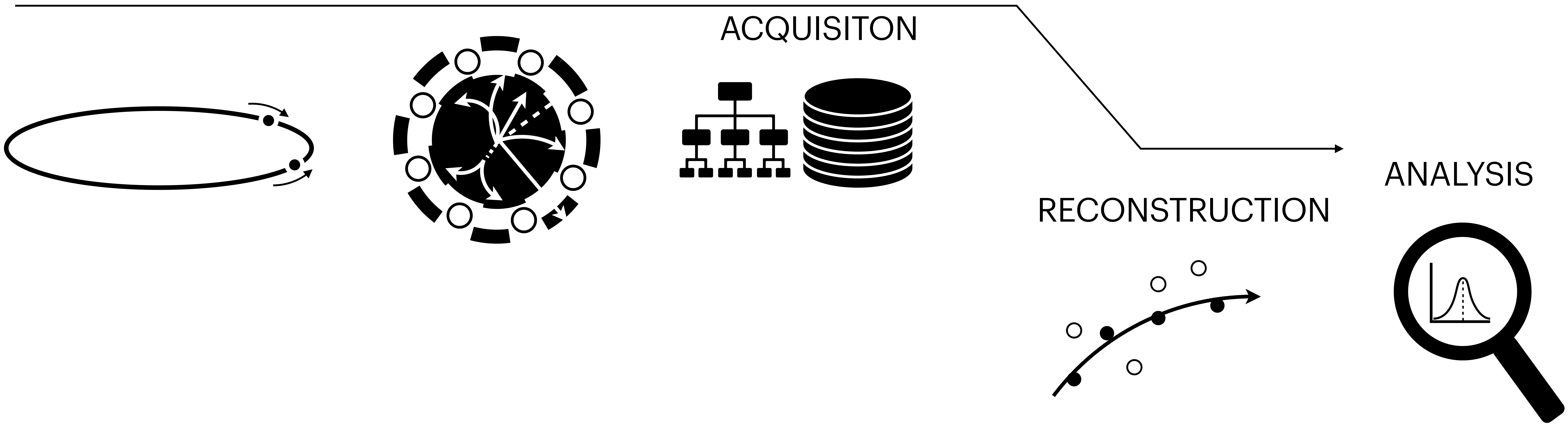


EXPERIMENT

TRIGGER & DATA
ACQUISITON

*collider centric view

# HEP landscape in a nutshell - data path



COLLIDER

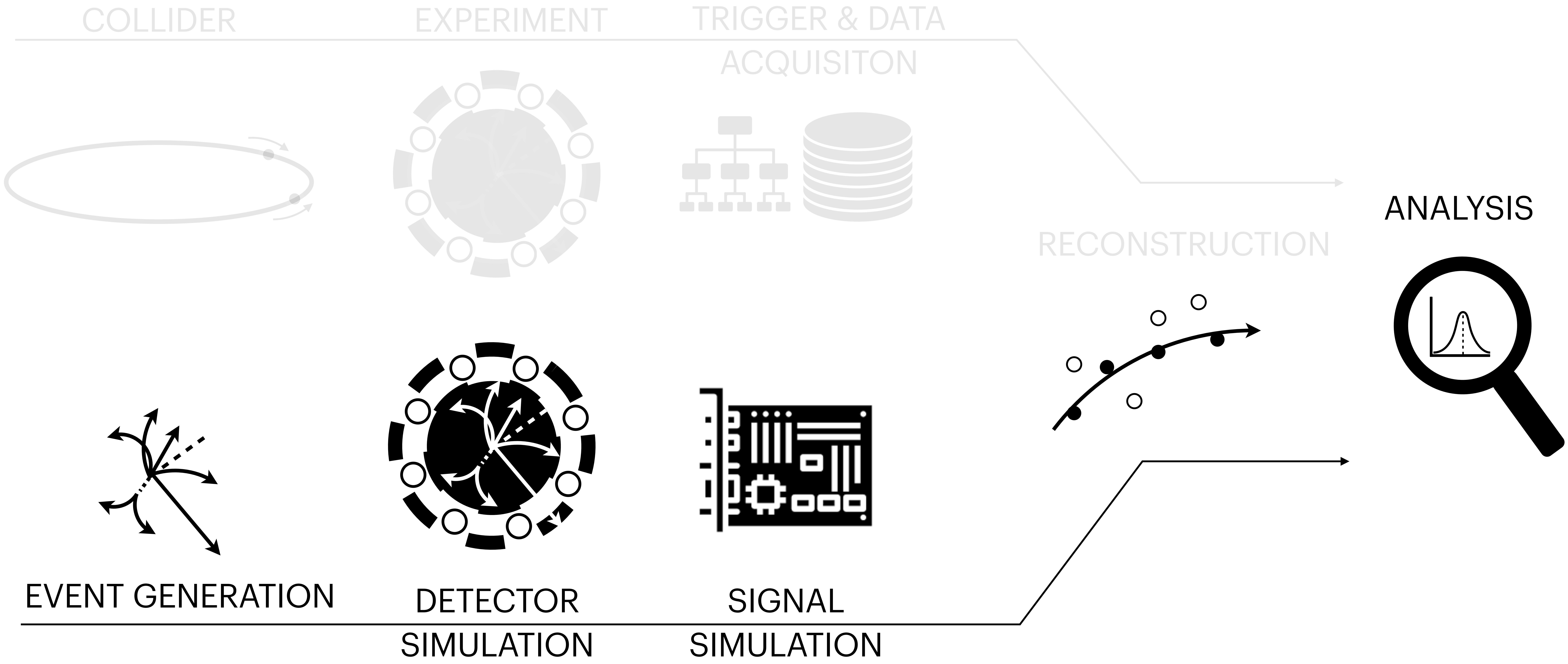
EXPERIMENT

TRIGGER & DATA ACQUISITON

RECONSTRUCTION

ANALYSIS

# HEP landscape in a nutshell - MC path



COLLIDER

EXPERIMENT

TRIGGER & DATA ACQUISITON

RECONSTRUCTION

ANALYSIS

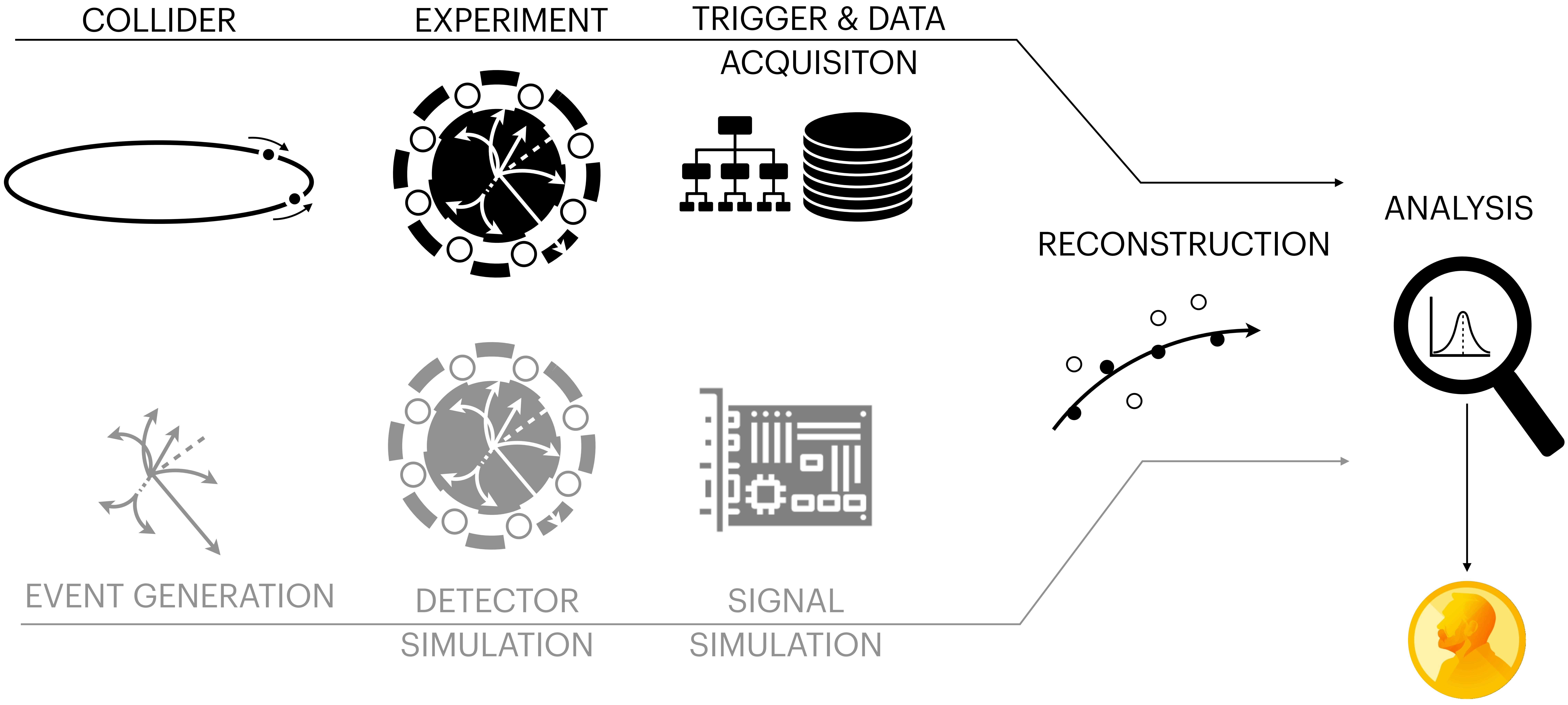
EVENT GENERATION

DETECTOR SIMULATION

SIGNAL SIMULATION

*collider centric view

# HEP landscape in a nutshell - success path



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*collider centric view

# HEP&ML: Data Analysis

CHEP 2018

23RD INTERNATIONAL CONFERENCE ON COMPUTING IN HIGH ENERGY AND NUCLEAR PHYSICS

9-13 July 2018
National Palace of Culture
Sofia, Bulgaria

Dedicated track all week: Machine Learning and Physics Analysis

ICHEP2018 SEOUL

XXXIX INTERNATIONAL CONFERENCE ON high Energy PHYSICS

JULY 4 - 11, 2018 COEX, SEOUL

18 contributions with Machine Learning in the Title

Machine Learning and the Physical Sciences

Workshop at the 33rd Conference on Neural Information Processing Systems (NeurIPS)

December 14, 2019

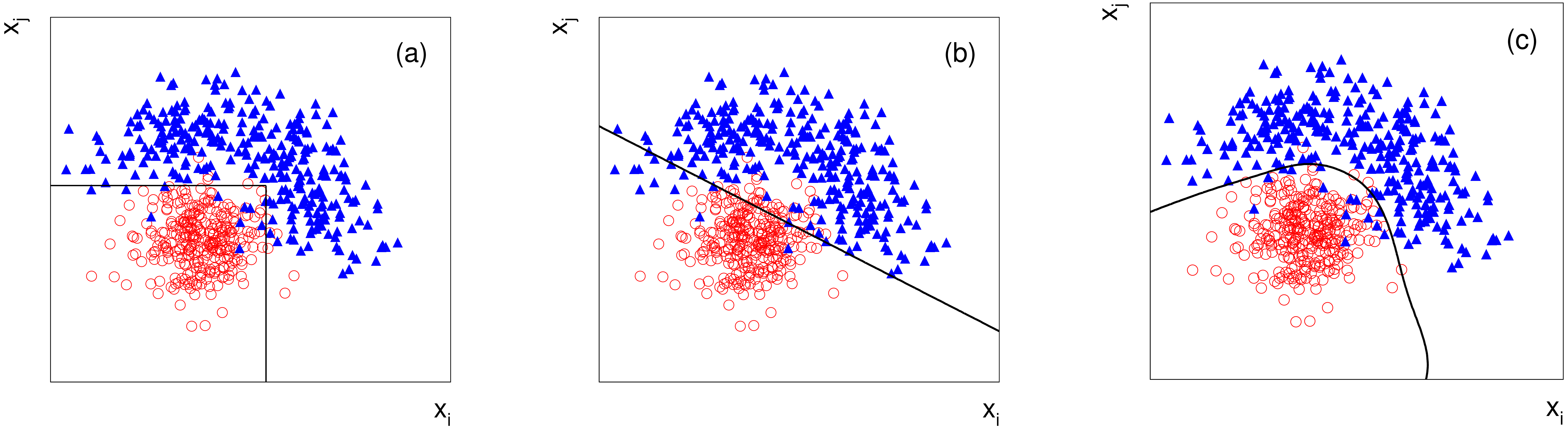
NeuRIPS: Machine Learning and the Physical Sciences

... and many, many more.

# HEP&ML: Data Analysis

## Potentials

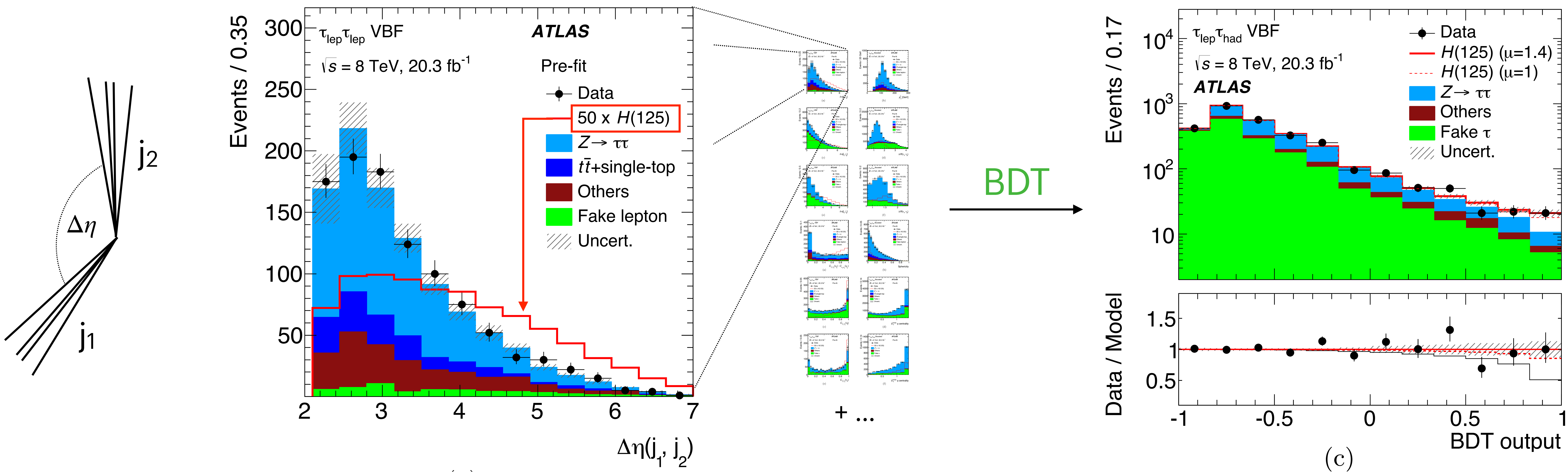
- Data analysis can profit hugely from ML techniques
- Most HEP analyses pose classification problem, e.g. signal (○) vs. background (▲)
  - Classical approach involved often parameter projection & cut (a)(b)
  - Trained classifiers do (in general) a better job (c)



# HEP&ML: Data Analysis

$H \to \tau^+\tau^-$

- Input is often multi-dimensional, separation at first sight poorly
  - perfect playground for advanced classifiers:
    - Boosted Decision Trees (BDT), Shallow/Deep Neural Networks (NN/DNN)



Evidence for Higgs Boson

[ arXiv:1501.04943 ]

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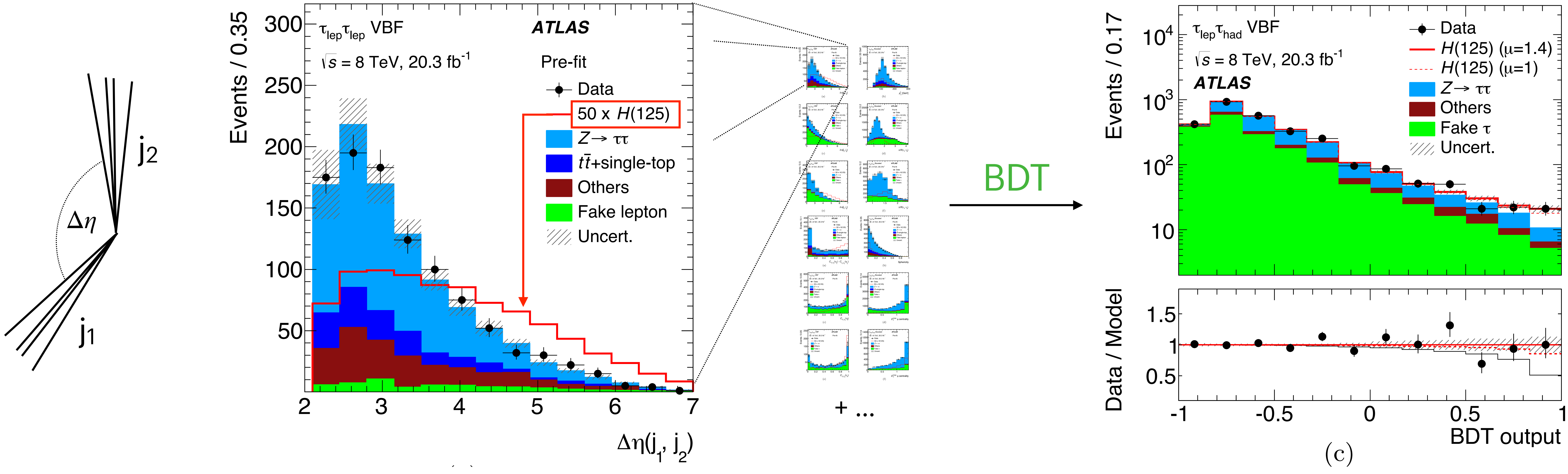

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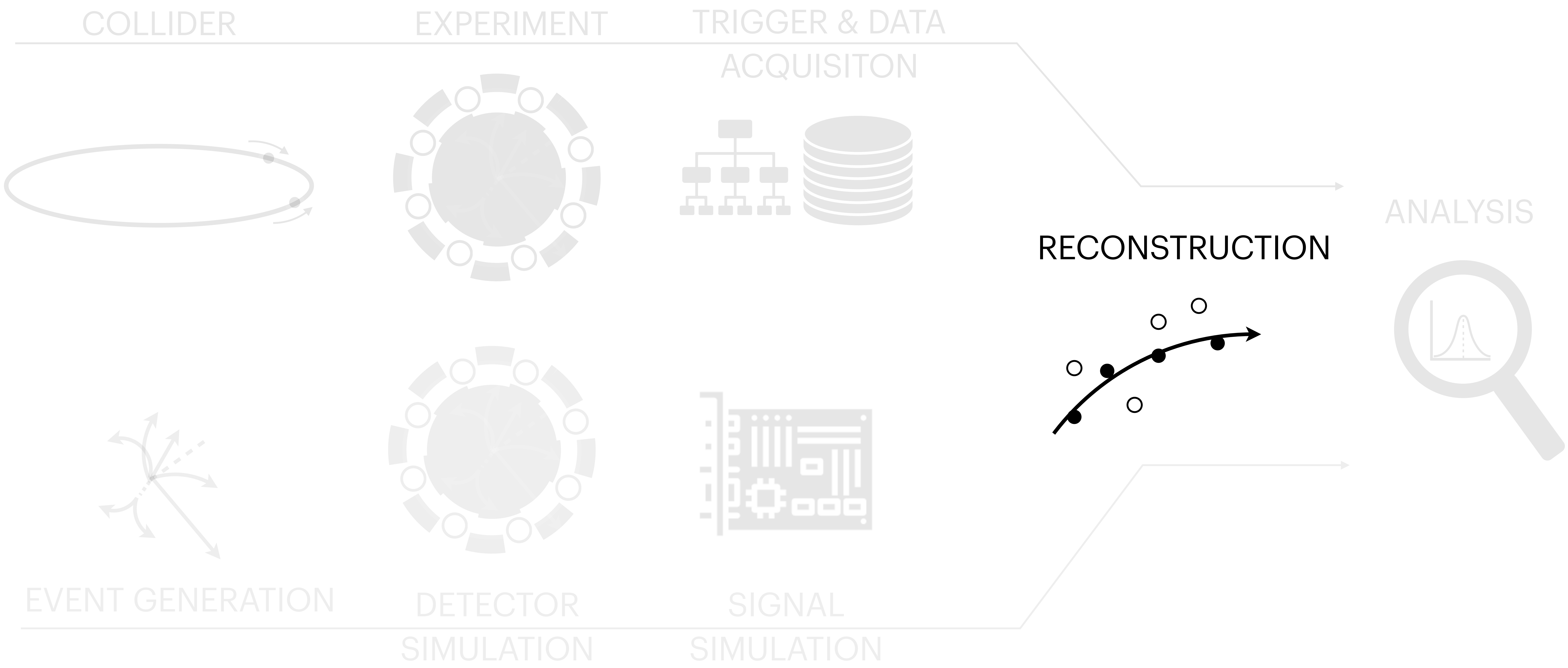
# HEP&ML: Data Analysis

Synergies and Challenges

- Many industry products are available in ML sector
  - Big tech players invest $$$ in algorithm development and SW/hardware optimisation (“free lunch” - not really)
- Huge pool of ML/DS experts
  - $H \to \tau^+\tau^-$ was put out as [ ML challenge ] on kaggle.com
- No out-of-the box solutions
  - Concerns regarding interpretability
  - Particular error reporting in HEP: $R = \nu \pm \sigma_{stat} \pm \sigma_{syst}$

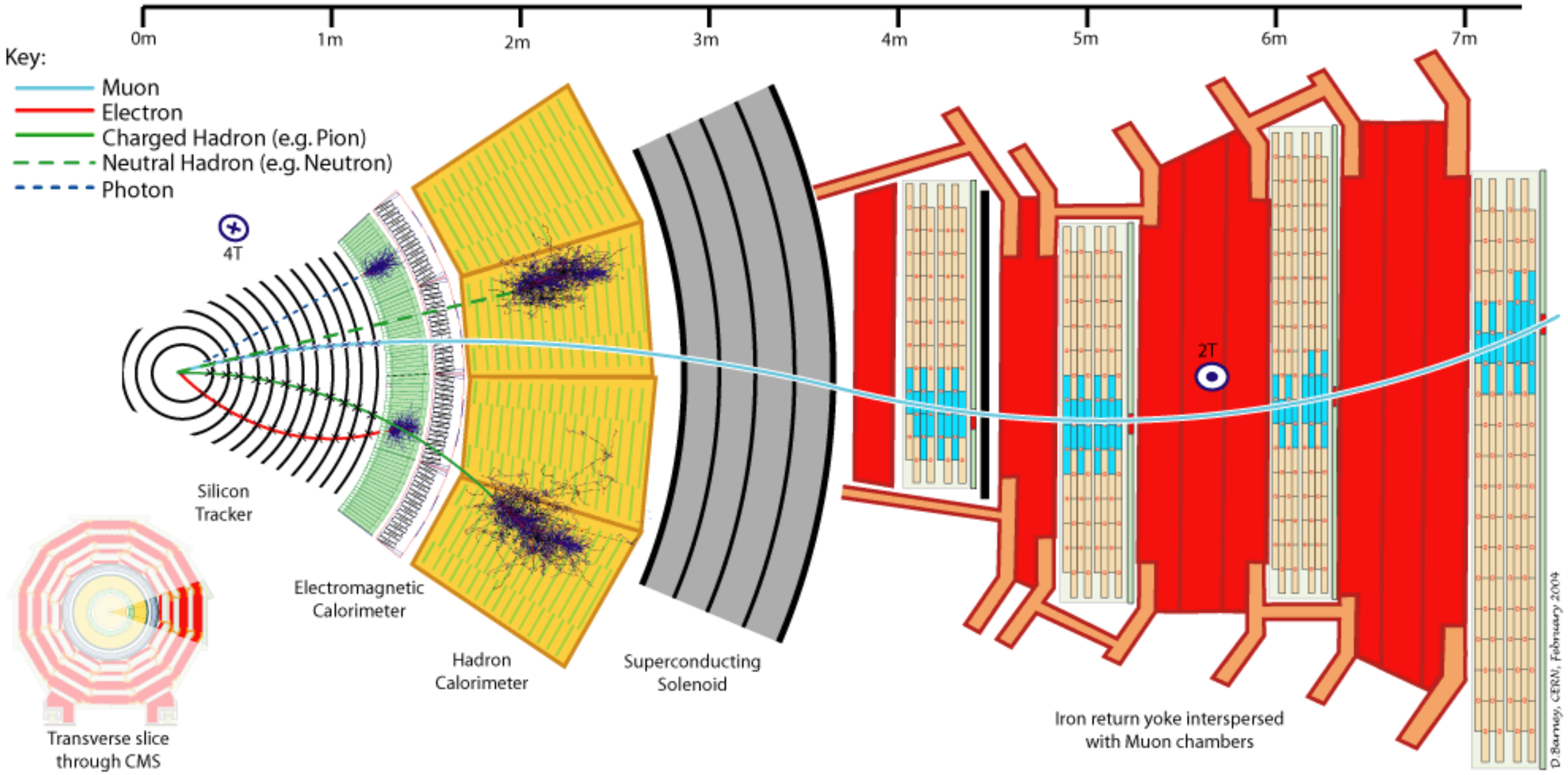
[ Higgs Machine Learning Challenge ]

# HEP&ML: Event Reconstruction



# Event Reconstruction

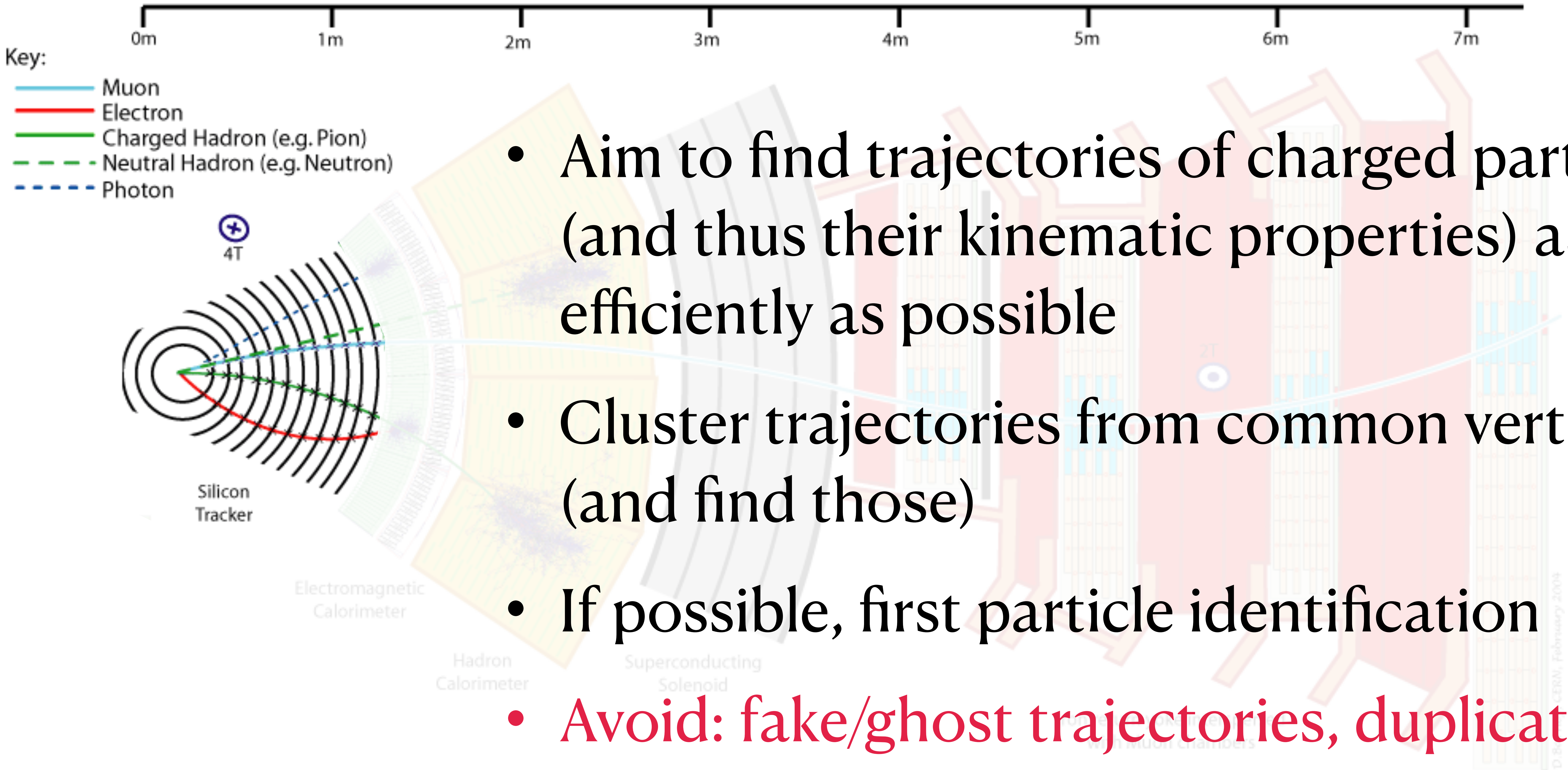
Particle and object reconstruction from “raw” input



[ Illustration: CERN ]

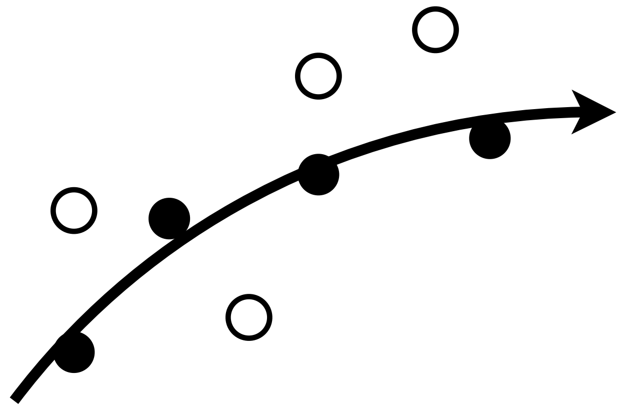
# Particle Tracking

Trajectory and vertex finding in tracking detectors



- Aim to find trajectories of charged particles (and thus their kinematic properties) as efficiently as possible
- Cluster trajectories from common vertices (and find those)
- If possible, first particle identification
- Avoid: fake/ghost trajectories, duplicates, …

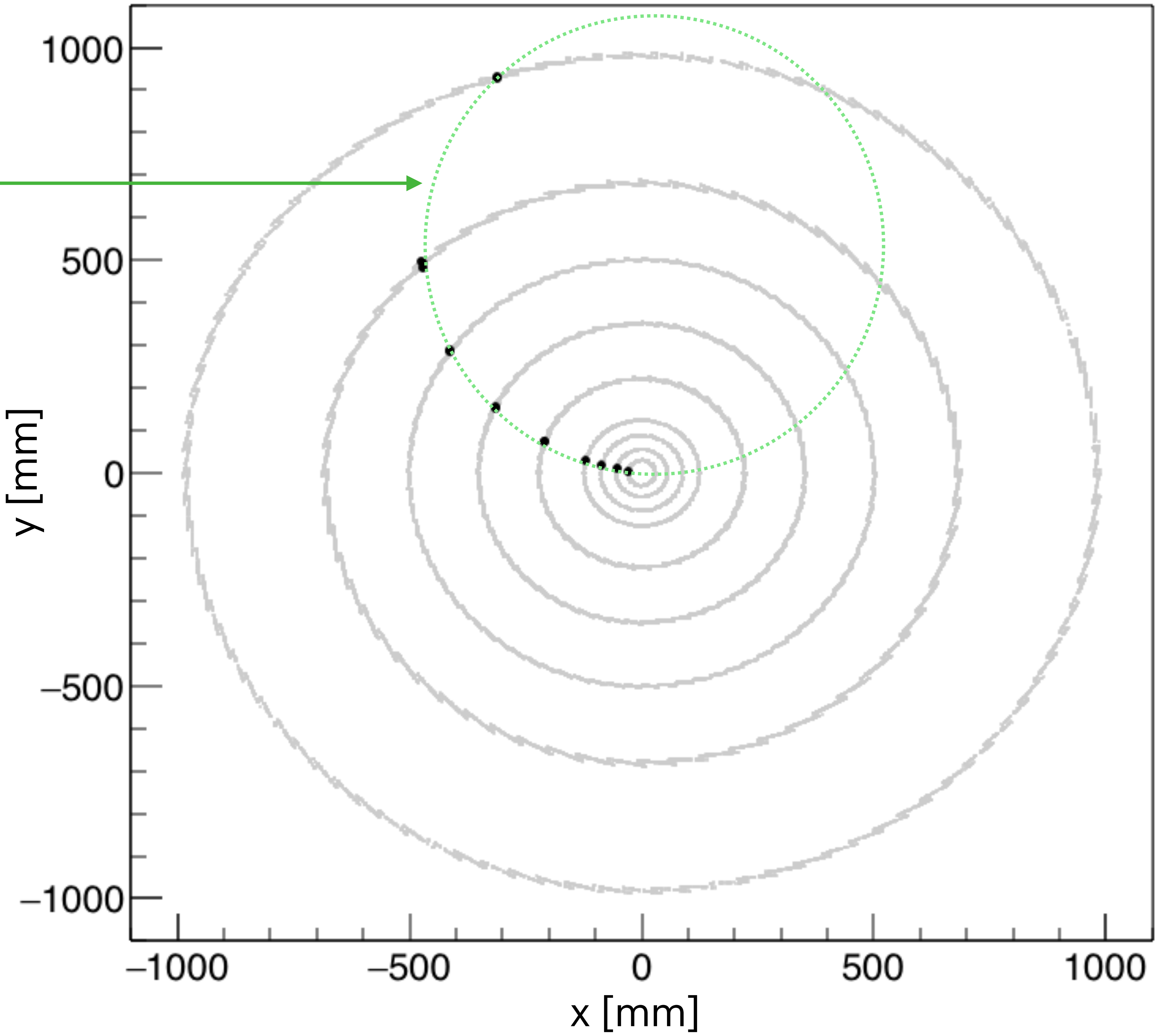
Particle Tracking Machine Learning Challenge [ Phase 1 ][ Phase 2 ]

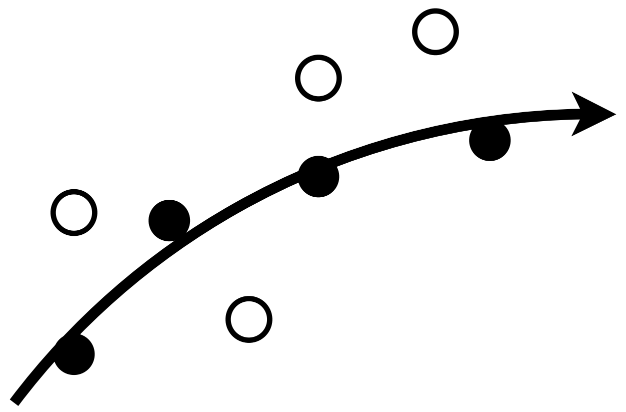


# Particle Tracking

Pattern recognition for particle detectors

- Typical pattern recognition problem
  - Effectively a clustering problem
- *Classical* approaches include
  - Global/conformal mapping
  - Track seeding & following
  - Combinatorial filtering





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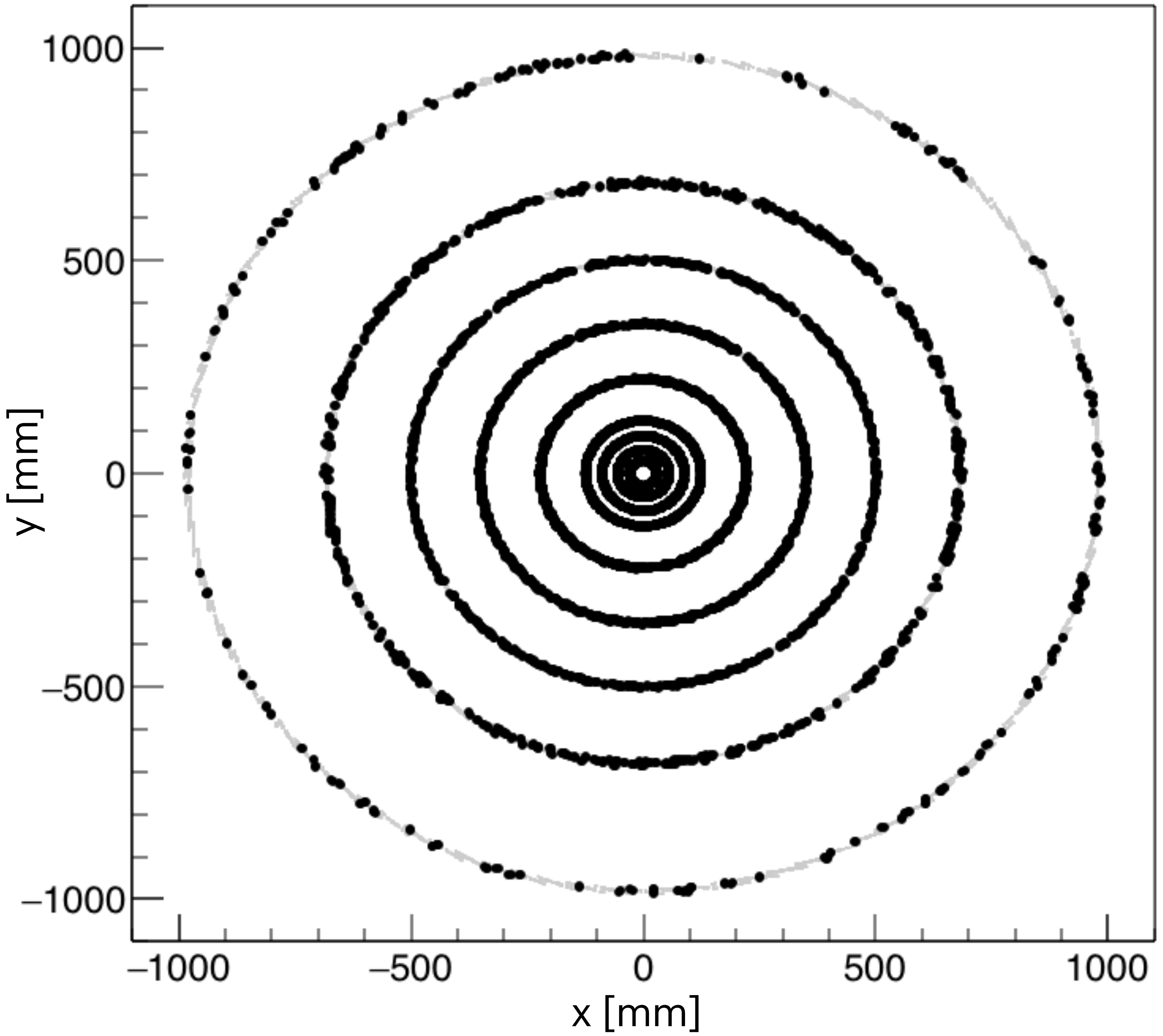
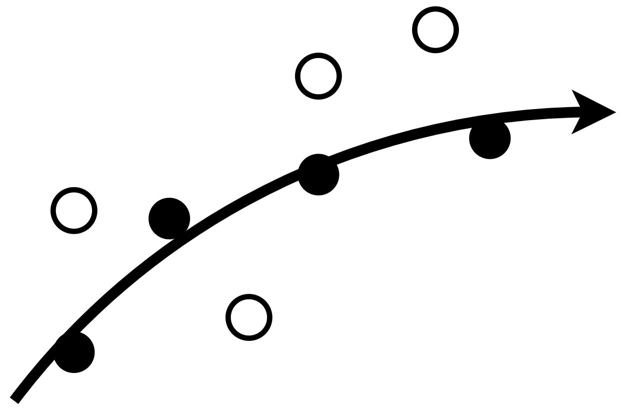
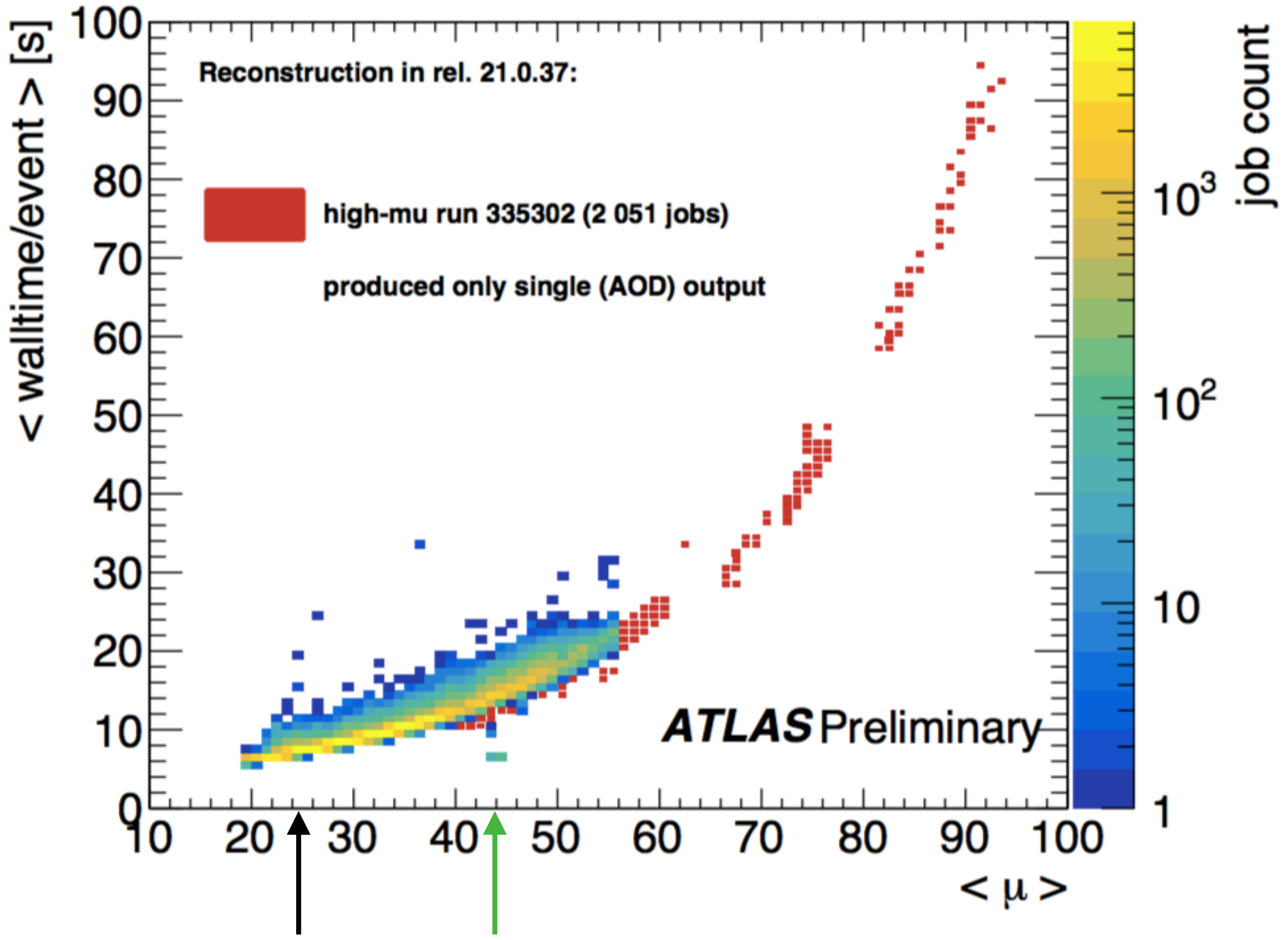




# Particle Tracking & Computing

- Combinatorial problem
- And it clearly scales
  like such



DESIGN/ACTUAL LUMINOSITY OF LHC
(+ DETECTORs, + ALGORITHMs)

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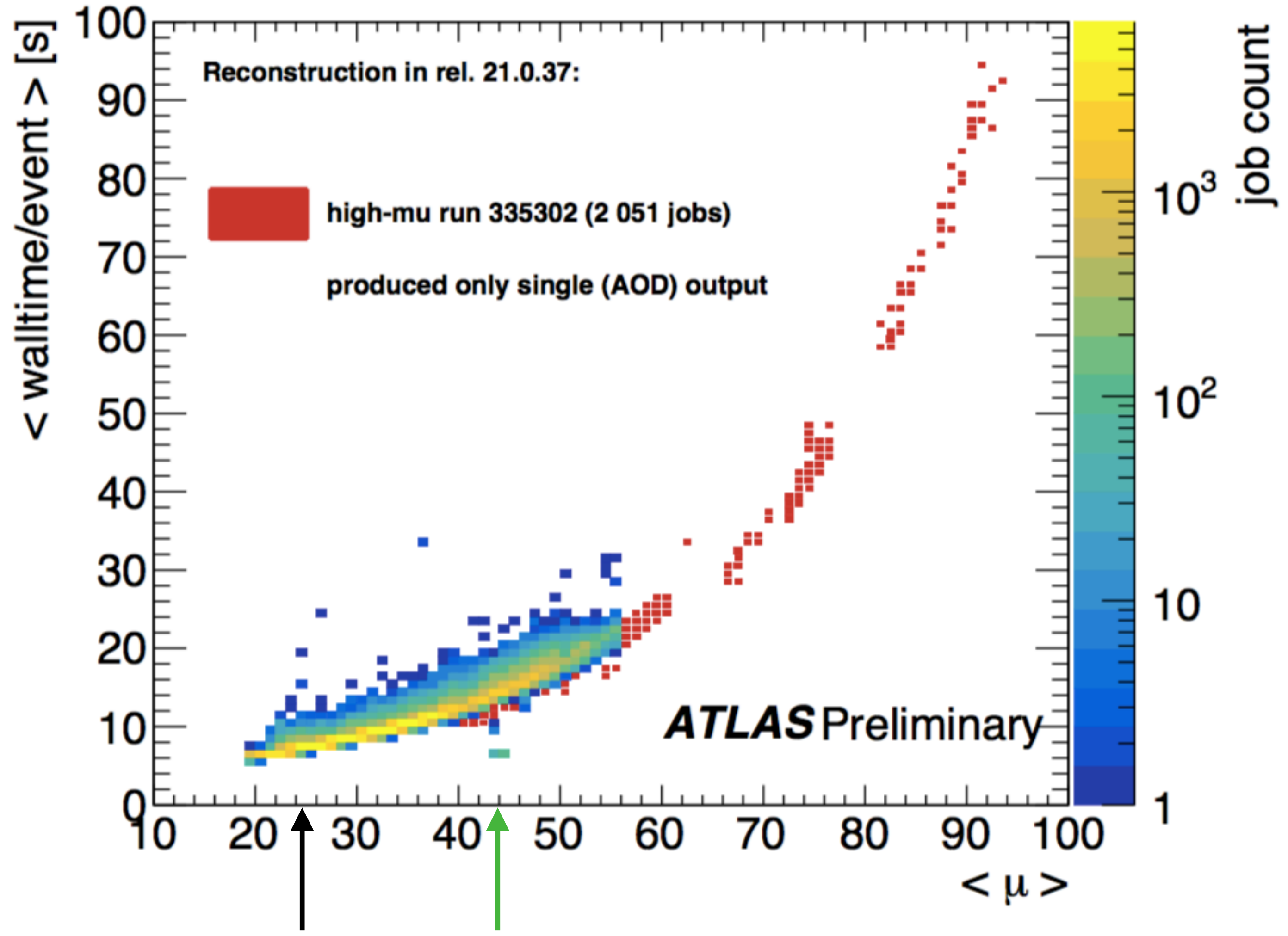

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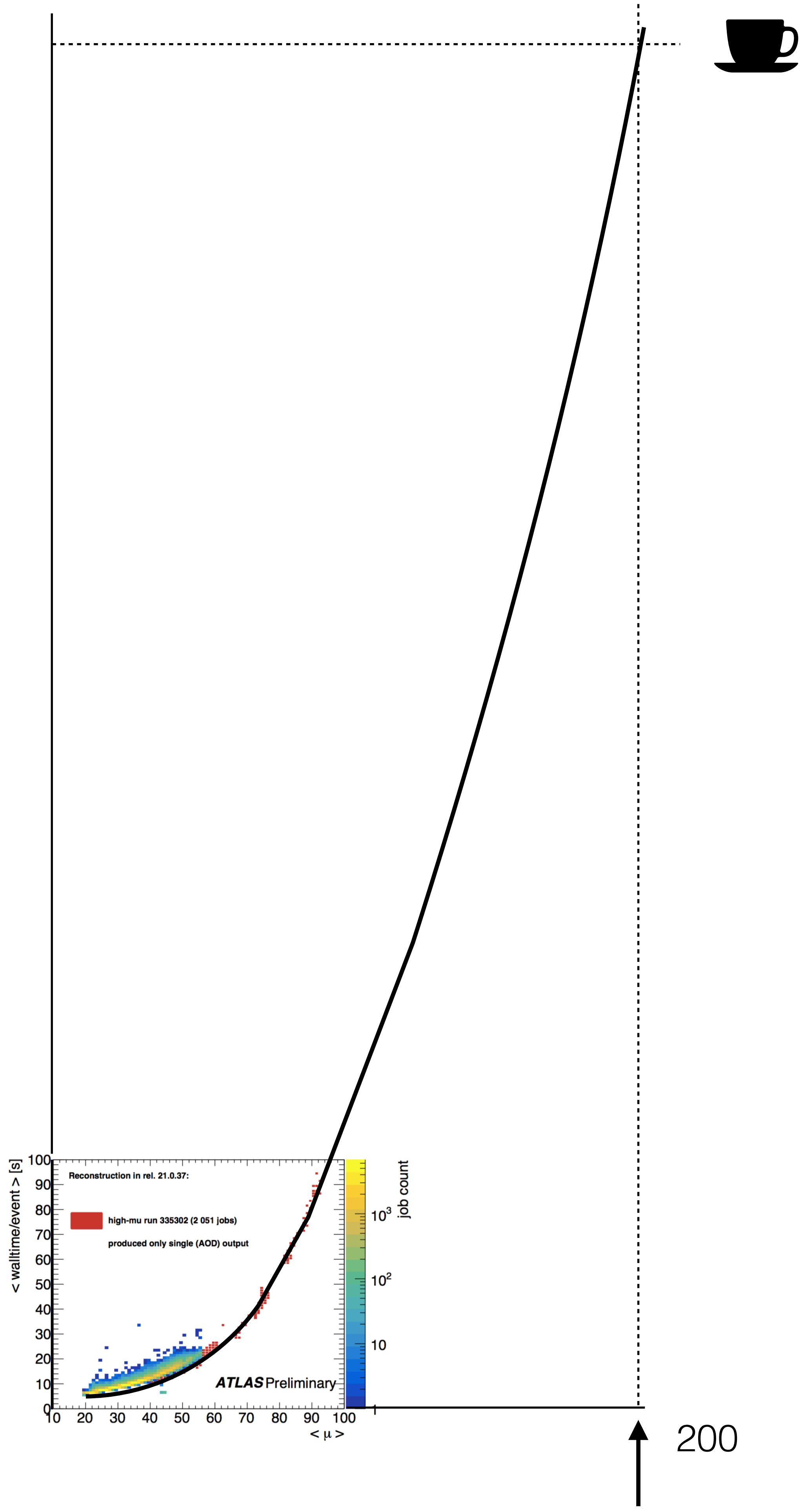

HIGH LUMINOSITY LHC (HL-LHC)
(EXP 2027)

VERY NAIVE SCALING: HL-LHC DETECTORS & ALGORITHMS PERFORM WAY BETTER!

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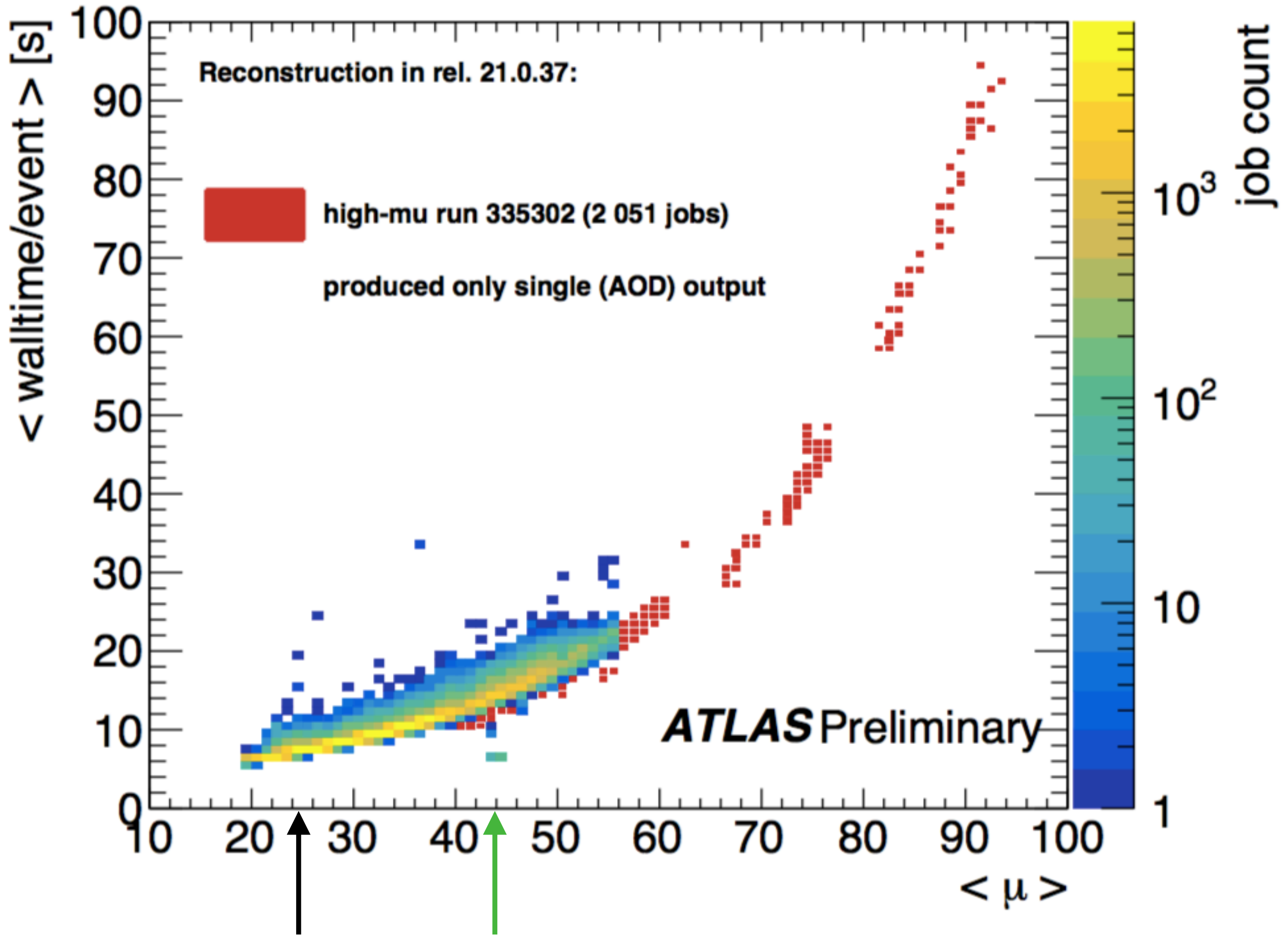

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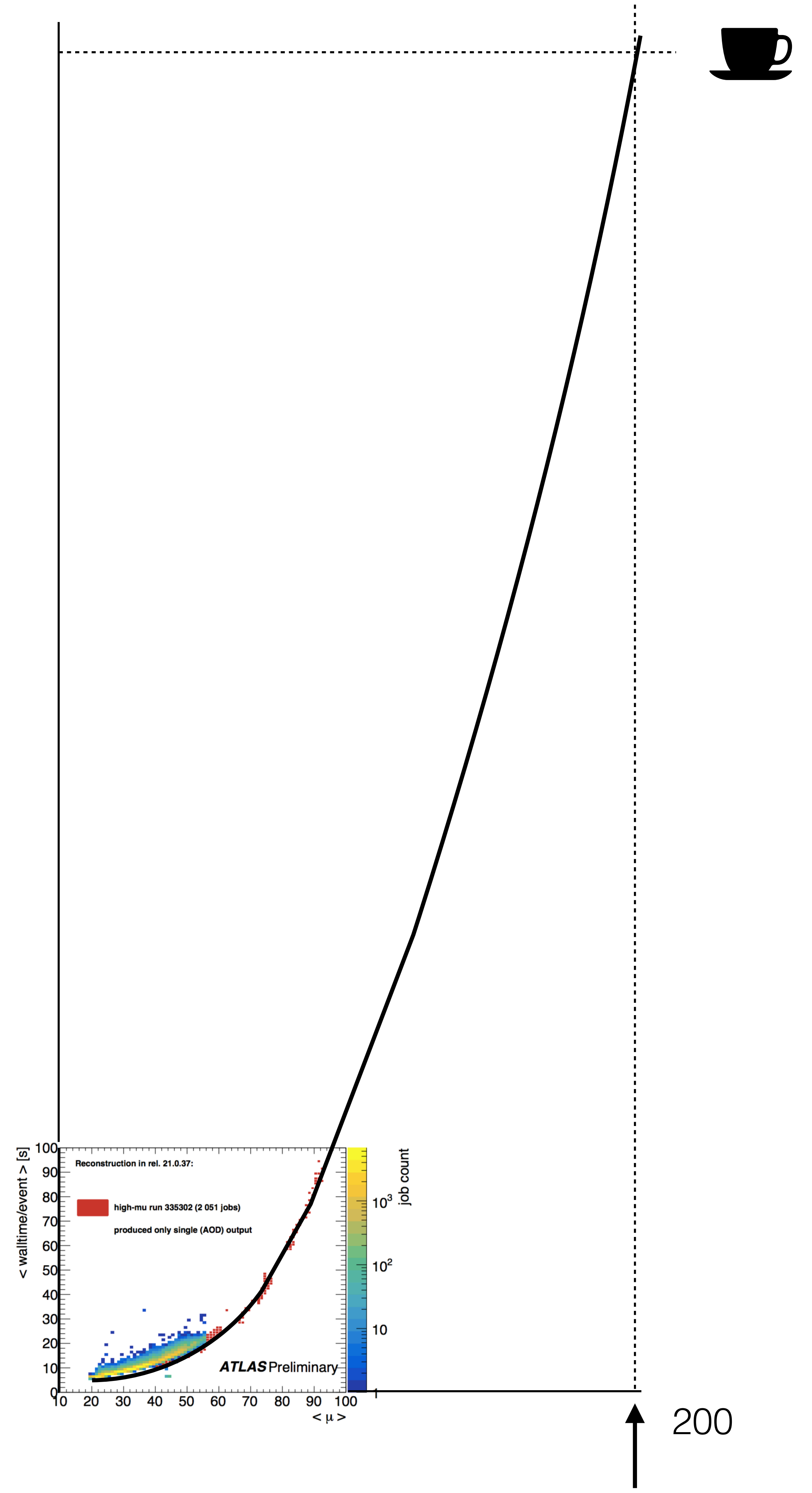

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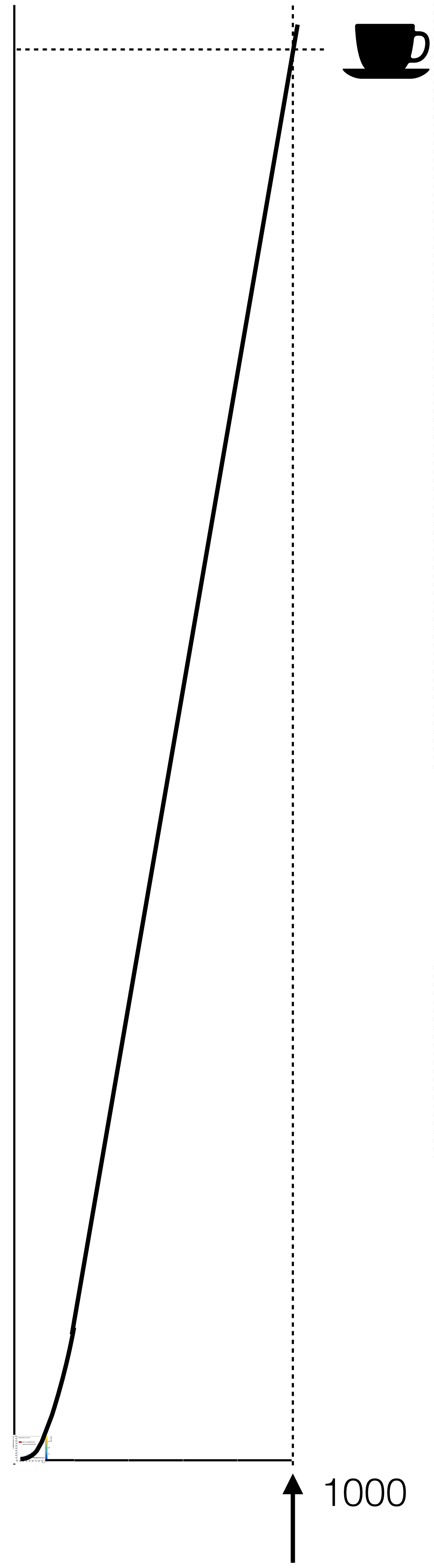
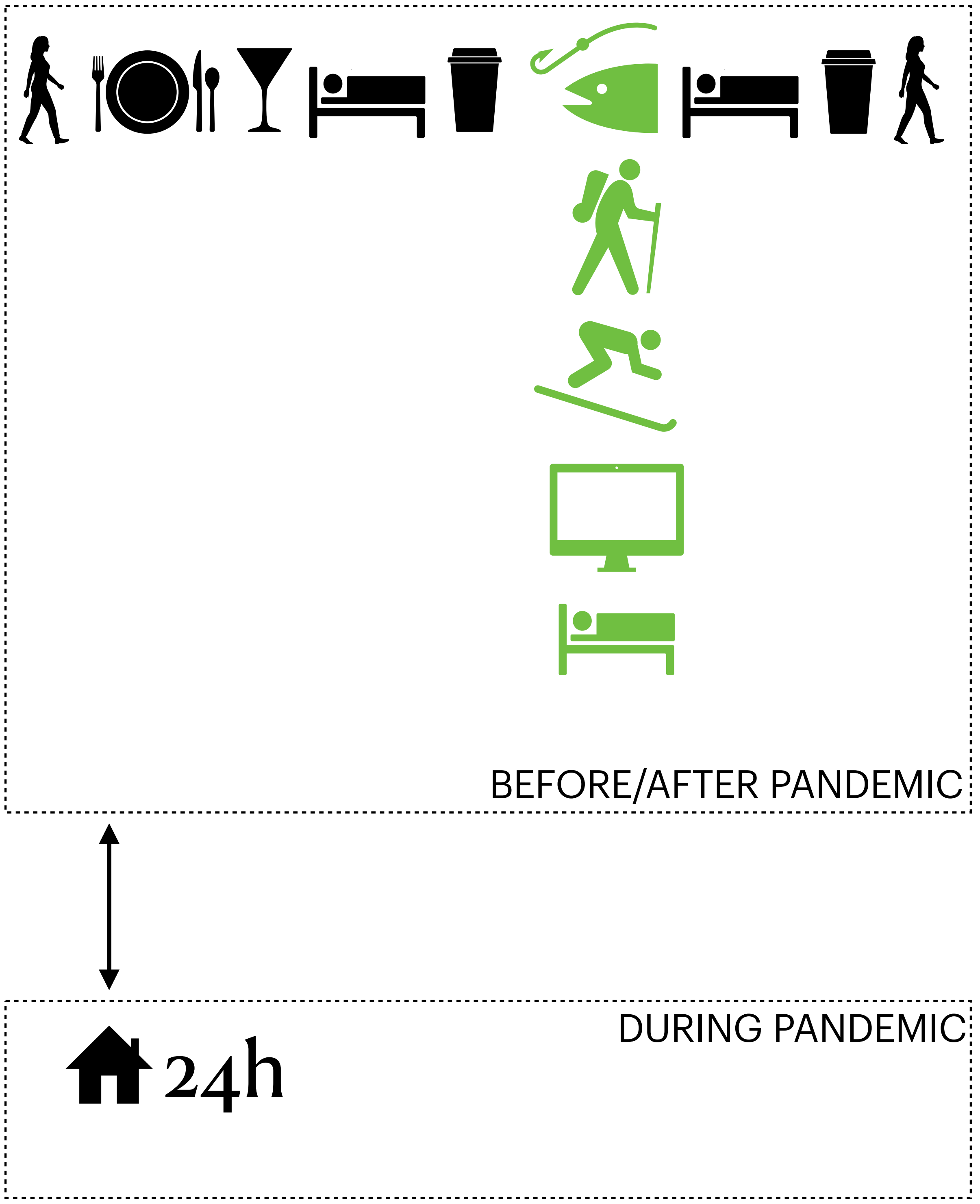


FCC-HH 25NS SCENARIO

(EXP ?)



VERY NAIVE SCALING: HL-LHC DETECTORS & ALGORITHMS PERFORM WAY BETTER!

# ML assisted track reconstruction

## Seed classification

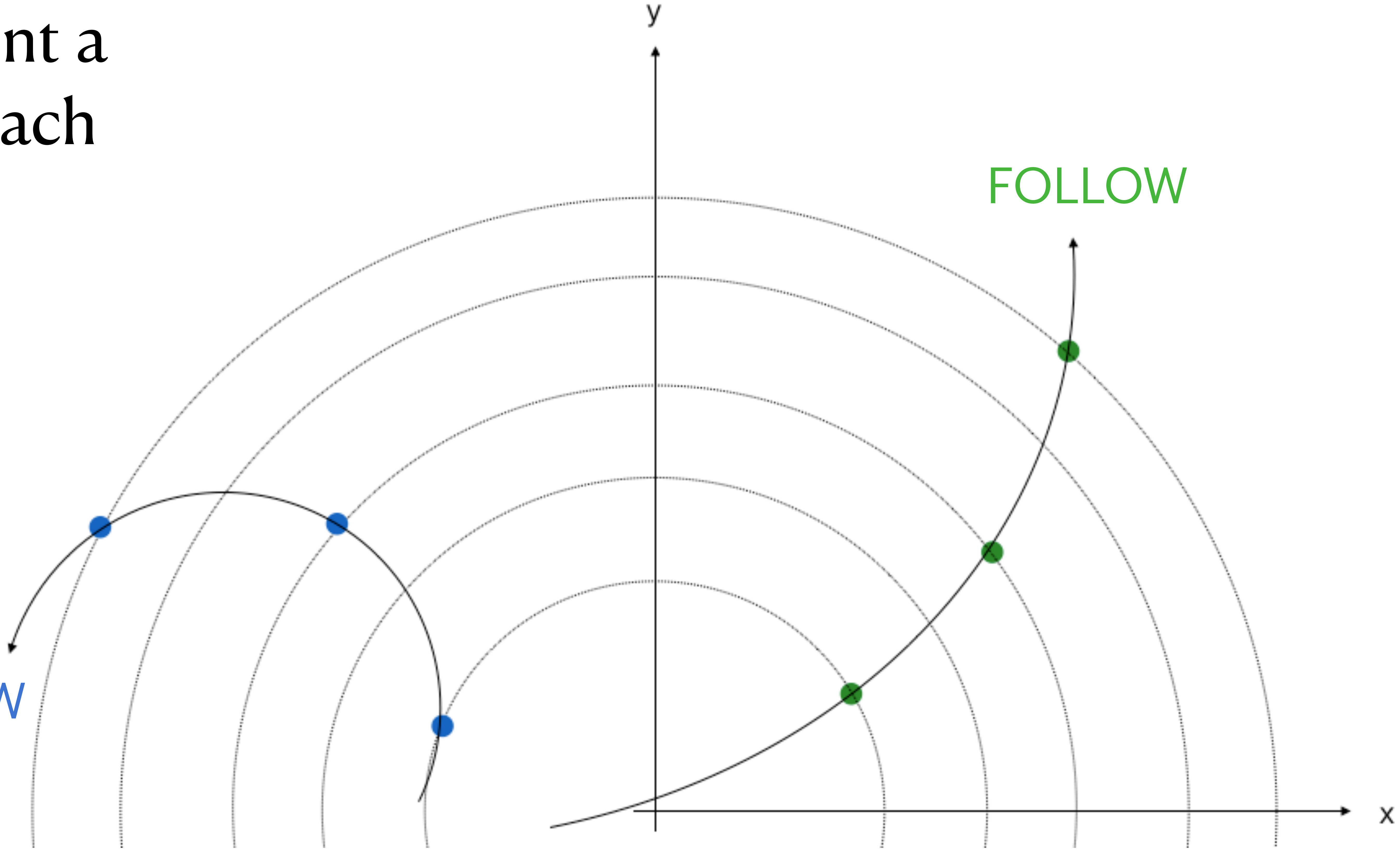
- Most LHC experiments implement a seeding & track following approach

↓

CPU INTENSIVE

↓

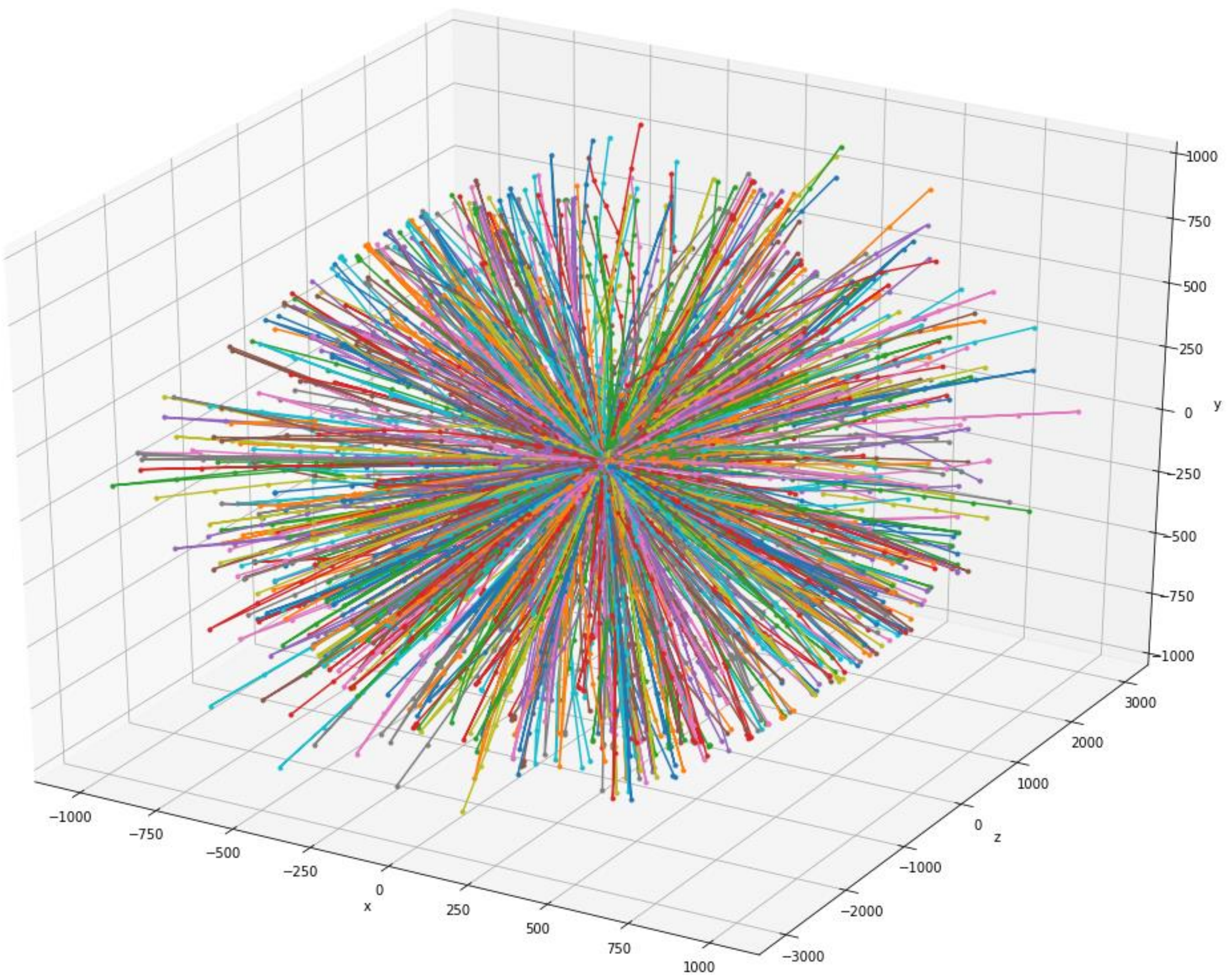
HIGHEST SEED PURITY REQUIRED

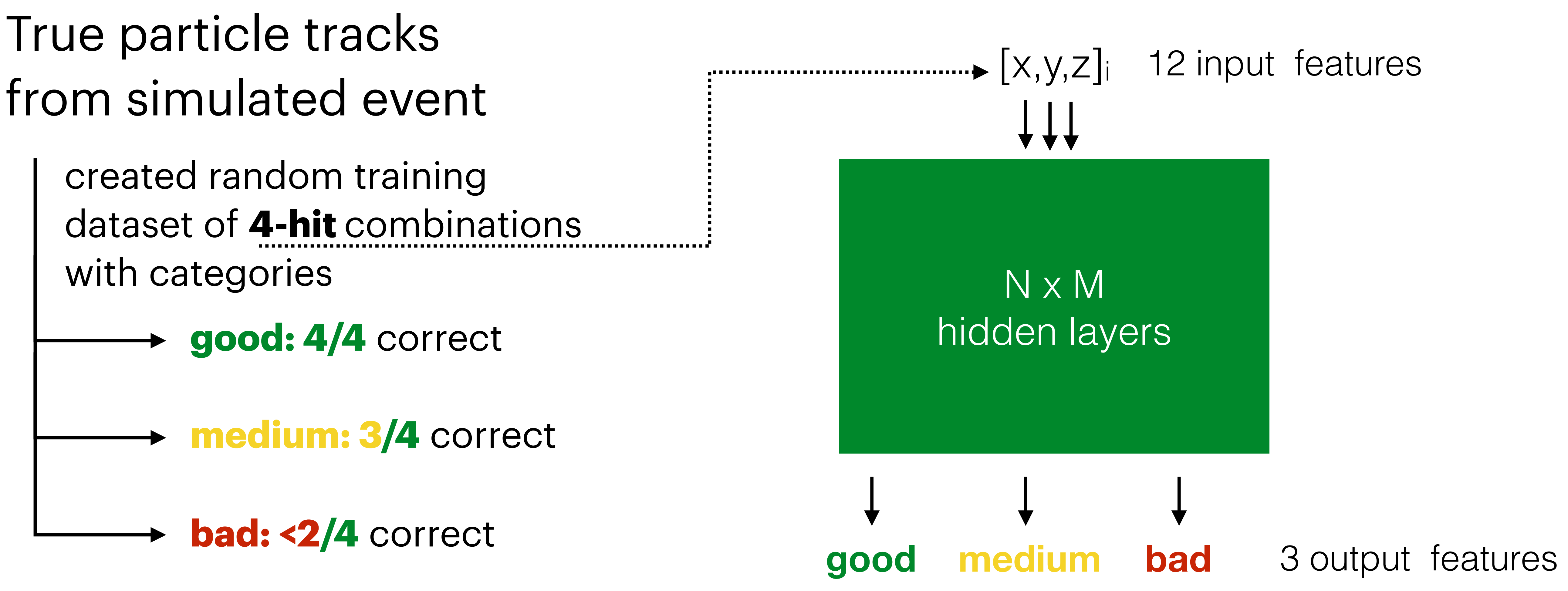


# ML assisted track reconstruction

## Seed classification

- Classification is perfect ML problem, replace cut & go technique





True particle tracks
from simulated event

created random training dataset of **4-hit** combinations with categories

- **good: 4/4** correct
- **medium: 3/4** correct
- **bad: <2/4** correct

$[x,y,z]_i$ 12 input features

N x M
hidden layers

**good** **medium** **bad** 3 output features

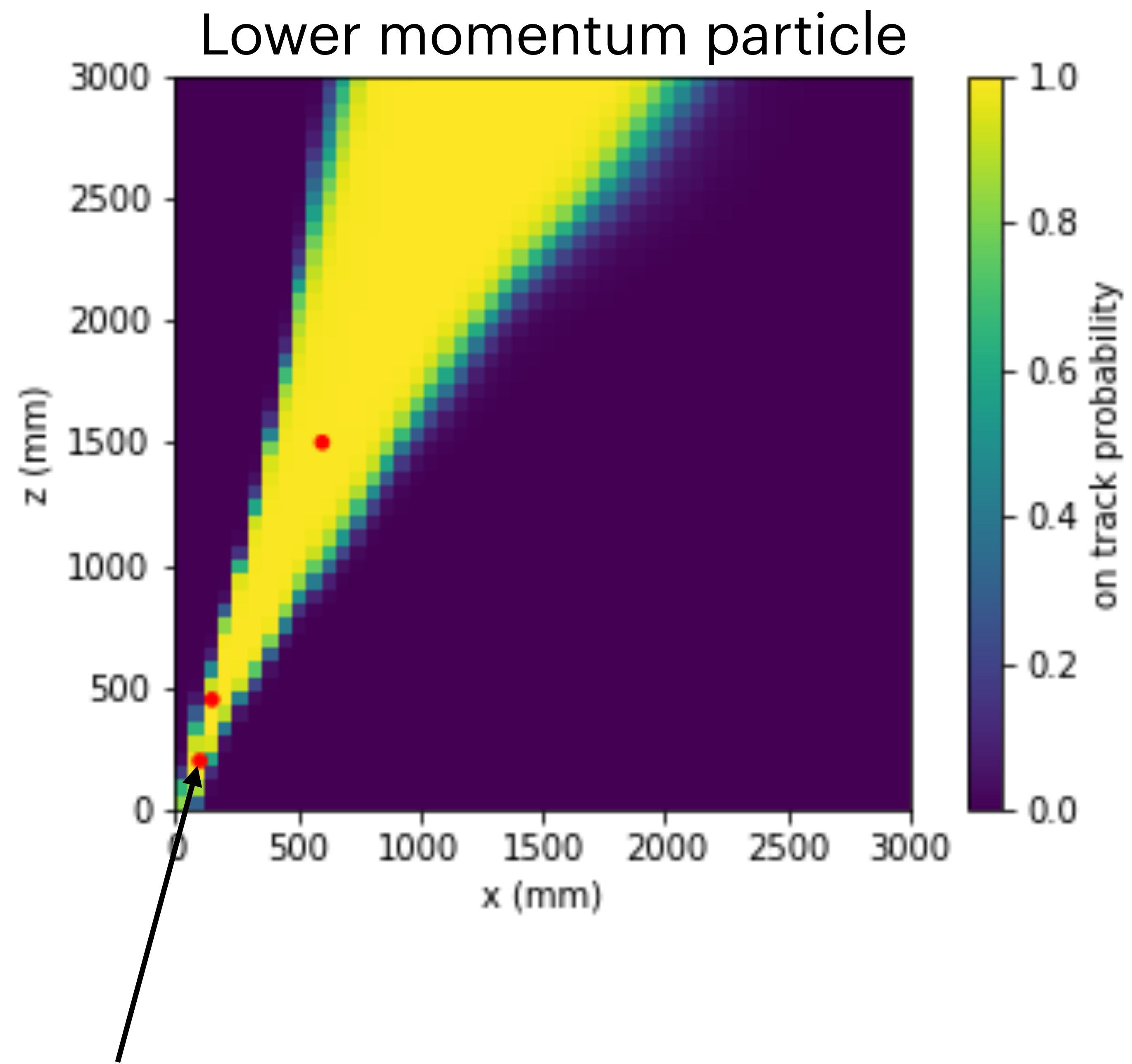
[ F. Dietrich, E. Knering, AS : Track Seed Classification using NNs ]

# ML assisted track reconstruction

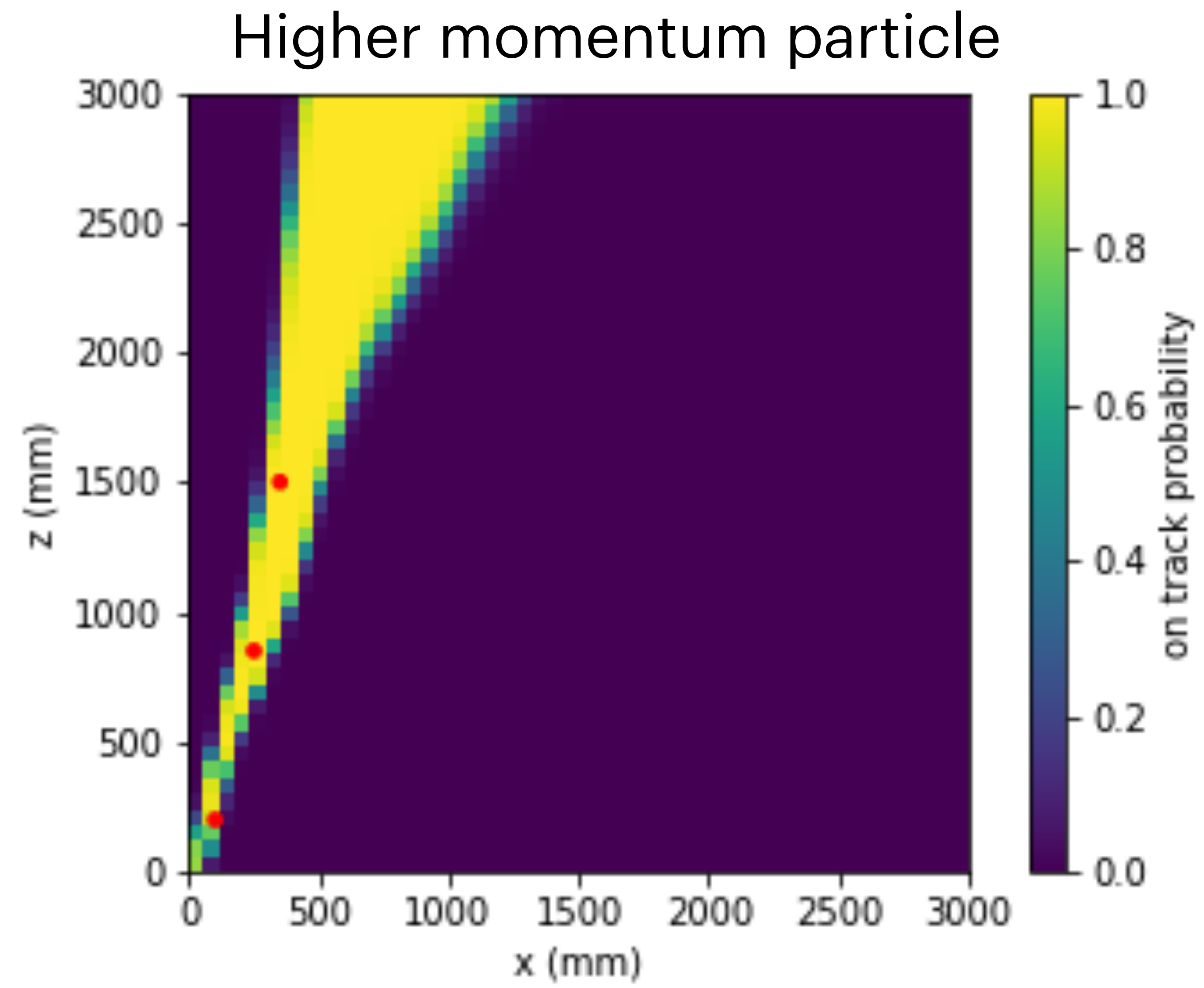
## Seed classification

- Powerful seed classification, here optimistic scenario
  - bad/medium training seeds created by distorting good seeds

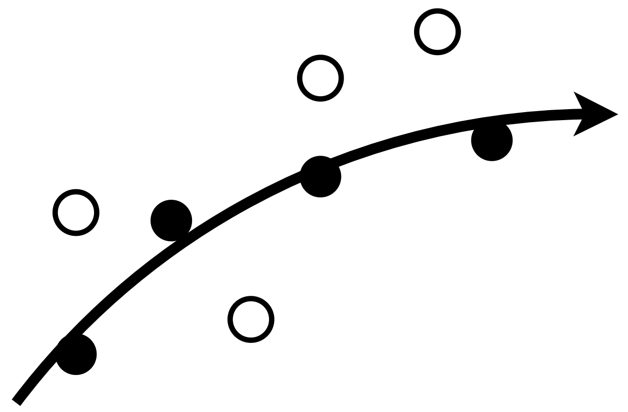
| | | Predicted Class | | |
|---|---|---|---|---|
| | | good | med | bad |
| Actual Class | good | 98.5% | 1.5% | 0.1% |
| | med | 3.5% | 95.7% | 0.8% |
| | bad | 0.2% | 3.2% | 96.7% |


Lower momentum particle

given hits


Higher momentum particle

[ F. Dietrich, E. Knering, AS : Track Seed Classification using NNs ]



# ML assisted track reconstruction

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NETWORK "LEARNED" PHYSICS OF MULTIPLE SCATTERING

Predicted Class

Actual Class

| | good | med | bad |
|---|---|---|---|
| good | 98.5% | 1.5% | 0.1% |
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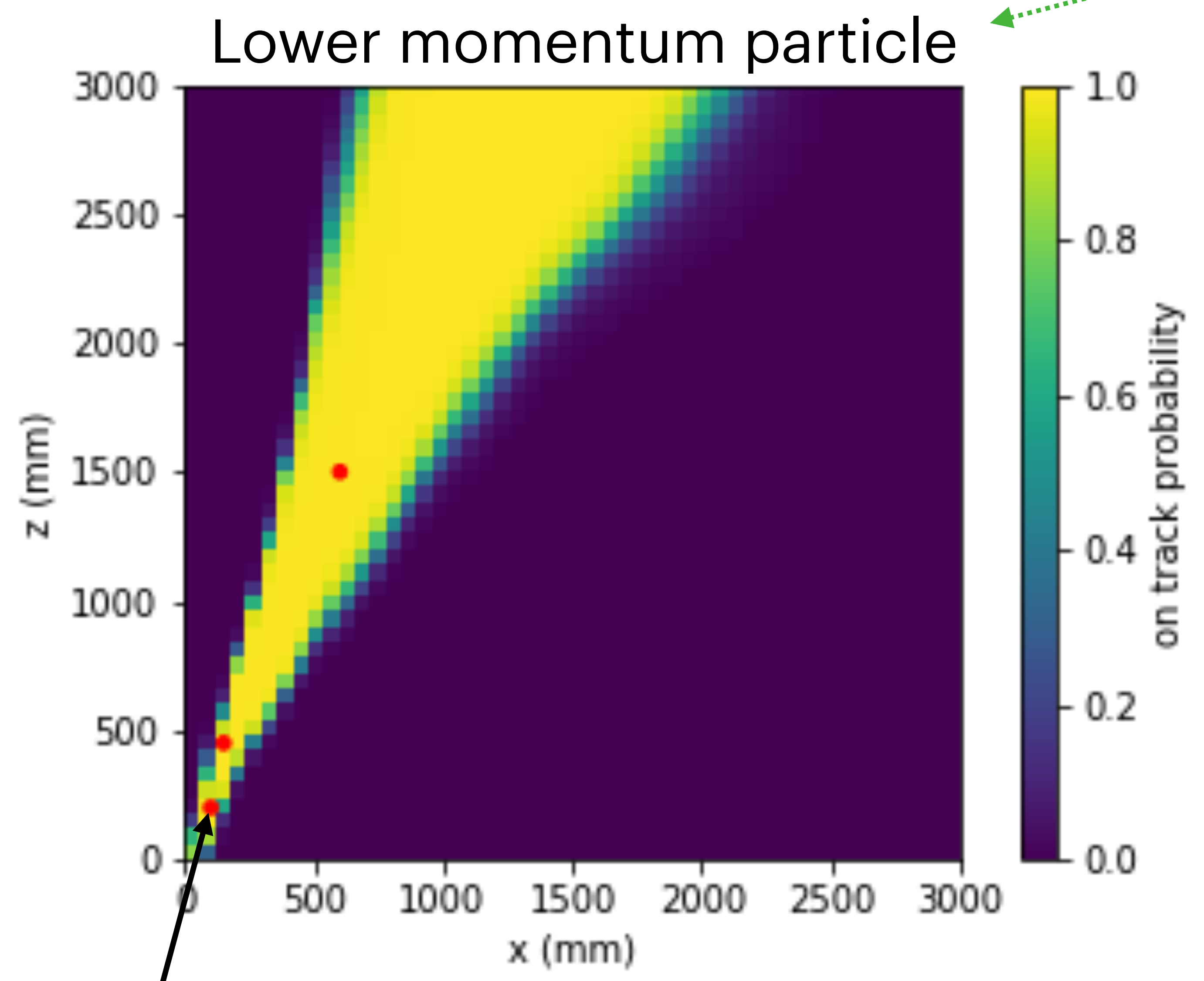

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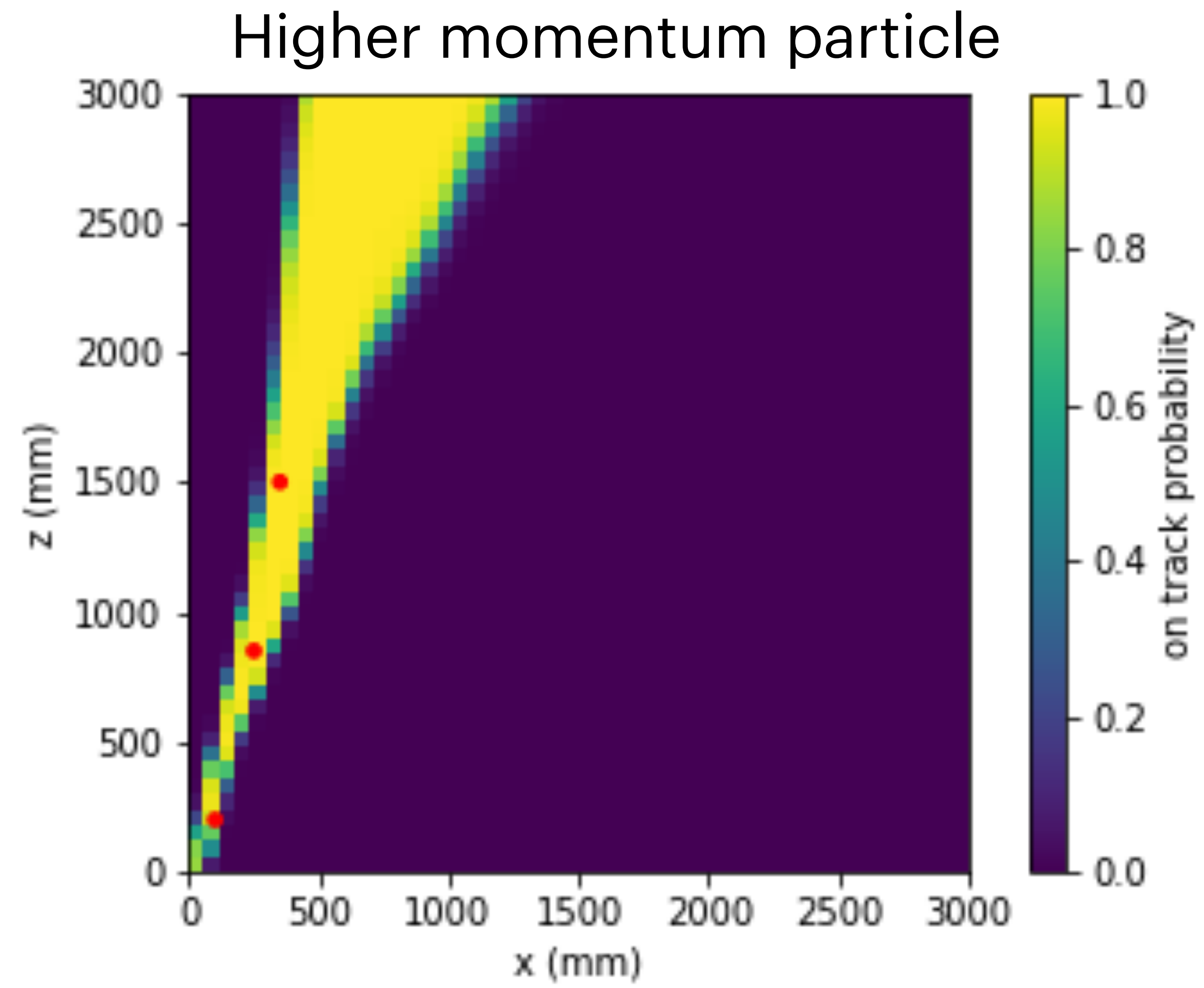
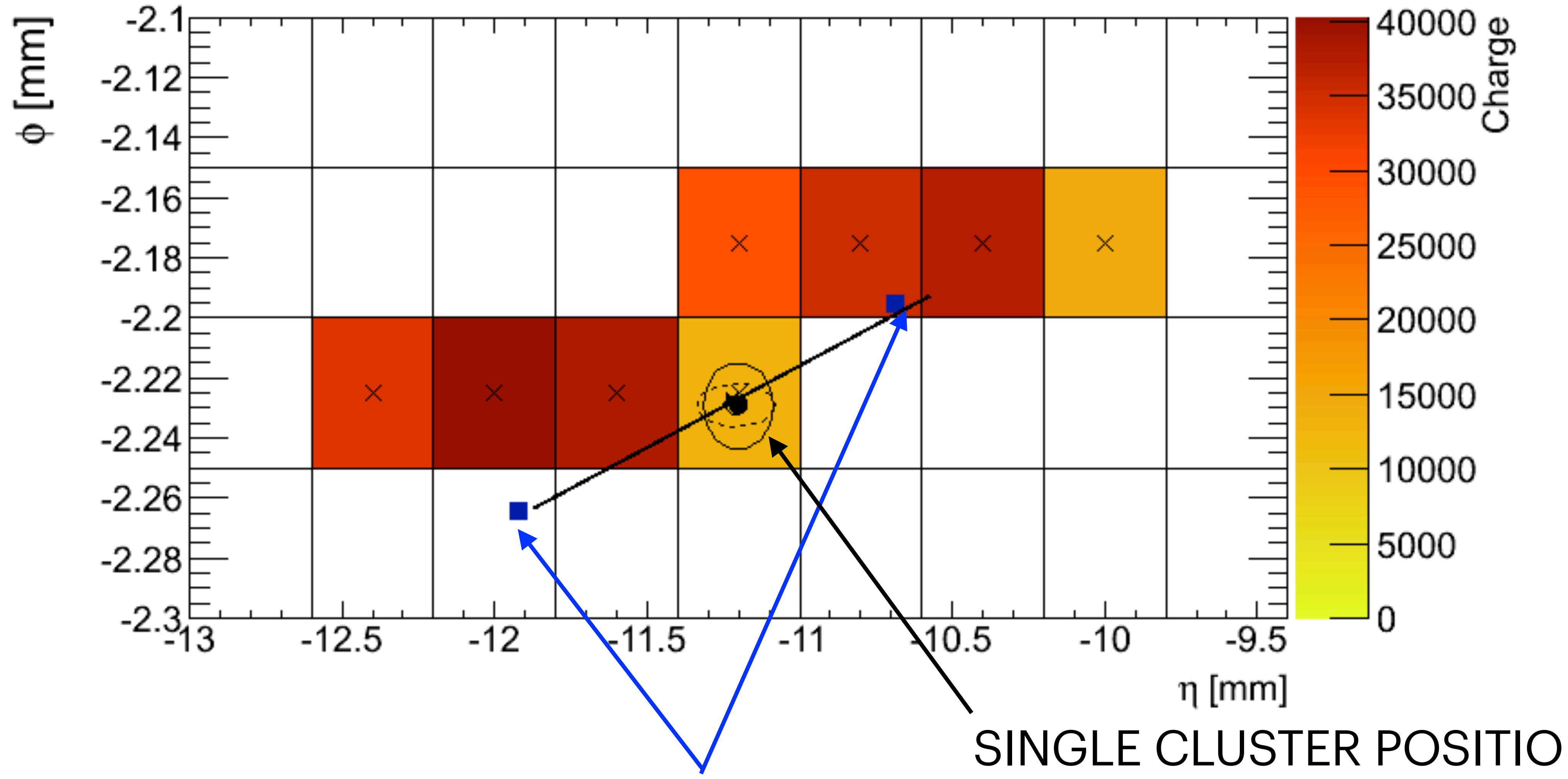


[ F. Dietrich, E. Knering, AS : Track Seed Classification using NNs ]

# ML assisted track reconstruction

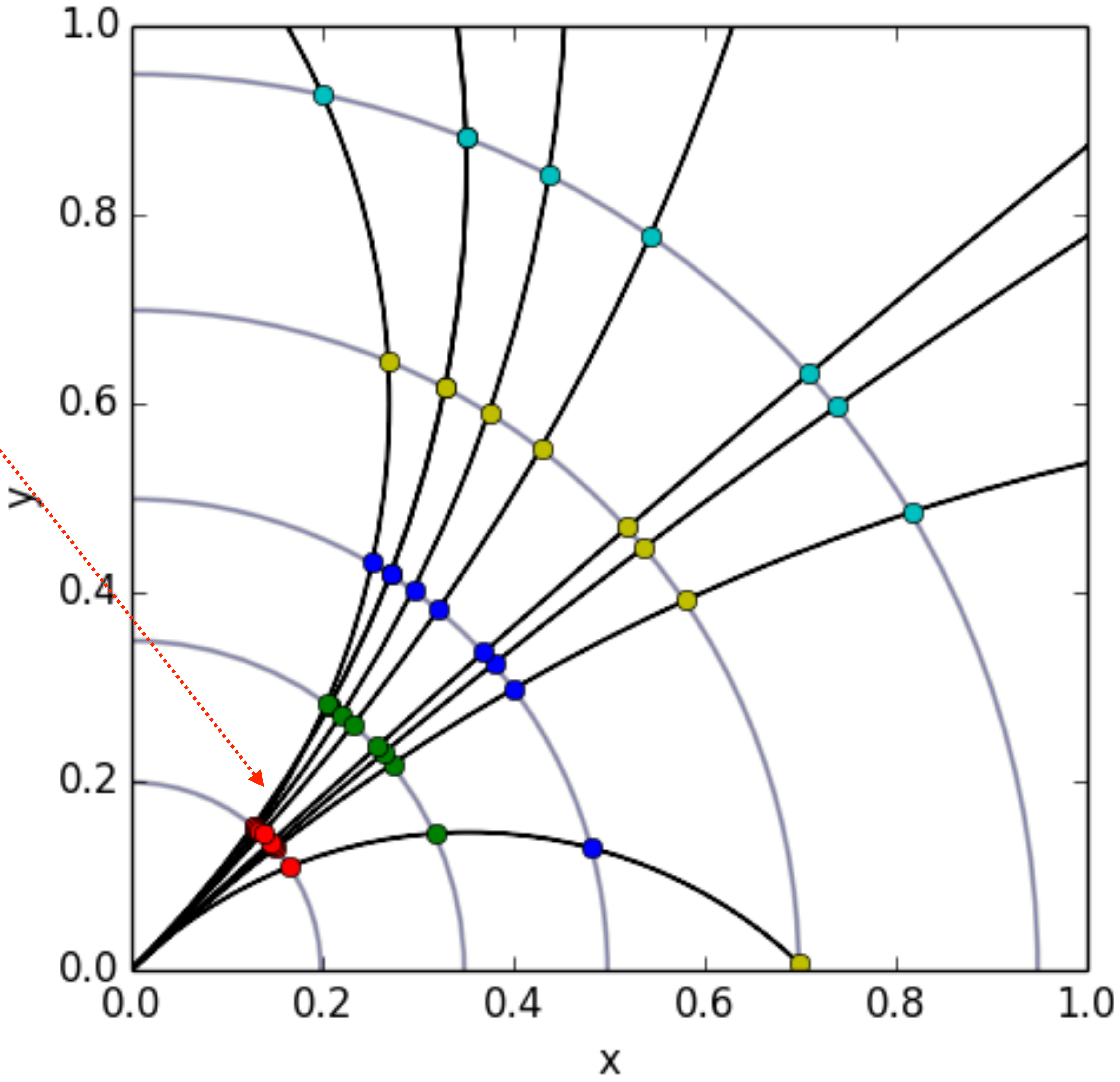
Particle tracking in dense environment

- Collimated final states can create local dense environments
- Unsupervised clustering may not resolve that



SINGLE CLUSTER POSITION

2 PARTICLE INTERSECTION

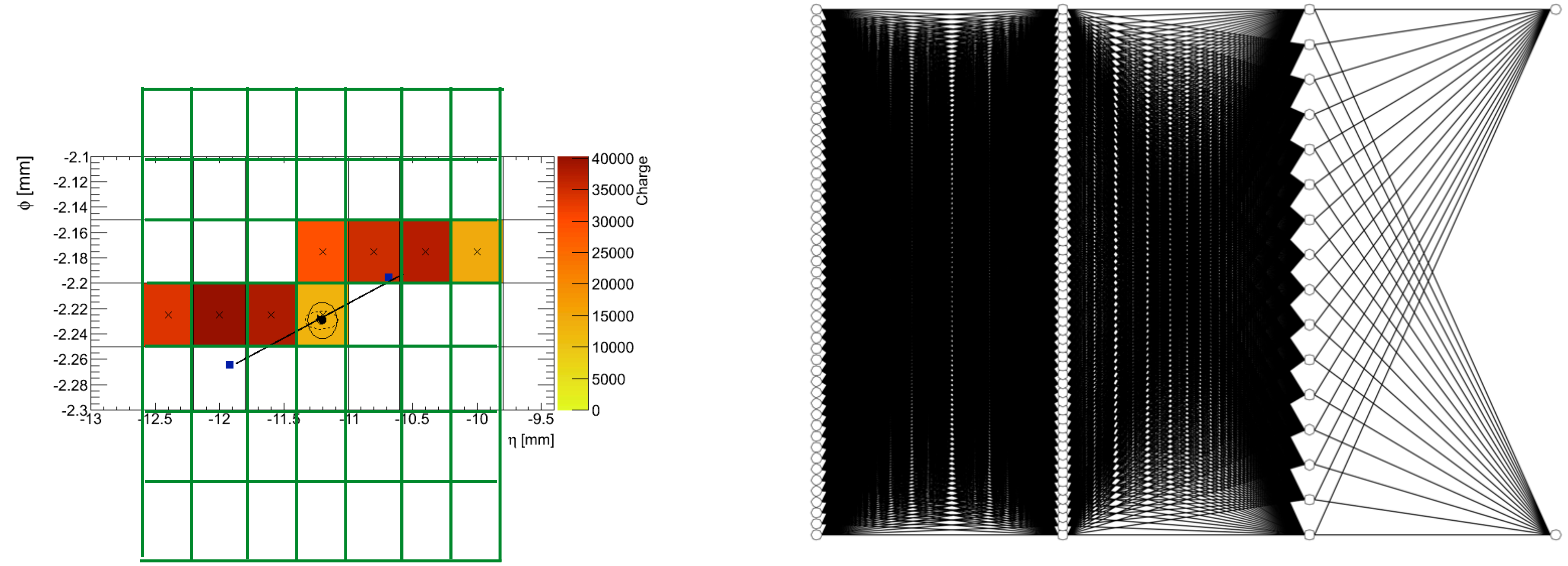


[ ATL-PHYS-2015-006 ]

# **ML** assisted track reconstruction

## Particle tracking in dense environment

- Use a set of NN to classify the probability if a cluster stems from 1,2 or more particles
  - NN trained on simulated data



7x7 pixel charge matrix → 49 input nodes → 2 hidden layers → 2 output layers

→ cluster compatible with 1 particle

→ cluster compatible with 2 and more particles

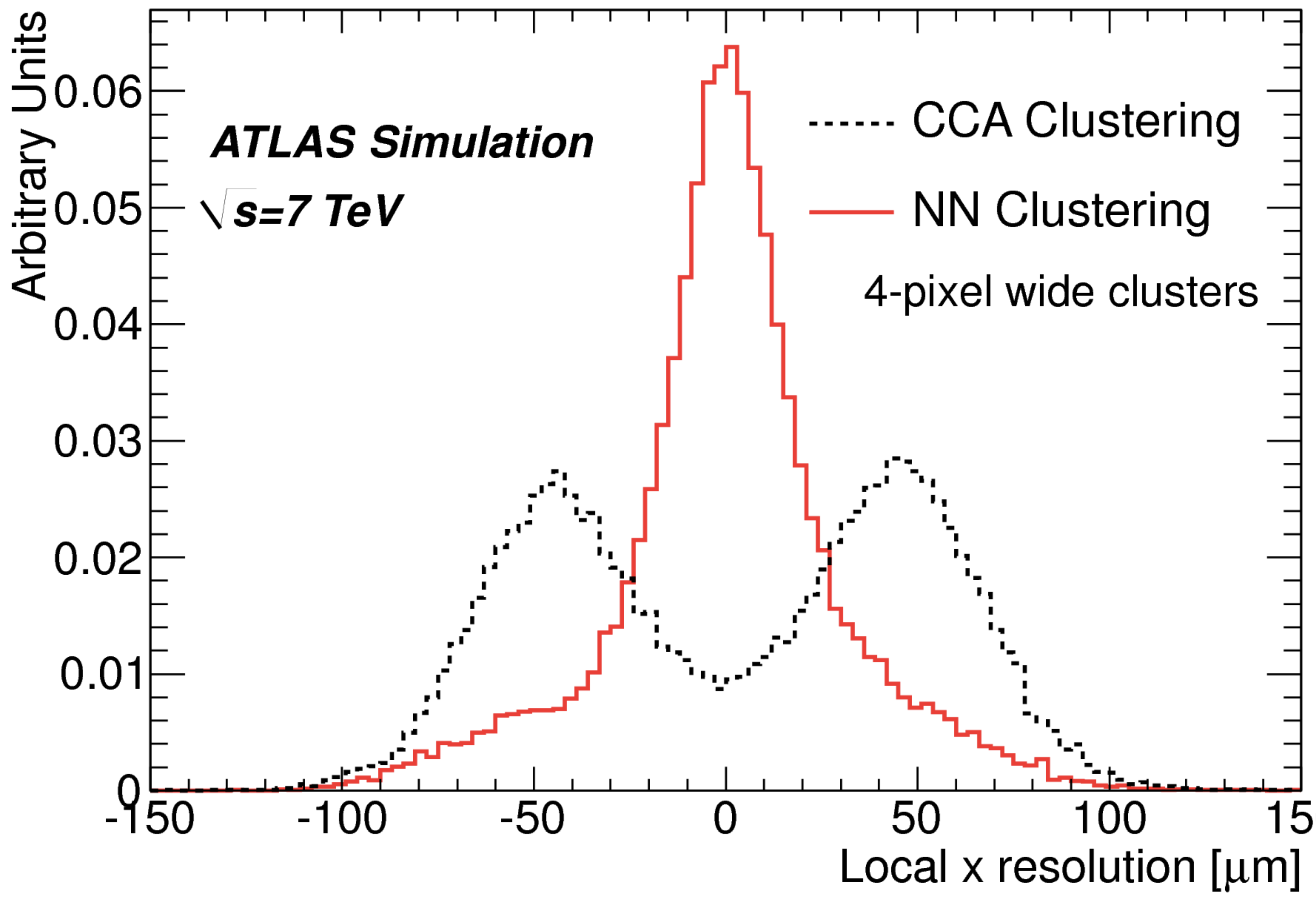
[ ATL-PHYS-2015-006 ]

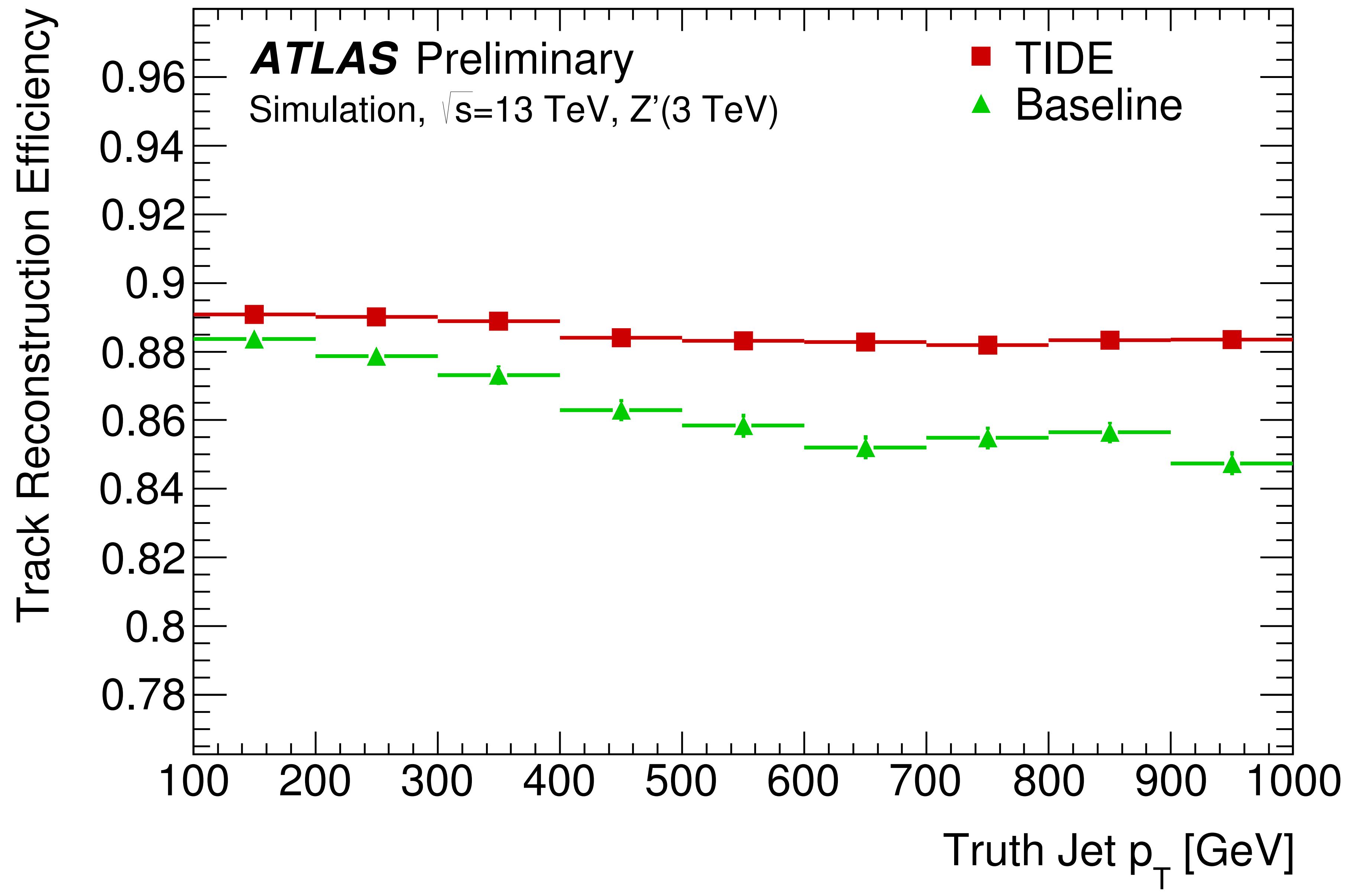
# ML assisted track reconstruction

Particle tracking in dense environment

- Use a set of NN to classify the probability if a cluster stems from 1,2 or more particles
  - NN trained on simulated data

What good is it if simulation does not describe reality adequately?



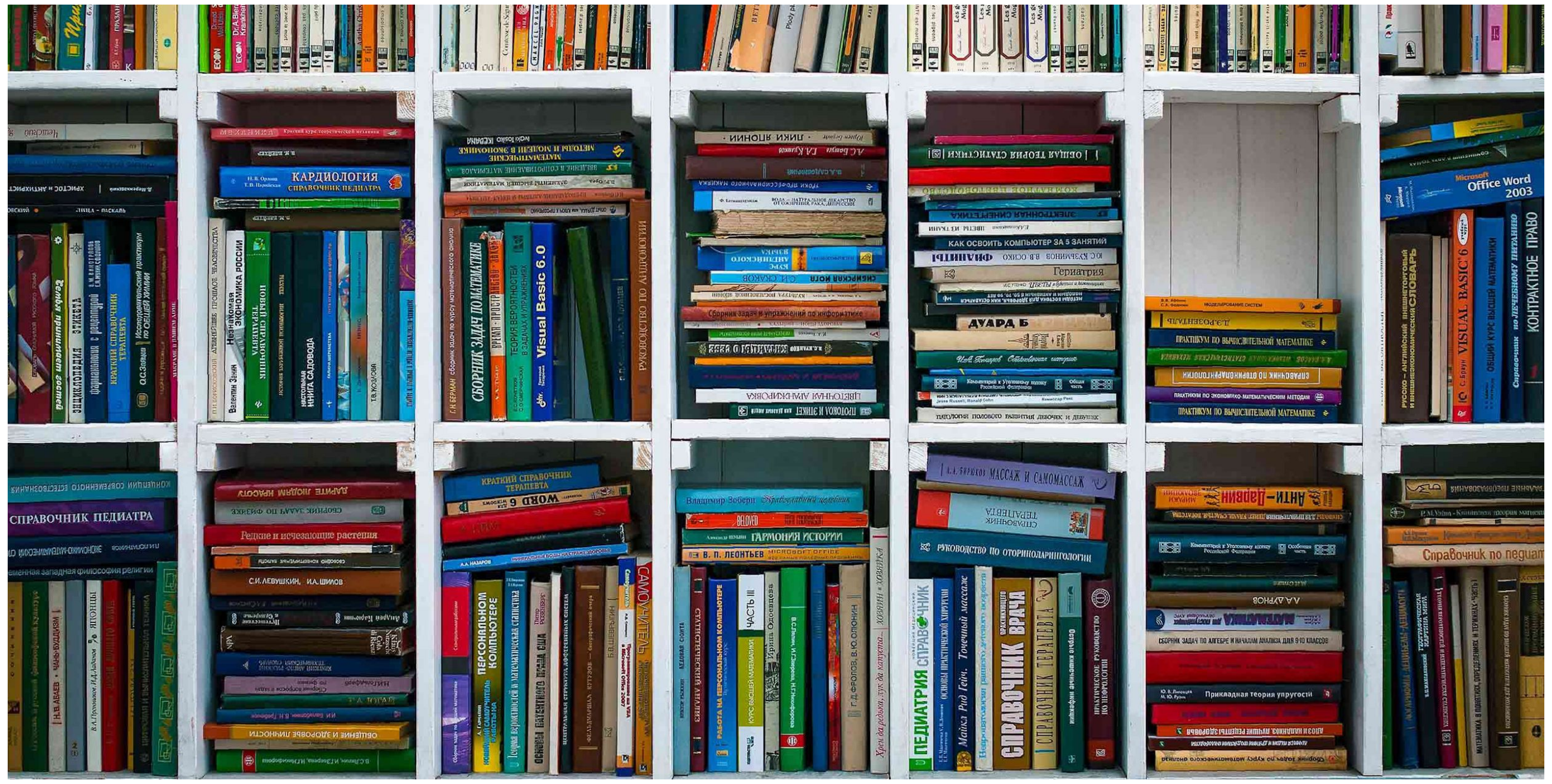


[ ATL-PHYS-2015-006 ]

# Music, Neighbours and Tracking

Hashing approaches for particle tracking

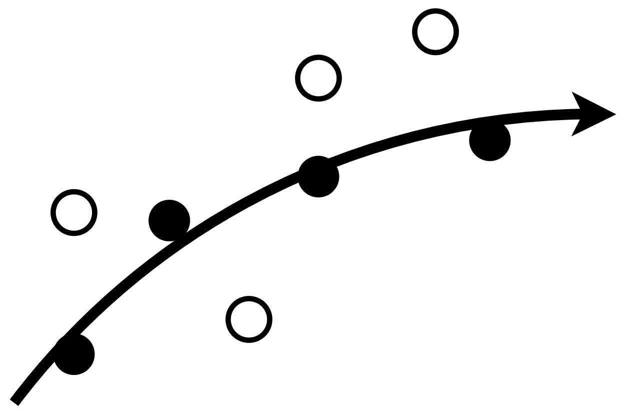
- Can we reduce the combinatorics of our problem by narrowing it down?
    - Using an optimal data structure could simplify your search significantly



**vs**

[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]

[ S. Amrouche, N. Calace, T. Golling, M. Kiehm. AS : Hashing & similarity learning ]



# Music, Neighbours and Tracking

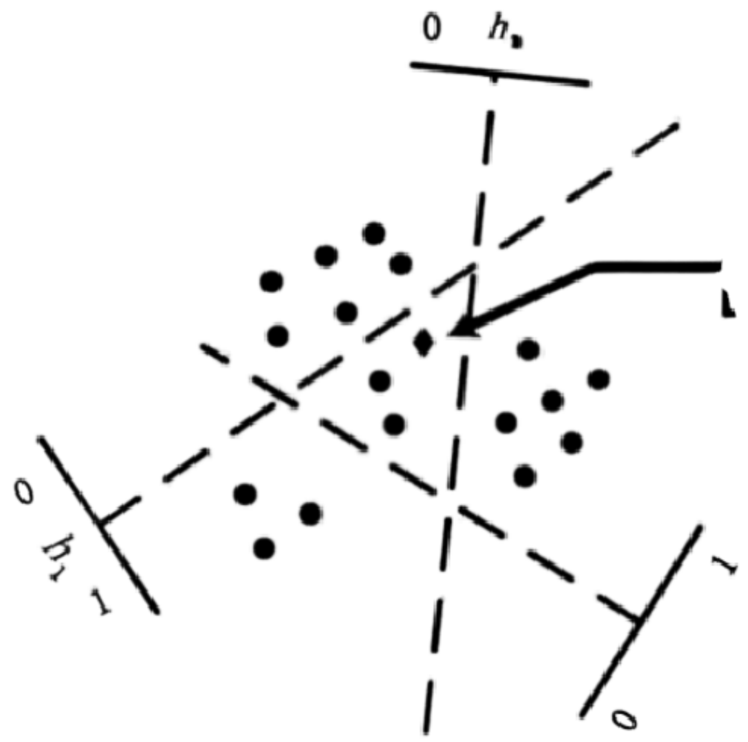
## Hashing approaches for particle tracking

- Perfect hash function would solve the tracking problem right away, but does not exist

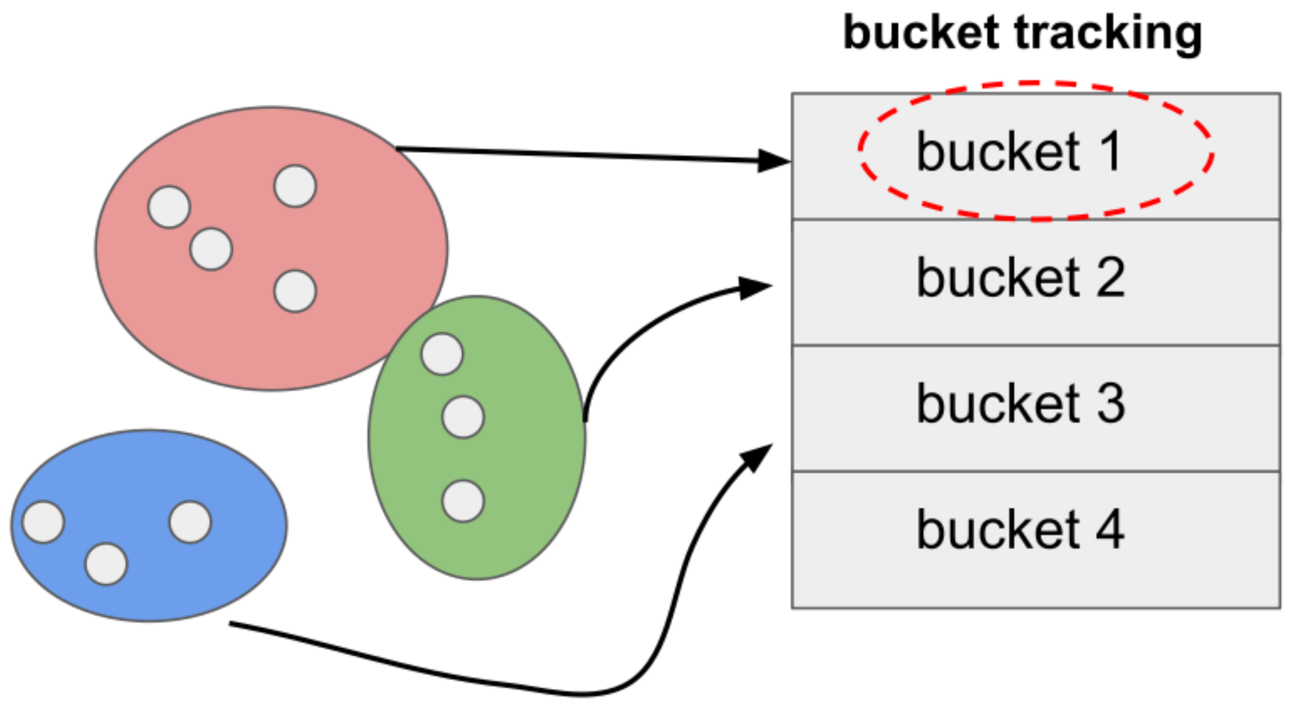
h(hit) = track number

- Approximate hashing, however, can be done

h(track 1 hit 0) = group x
h(track 1 hit 1) = group x
h(track 0 hit 1) = group x



RADNOM
PROJECTIONS

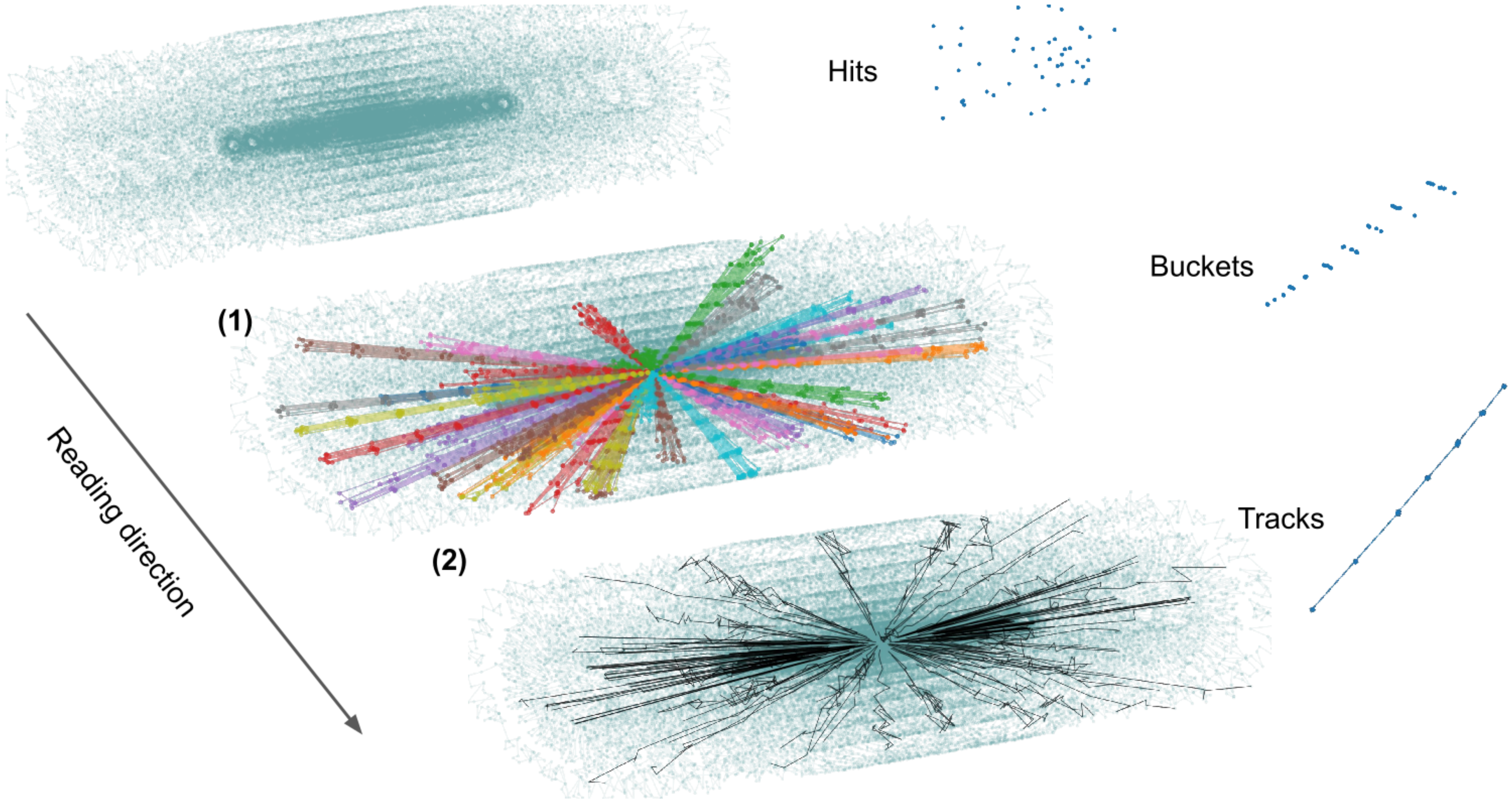


APPROXIMATE
NEAREST
NEIGHBOURS

[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]
[ S. Amrouche, N. Calace, T. Golling, M. Kiehm. AS : Hashing & similarity learning ]

# Music, Neighbours and Tracking

Hashing approaches for particle tracking



[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]
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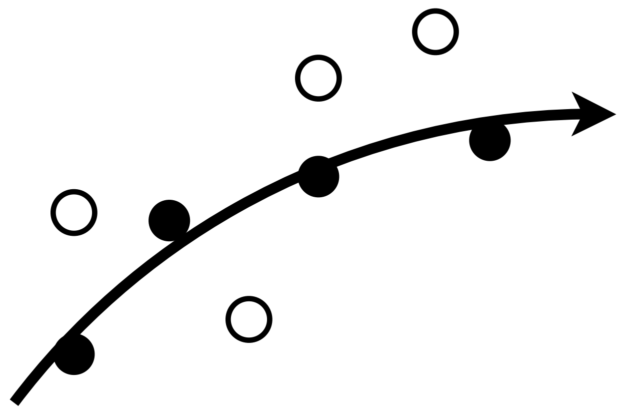


# Music,

seed

approximate

nearest neighbours

Copenhagen

asalzburger

Copenhagen
RADIO

PLAYLIST

**Copenhagen Radio**

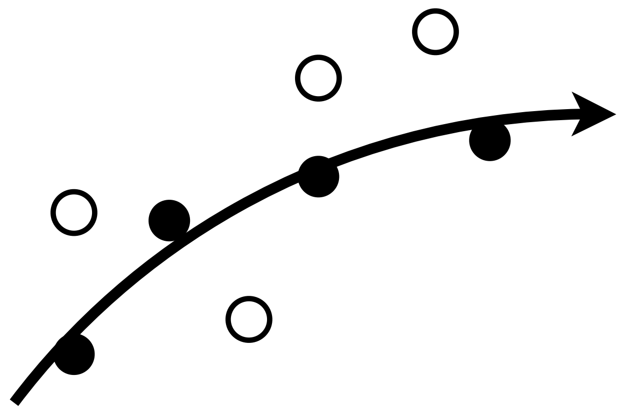
With Jack Vallier, Wrabel, Tom Odell, Jeremy Zucker and more

Created by **Spotify** • 50 songs, 2 hr 52 min

| TITLE | ARTIST | ALBUM | |
|---|---|---|---|
| Copenhagen | Jack Vallier | Changes | 3:02 |
| hurts like hell | Wrabel | hurts like hell | 3:57 |
| Sometimes | Kodaline | Sometimes | 3:48 |
| Before You Go - Piano Version | Lewis Capaldi | Before You Go (Piano Ver... | 3:39 |
| i'm lonely | Luz | i'm lonely | 3:01 |
| Beautiful & Brutal | Plested | Beautiful & Brutal | 3:31 |
| 25 in Barcelona EXPLICIT | JP Saxe | Hold It Together | 3:13 |
| Homesick | Declan J Donovan | Homesick | 3:02 |
| I miss you, I'm sorry | Gracie Abrams | I miss you, I'm sorry | 2:48 |
| smiling when i die | Sasha Sloan | smiling when i die | 3:26 |

[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]

[ S. Amrouche, N. Calace, T. Golling, M. Kiehm. AS : Hashing & similarity learning ]



# Music, Neighbours and Tracking

Hashing approaches for particle tracking

Tree-based

Hashing-based

Quantization

Relative Neighborhood Graphs

Navigable Small-World Networks

RADNOM ROJECTIONS

**KD-tree** **R-tree** **VA-file** **Locality Sensitive Hashing** **Product Quantization**

n(track 1 hit 0) = group x

bucket tracking

bucket 1

bucket 3

o hit 1) = group x

APPROXIMATE NEAREST NEIGHBOURS

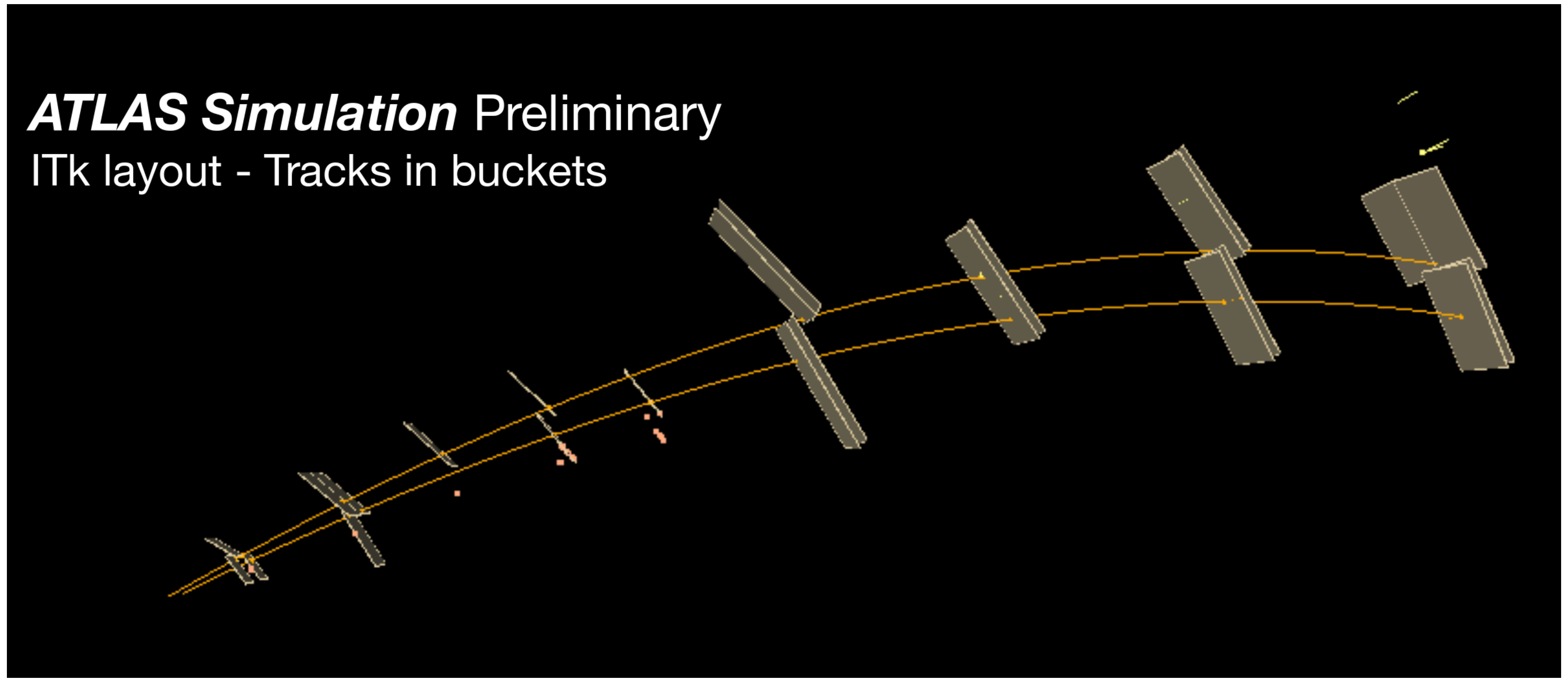
- Our initial choice was the [ annoy ] library from [ spotify ]
- Recently testing [ faiss ] from facebook research (mainly for GPU backend)
- The use of open source industry products is a real asset of ML for HEP

[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]

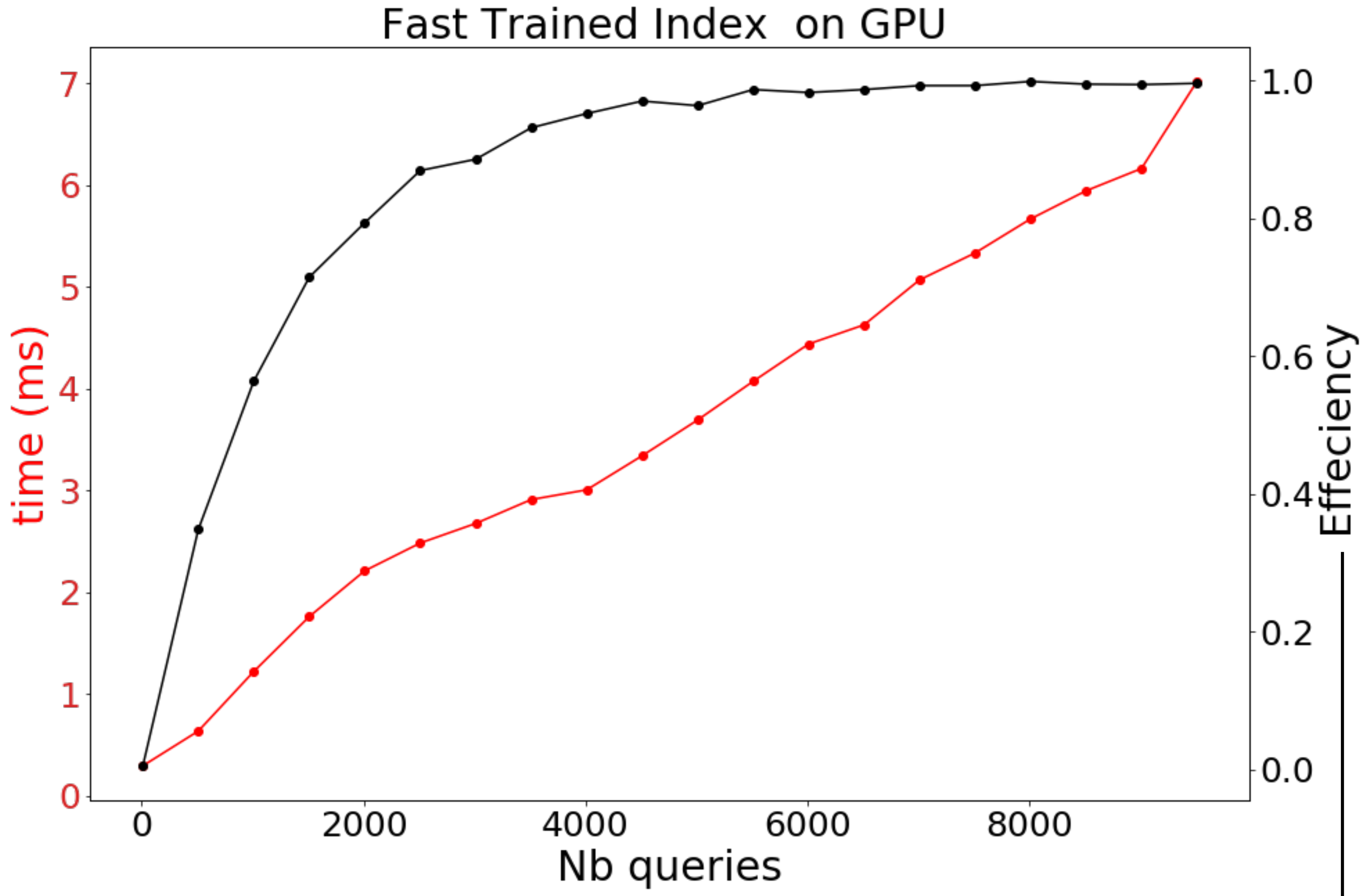
[ S. Amrouche, N. Calace, T. Golling, M. Kiehm. AS : Hashing & similarity learning ]

# Music, Neighbours and Tracking

Hashing approaches for particle tracking



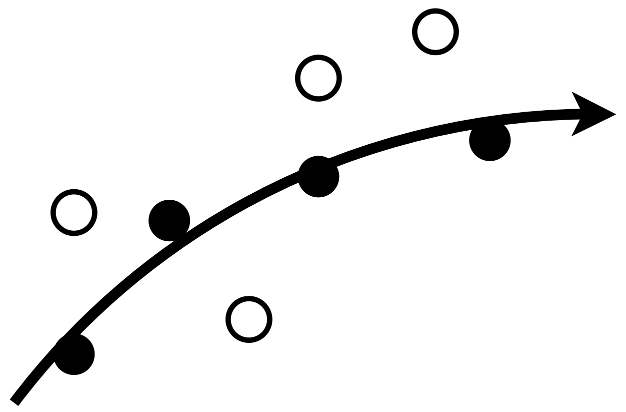
These tracks are brought to you by



To find a bucket with at least 4/hits of the track contained
(good enough for track seeding)

[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]

[ S. Amrouche, N. Calace, T. Golling, M. Kiehm. AS : Hashing & similarity learning ]



# Tracking & metric learning

Are we searching/clustering in the right space?

- Mapping data into a different representation was one classical approach to track finding (hough transform, conformal mapping) → REQUIRED ANALYTICAL TRANSFORM
- Can we learn a better way to look at tracks?

HUMAN

Fig 1 Transverse view (x/y)

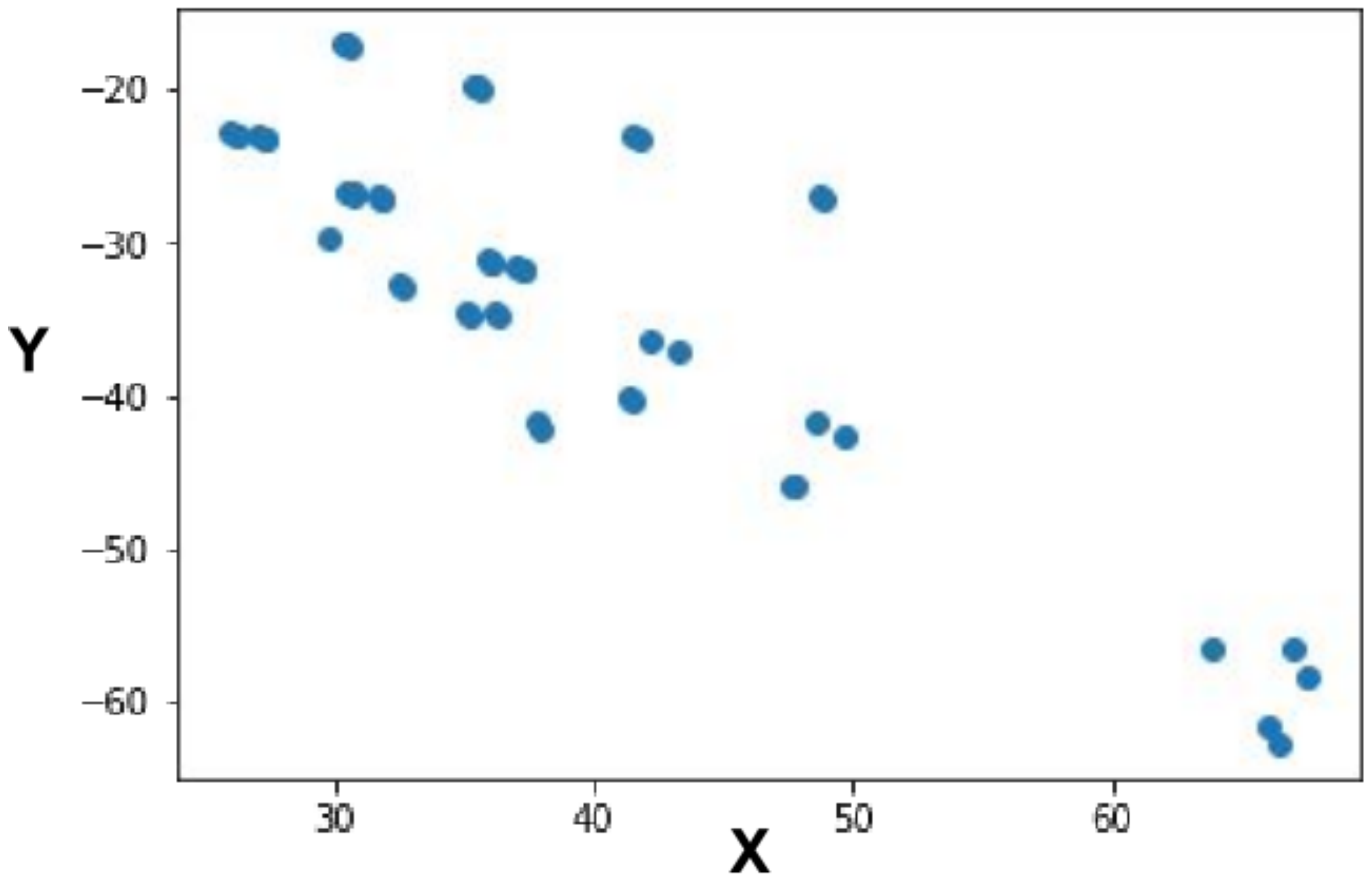
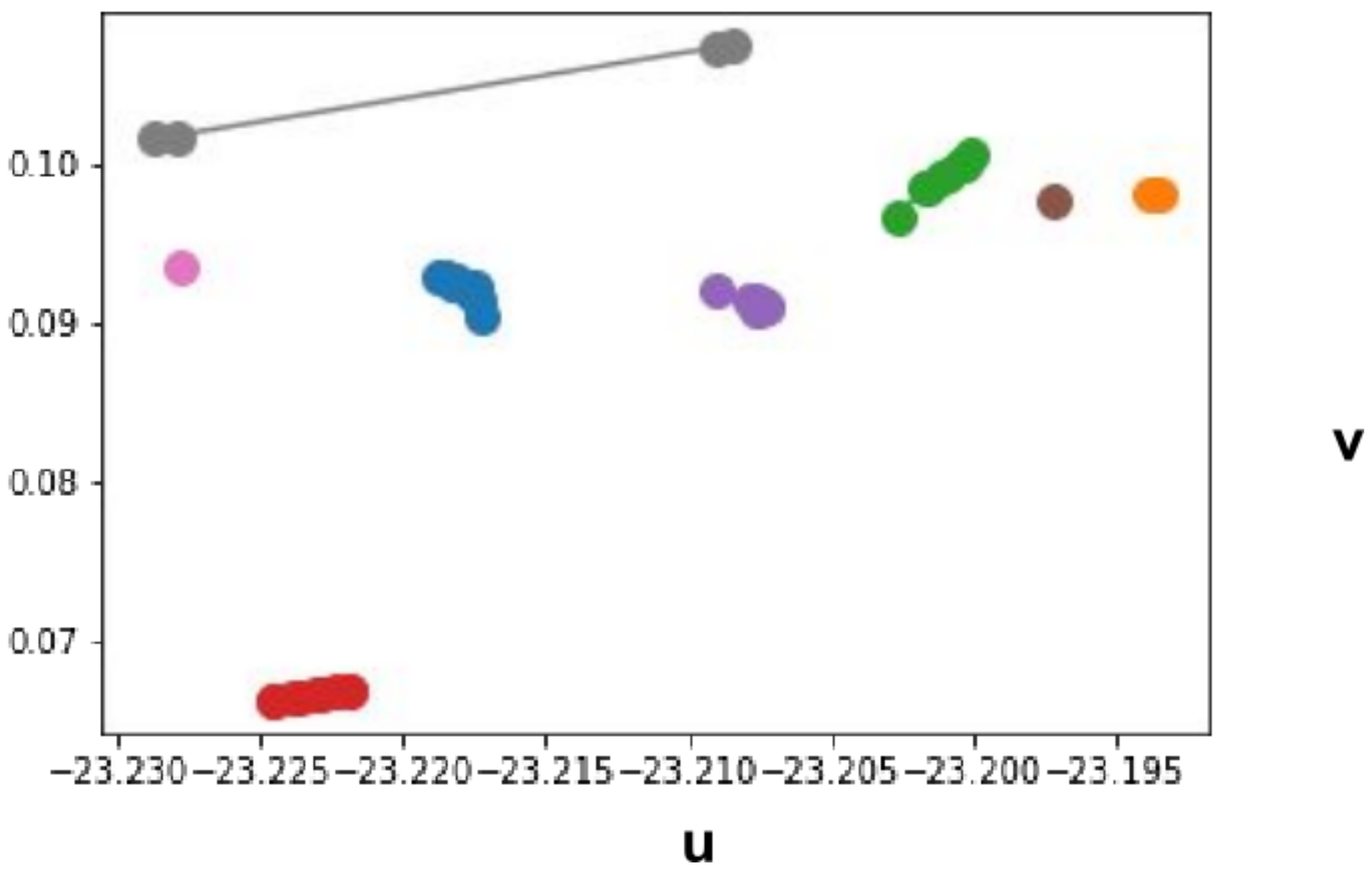


Fig 2  Learned (u/v) space



ML AGENT

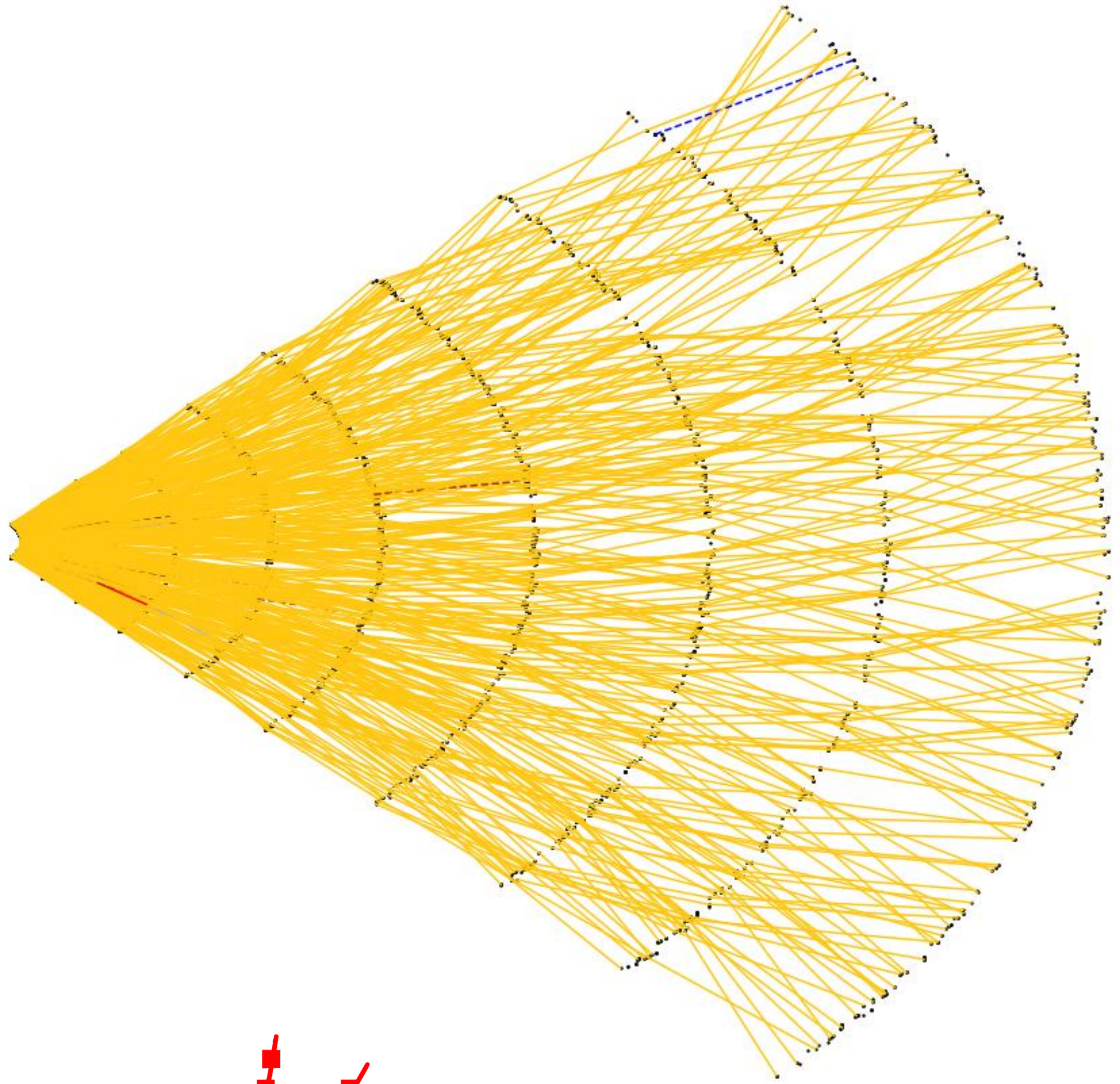
[ S. Amrouche, T. Golling, M. Kiehn, AS: Music, Neighbours & Tracking ]

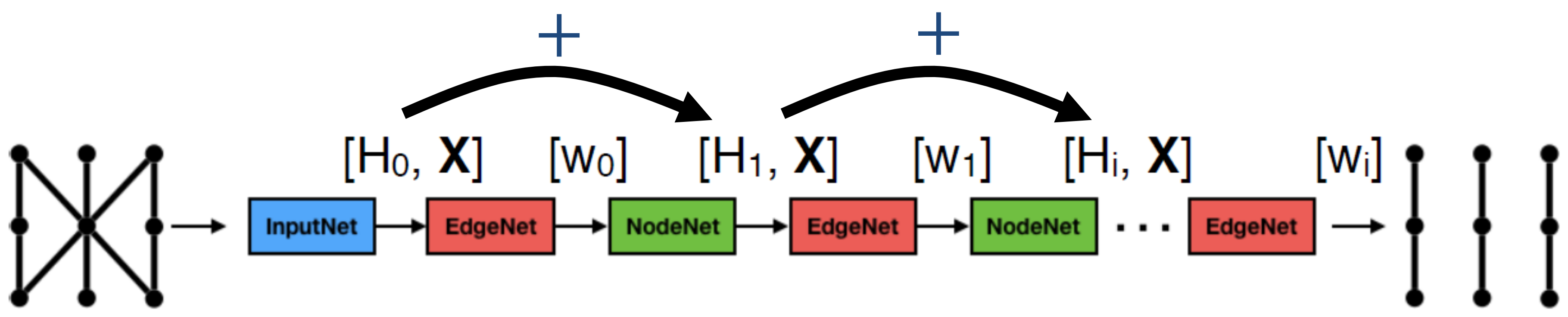
[ S. Amrouche, N. Calace, T. Golling, M. Kiehm. AS : Hashing & similarity learning ]

# End-to-end Tracking attempts

The “my job is done by a machine” scenario

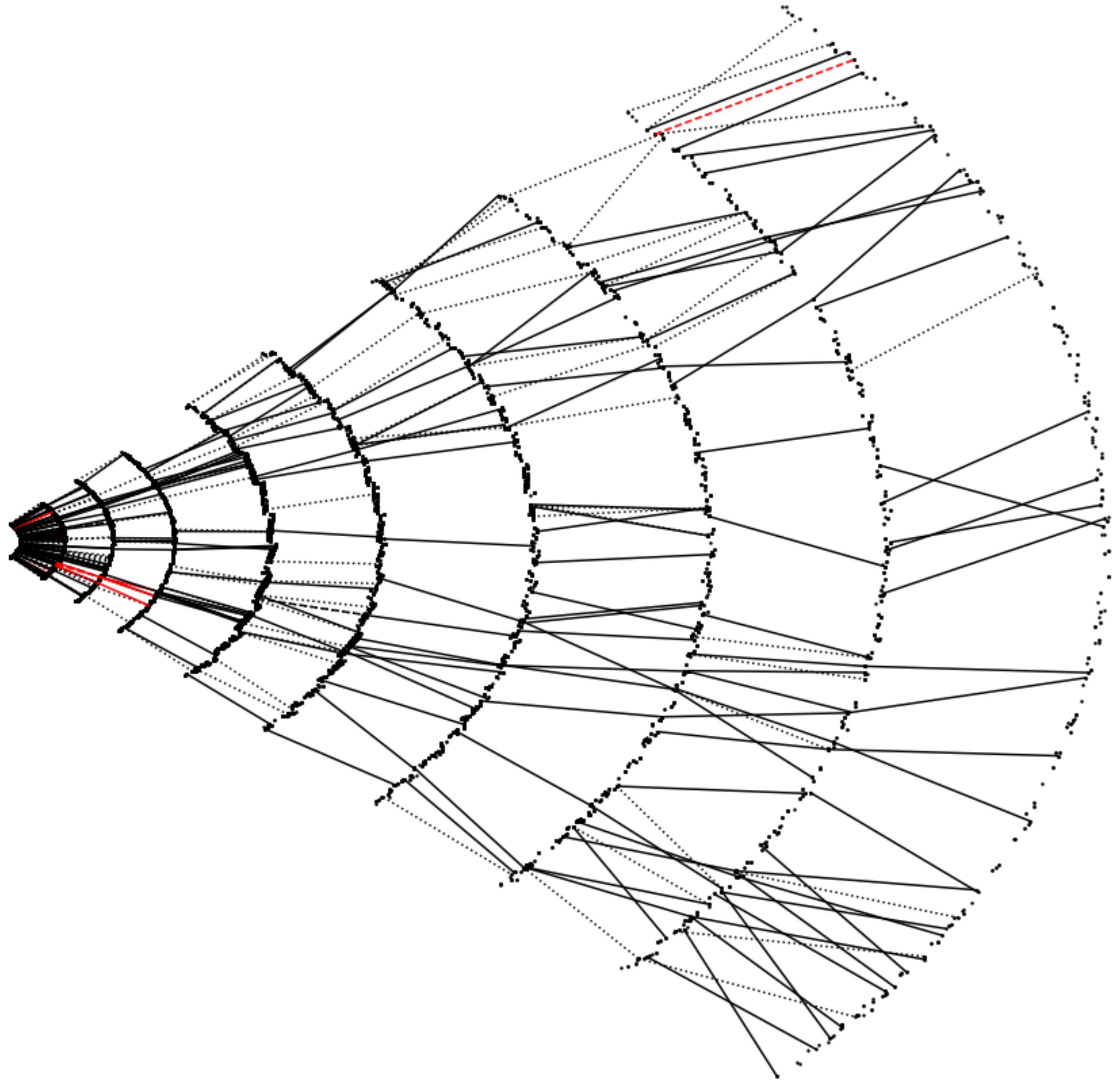
- Exa.TrkX project applies a Graph Neural Network (GNN) approach
    - Build nodes and edges, classify edges [0, 1] and eventually drop them





- Attention Message Passing with Residuals

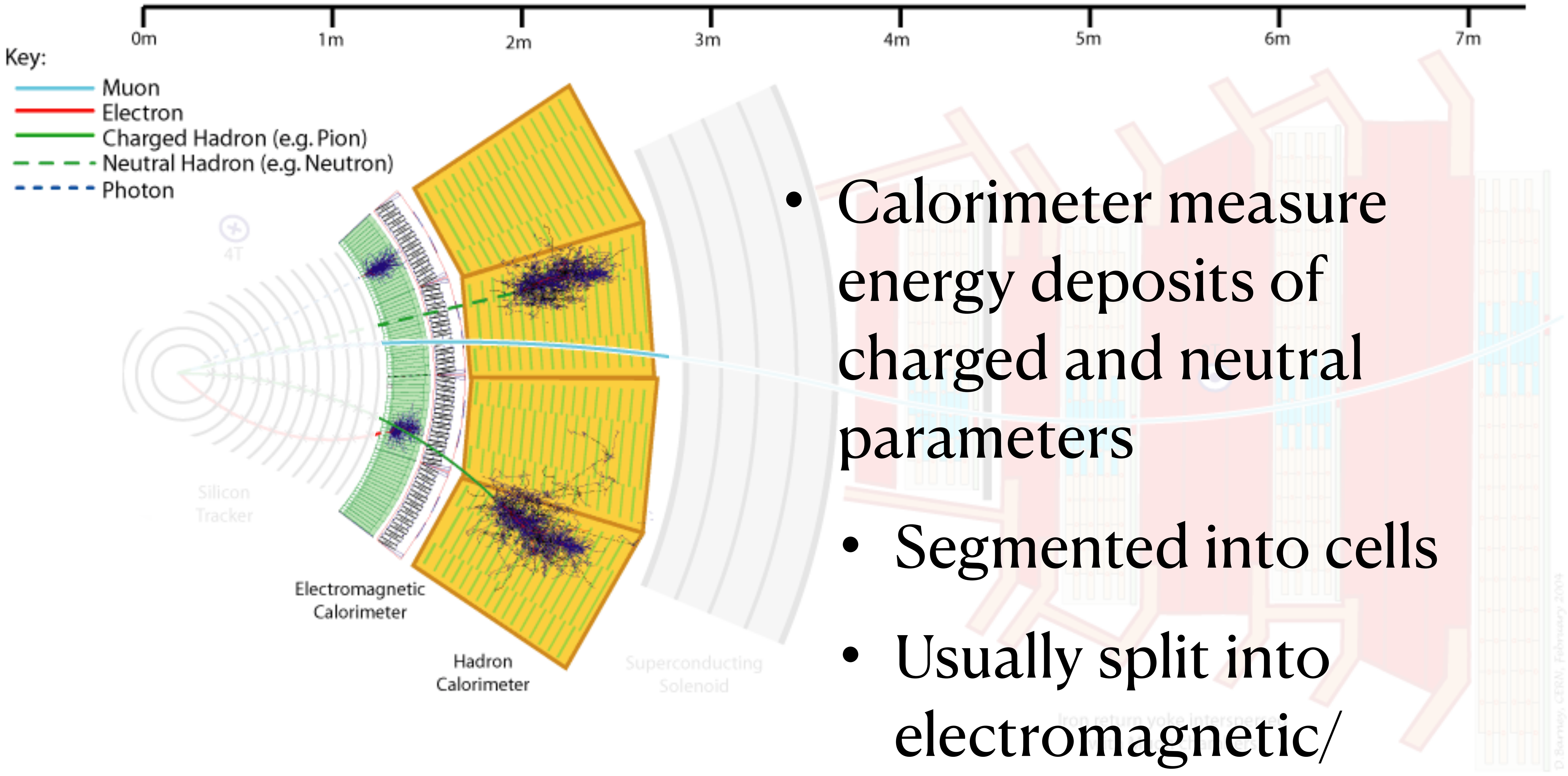
Kipf, Thomas N., and Max Welling. "Semi-supervised classification with graph convolutional networks." *arXiv preprint arXiv:1609.02907* (2016).



Particle Tracking Machine Learning Challenge [ Phase 1 ][ Phase 2 ]

# Calorimeter & Jets

Jet clustering & particle identification

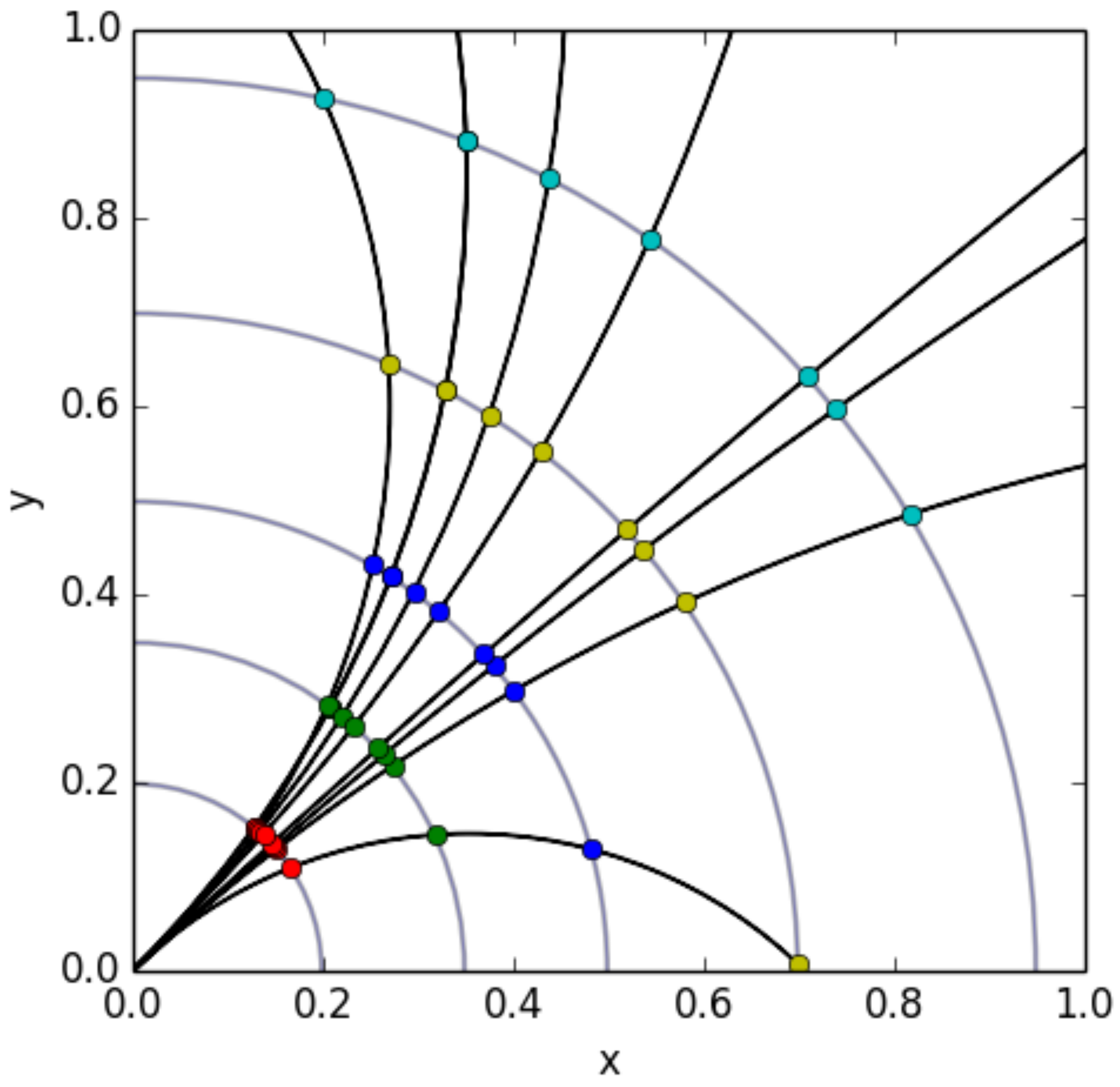


- Calorimeter measure energy deposits of charged and neutral parameters
  - Segmented into cells
  - Usually split into electromagnetic/ hadronic part

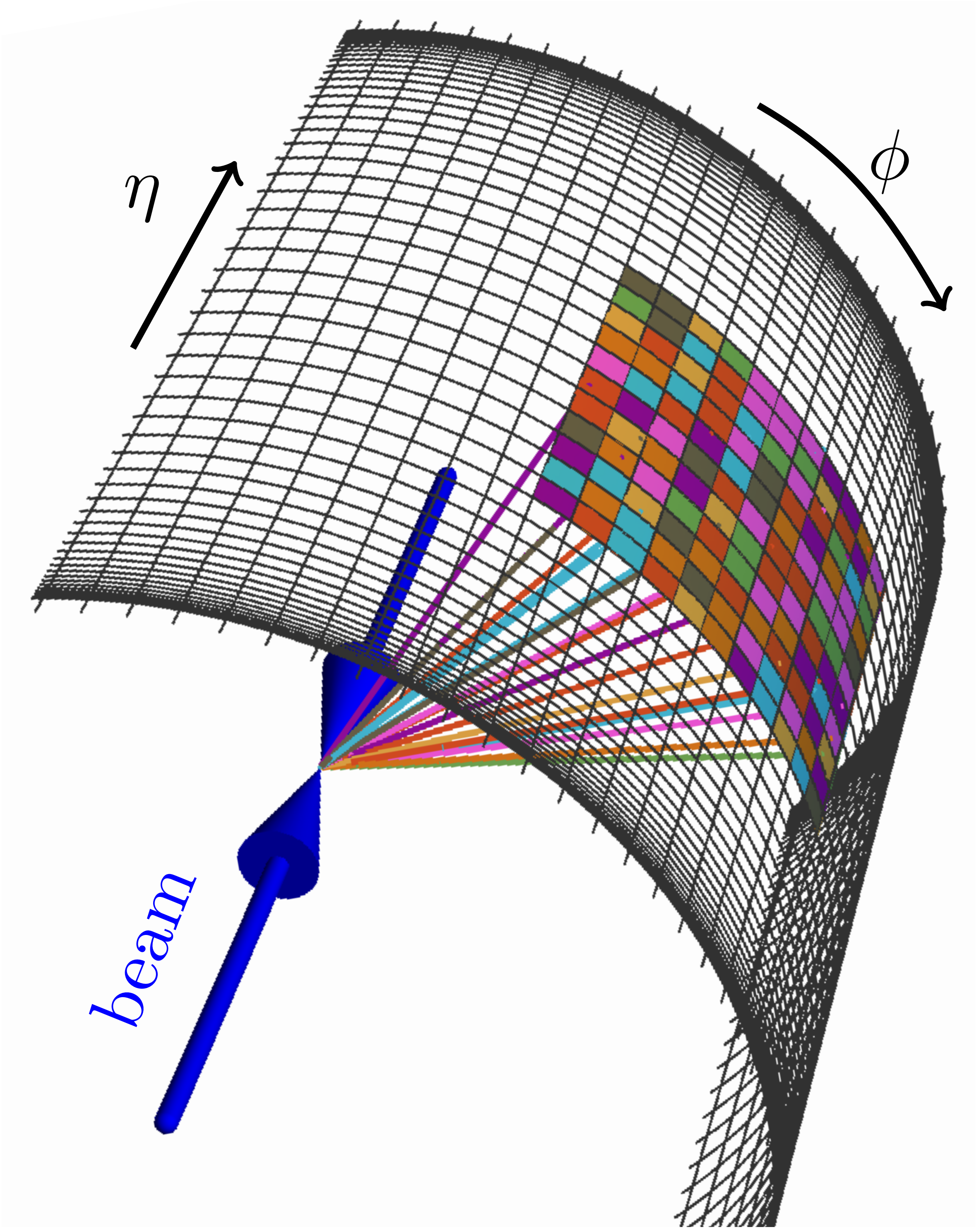
# Calorimetry & Jet reconstruction

Clustering and object identification

- Calorimeters measure energy deposits of charged and neutral parameters
  - Segmented into cells
  - Usually split into electromagnetic/ hadronic part
- Image representation very intuitively



Tracking view

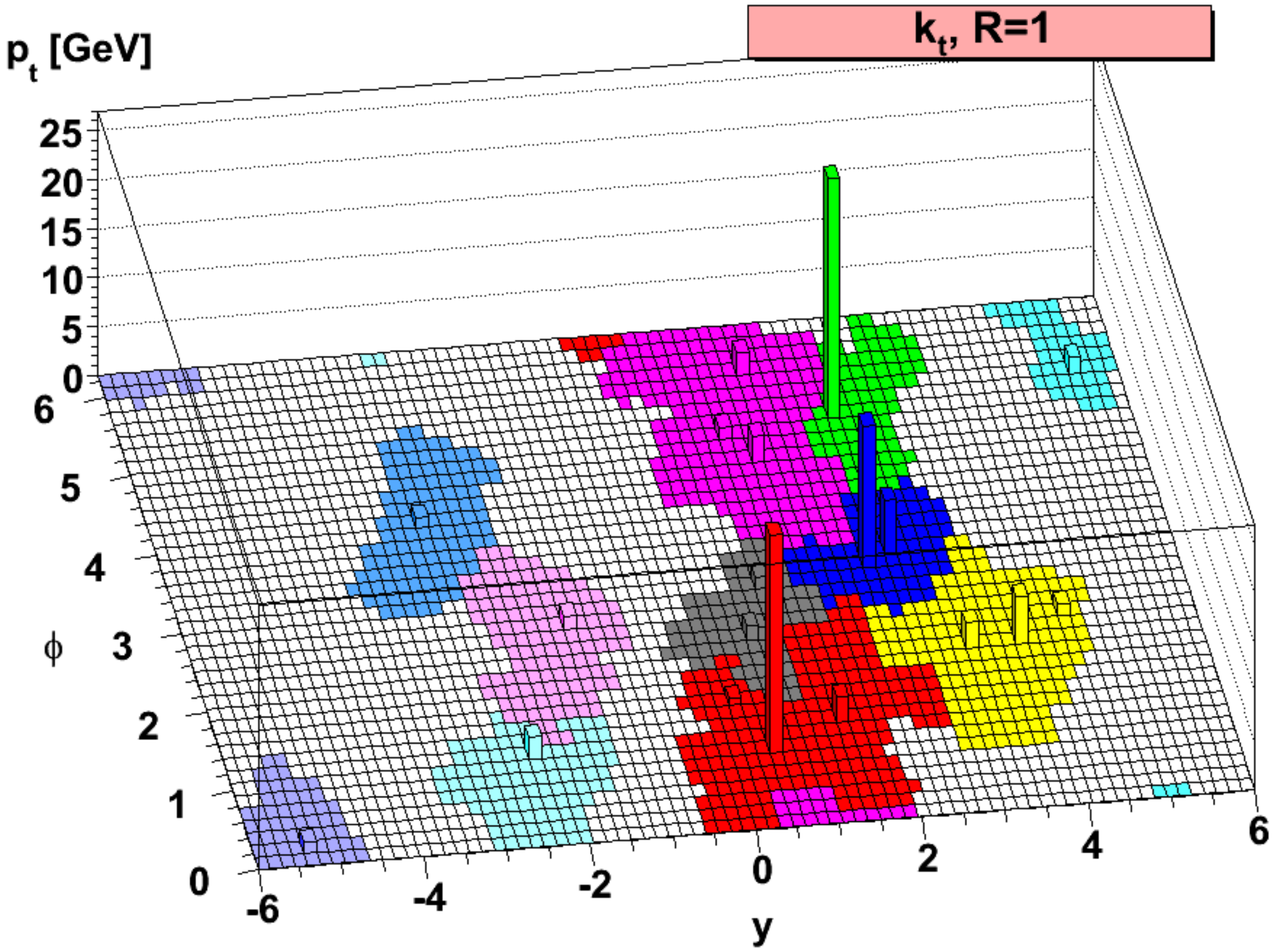


Calorimeter view

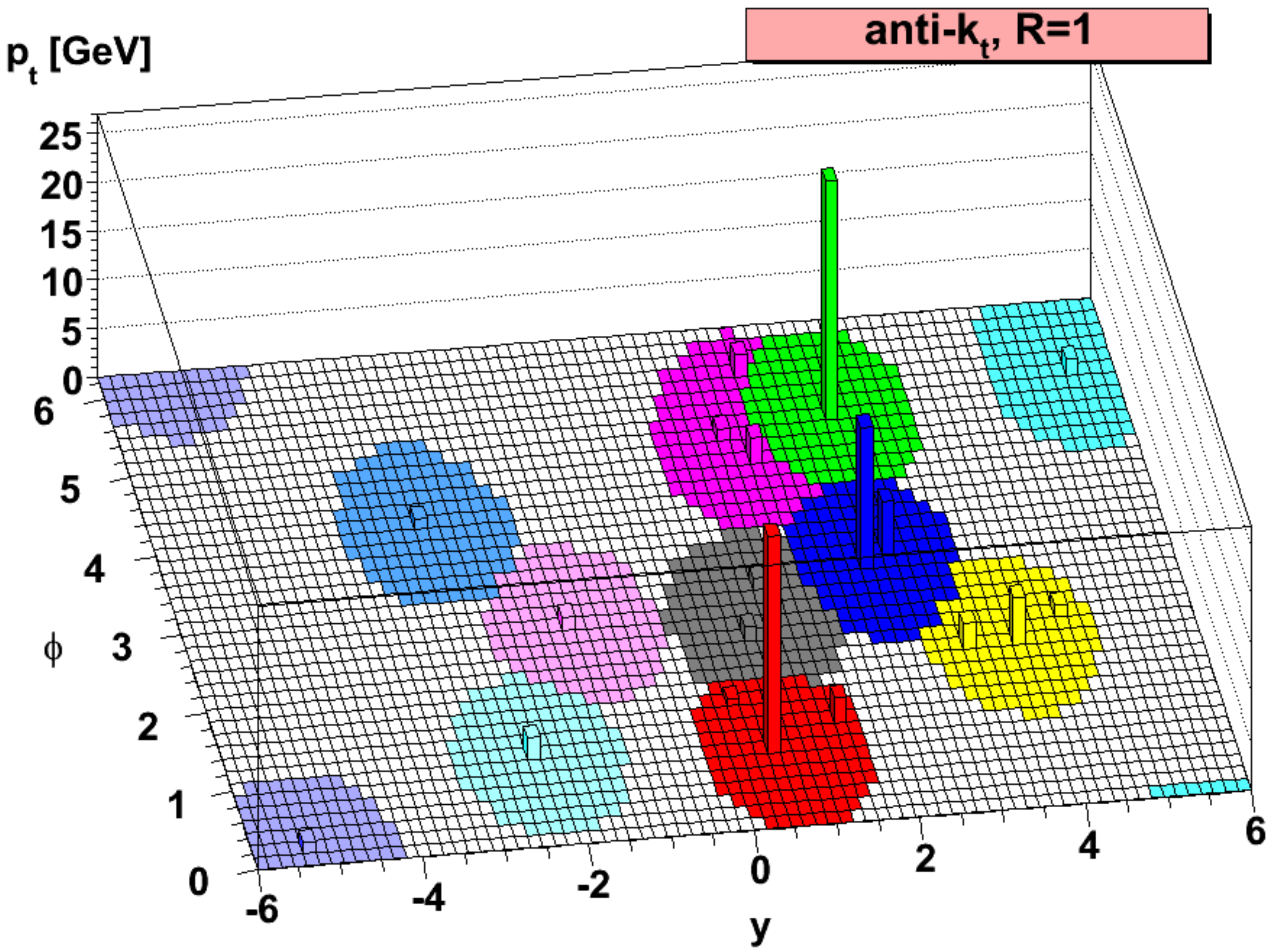
# Calorimetry & Jet reconstruction

## Clustering and object identification

- Clustering & jet building is unsupervised learning



$k_t$ clustering algorithm

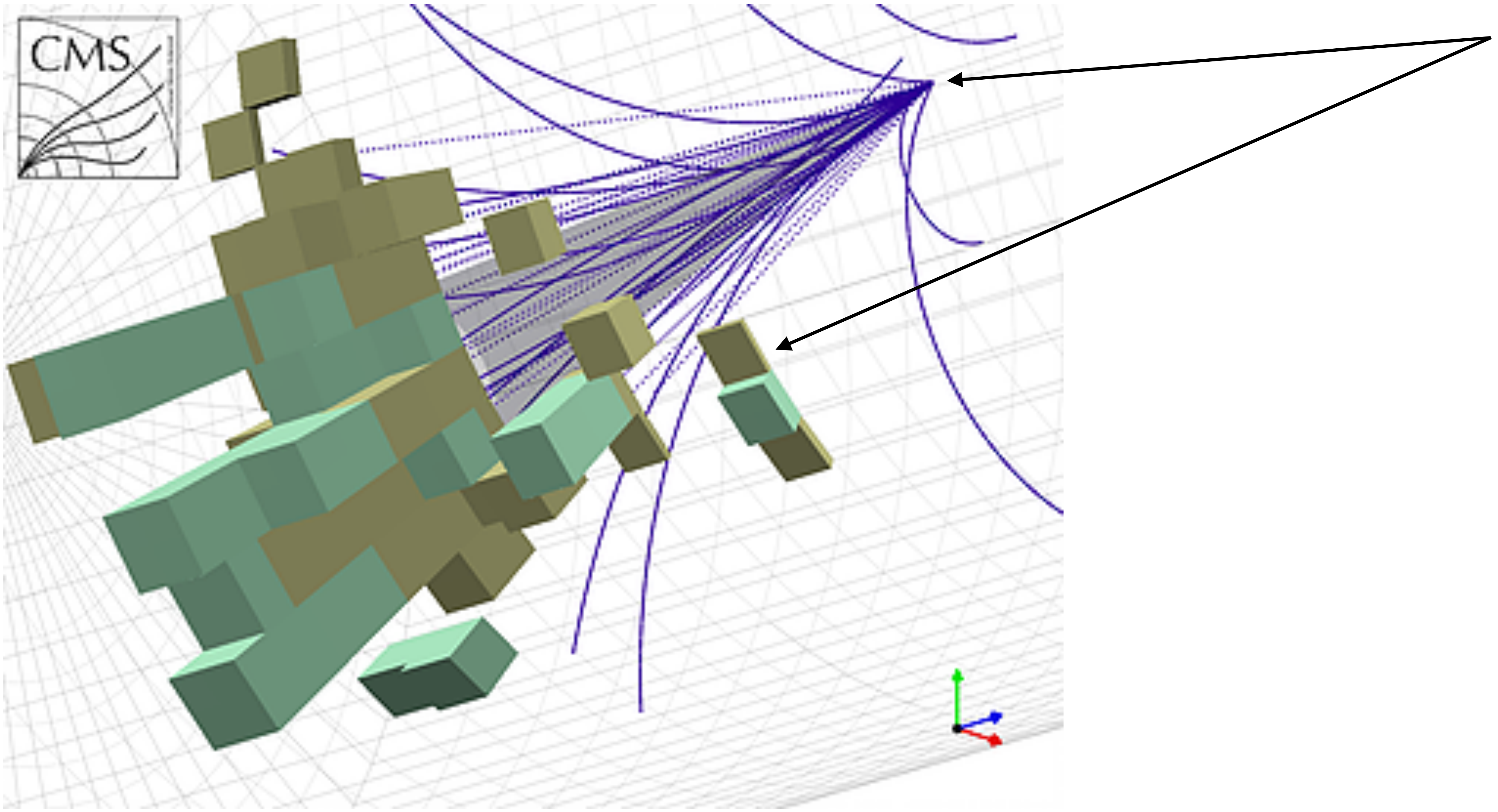


anti-$k_t$ clustering algorithm

# Calorimetry & Jet reconstruction

Clustering and object identification

- Many, many input variables



- Each line (track) or box (energy deposit, cluster) represents several input features

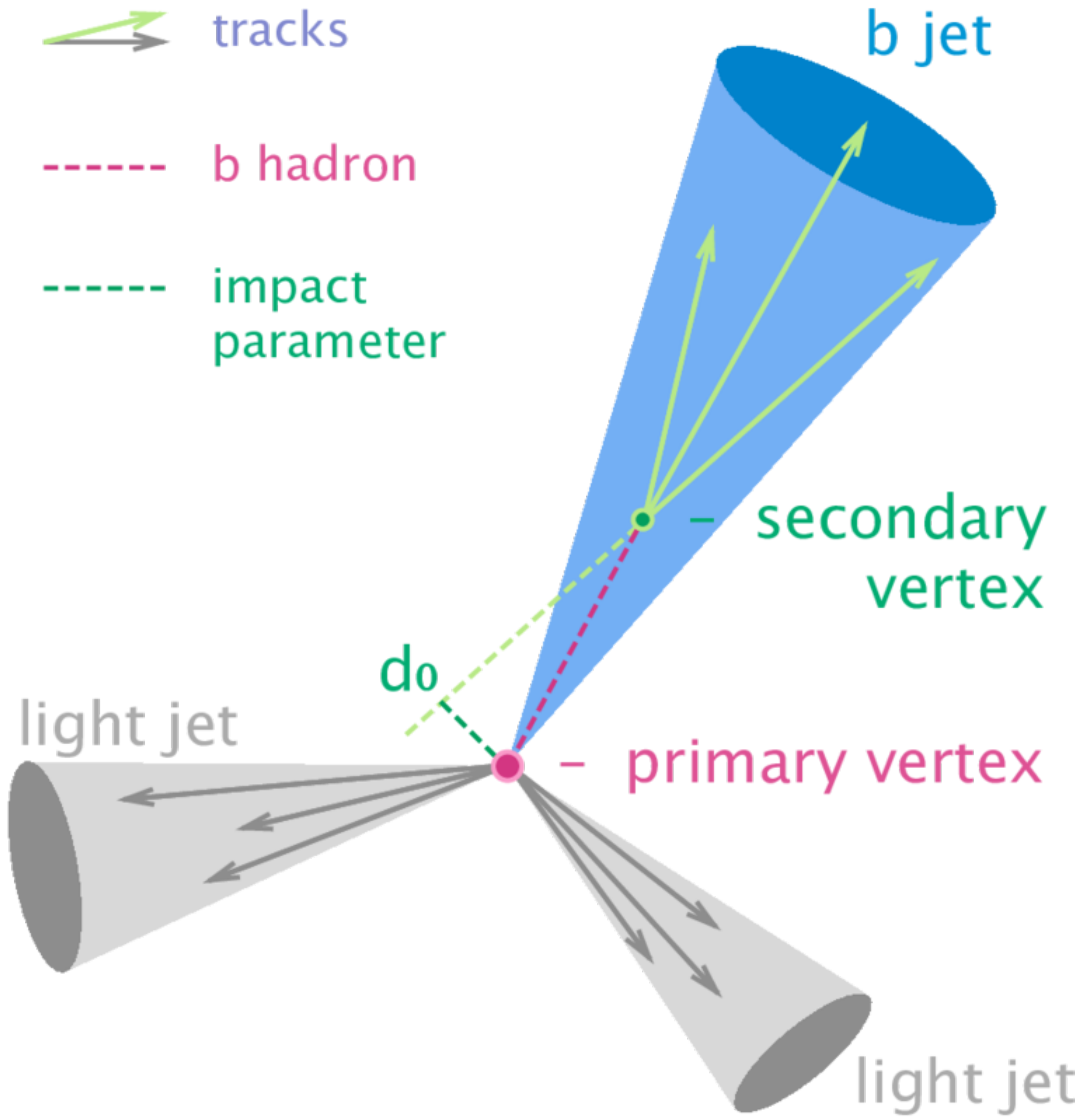
O (1000) input features

- Those input features look differently for different jet types: q (flavour), g

# Jet tagging: which flavour of q

## Classification problems

- Most commonly known and applied taggers aim to identify jets from b-quarks



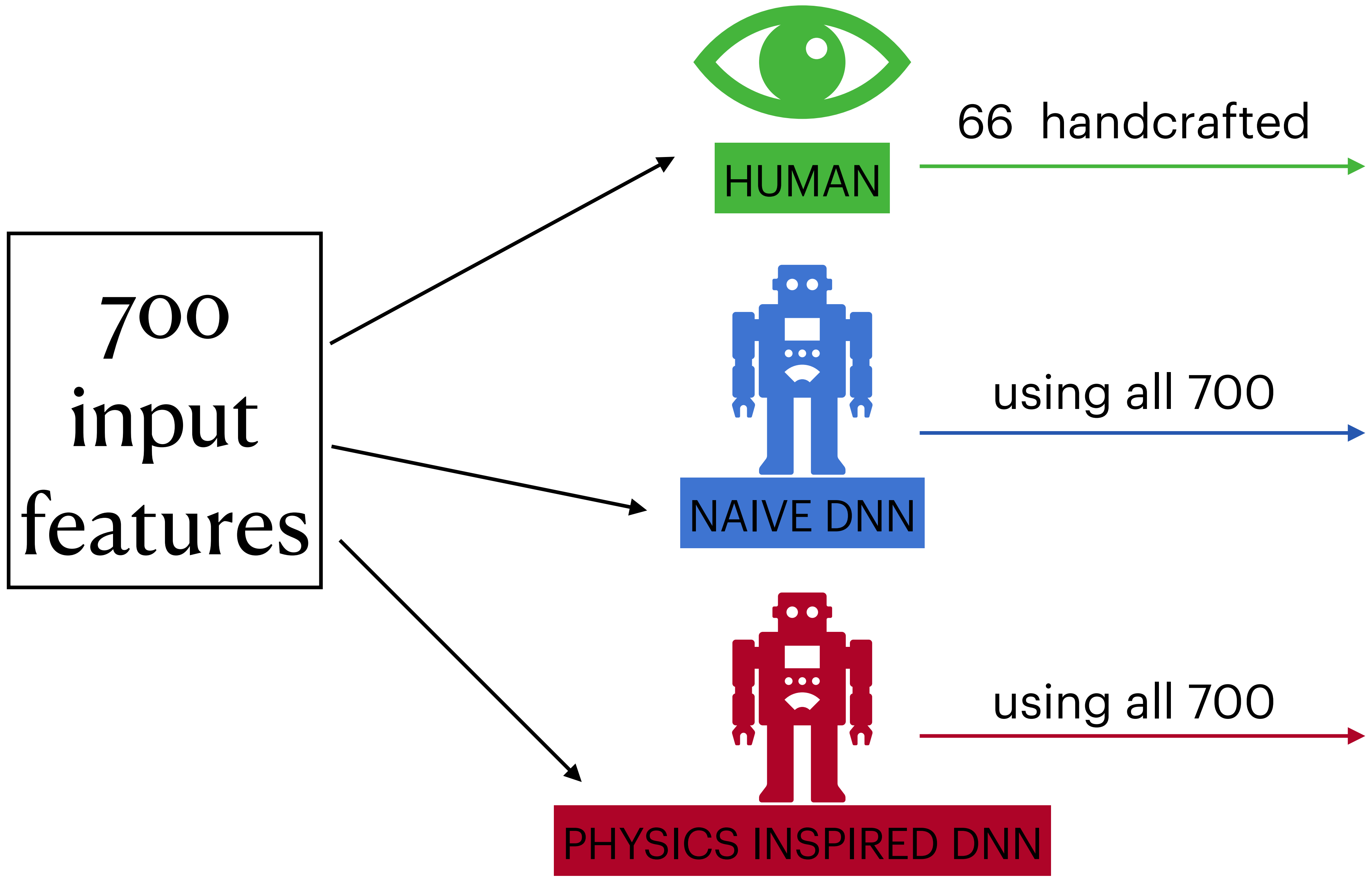
- Most state-of-the-art b-tagger use ML to exploit a variety of features
  - Finite lifetime of b-quark generates secondary vertex & displaced tracks
  - Eventually leptons in final state
  - Slightly wider jet structure from kinematics

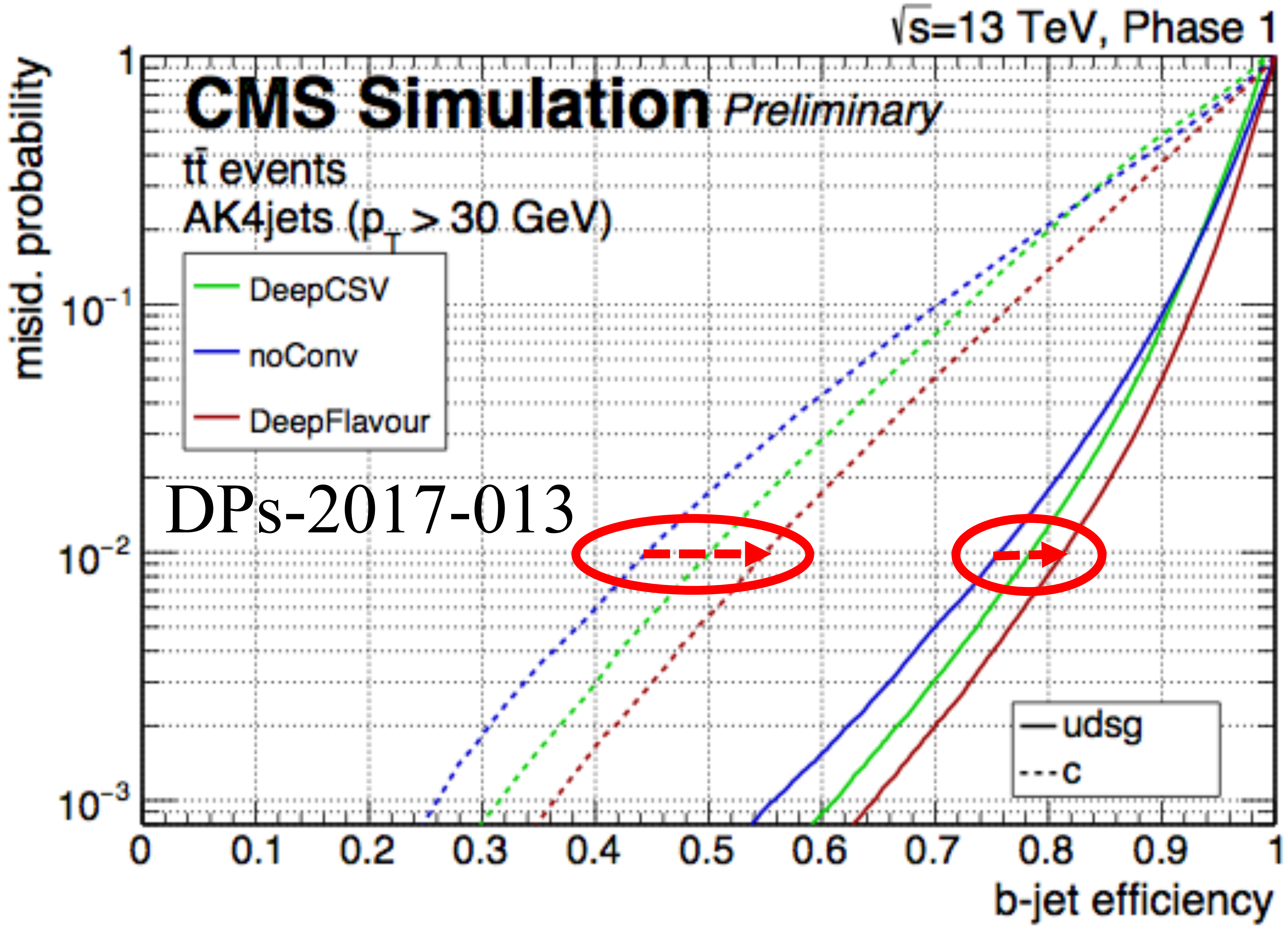
[ Image: Nazar Bartosik ]

# Jet tagging: which flavour of q

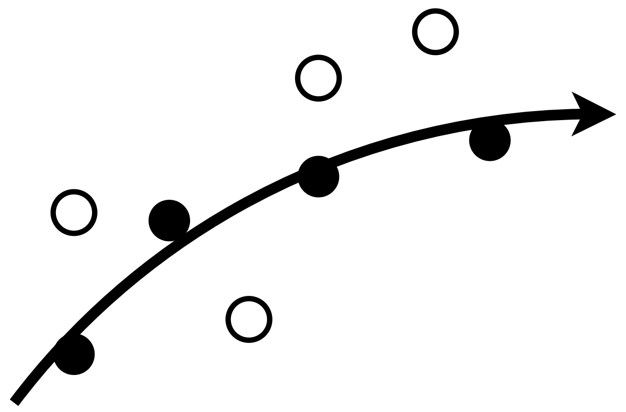
## Classification problems

- The network architecture is not unessential in this context





[ M Stoye: DeepJet ]



# Jet tagging: q/g separation

## Clustering and object identification

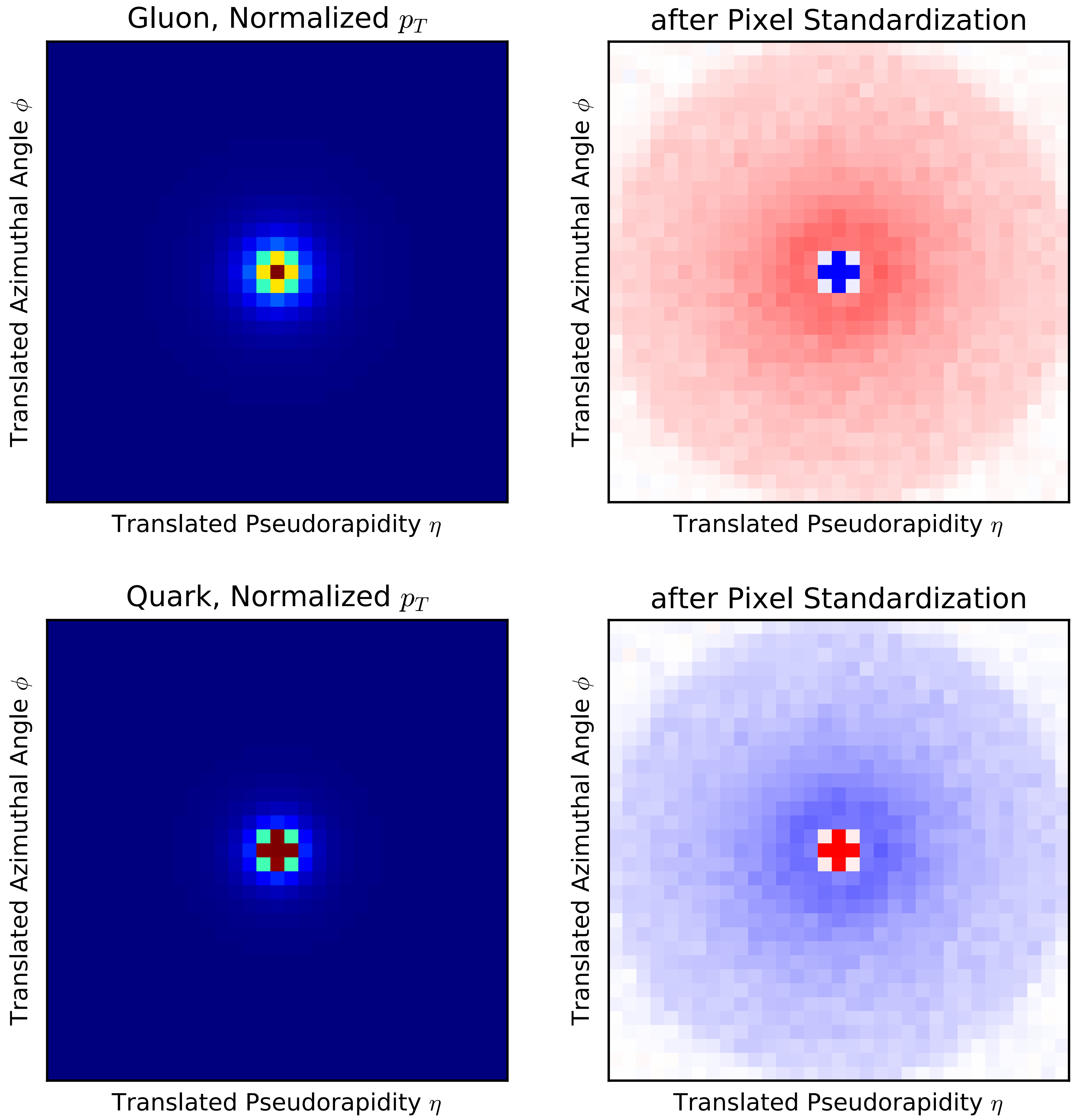
- Jets from quarks & gluons result in different topologies (*“images”*)

- Jet images augmented with *color information:*

RED: transverse momenta of charged particles

GREEN: transverse momenta of neutral particles

BLUE: charged particle multiplicity



Source:
arxiv.org:612.01551

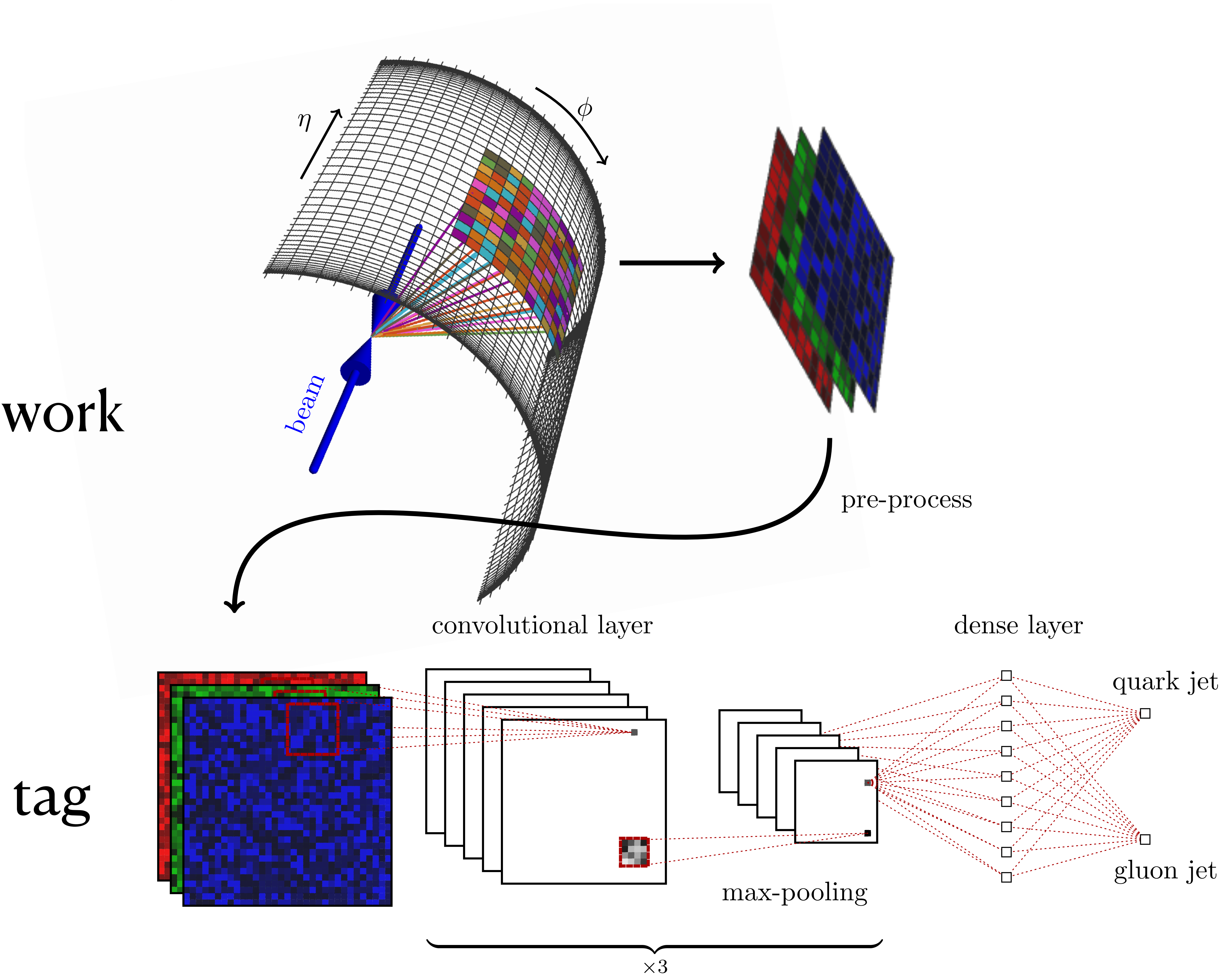
# Jet tagging: q/g separation

Clustering and object identification

- Jets from quarks & gluons result in different topologies (*“images”*)

- Fed into Convolutional Neural Network
  - Max pooling
  - Dense layers

- Output interpreted as quark/gluon tag

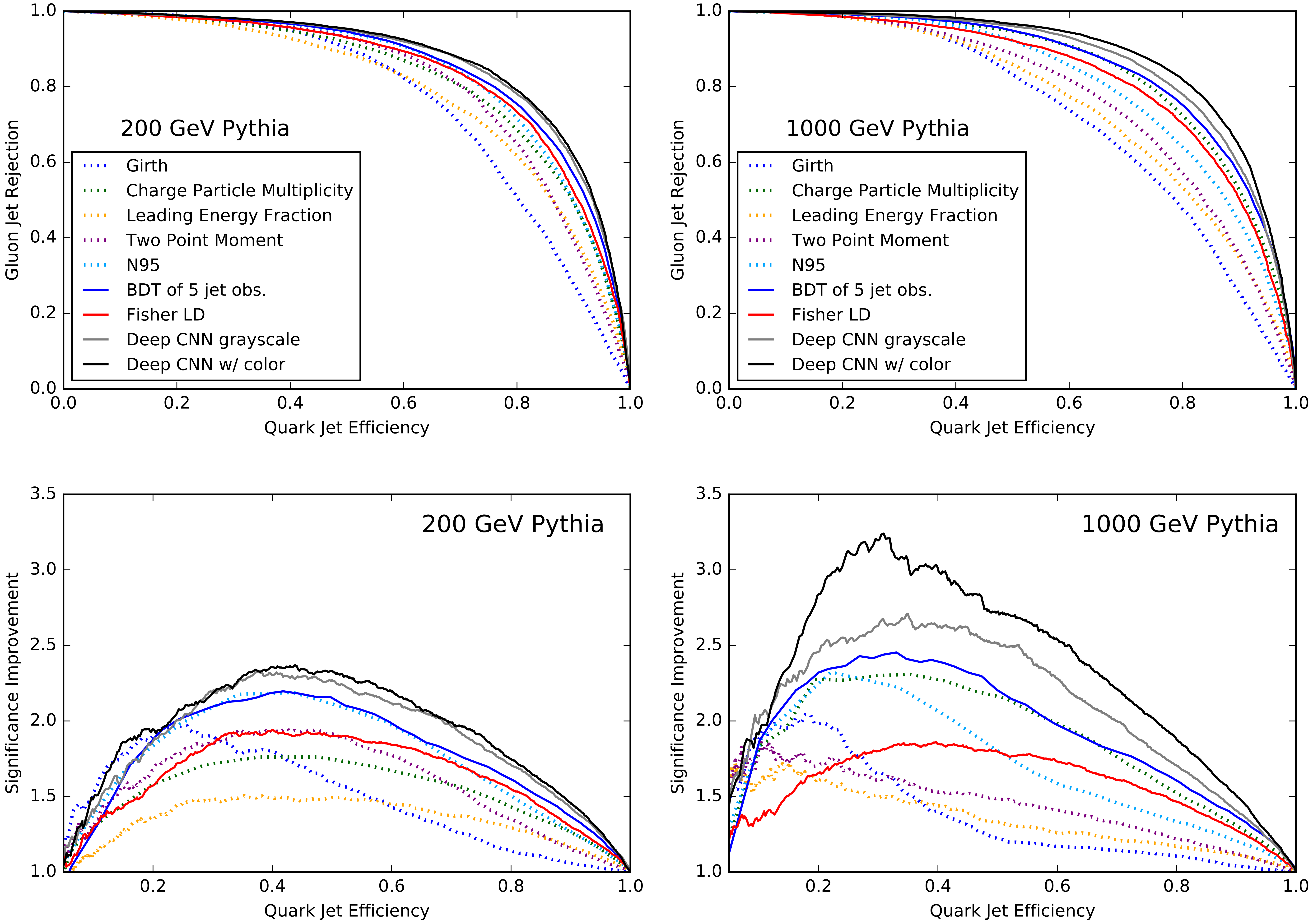


Source:
arxiv.org:612.01551

# Jet tagging: q/g separation

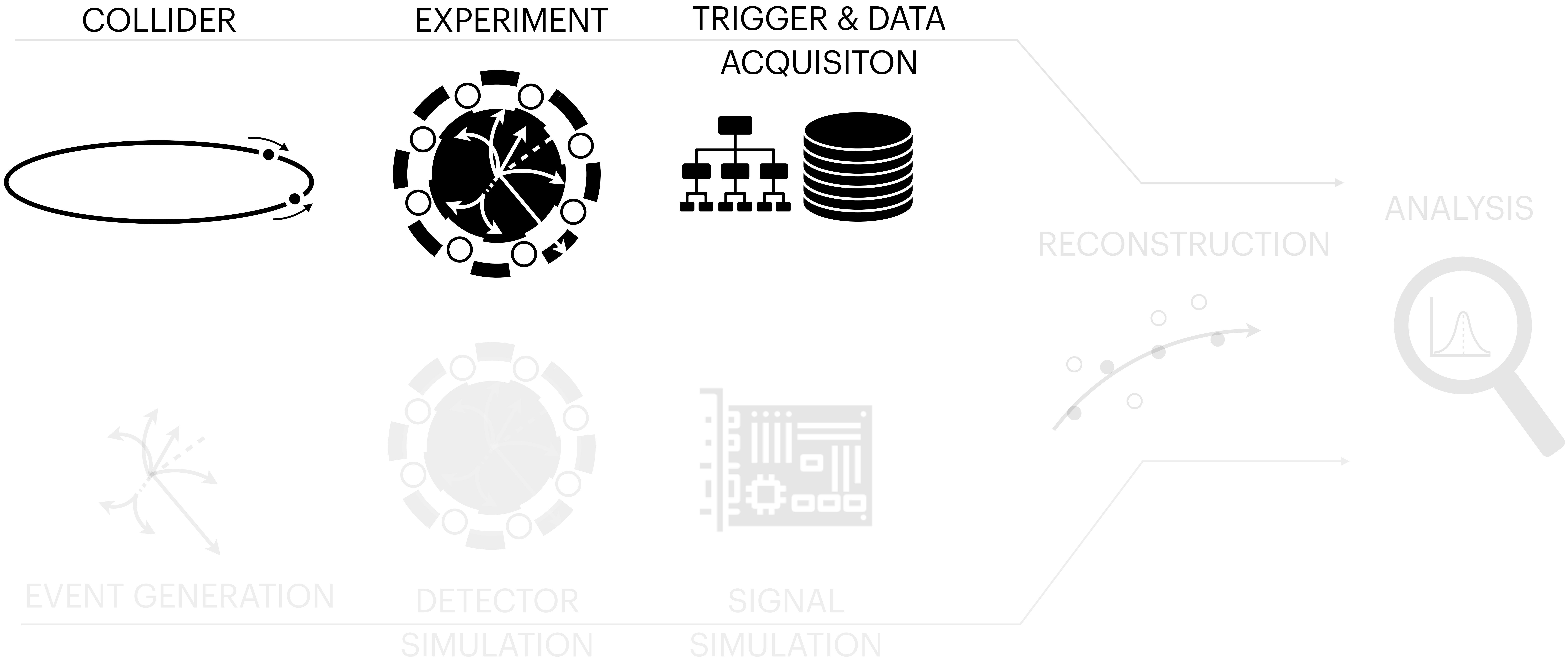
## Clustering and object identification

- CNN classification shows extremely strong ROC curve
- Adding "color" enhances that even more



Source:
arxiv.org:612.01551

# HEP&ML: Operation



COLLIDER

EXPERIMENT

TRIGGER & DATA ACQUISITON

RECONSTRUCTION

ANALYSIS

EVENT GENERATION

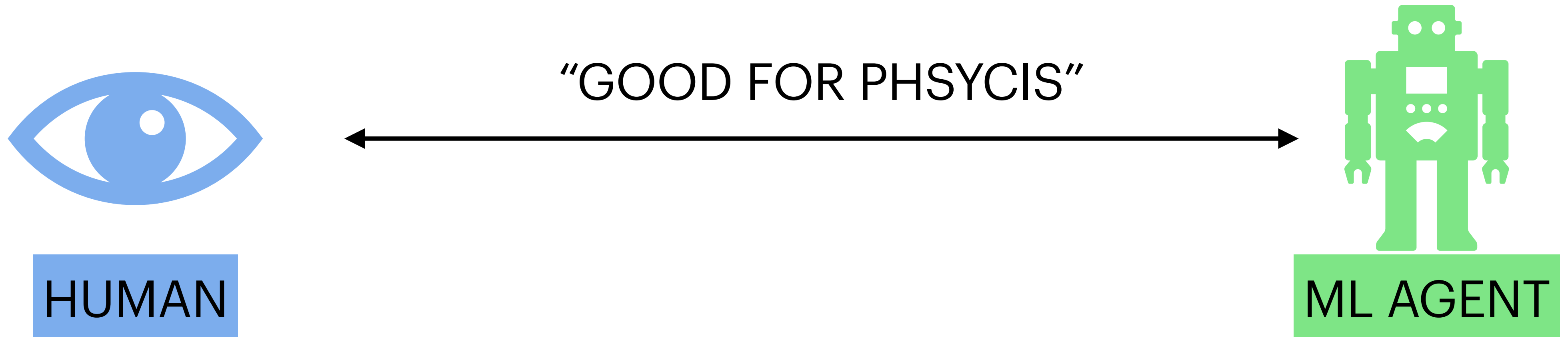
DETECTOR SIMULATION

SIGNAL SIMULATION

# Data Quality Monitoring (DQM)

## Anomalie Detection

- DQM is essential for detector operation, guarantees high quality data
- Has been (is) often done with human intervention (shifters)



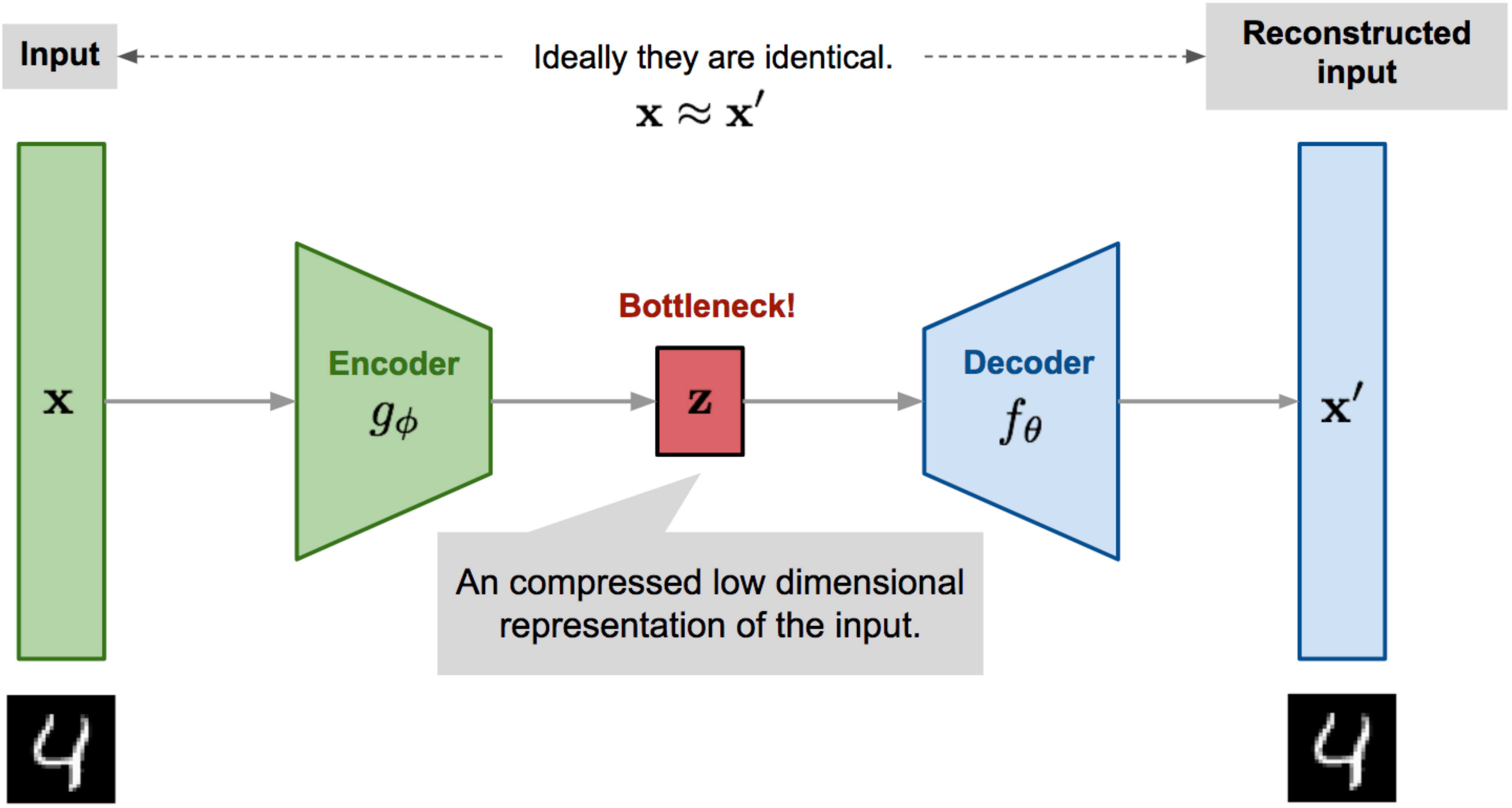
FASTER RESPONSE TIME
INTERPRETABILITY INCREASES
**+ IT IS A BORING JOB TO A BE SHIFTER**

- A lot of data (40 MHz collision, $10^8$ channels), but sparse (anomalies even sparser)

# Data Quality Monitoring (DQM)

## Anomalie Detection

- Auto-encoders are networks that aim (sparse) to map the input data to output data through a compressed representation



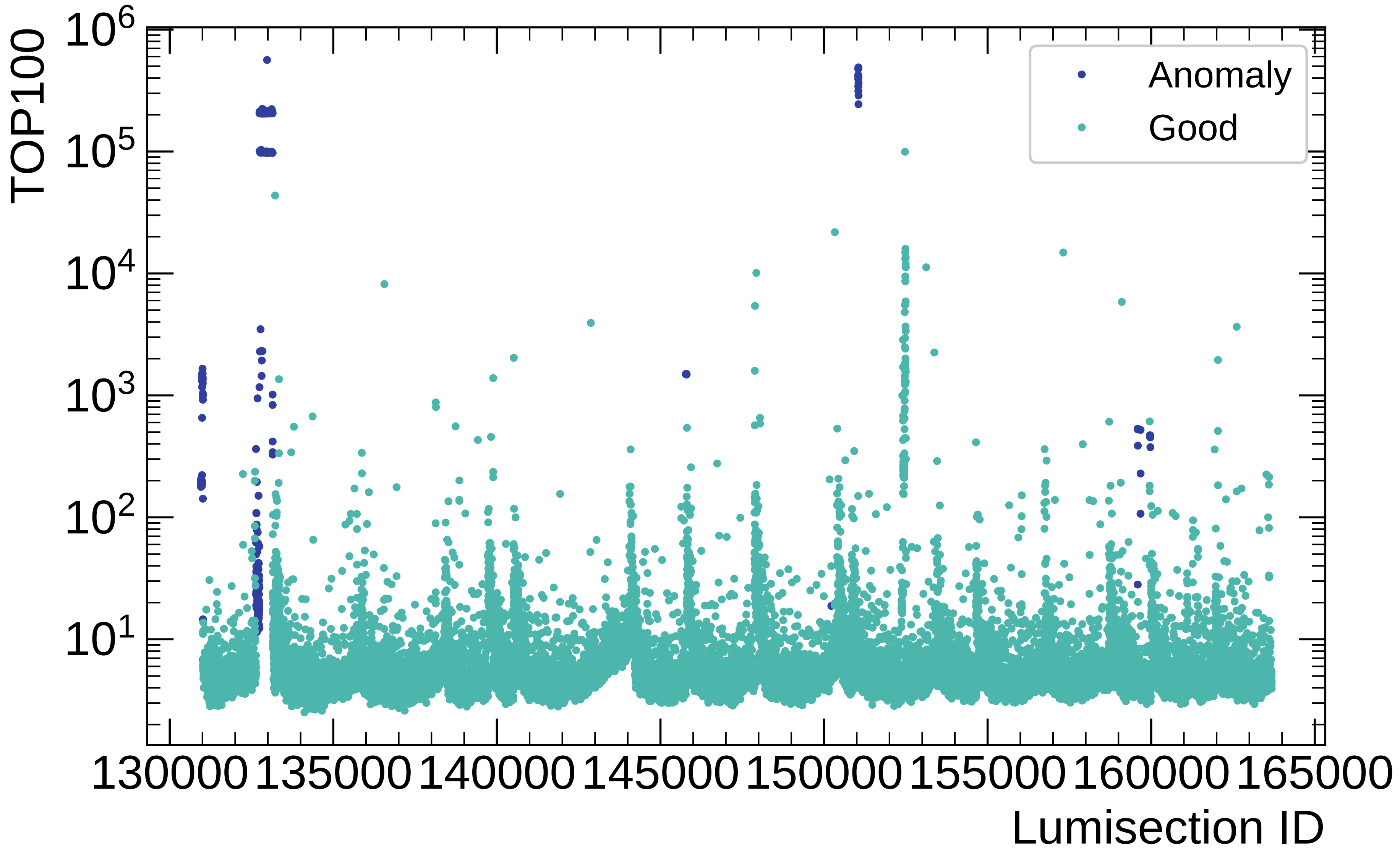
[ Lilian Weng: From Autoencoder to Beta-VAE ]

# Data Quality Monitoring (DQM)

## Anomalie Detection

- Auto-encoders are networks that aim (sparse) to map the input data to output data through a compressed representation
  - Trained only on a “good” selection will result in sub-optimal output on anomalies
  - Least squares of 100 worst reconstructed features

$$TOP100 = \frac{1}{100}\sum_{i=1}^{100} sorted(X_i - \hat{X}_i)^2$$



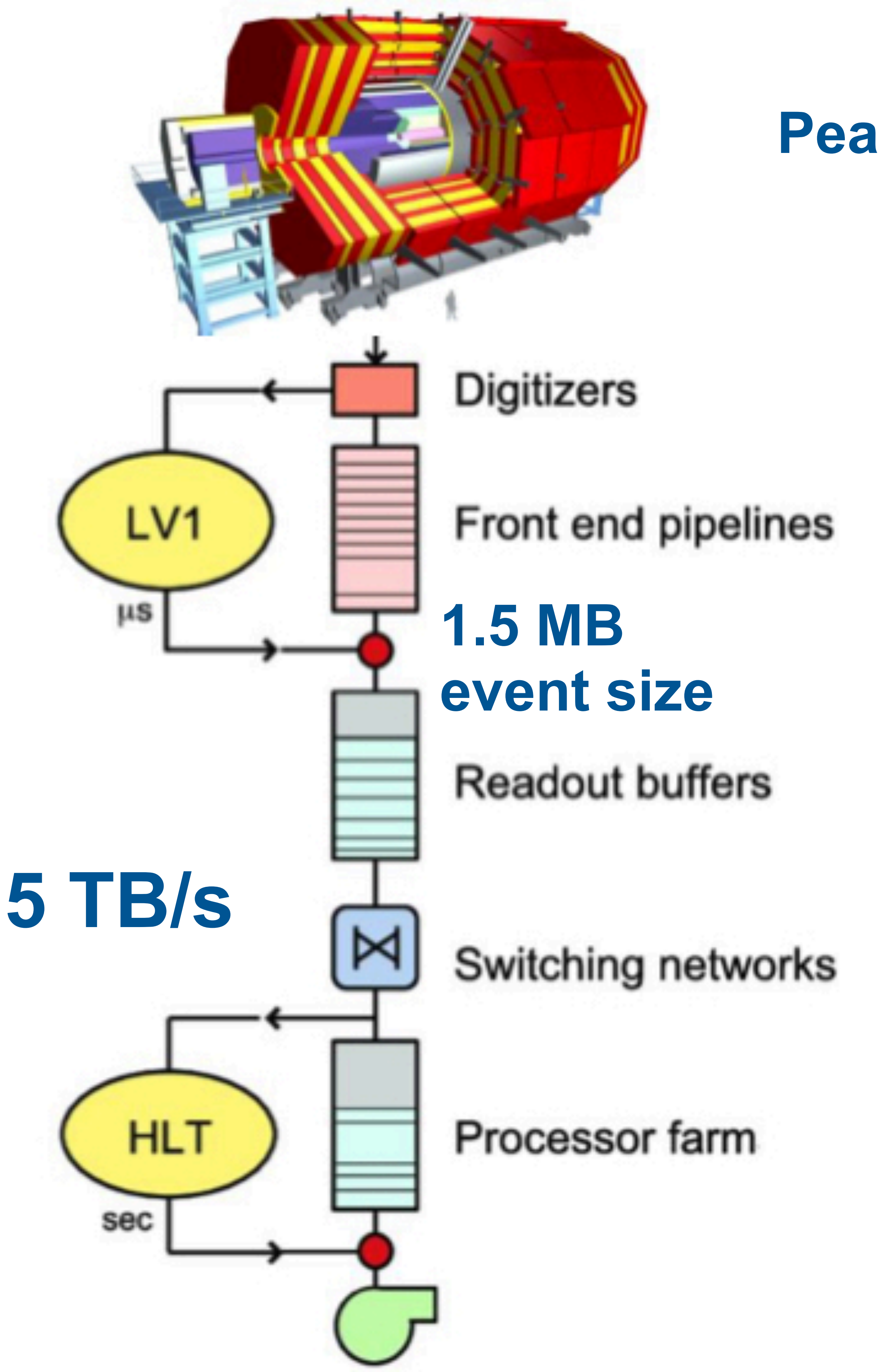
[ A. Pole, Anomalie Detection in CMS, CHEP2018 ]

# Triggering using ML

## Fast trigger detection / scouting

- LHC experiments deploy complicated triggering systems to filter “interesting” events
- Data scouting is one of the strategies
  - Trigger objects fed into a multi-layer perception network to model offline parameters for muons
  - Goal to run on FPGAs in real-time

**Phase 0&1: 2008 - 2024**



**Peak pile-up 60**

**40 MHz**

**1.5 MB event size**

**100 KHz**

**0.15 TB/s**

**2 KHz**

[ D. Golubović/CMS: 40 MHz scouting at CMS ]

# Triggering using ML

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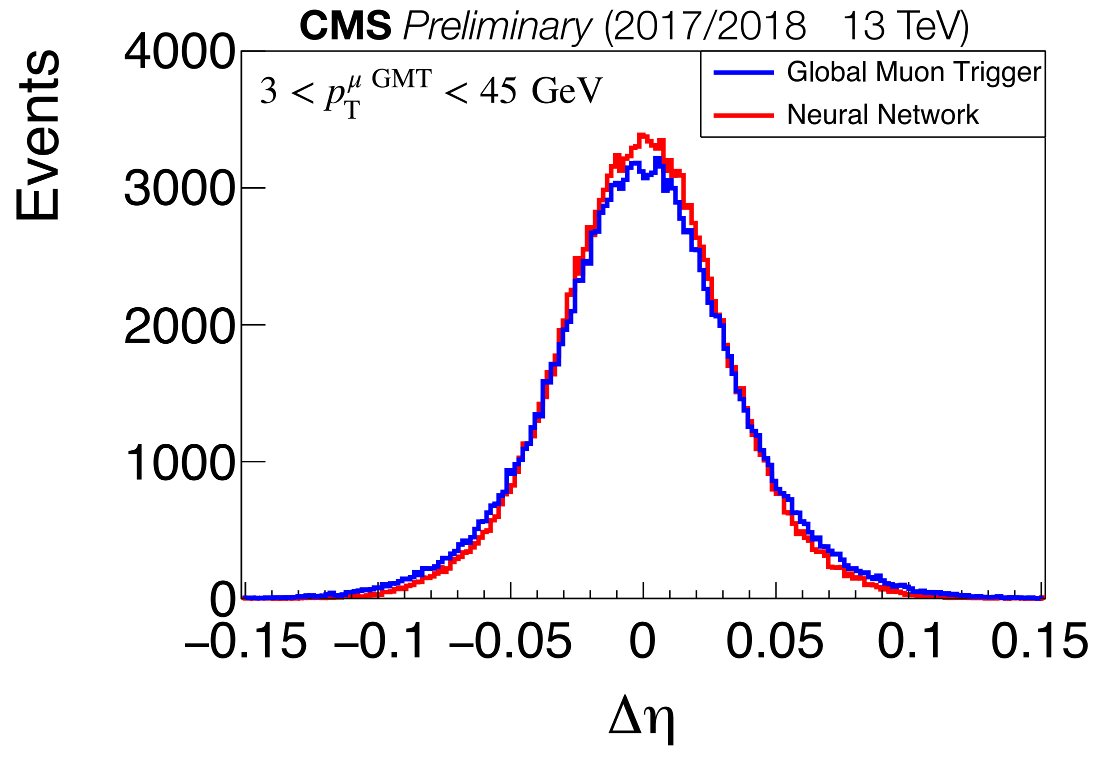
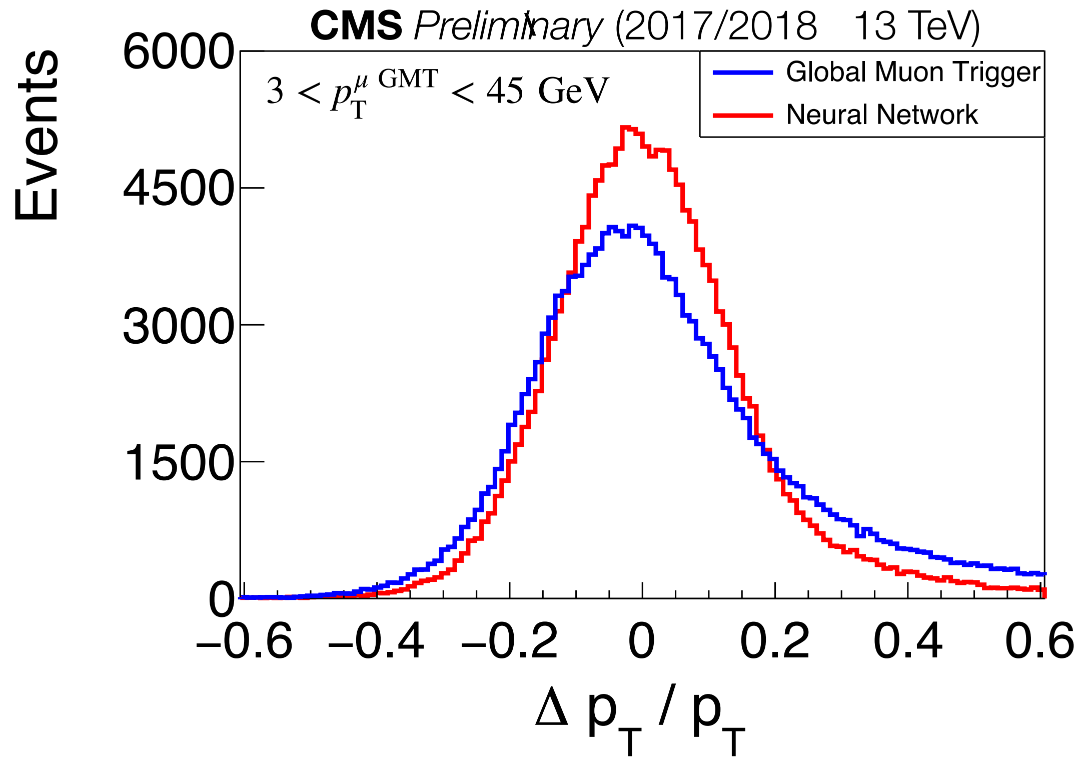
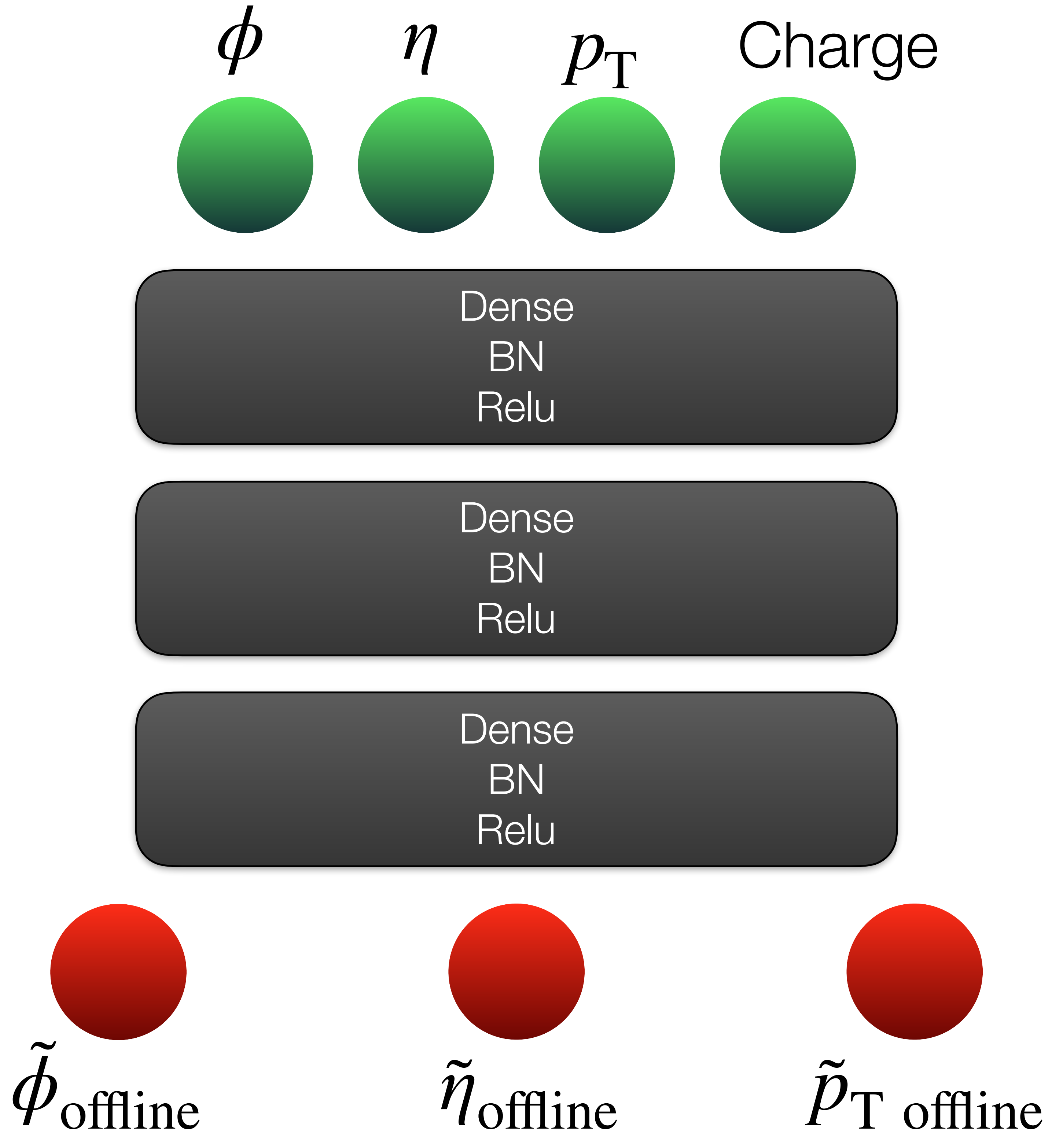






TRAIN ON GPU / RUN ON FPGA

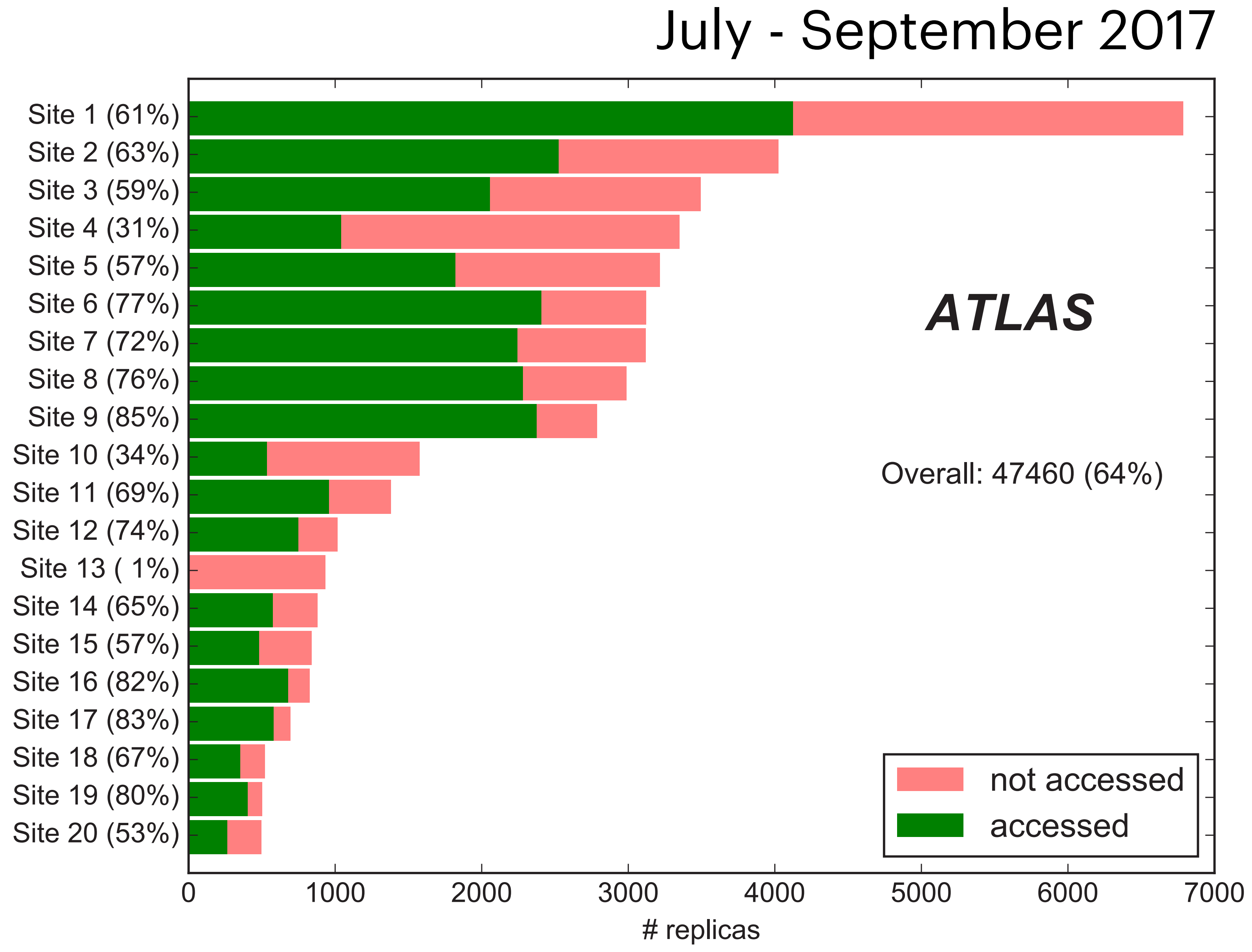
[ D. Golubović/CMS: 40 MHz scouting at CMS ]

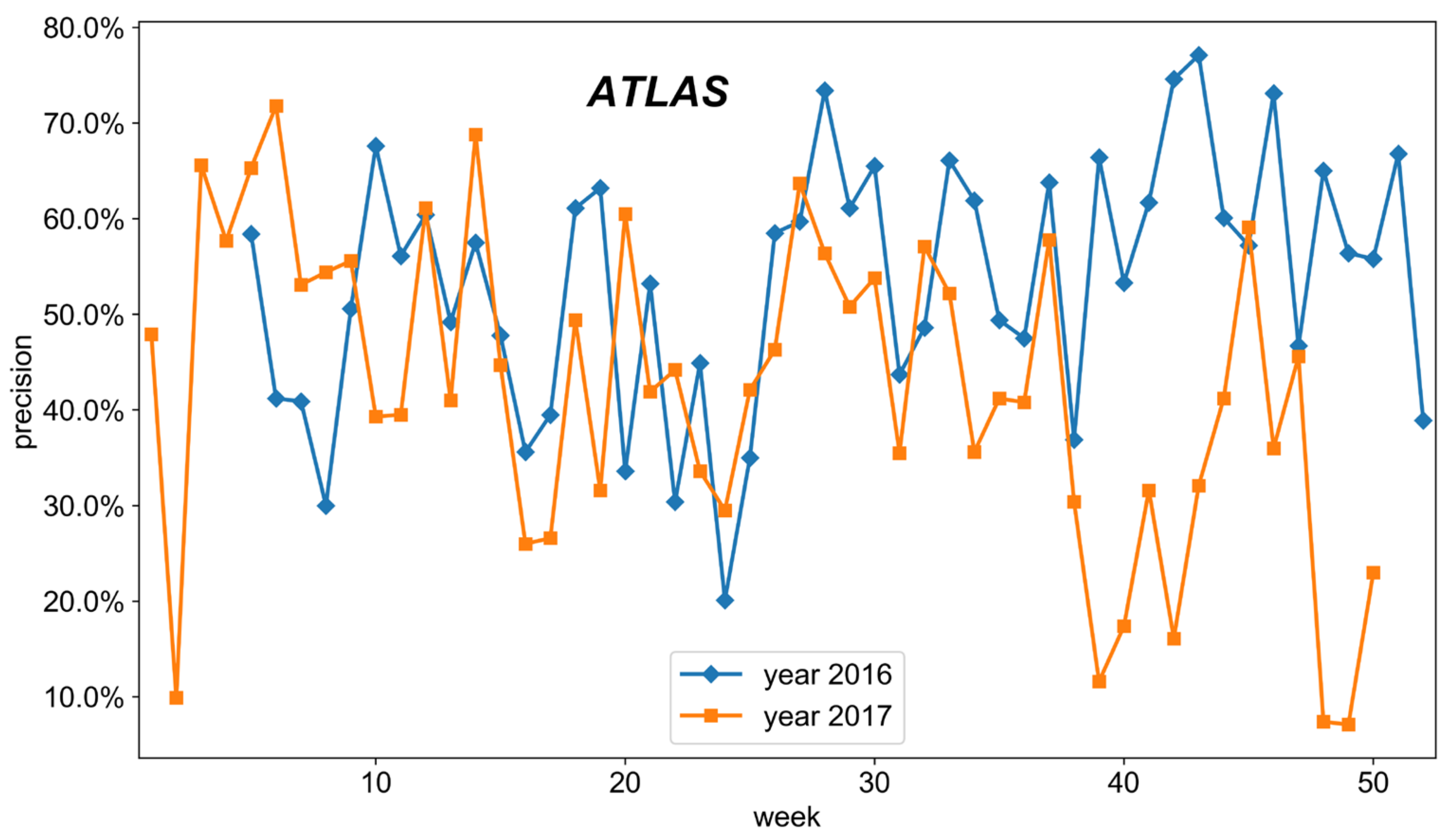
# **Intelligent** Computing operation

## Data popularity prediction

- HEP lives from distributed data storage & processing
  - Non-trivial problem, as data storage & CPU is expensive
  - Predicting popularity of a data set could help optimising computing resources, using meta data to predict popularity with AdaBoost

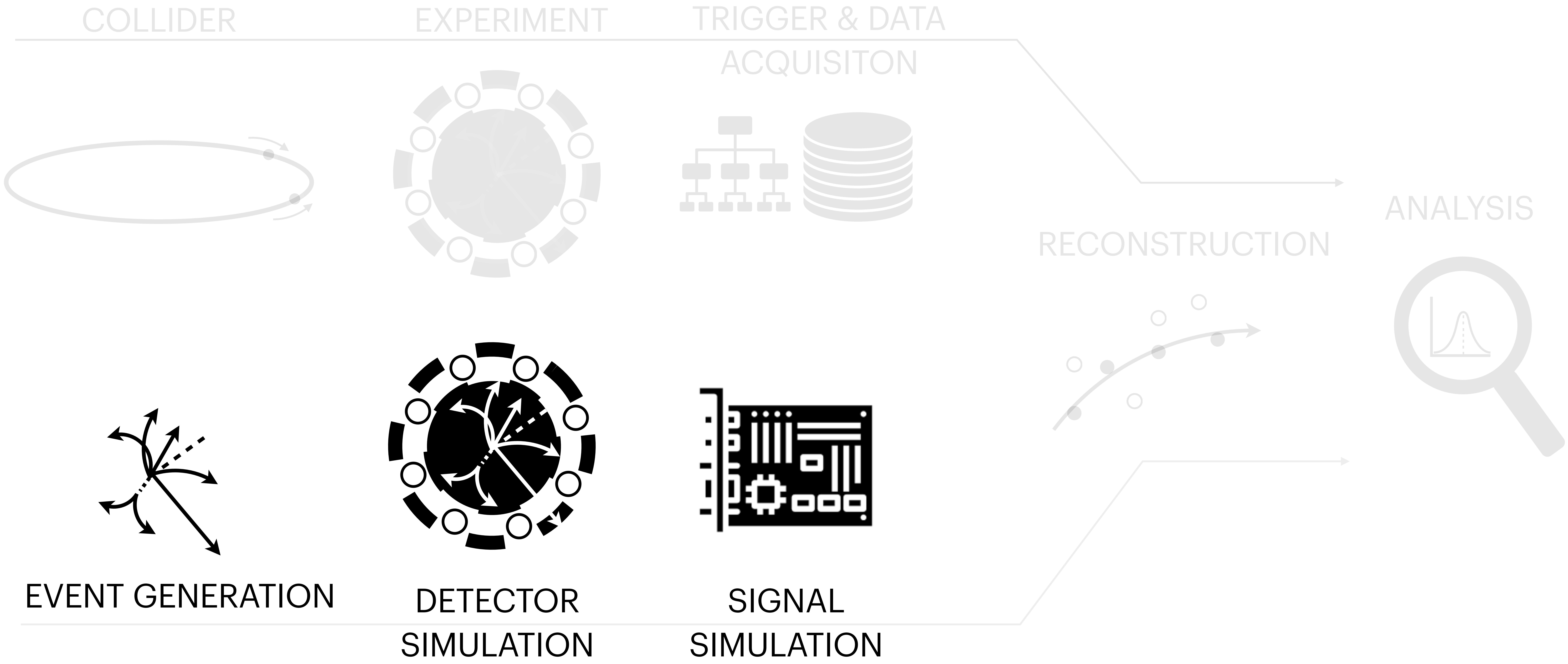
- Intelligent computing operation is an upcoming topic
  - Aim is to optimise resource usage & minimise failures





[ Performance and Impact of dynamic data placement in ATLAS ]

# HEP&ML: Simulation



COLLIDER

EXPERIMENT

TRIGGER & DATA ACQUISITON

RECONSTRUCTION

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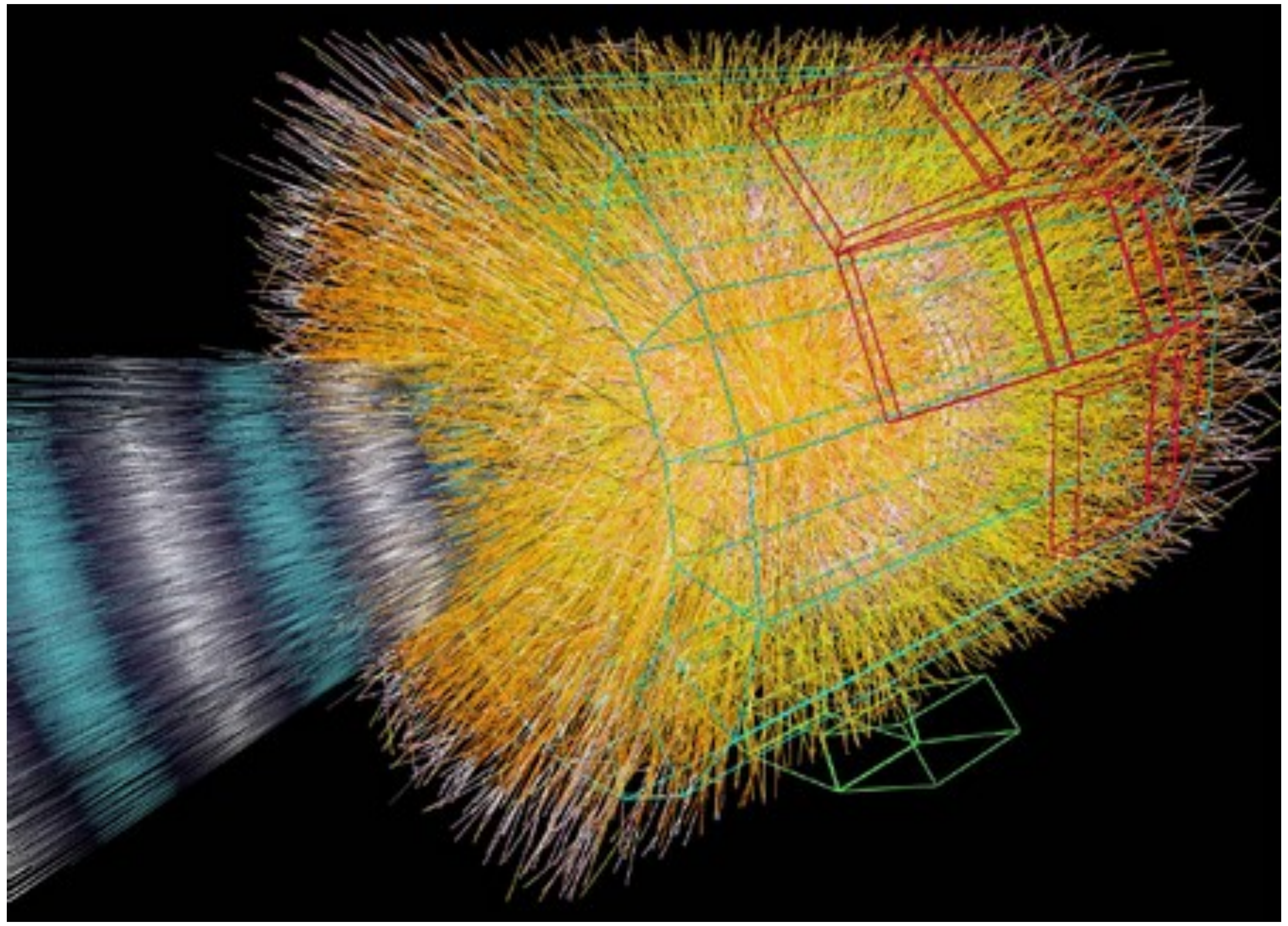
SIGNAL SIMULATION

# Detector Simulation

Monte Carlo data production

- HEP relies a lot (too much?) in Monte Carlo simulation
- Full (& very precise) detector simulation toolkit Geant4, very CPU hungry
  - Fast simulation techniques are often good enough
  - But how to sample something as complex as this?



[ Image : ALICE CERN ]

# Detector Simulation

Monte Carlo data production

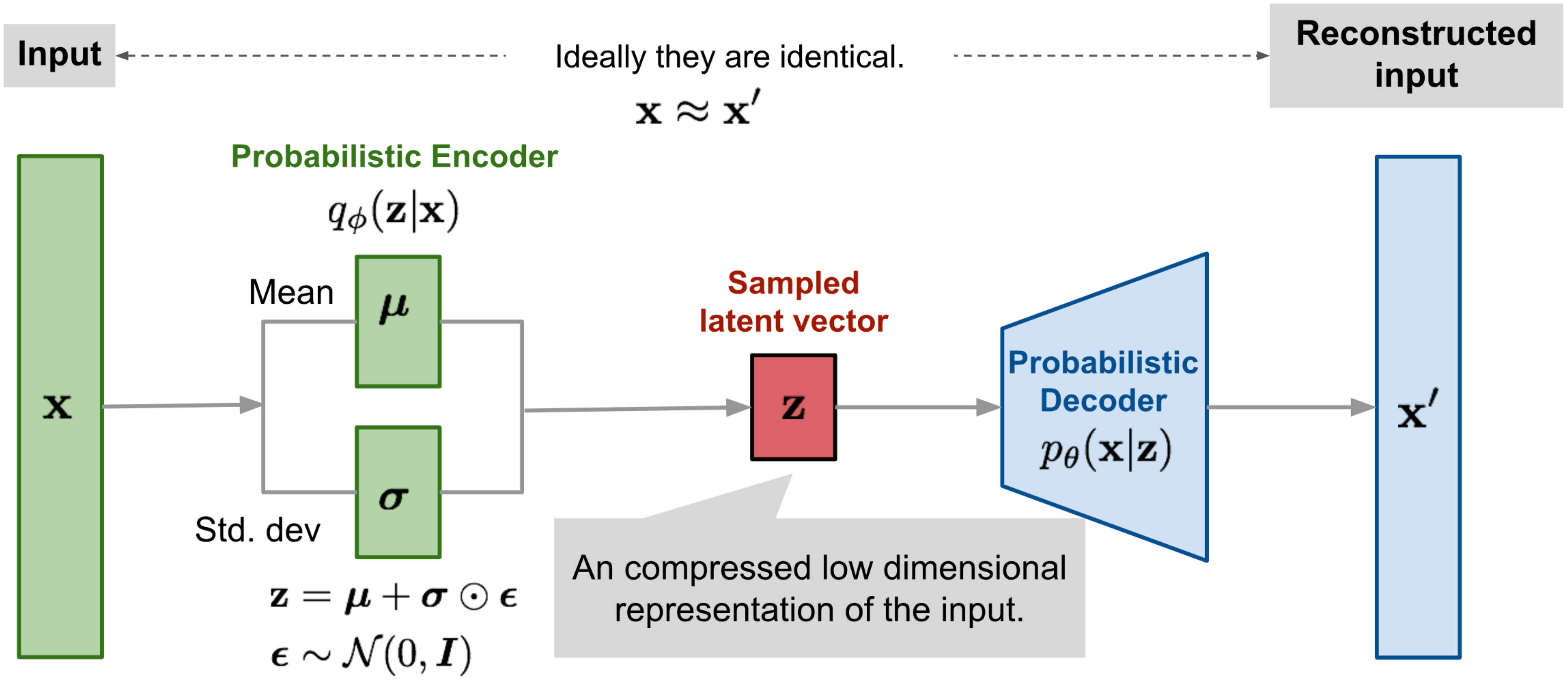
- HEP relies a lot (too much?) in Monte Carlo simulation
- Full (& very precise) detector simulation toolkit Geant4, very CPU hungry
  - Fast simulation techniques are often good enough
  - But how to sample something as complex as this?
- Generative Adversarial Network (GAN)

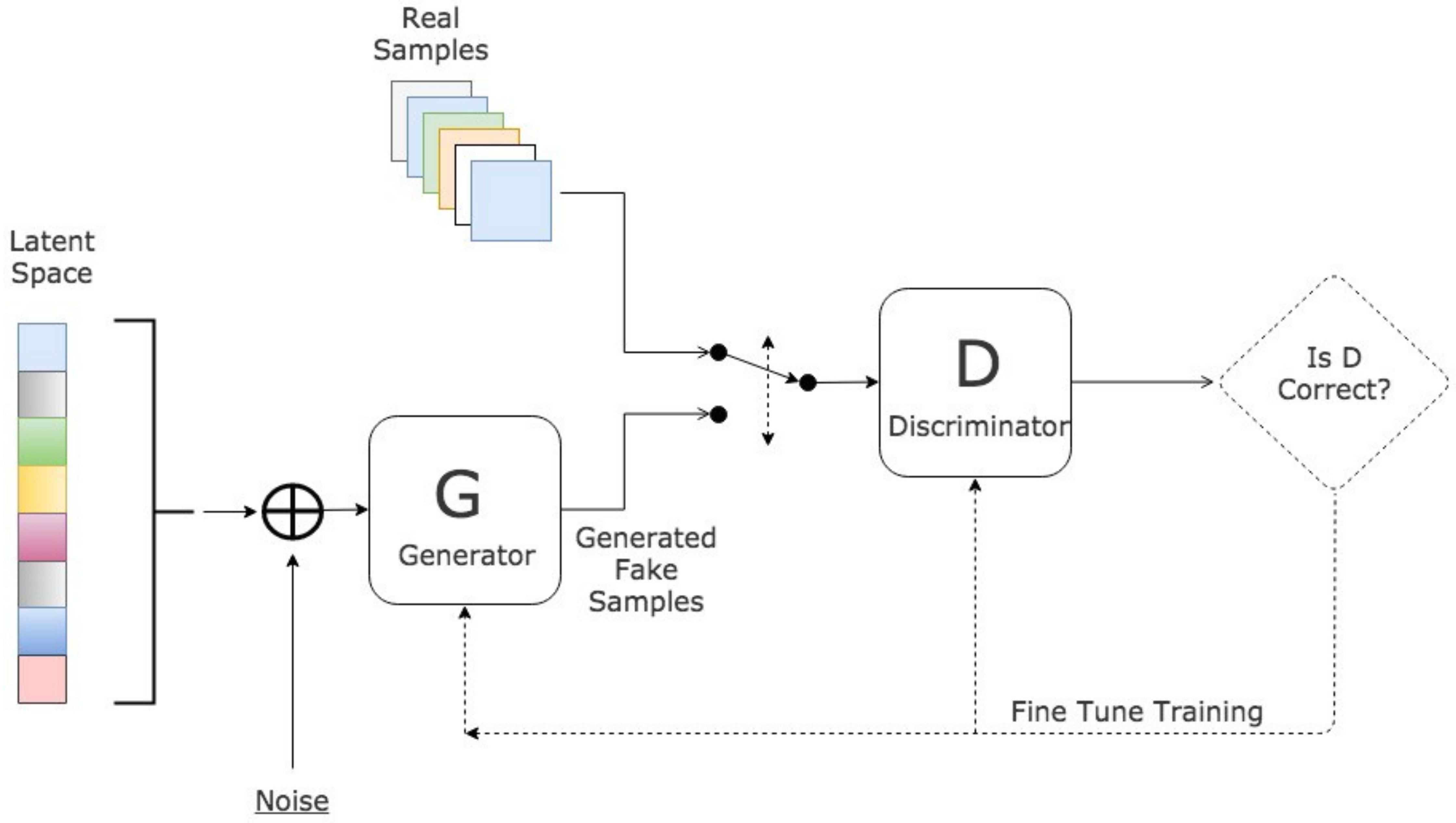
[ www.thispersondoesnotexit.com ]

# Detector Simulation

Fast simulation techniques

- Variational Auto-Encoder (VAE)
- Generative Adversarial Network (GAN)





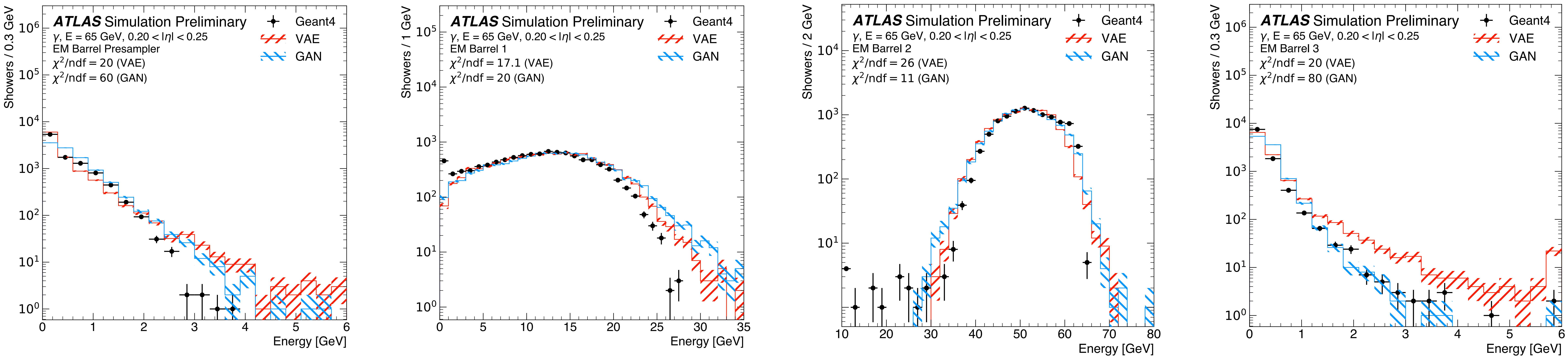
[ Lilian Weng: From Autoencoder to Beta-VAE ]

[ I. Goodfellow et al: Generative Adversarial Nets ]

# Detector Simulation

Fast simulation techniques

- Variational Auto-Encoder (VAE)
- Generative Adversarial Network (GAN)

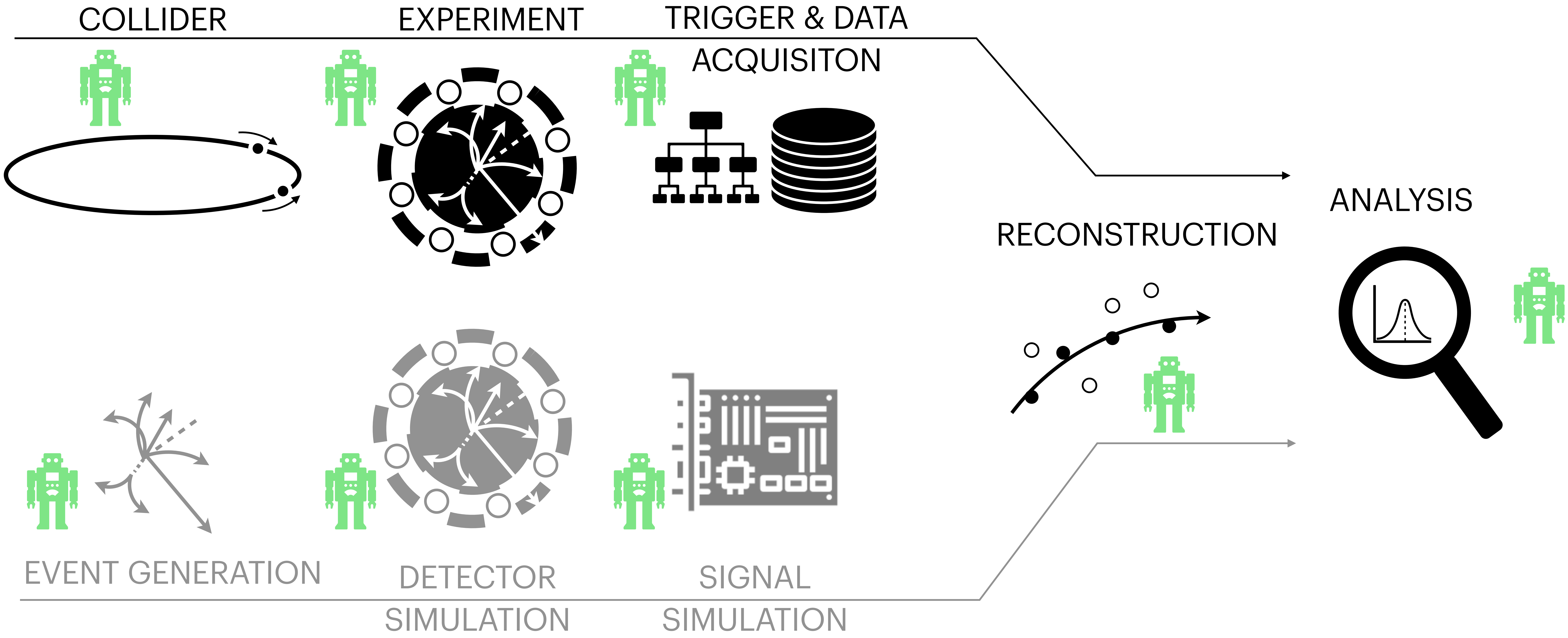


- Very promising results at a fraction of the CPU cost, similar study quotes ~1/1000

[ ATL-SOFT-PUB-2018-001 ]
[ S. Vallecorsa , F. Carminati , G. Khattak : 3D convolutional GAN for fast simulation ]

# Conclusion

ML IS EVERYWHERE IN HEP



COLLIDER

EXPERIMENT

TRIGGER & DATA ACQUISITON

RECONSTRUCTION

ANALYSIS

EVENT GENERATION

DETECTOR SIMULATION

SIGNAL SIMULATION

# Conclusion

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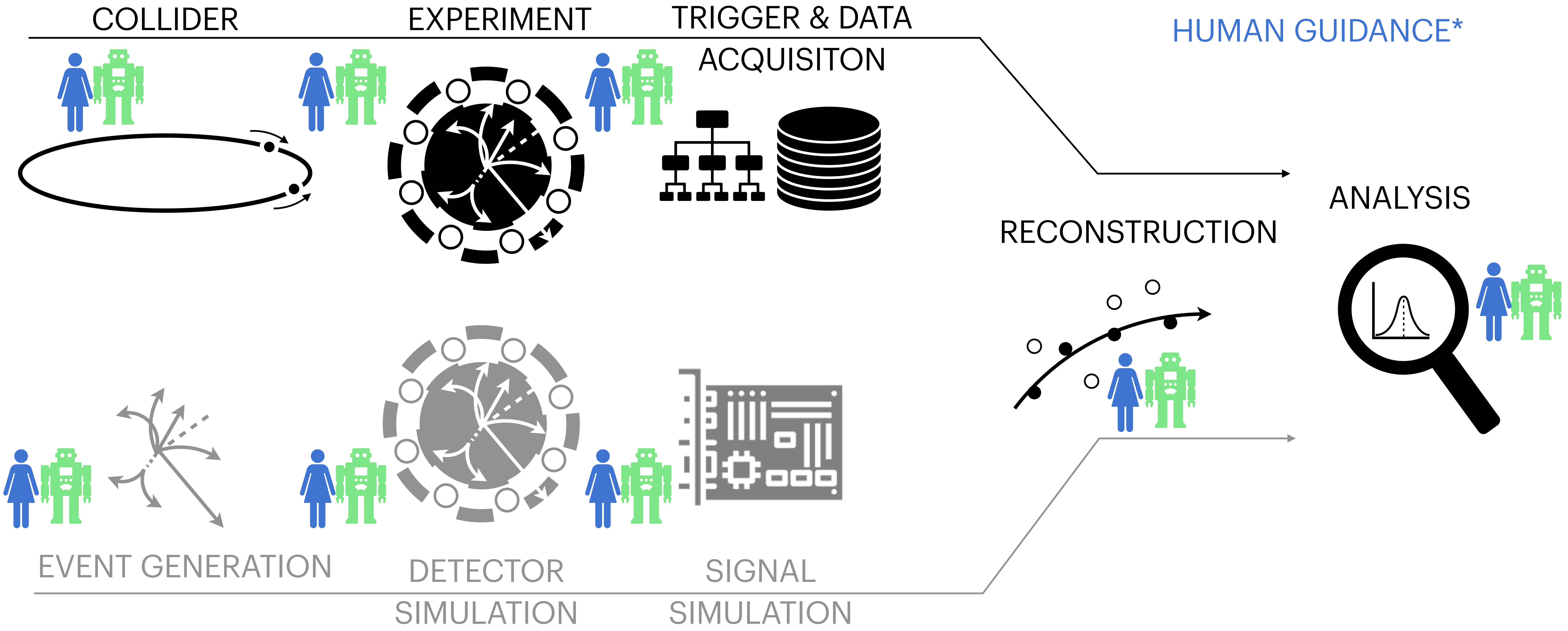
AND IT WORKS BEST WITH HUMAN GUIDANCE*



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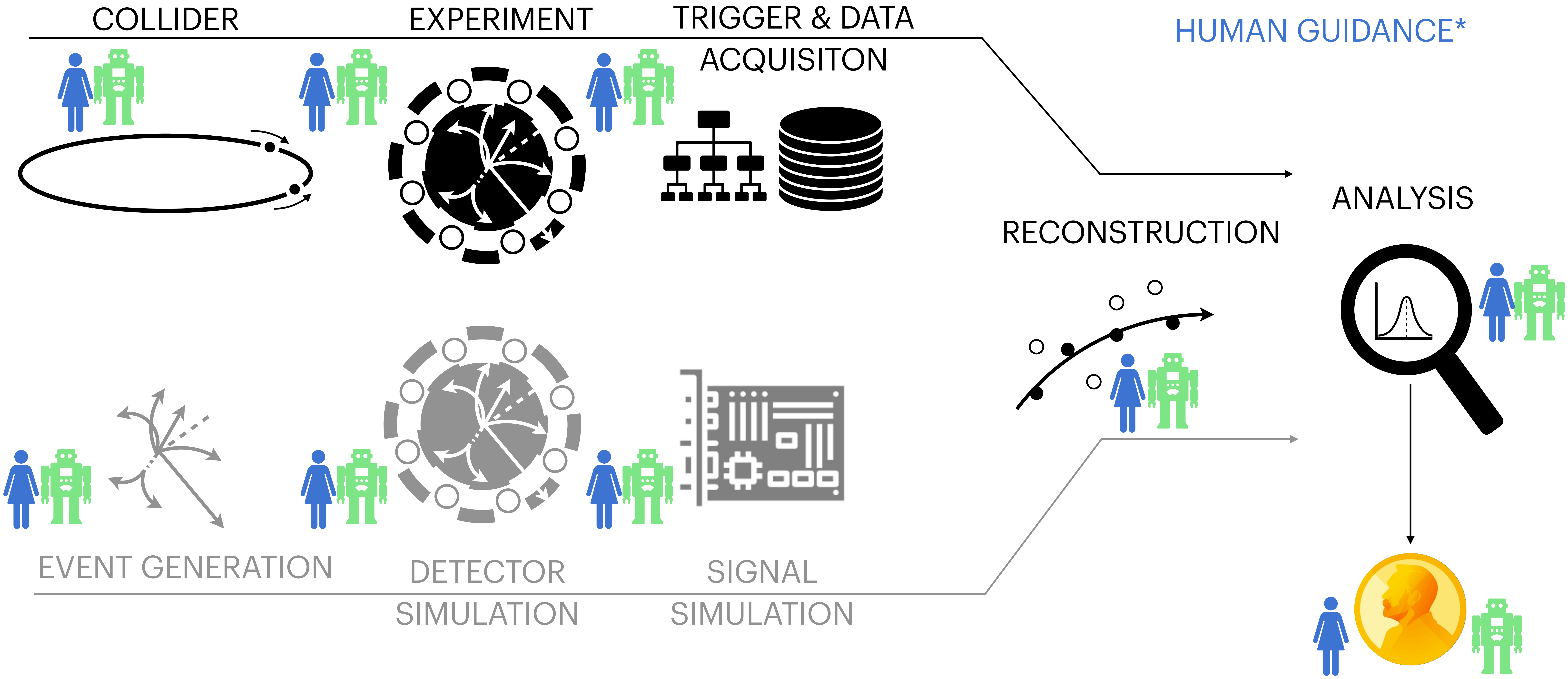

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