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U.S. DEPARTMENT OF  
**ENERGY**

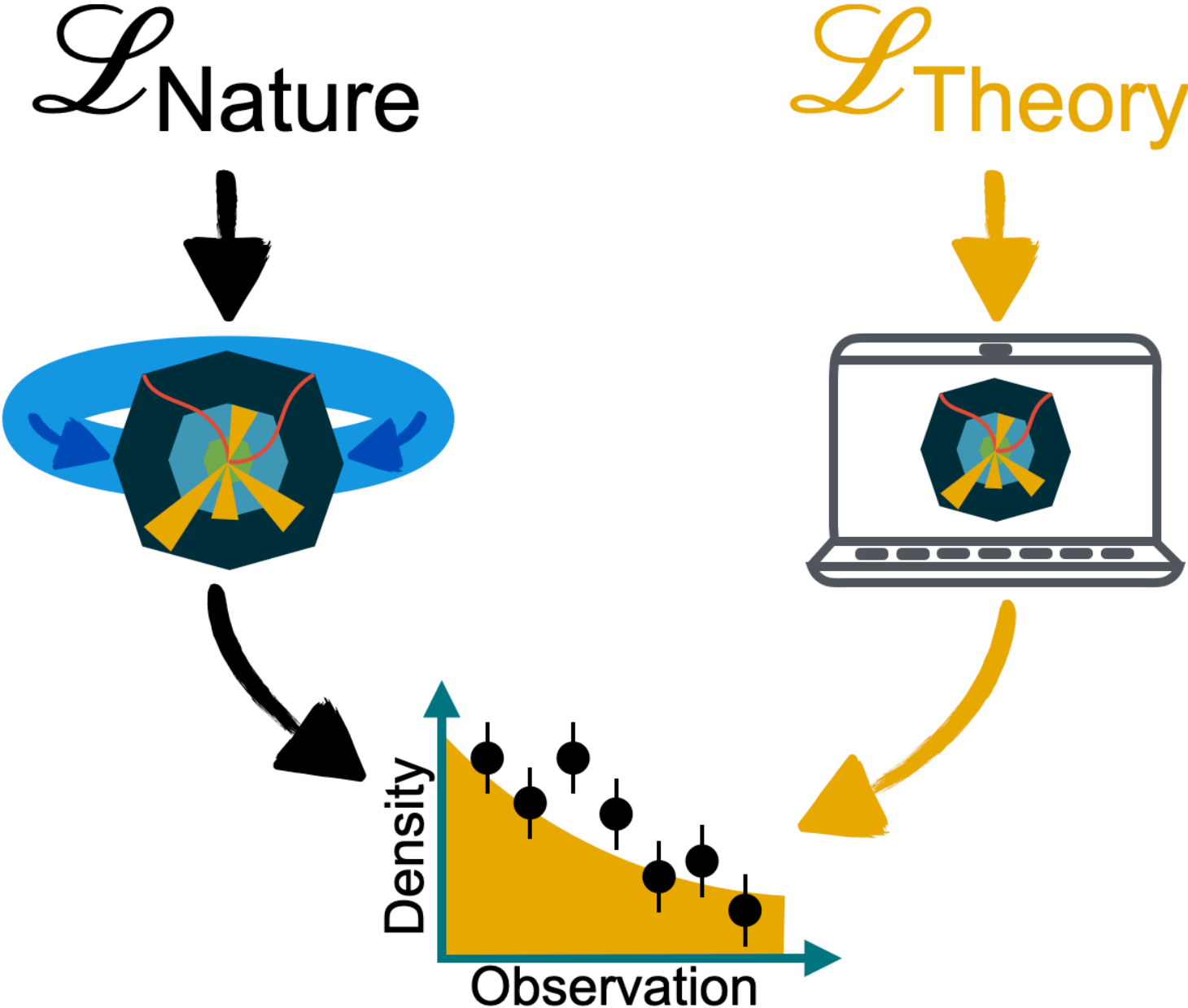
Office of Science

# Machine Learning for HEP Data Analysis

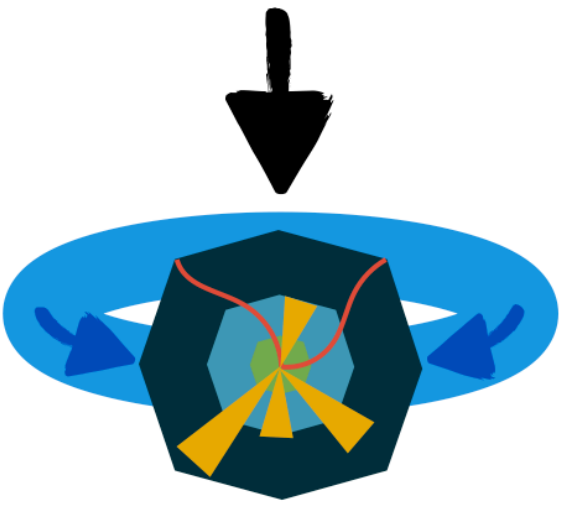
**Dennis Noll**

FCC Week 2024

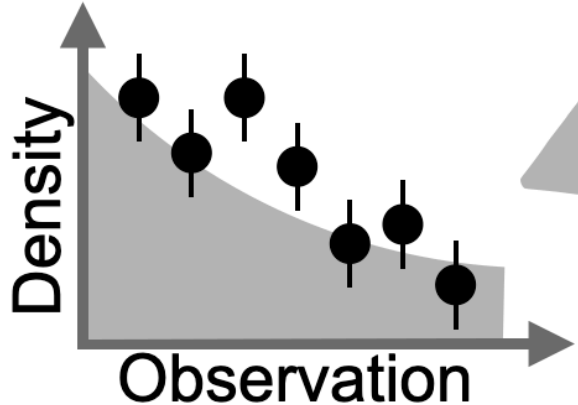
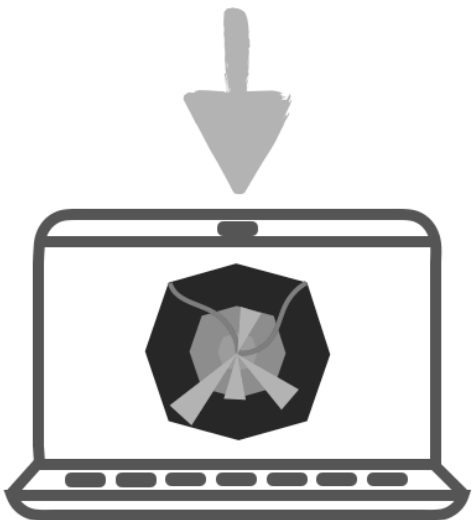
June 13, 2024



$\mathcal{L}$  Nature



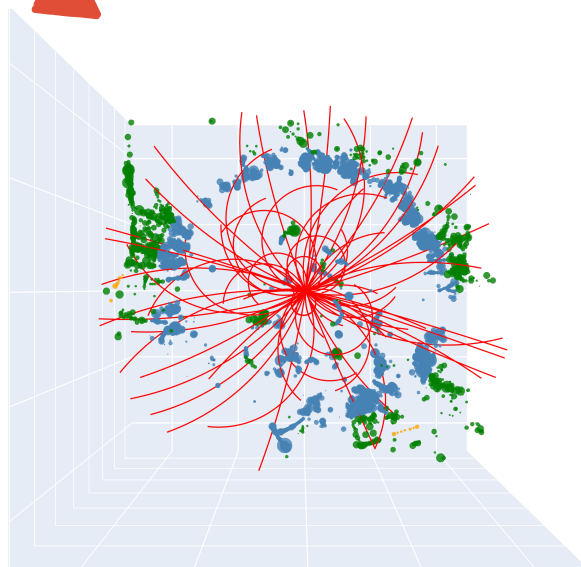
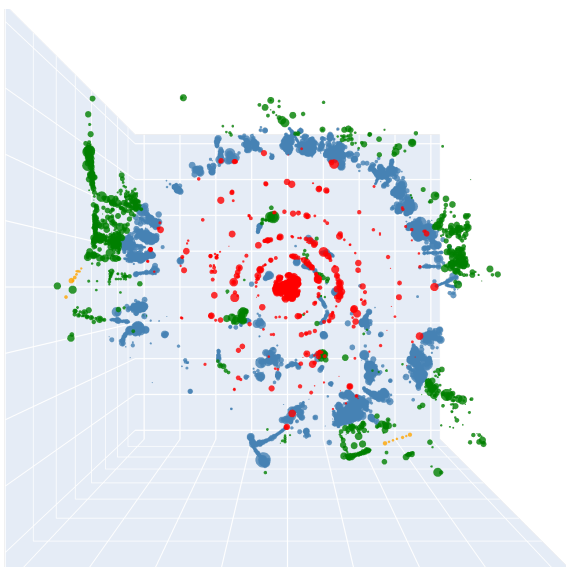
$\mathcal{L}$  Theory



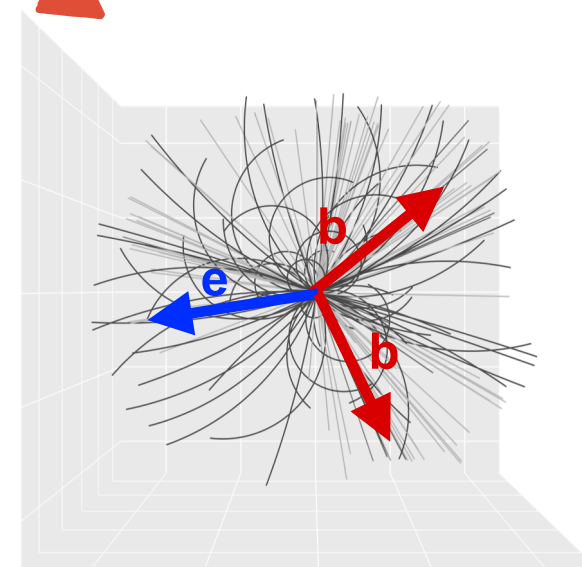
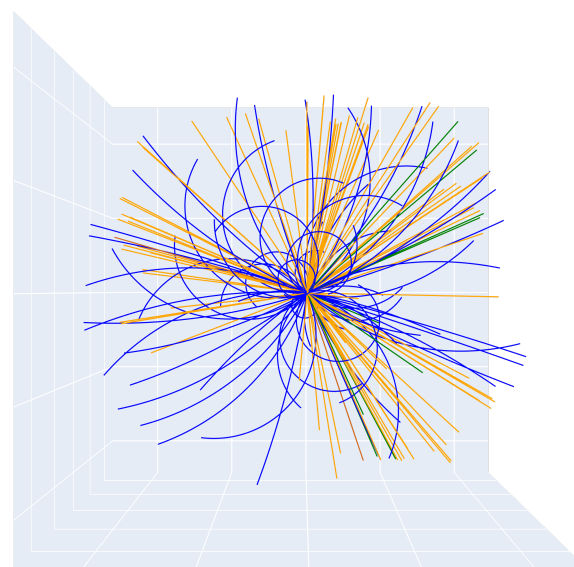
# Introduction - Experiment

[2]

1. Tracking



3. Tagging



2. Particle Flow



4. Calibration



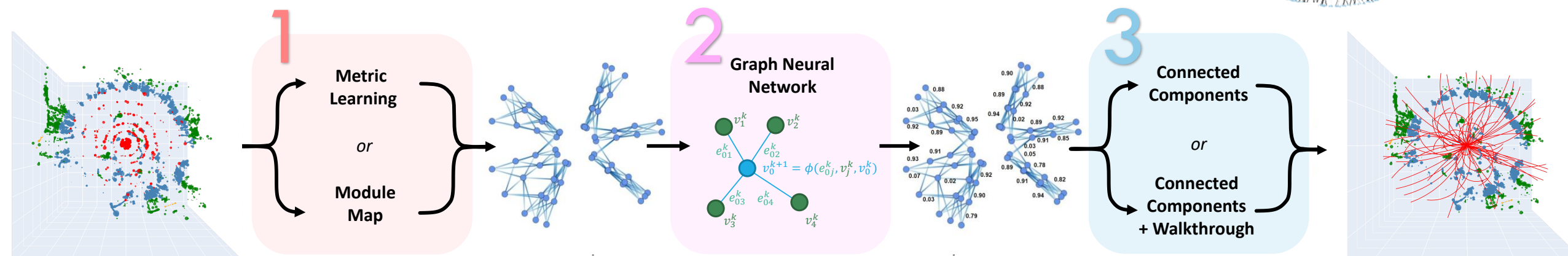
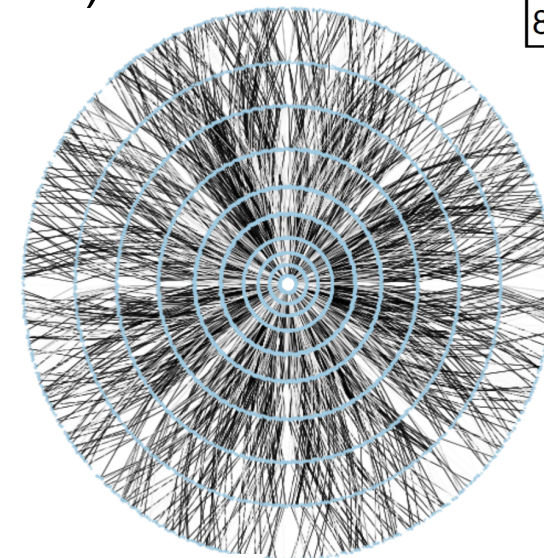


# Experiment - 1. Tracking

[3]

- Charged particles leave hits in tracker along their path (up to ~5000 per event)
- Turn tracker hits into tracks with graph-based ML
- Using ExaTrkX algorithm:
  1. Construct graph of hits
  2. Label graph edges
  3. Segment graph into tracks

8

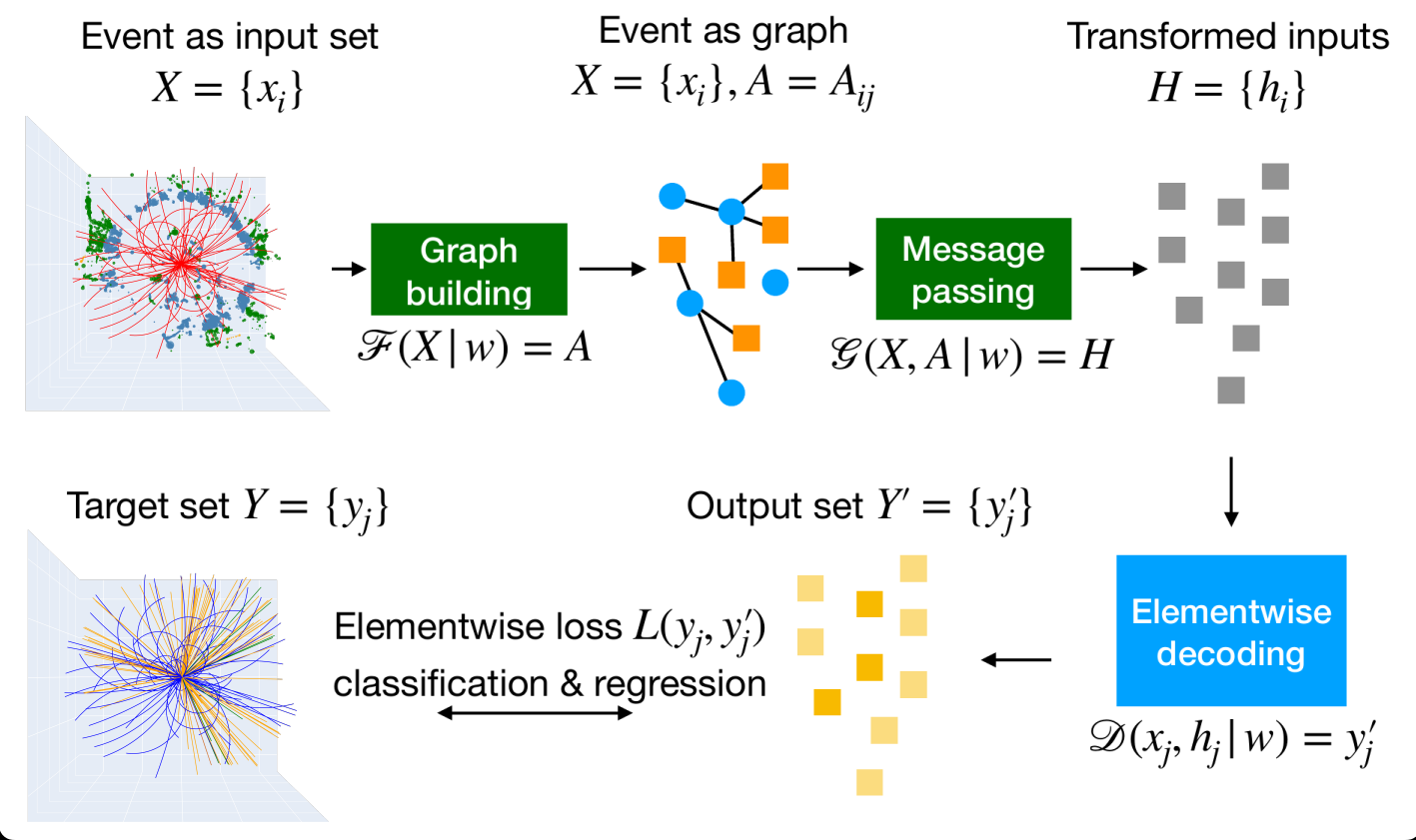


# Experiment - 2. Particle Flow

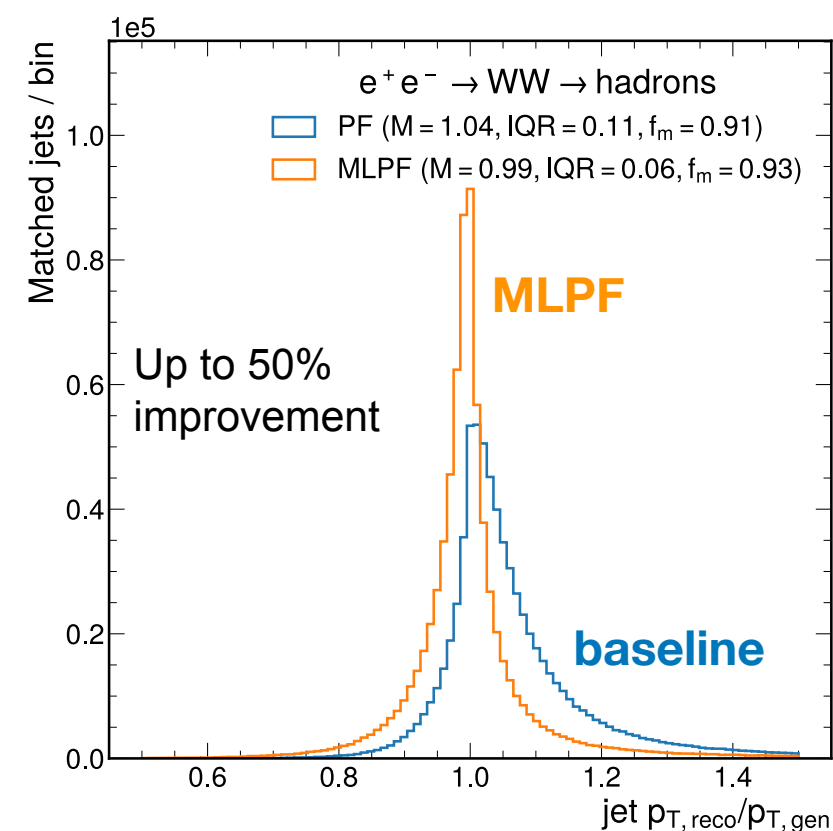
[2,4]

- Turn tracks and calorimeter clusters into particles
- Use granular detector layout optimally
- Different graph-based approaches ML approaches exist ([MLPF](#), [HGPflow](#), ...)

## MLPF Method



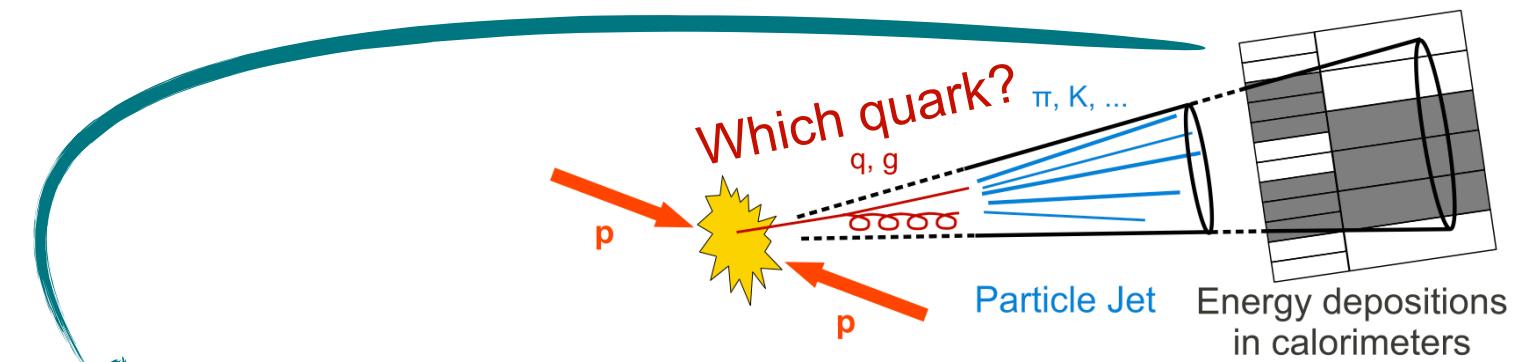
## MLPF Result



# Experiment - 3. Tagging

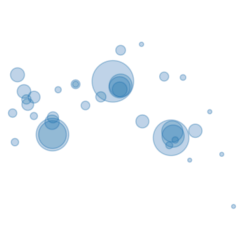
[5]

- Quarks from the hard interaction initiate jets in the detector
- Determine which type of quark initiated the jet (tagging)



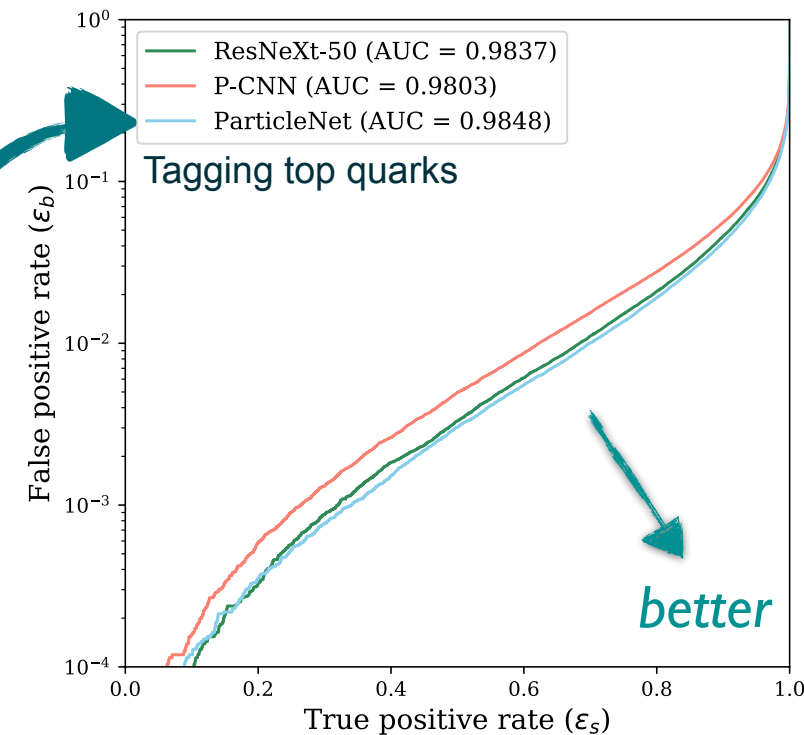
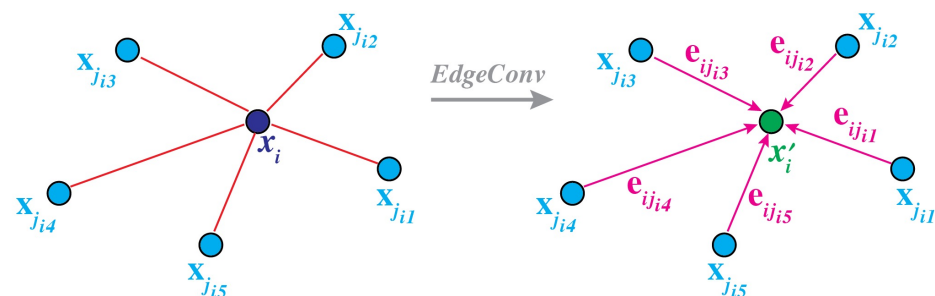
## Jet as Point Cloud

simulated top quark jet  
anti- $k_T$ ,  $R = 0.8$ ,  $p_T = 600$  GeV



Representation in  $(\eta, \phi)$  - plane

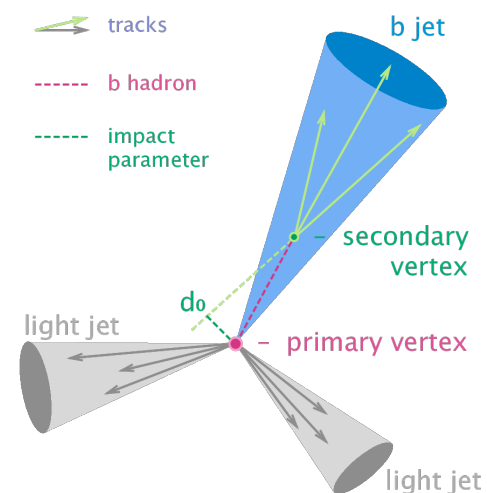
## ParticleNet



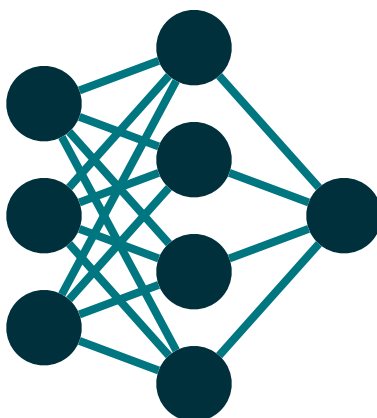
# Experiment - 4. Calibration

[6]

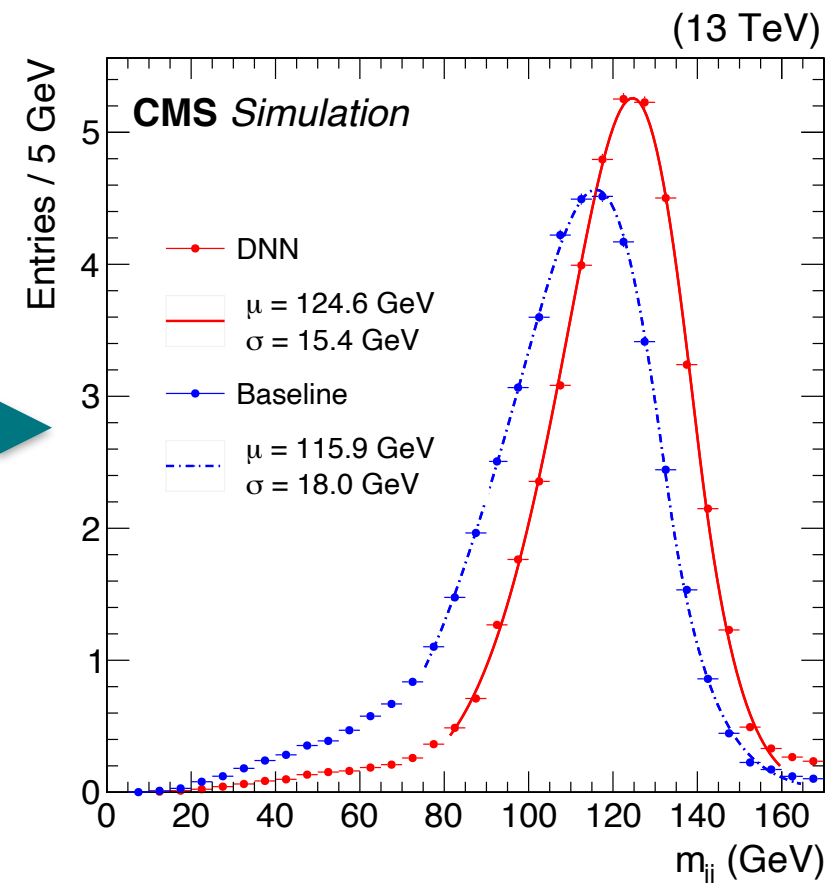
- Jets from b-quarks have large invisible (neutrino) contribution
- Calibrate the momentum of the jets with feed forward DNN regression
- Improved di-jet resolution by  $\sim 15\%$  compared to baseline

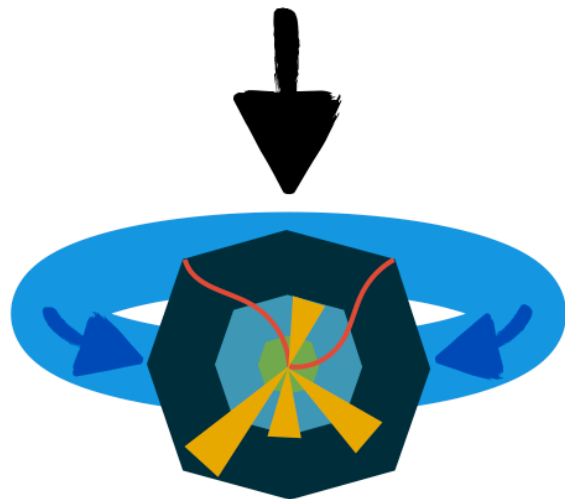


- Jet kinematics
- Jet composition
- PU info



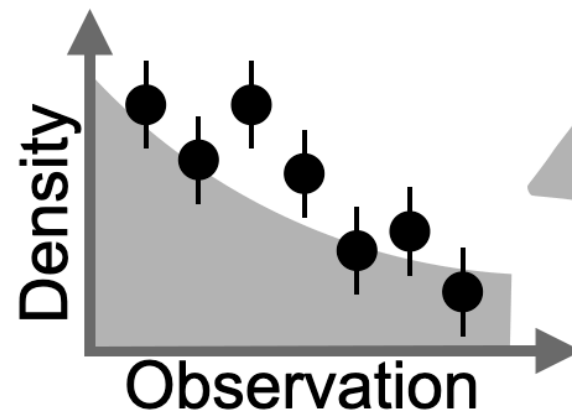
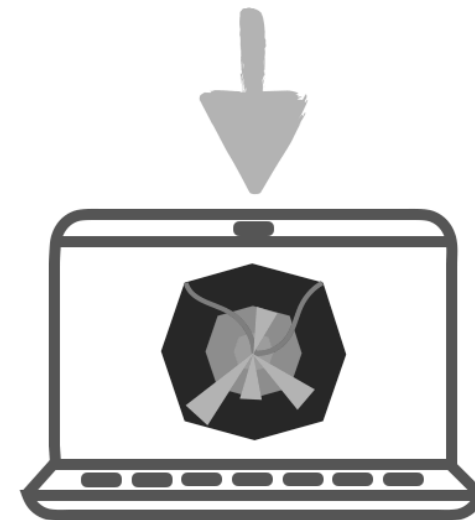
$$\frac{p_{T,true}}{p_{T,reco}}$$

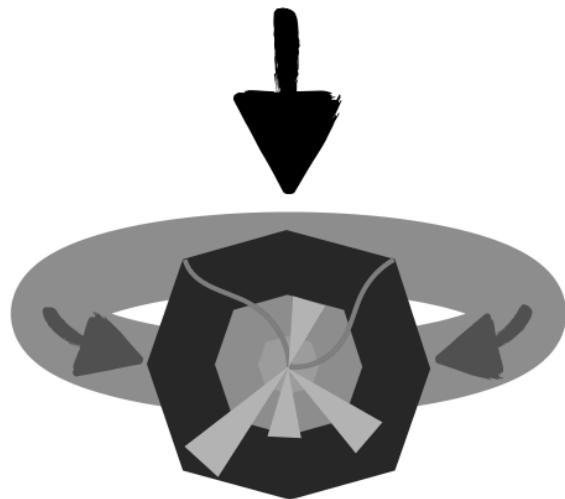
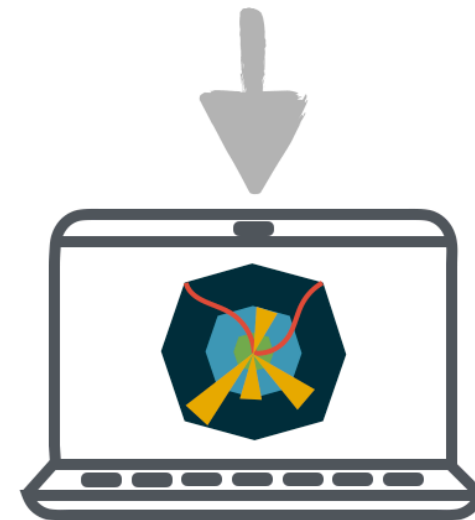


$\mathcal{L}$  Nature

Experiment:

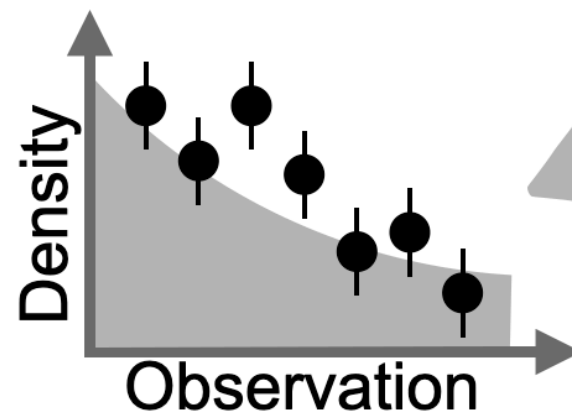
- Tracking
- MLPF
- Tagging
- Calibration

 $\mathcal{L}$  Theory

$\mathcal{L}$  Nature $\mathcal{L}$  Theory

Experiment:

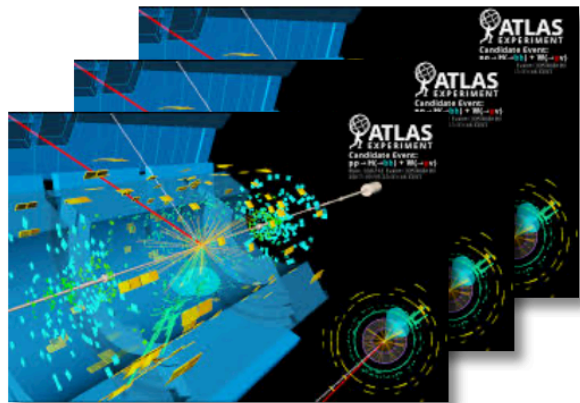
- Tracking
- MLPF
- Tagging
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# Simulation - Introduction

[1]

- Experiments spend significant computing budget on simulations
- Can make simulations much more efficient using ML
- **Simulations have different levels (full detector vs. particles), data types, complexities, ...**

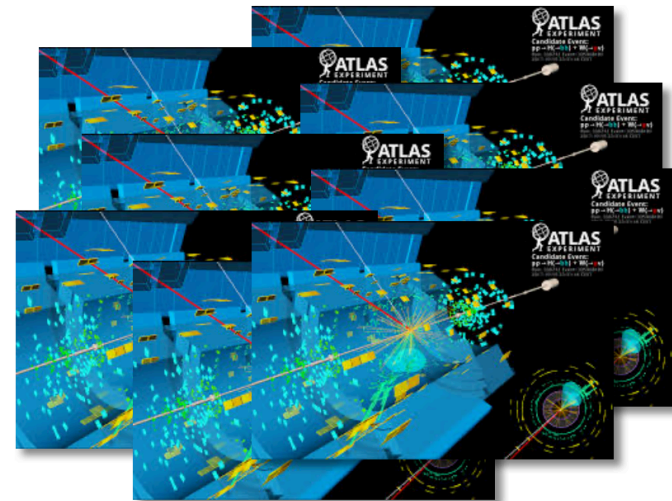


Simulation /  
Recorded Data



## Generative Model

- GANs
- Variational AEs
- Normalizing Flows
- Diffusion Models
- ...



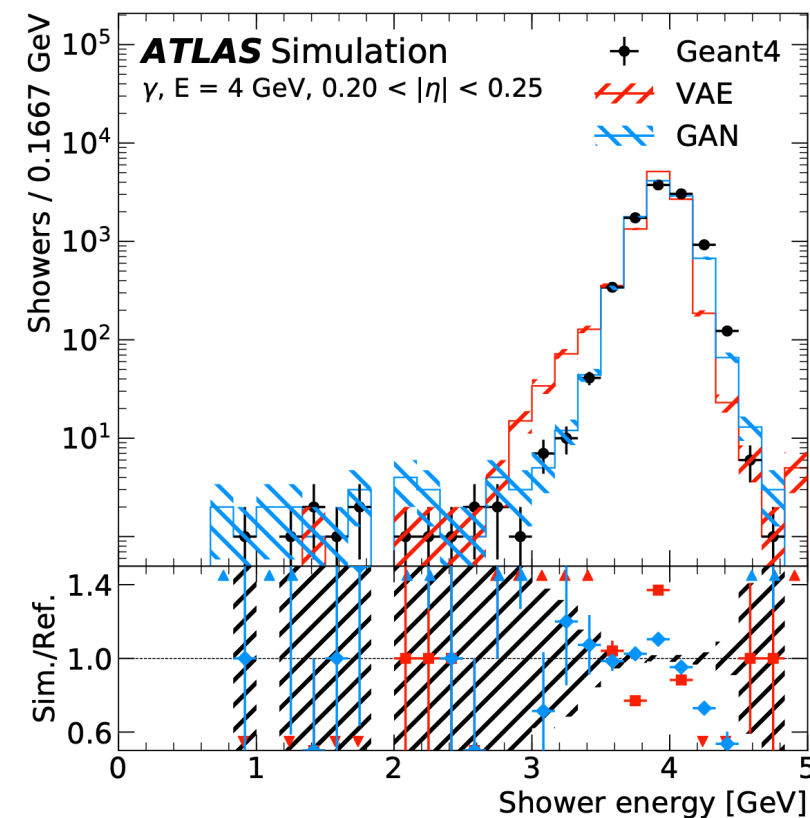
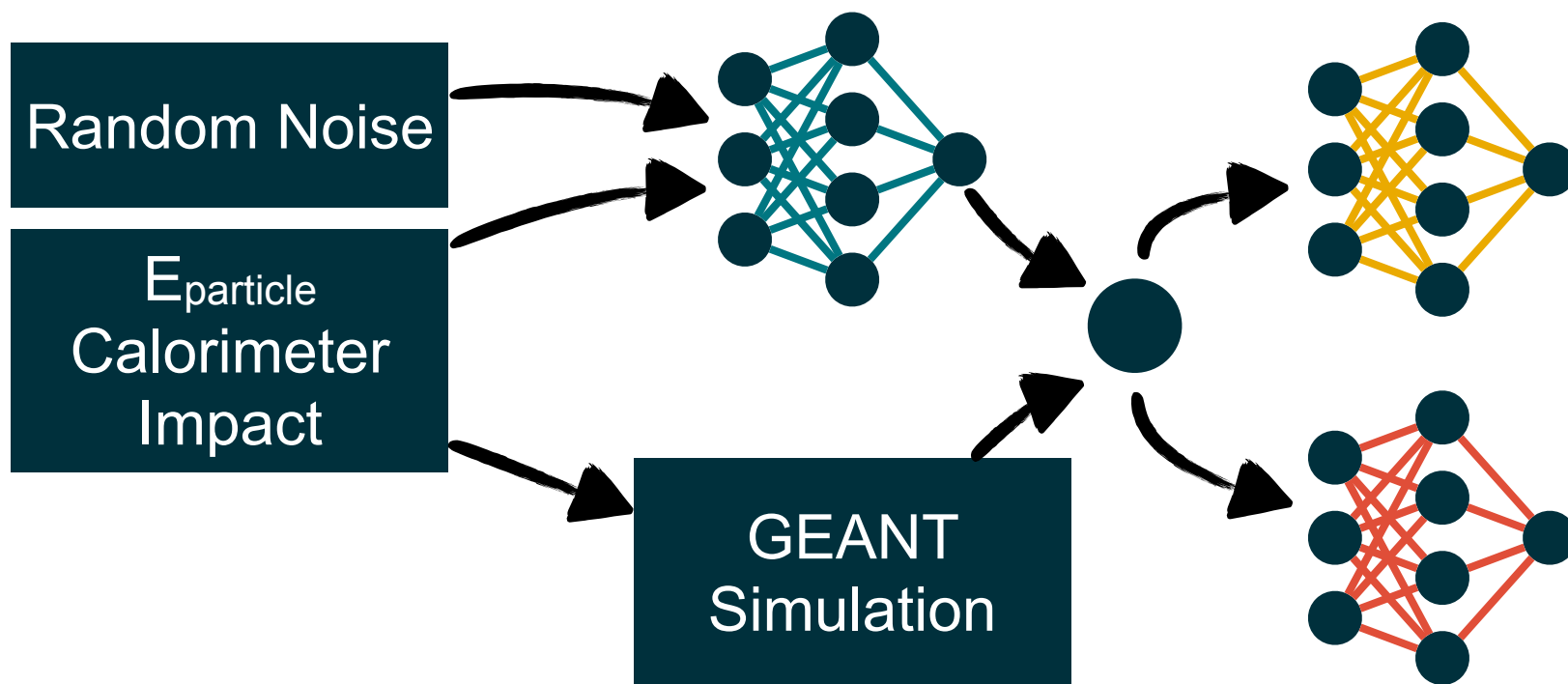
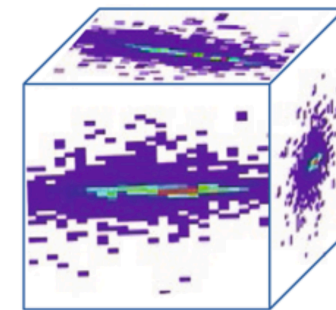
Oversampled



# Simulation - Detector Level (Showers)

[7]

- Simulate regular spatial shower profiles with ML
- Using generative adversarial networks (GANs)
- Parametrized by particle energy, calorimeter configuration, impact point
- Three networks: **Generator**, **Critic**, **Energy Critic**



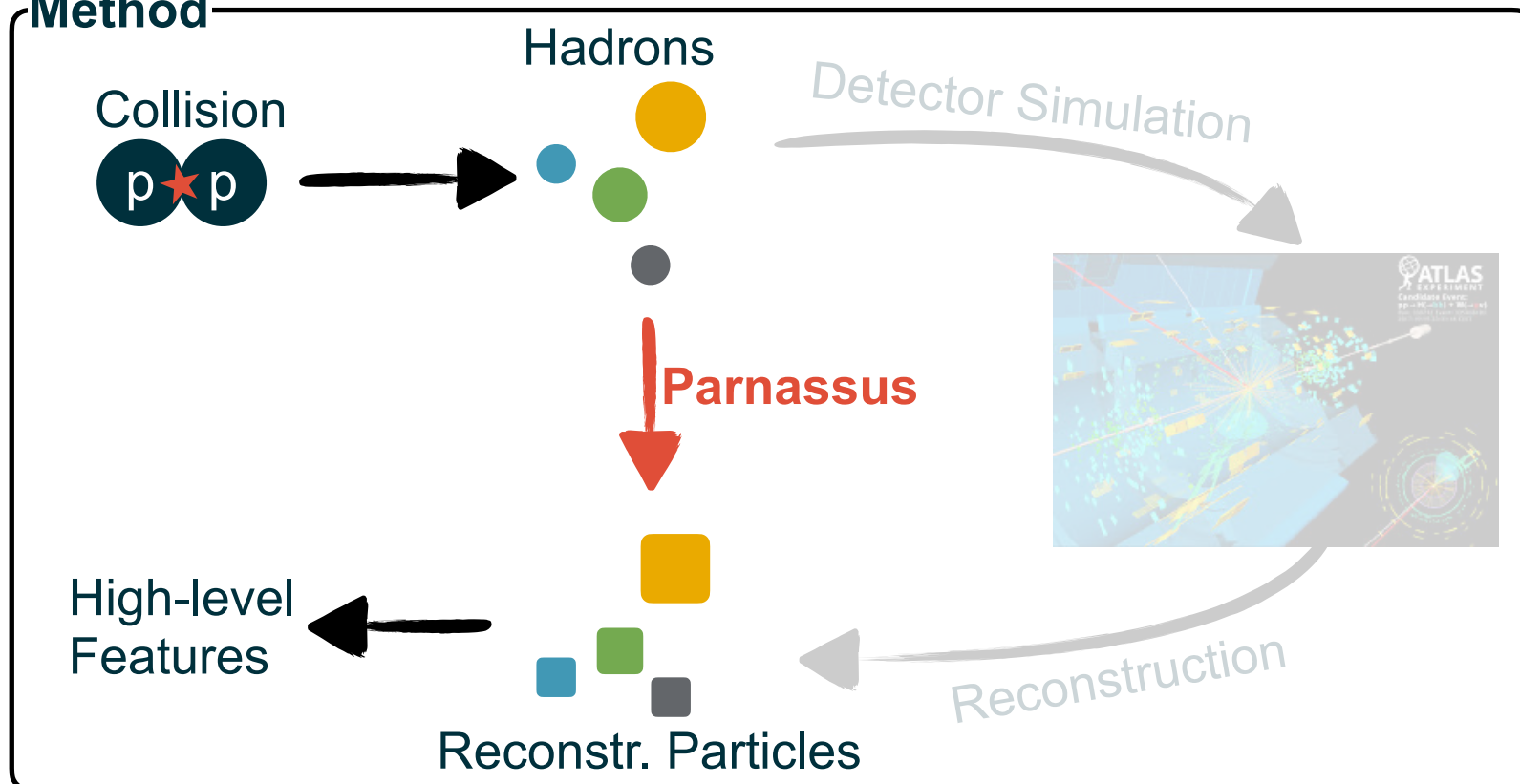


# Simulation - Particle Level

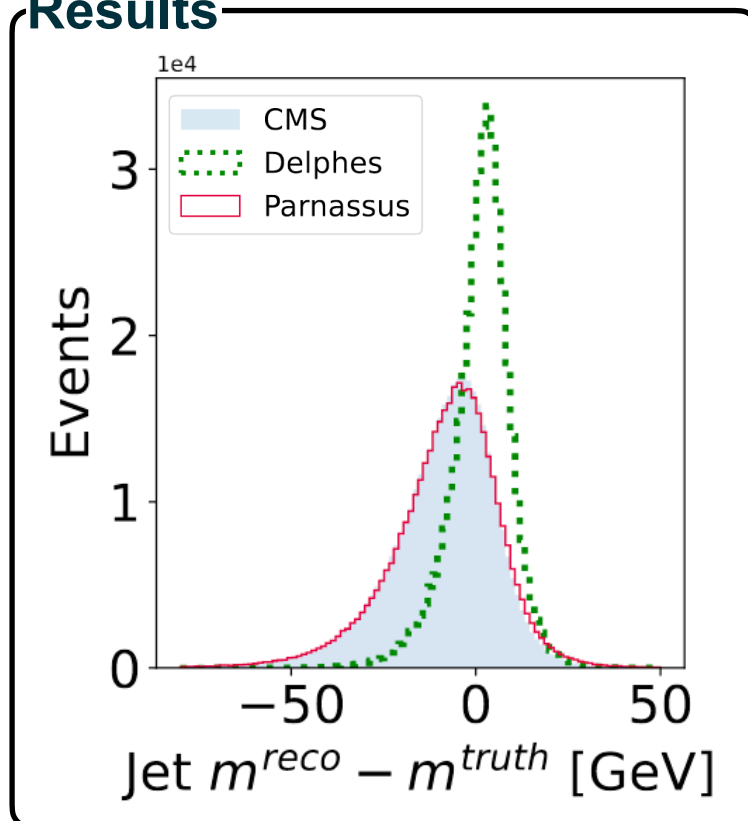
[8]

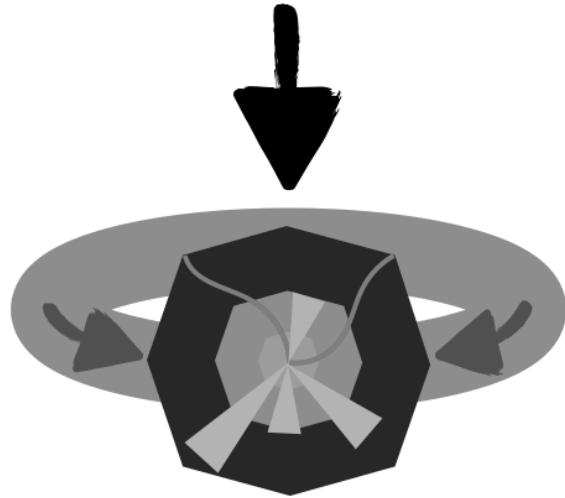
- Skip detector simulation and directly model reconstructed particles
- New ML method **Parnassus** [8]:
  - Normalizing Flow with Neural Ordinary Differential Equations
  - Transformer architecture (particle relations)

## Method



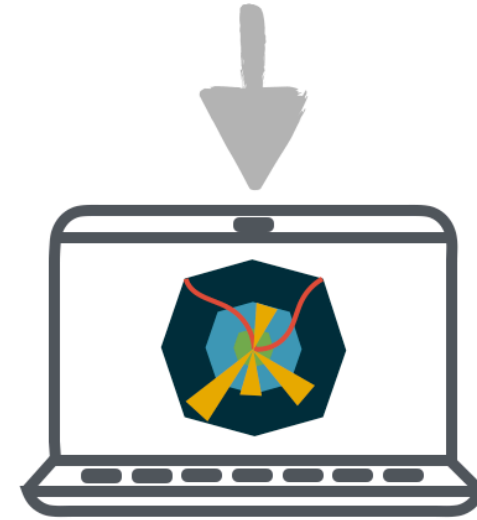
## Results



$\mathcal{L}$  Nature

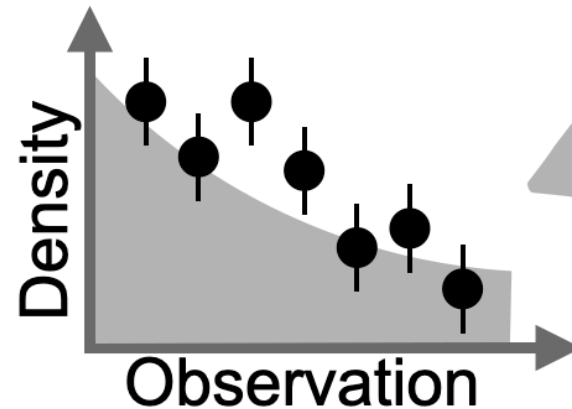
Experiment:

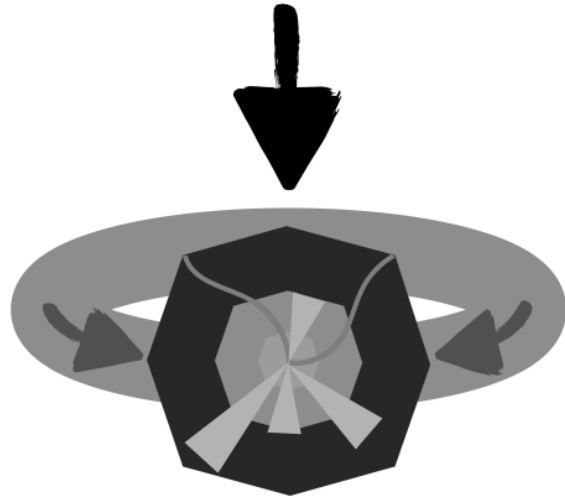
- Tracking
- MLPF
- Tagging
- Calibration

 $\mathcal{L}$  Theory

Simulation:

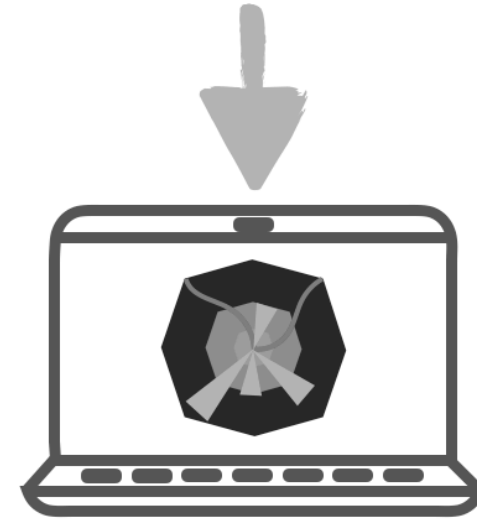
- Shower-level
- Particle-level



$\mathcal{L}$  Nature

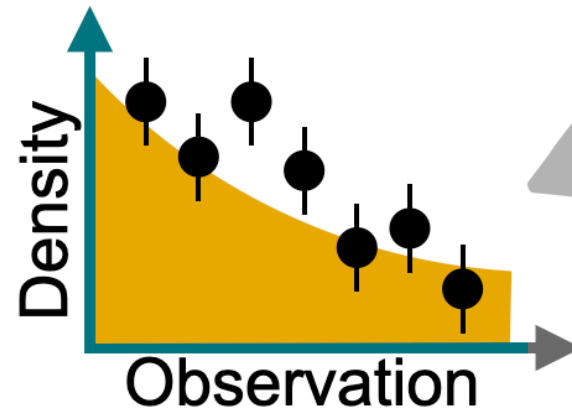
Experiment:

- Tracking
- MLPF
- Tagging
- Calibration

 $\mathcal{L}$  Theory

Simulation:

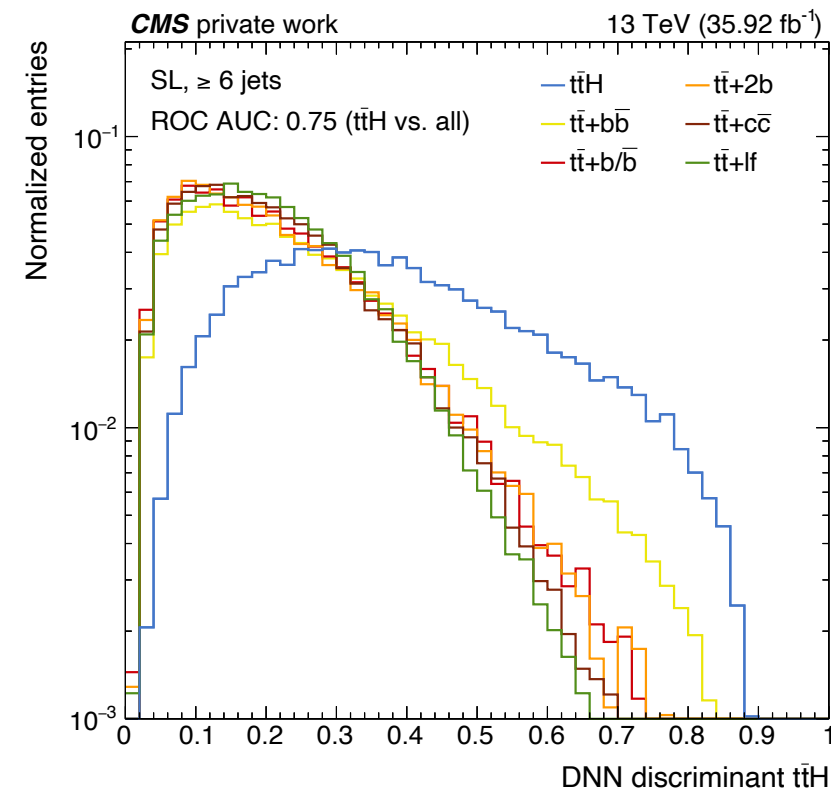
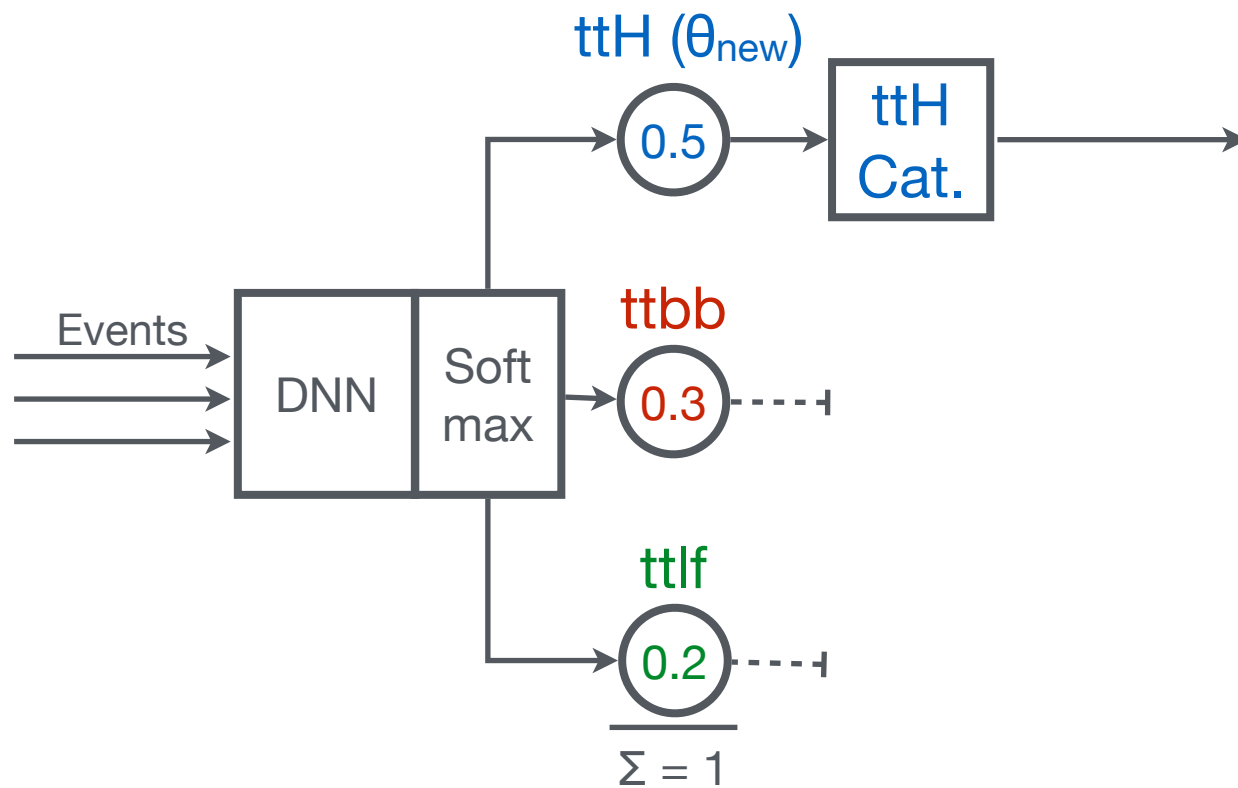
- Shower-level
- Particle-level



# Regular Analysis

[9]

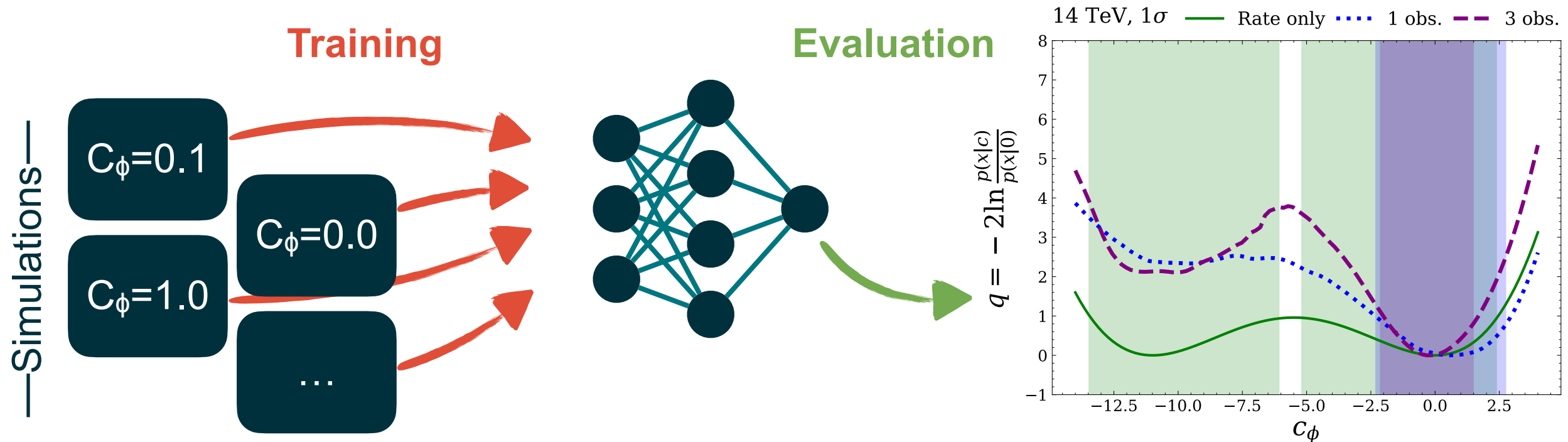
- Challenge: Decrease dimensionality of data ( $x$ ) but keep physics information
- Optimal feature is probability of a new model  $p(x|\theta_{\text{new}})$  vs  $p(x|\theta_{\text{old}})$
- Multi-class classification trained with categorical cross-entropy (e.g.  $t\bar{t}H$  measurement)



# Simulation-Based Inference (SBI)

[10,11]

- Techniques to directly infer  $p(\theta|x)$  without using summary statistics / histograms
- Train networks to directly model likelihood ratio:
  - Trained via simple classification (e.g.  $p(x|\theta_{\text{BSM}}) / p(x|\theta_{\text{SM}})$ )
  - DNN can use low or high-dimensional data  $x$



# Anomaly Detection (AD)

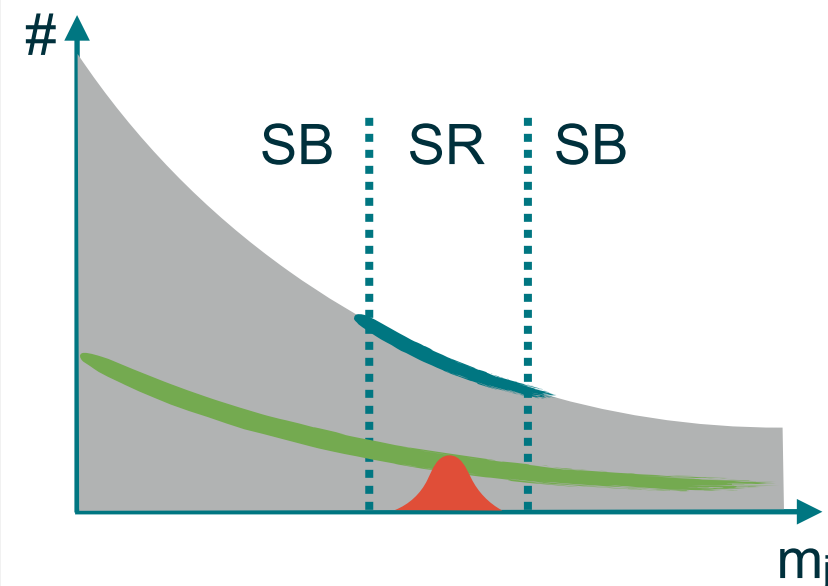
[12,13]

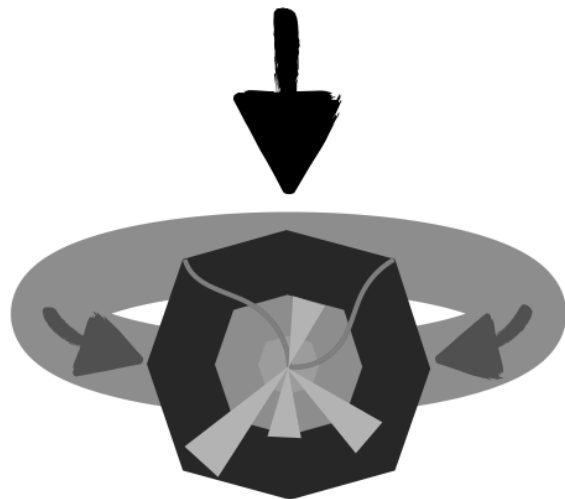
- Search for BSM in a model agnostic way
- Let machine figure out:
  - Interesting parts of phase space
  - How to look at them

2 Approaches	Assumption	Drawback
Unsupervised ML	Signal is rare	Not universal [14]
Weakly Supervised ML	Signal is peak	Need Bkg. Est.

## Weakly Supervised AD in a Nutshell:

1. Define SR/SB
2. ML Bkg. Estimate
3. ML Class. ■ vs. ■
4. Bump Hunt



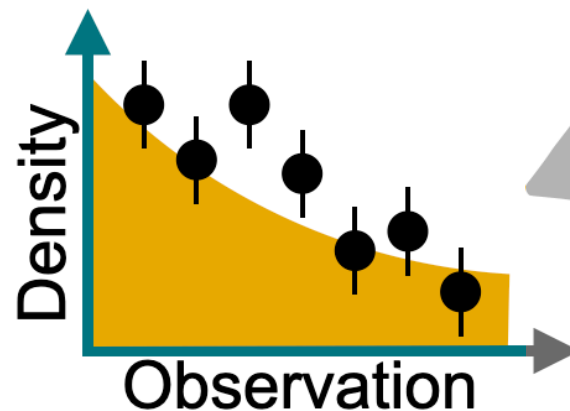
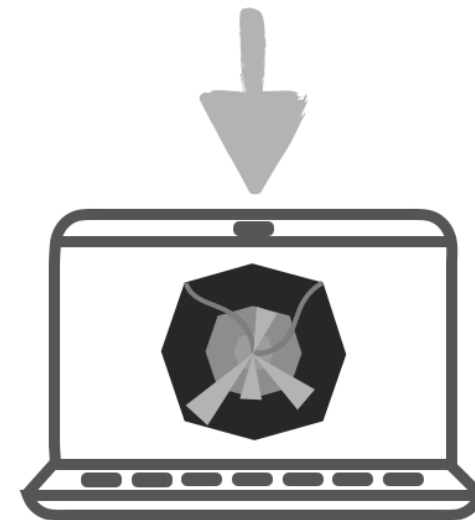
$\mathcal{L}_{\text{Nature}}$ 

Experiment:

- Tracking
- MLPF
- Tagging
- Calibration

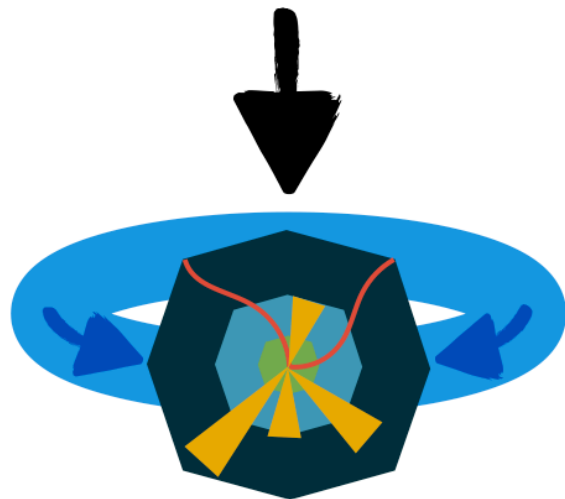
Comparison:

- Classification
- SBI
- AD

 $\mathcal{L}_{\text{Theory}}$ 

Simulation:

- Shower-level
- Particle-level

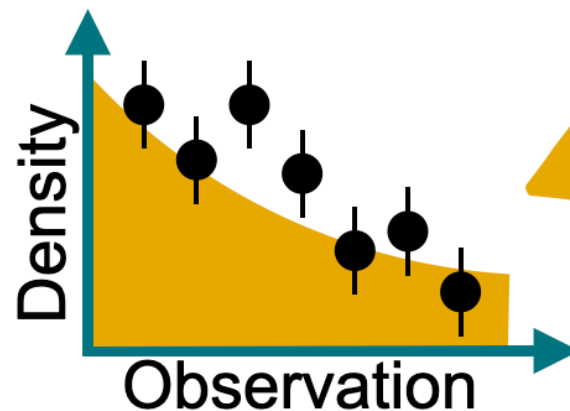
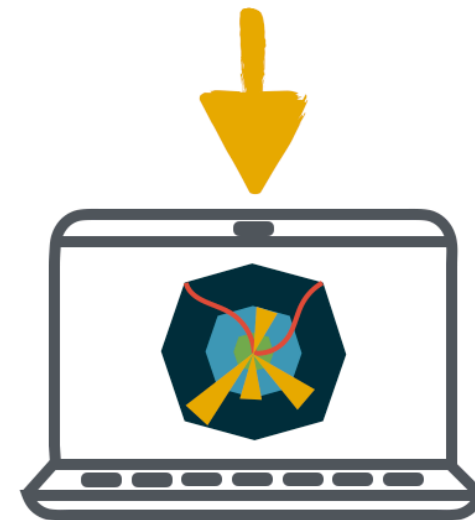
$\mathcal{L}_{\text{Nature}}$ 

Experiment:

- Tracking
- MLPF
- Tagging
- Calibration

Comparison:

- Classification
- SBI
- AD

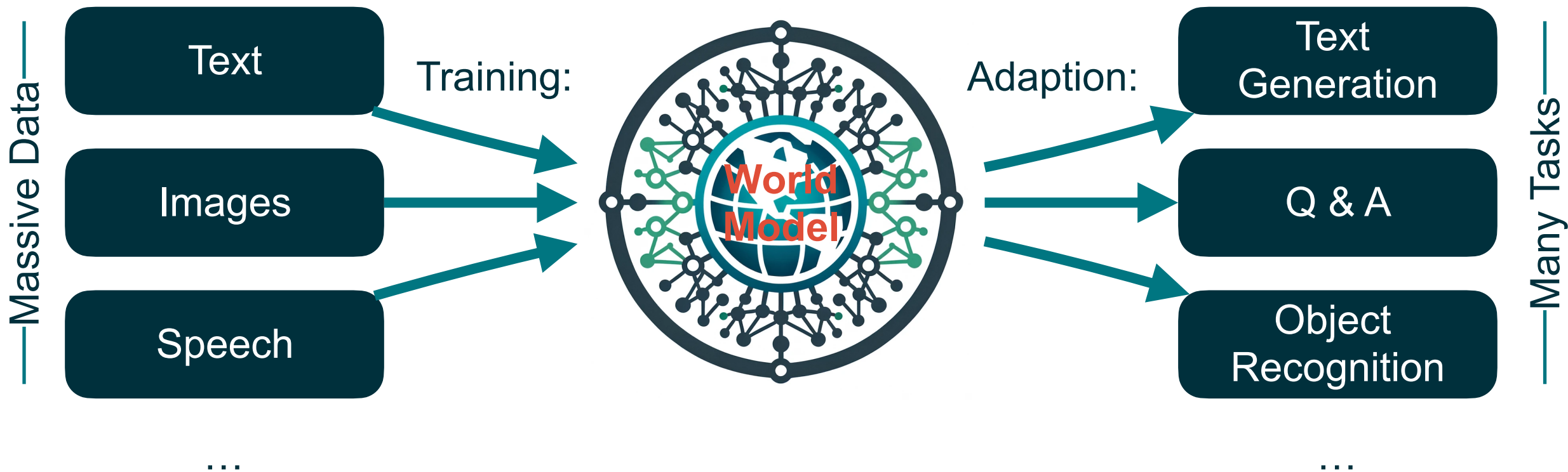
 $\mathcal{L}_{\text{Theory}}$ 

Simulation:

- Shower-level
- Particle-level



# Foundation Models (Motivation)

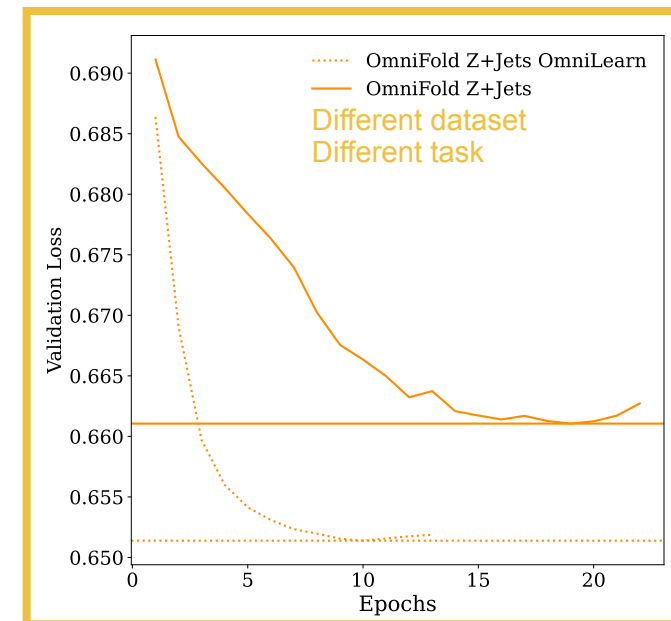
**[15]**

# Foundation Models (Physics - OmniLearn)

[16]



- OmniLearn:
  - Train foundation model for many jet-related tasks
  - Transformer model with Graph-attention networks
- Learns general World (Jet) Model
- Adaption better and more cost-efficient than training from scratch



$\mathcal{L}_{\text{Nature}}$

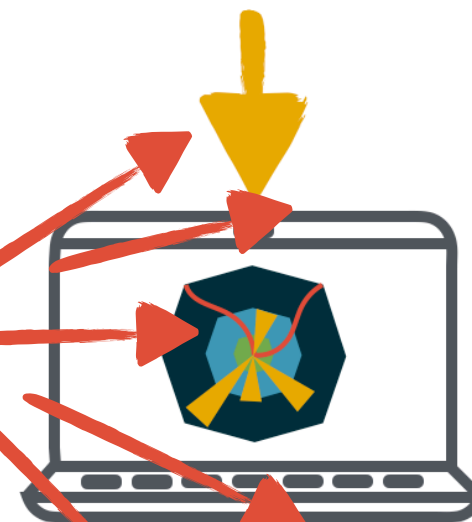
$\mathcal{L}_{\text{Theory}}$

Experiment:

- Tracking
- MLPF
- Tagging
- Calibration



ML

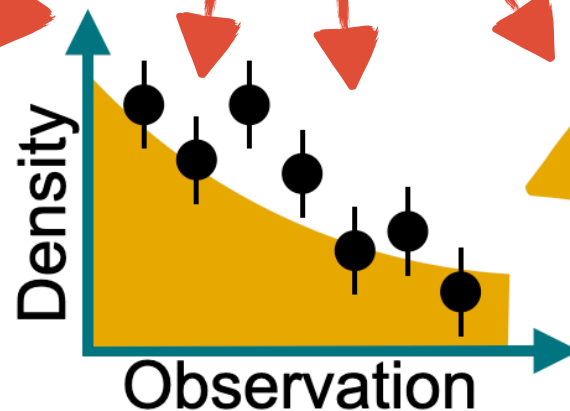


Simulation:

- Shower-level
- Particle-level

Comparison:

- Classification
- SBI
- AD



Foundation Models

# Contact

- First year postdoc at Berkeley Lab
- Since >7 years working in data analysis for CERN experiments
  
- **Physics:** Higgs, Anomaly Detection
- **Deep Learning:** Supervised, Unsupervised, Reinforcement
- **Computing:** Fast O(TB) Data Processing & Computing Pipelines



# Citations

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4. Di Bello et al., Reconstructing particles in jets using set transformer and hypergraph prediction networks, *Eur.Phys.J.C* 83 (2023) 7, 596
5. Qu, H., & Gouskos, L. (2020). Jet tagging via particle clouds. *Physical Review D*, 101(5), 056019. DOI: 10.48550/arXiv.1902.08570
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15. Rick Merrit (NVIDIA), What Are Foundation Models? <https://blogs.nvidia.com/blog/what-are-foundation-models/>
16. Vinicius Mikuni, Benjamin Nachman, OmniLearn: A Method to Simultaneously Facilitate All Jet Physics Tasks, <https://arxiv.org/abs/2404.16091>