

ML in Particle Physics

Prof. Gregor Kasieczka
Email: gregor.kasieczka@uni-hamburg.de
Twitter/X: [@GregorKasieczka](https://twitter.com/GregorKasieczka)
PHYSTAT — Statistics meets ML, Imperial
10.9.2024

CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE

U+H

Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG


KISS
CDCS
CENTER FOR DATA AND COMPUTING
IN NATURAL SCIENCES


FSP
CMS


PUNCH
4NFDI

DASHH


PIER
Partnership of
Universität Hamburg and DESY

GEFÖRDERT VOM


Bundesministerium
für Bildung
und Forschung

**Emmy
Noether-
Programm**
Deutsche
Forschungsgemeinschaft
DFG

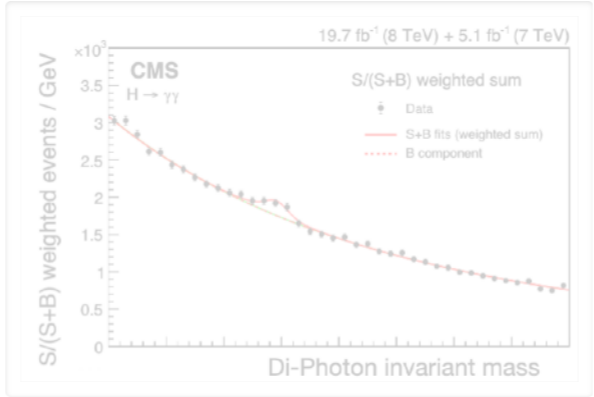
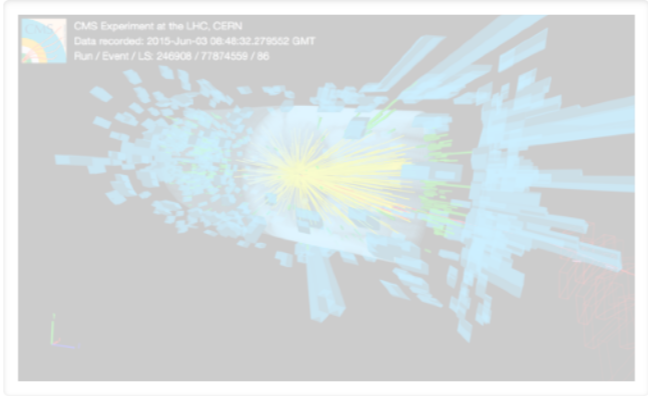
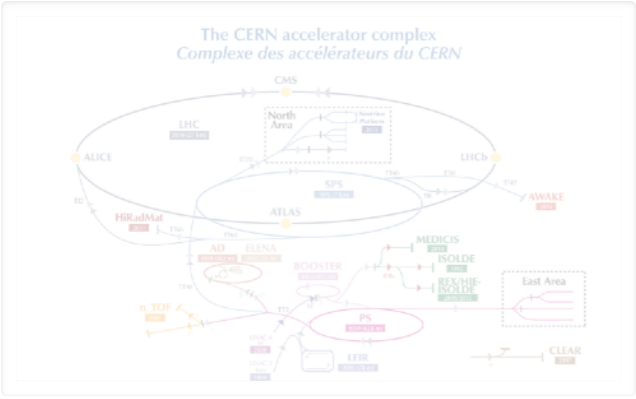

To consult the statistician after an experiment is finished is often merely to ask him to conduct a post mortem examination. He can perhaps say what the experiment died of.



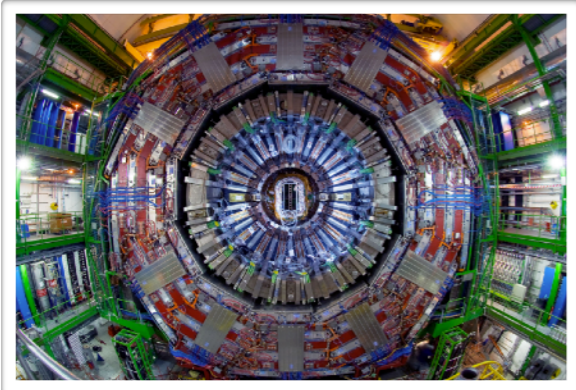
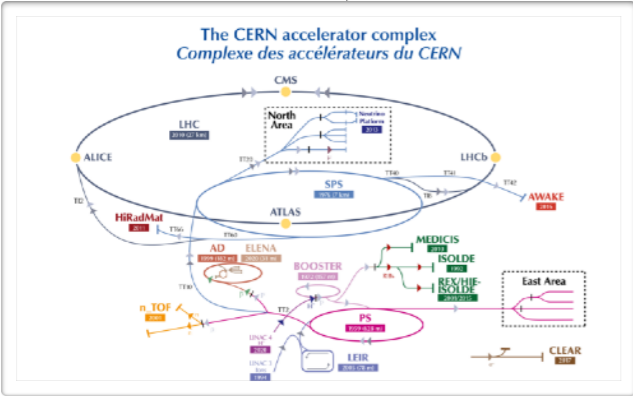
Ronald Fisher

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

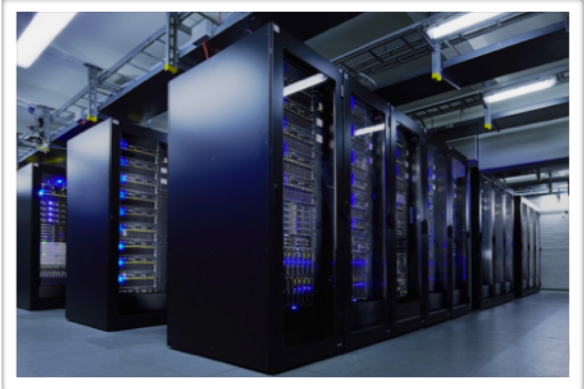
First principle, quantum theoretical model



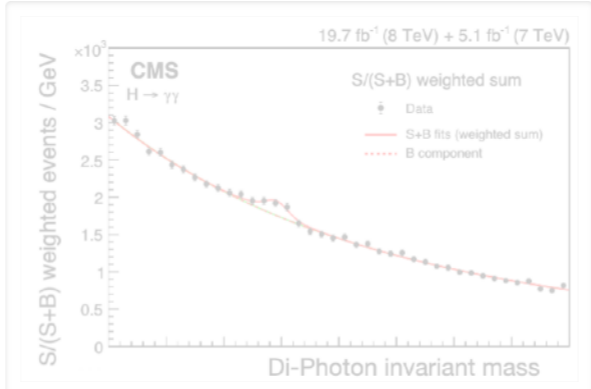
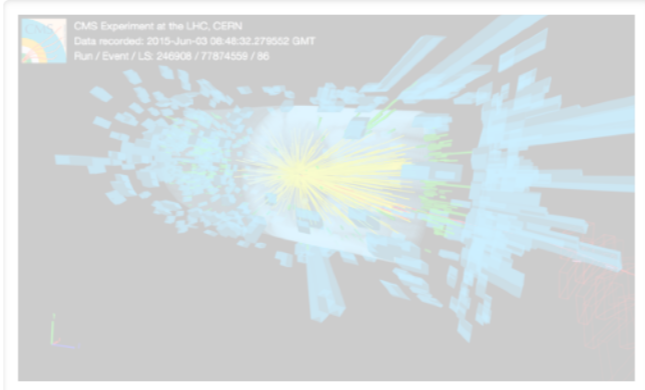
$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$



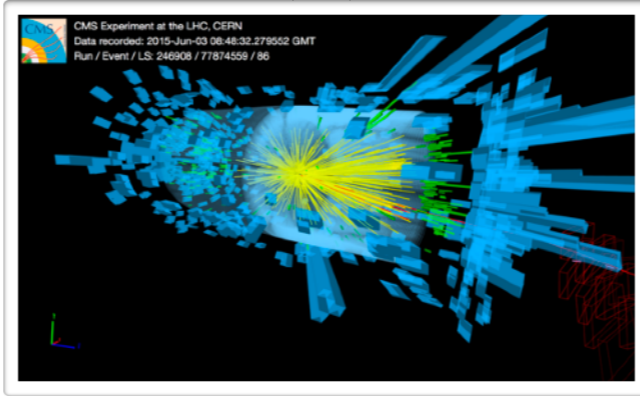
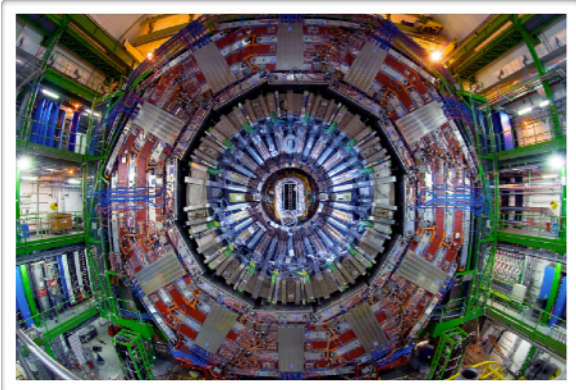
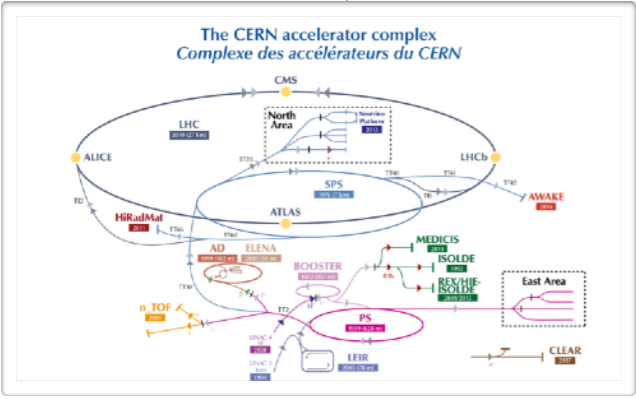
Colliders with 40 million events/second, detectors with 100 million read-outs,



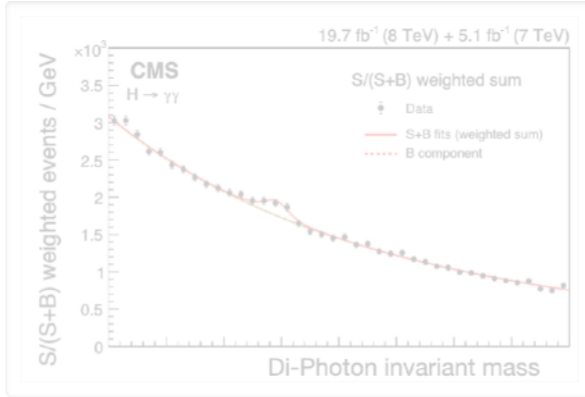
and massive theory-driven simulation codes



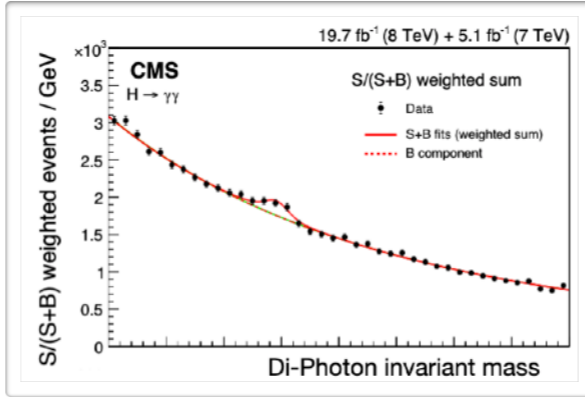
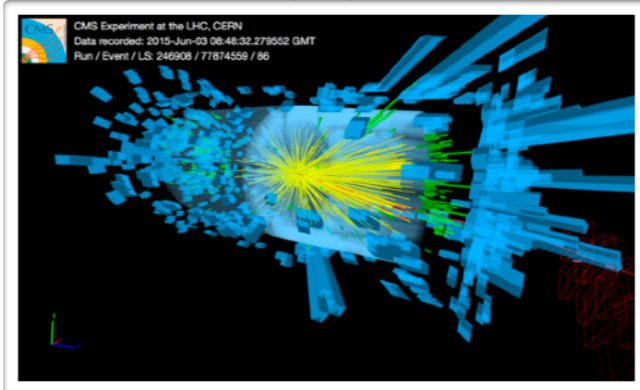
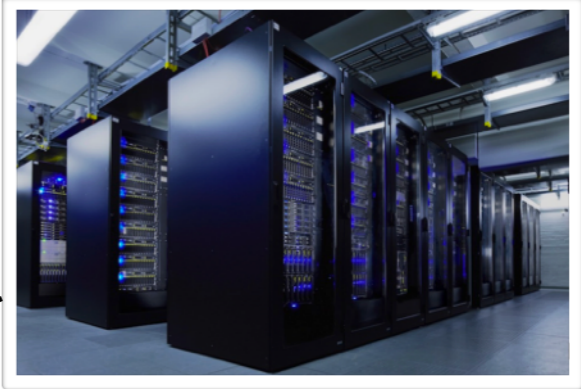
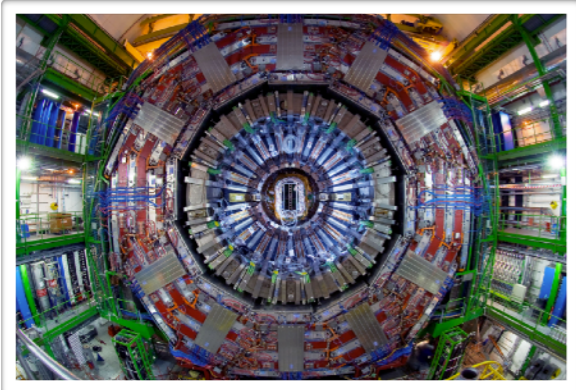
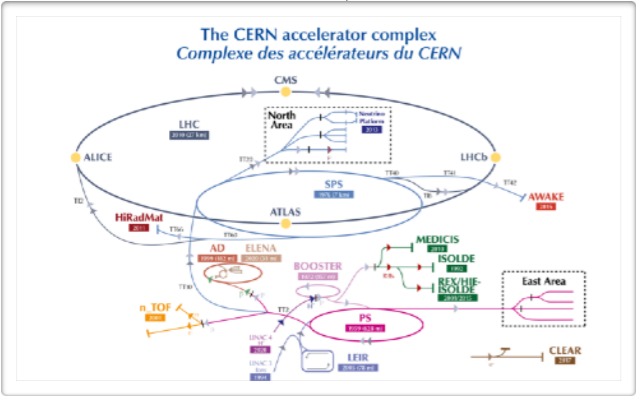
$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$



Complex reconstruction chain to turn low-level read-outs into high-level physics objects

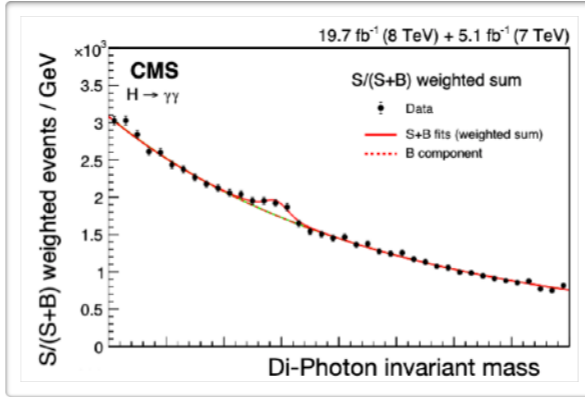
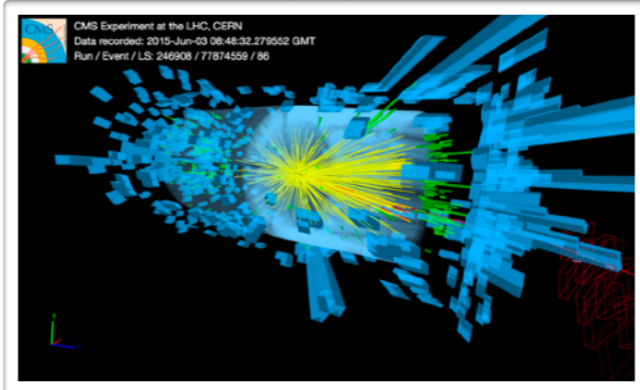
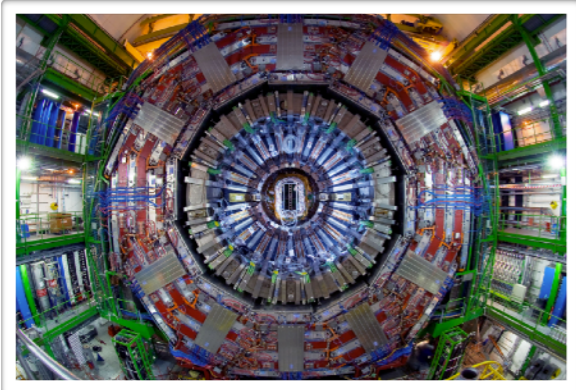
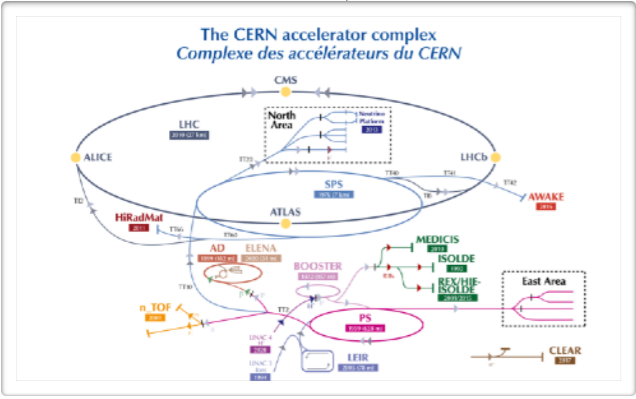


$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

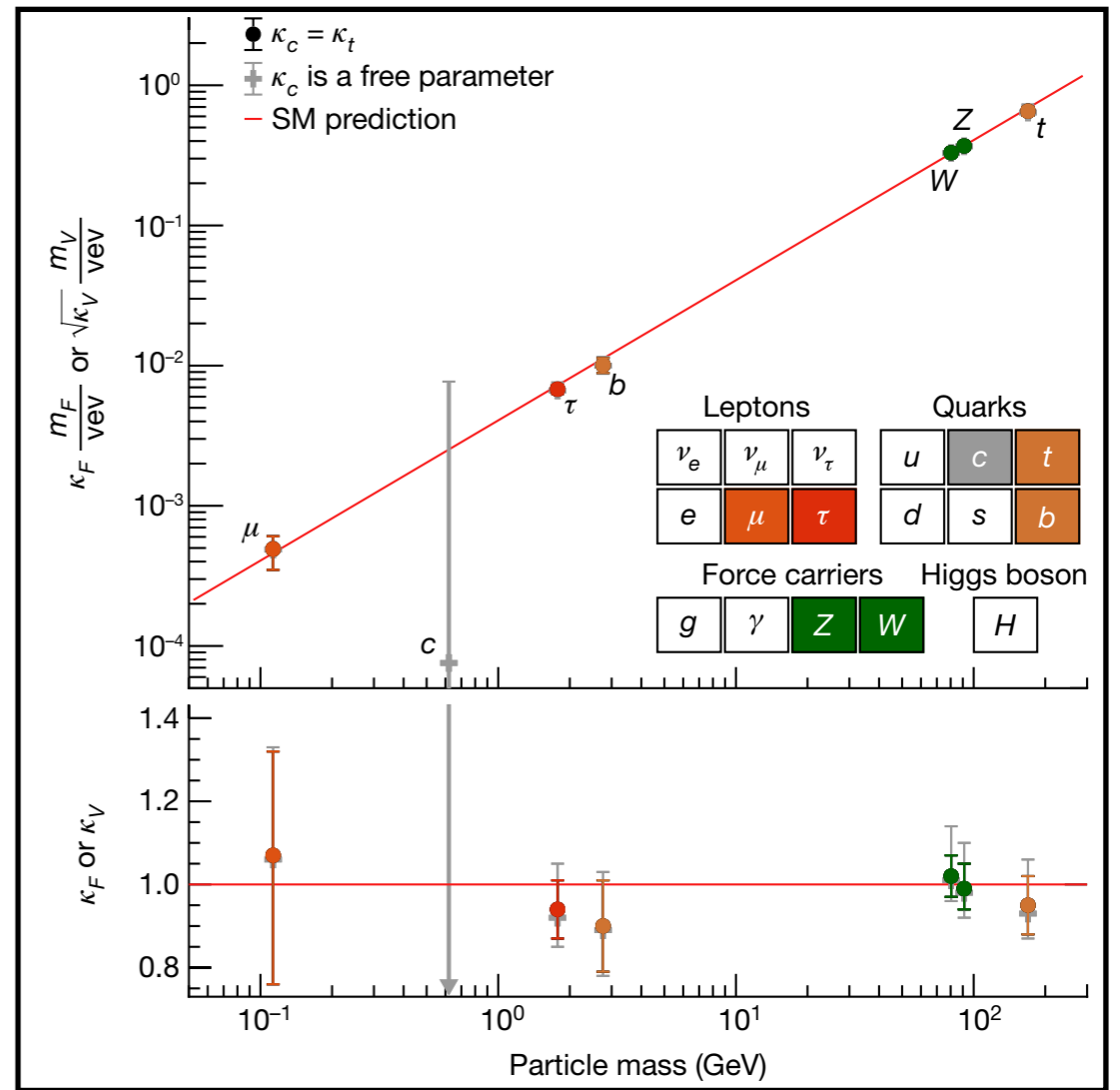
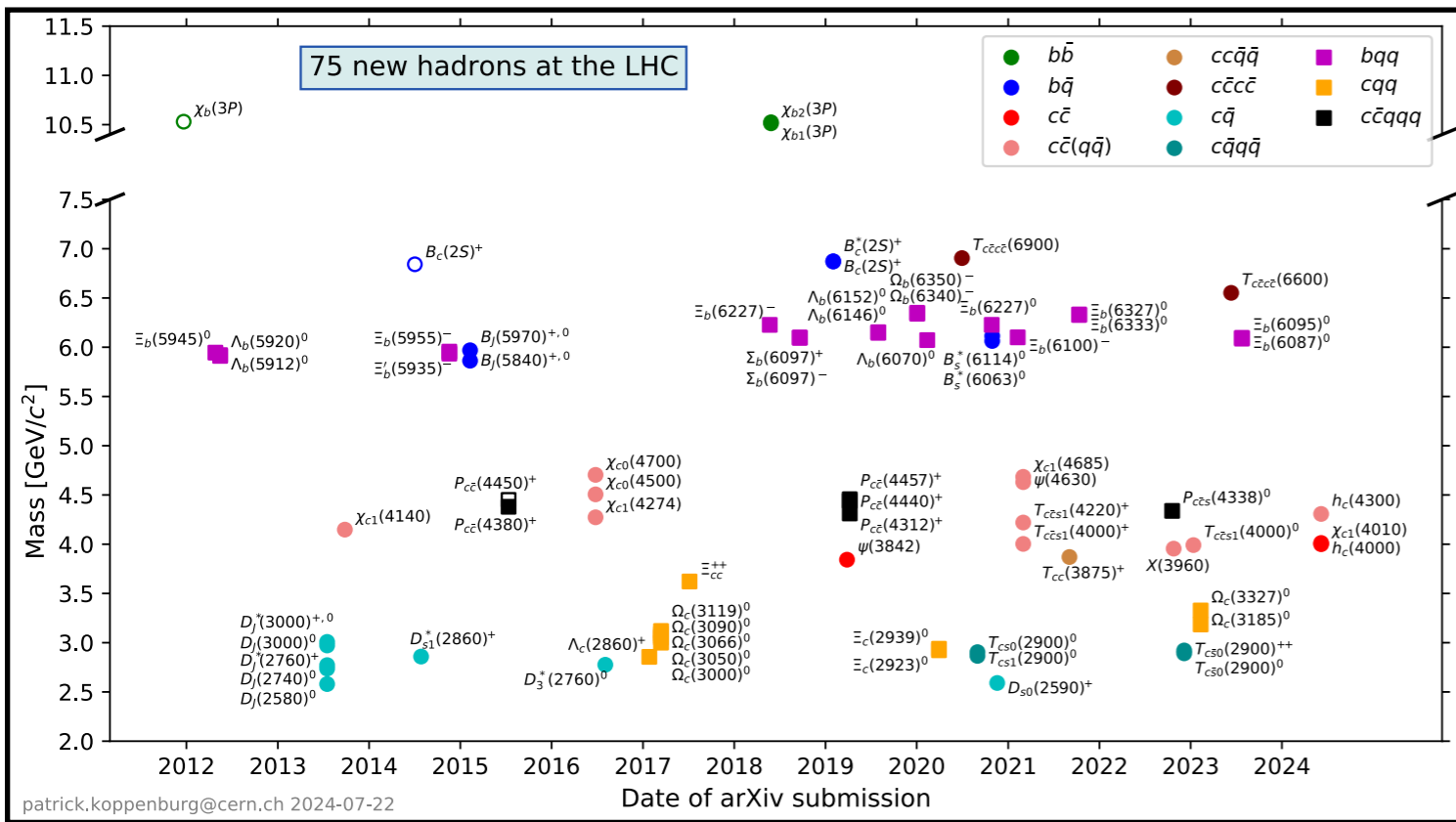


Aggregate events, define phase space regions of interest & relevant summary statistics followed by sophisticated final statistical analysis

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

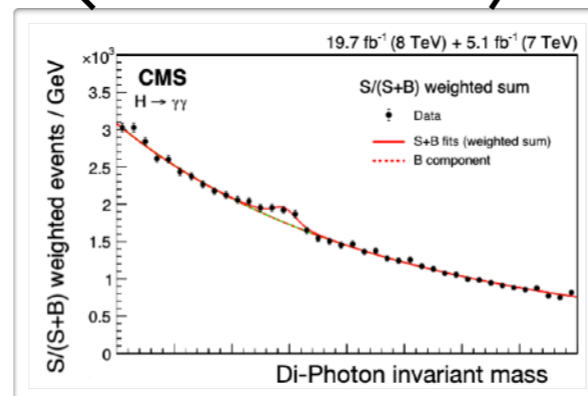


Sophisticated final statistical analysis



Discover new particles

Measure fundamental properties of nature



Sophisticated final statistical analysis

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

AI

Inference

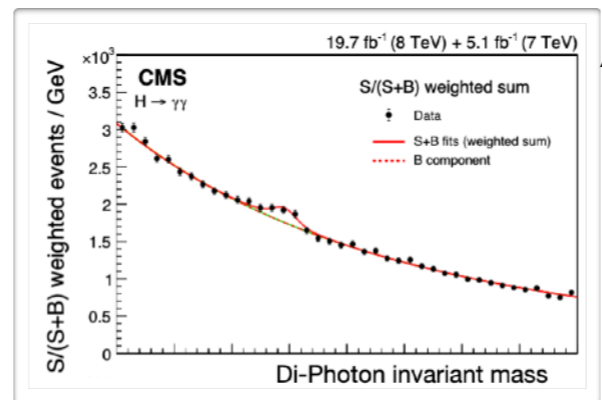
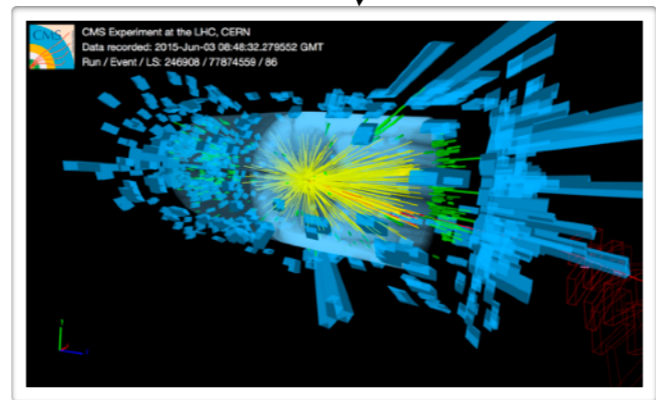
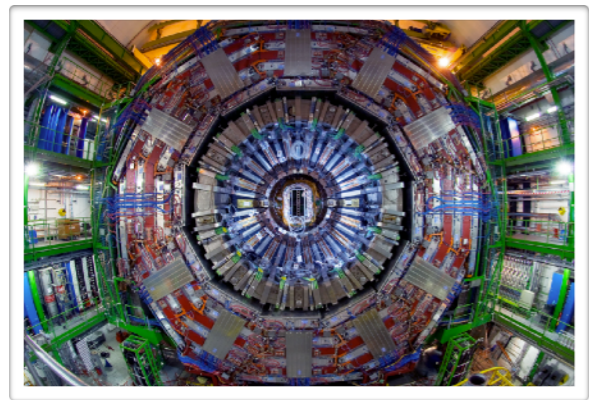
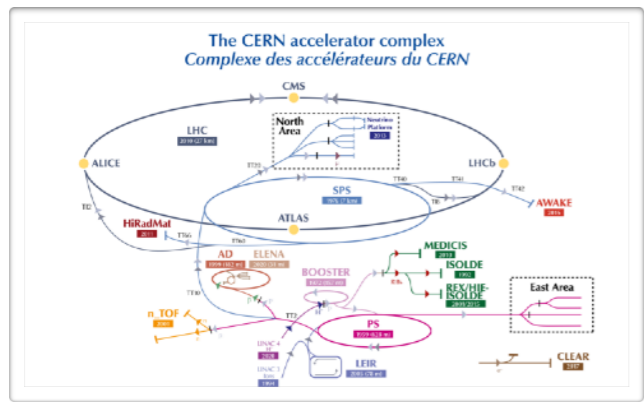
Experiment Design

Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection



AI/ML models are studied for **all aspects** of experimental particle physics

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

AI

Inference

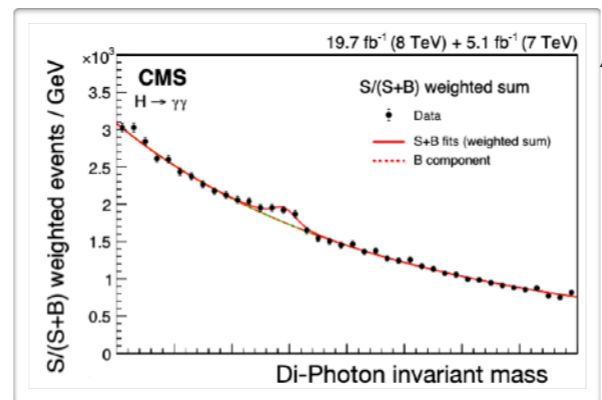
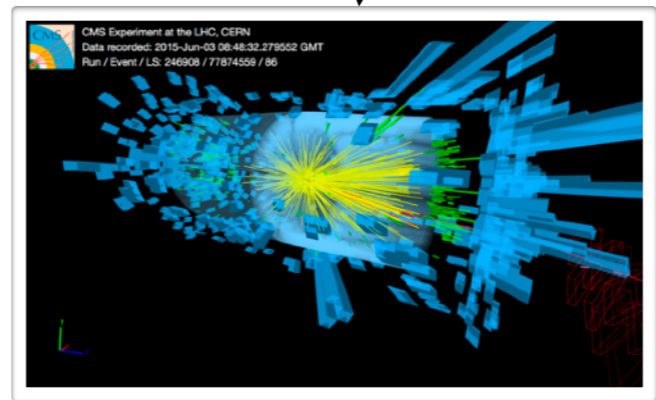
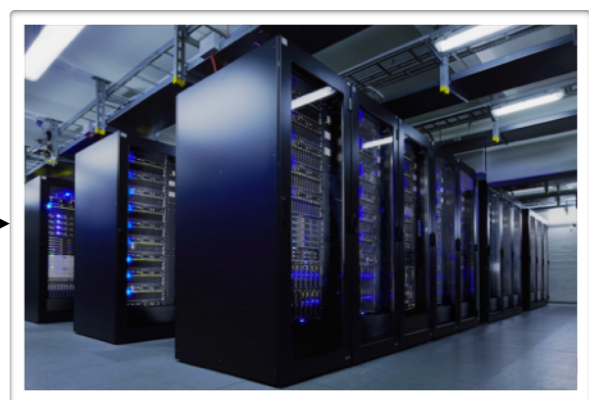
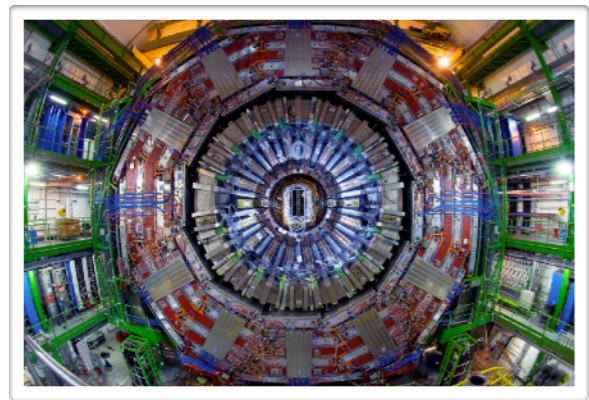
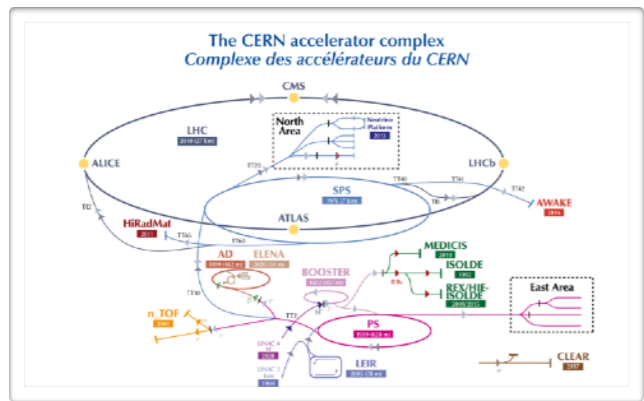
Experiment Design

Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection



AI/ML models are studied for **all aspects** of experimental particle physics

and **interesting statistical problems** lurk everywhere

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

Inference

Experiment Design

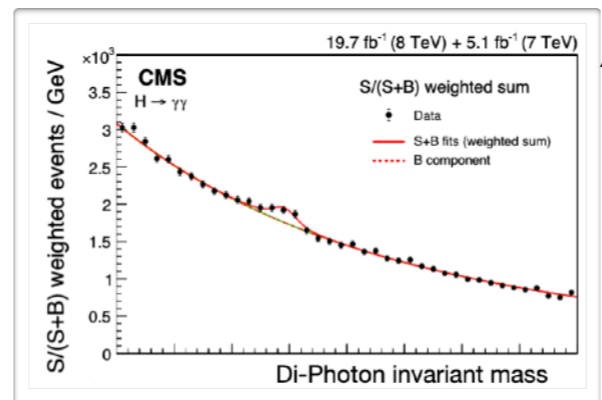
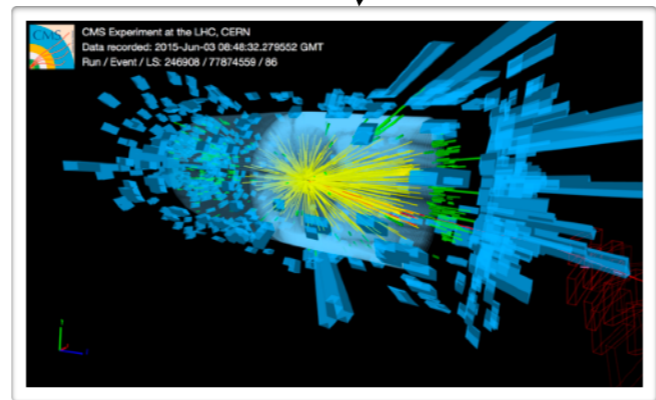
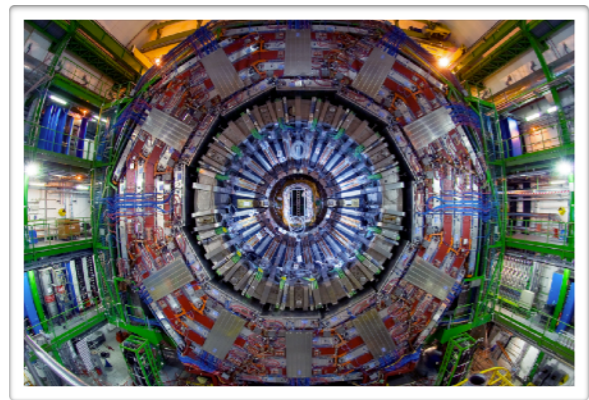
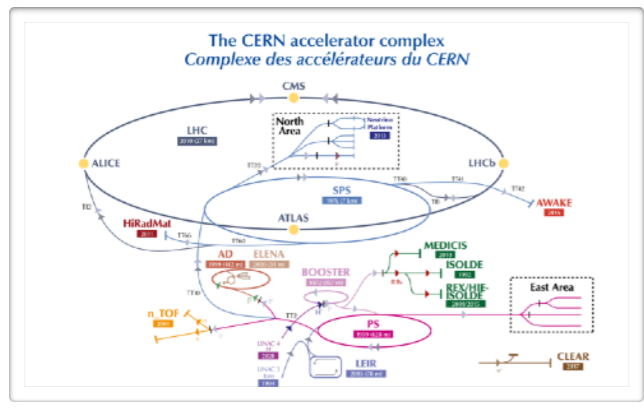
Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection

AI



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

AI

Inference

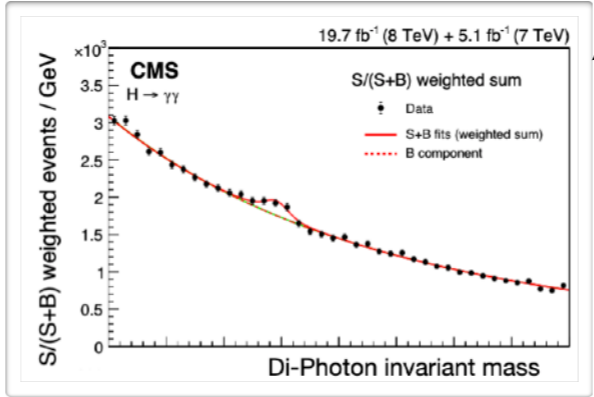
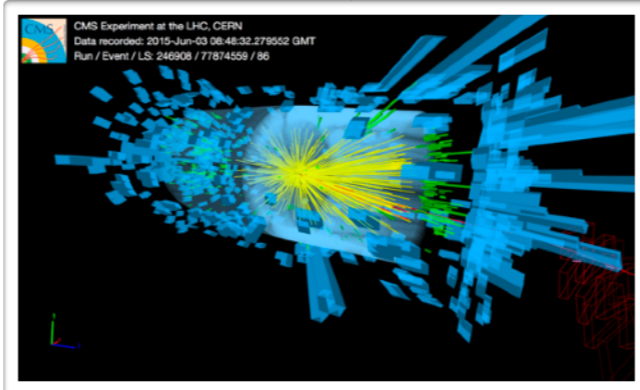
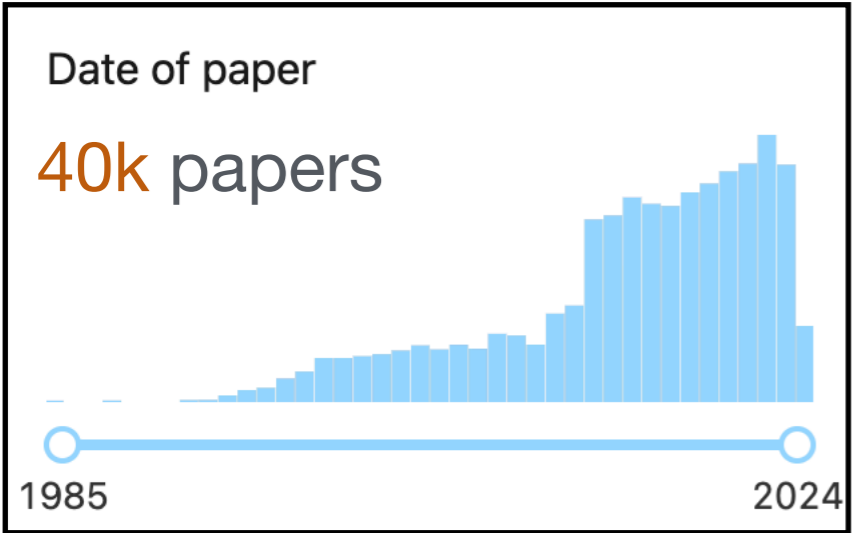
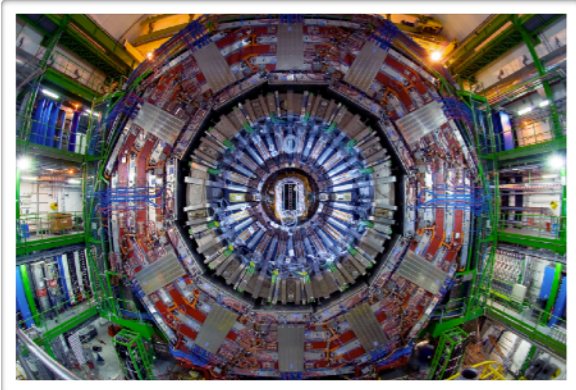
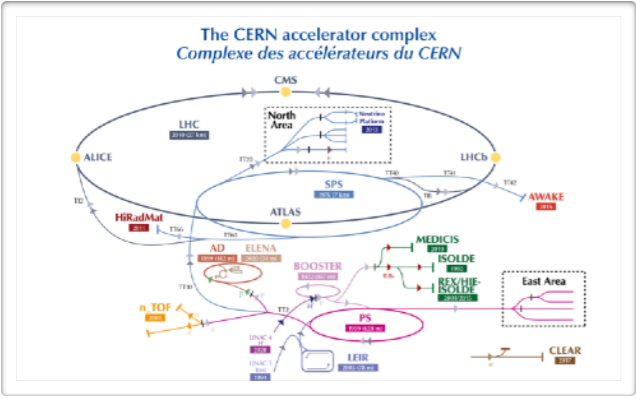
Experiment Design

Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection



Apologies - there will be some selection bias.

Particle Data Primer

“Data Data”

Particle collisions with ~ 1 MB/event happen at a **rate of 40 MHz**

Distill to ~ 1 kHz via lossy, irreversible filtering algorithms (Trigger)

Samples i.i.d. from physics distribution (e.g. the Standard Model + potential new physics)

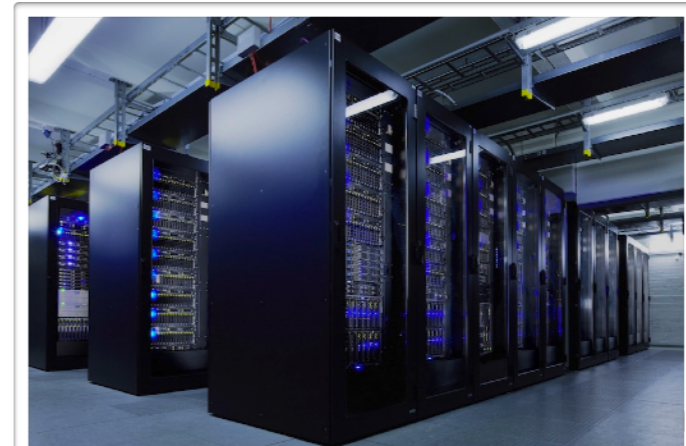


“Simulated Data”

Based on first-principle mathematical model of physical theory and detector interaction

Full control over which process occurs

Uncertainty in detector calibration and natural constants encoded by **performing multiple simulations**, one per set of parameter values



Particle Data Primer

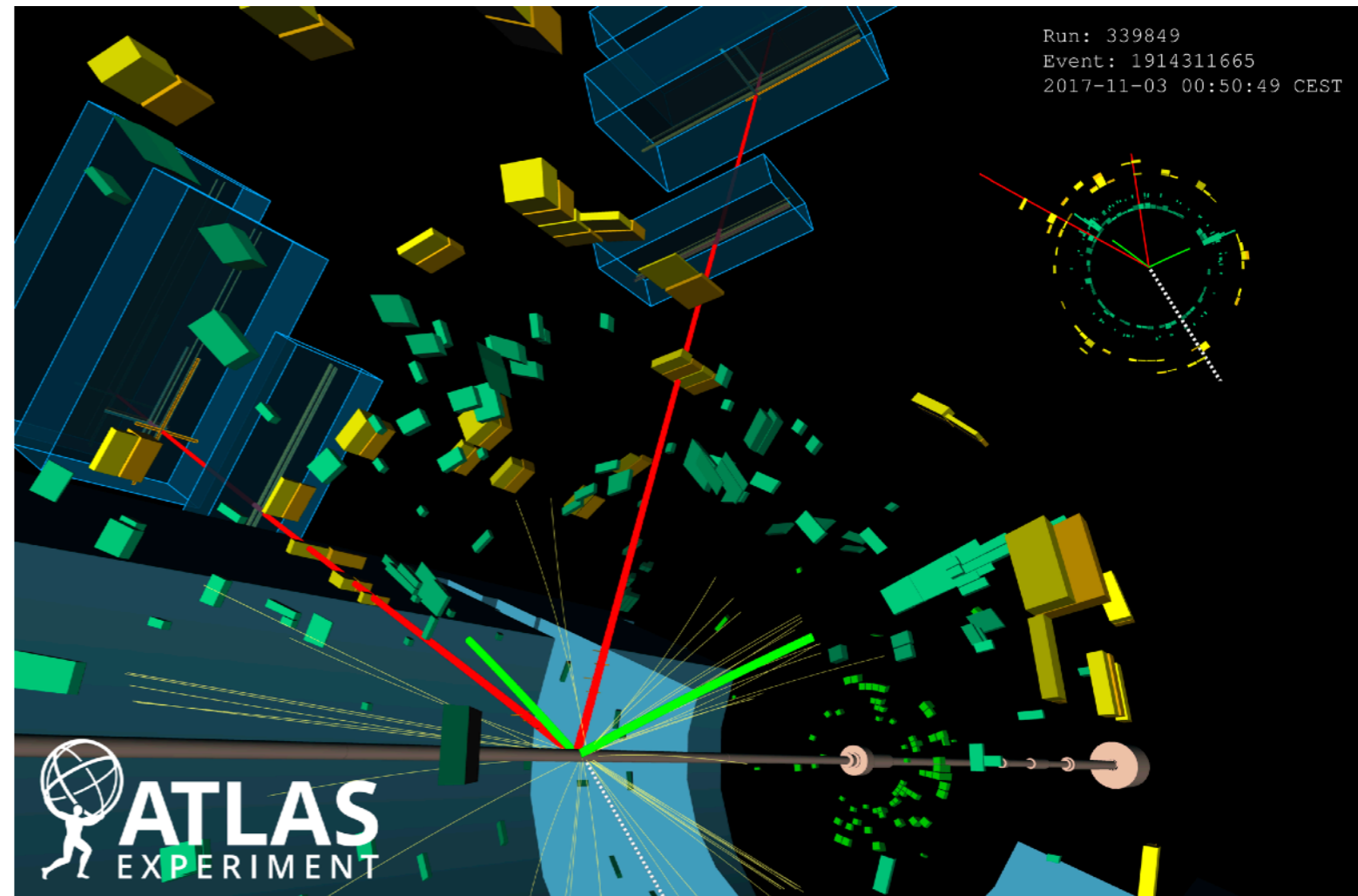
Both types of data share **common format** and reconstruction software

Different ways of representation (all aligned with physical interpretation):

- low-level readouts in $\sim 100\text{M}$ channels
- 10s-100s of intermediate four-vectors
- $O(10)$ high-level features

Message passing/attention-based models

One collision/event = “one image”



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

AI

Inference

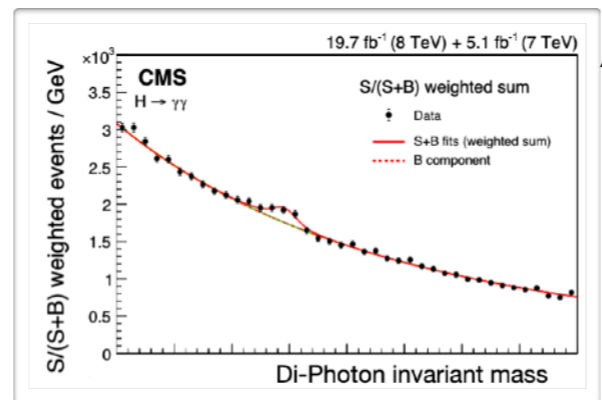
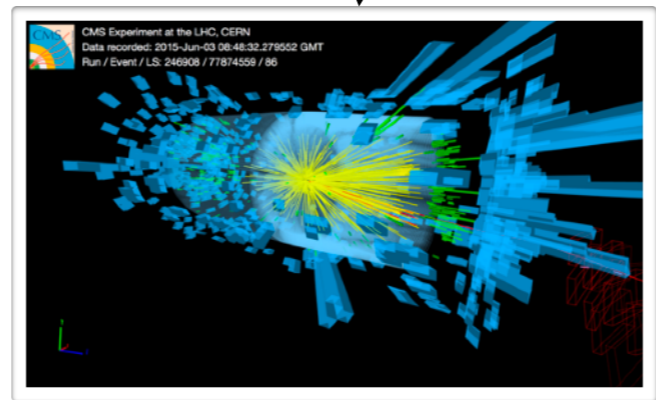
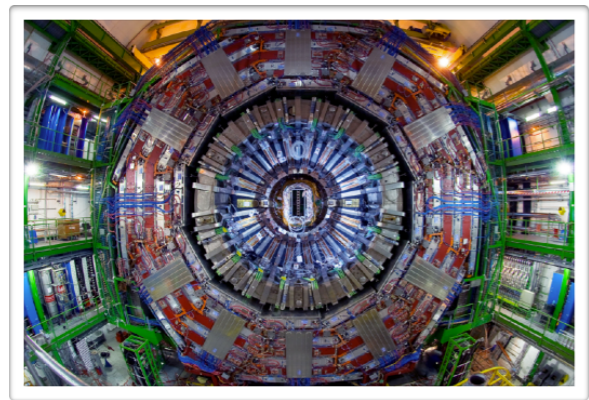
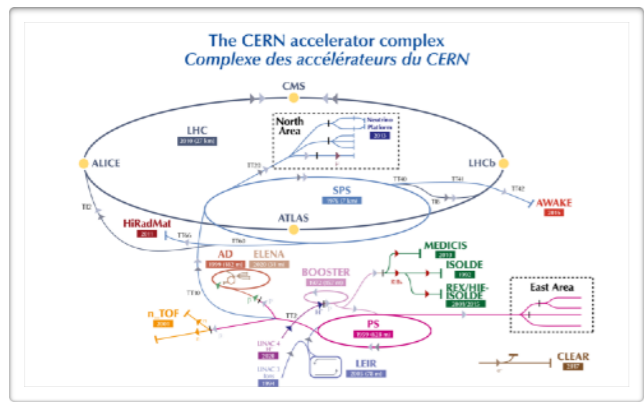
Simulation

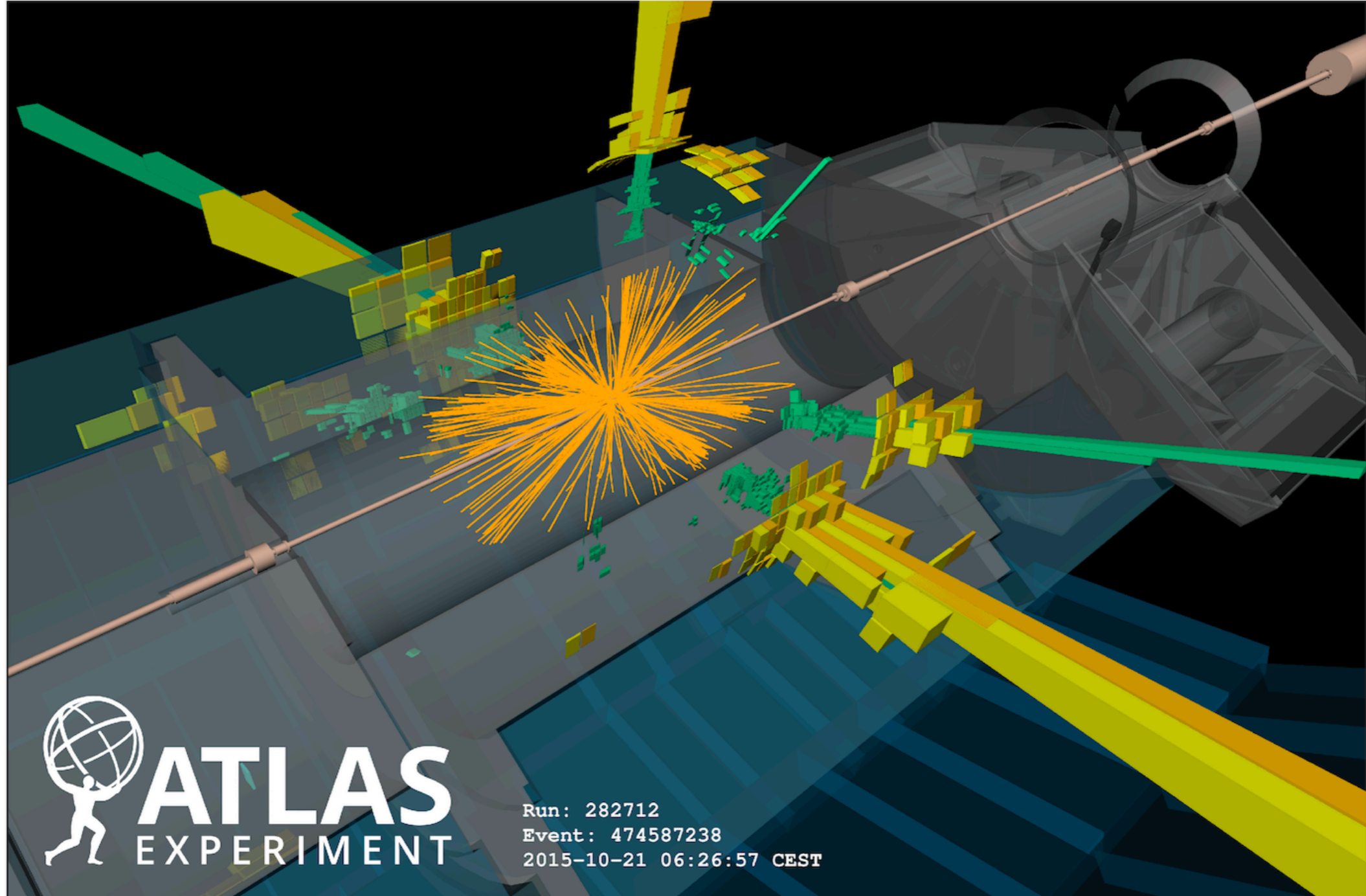
Experiment Design

Triggers

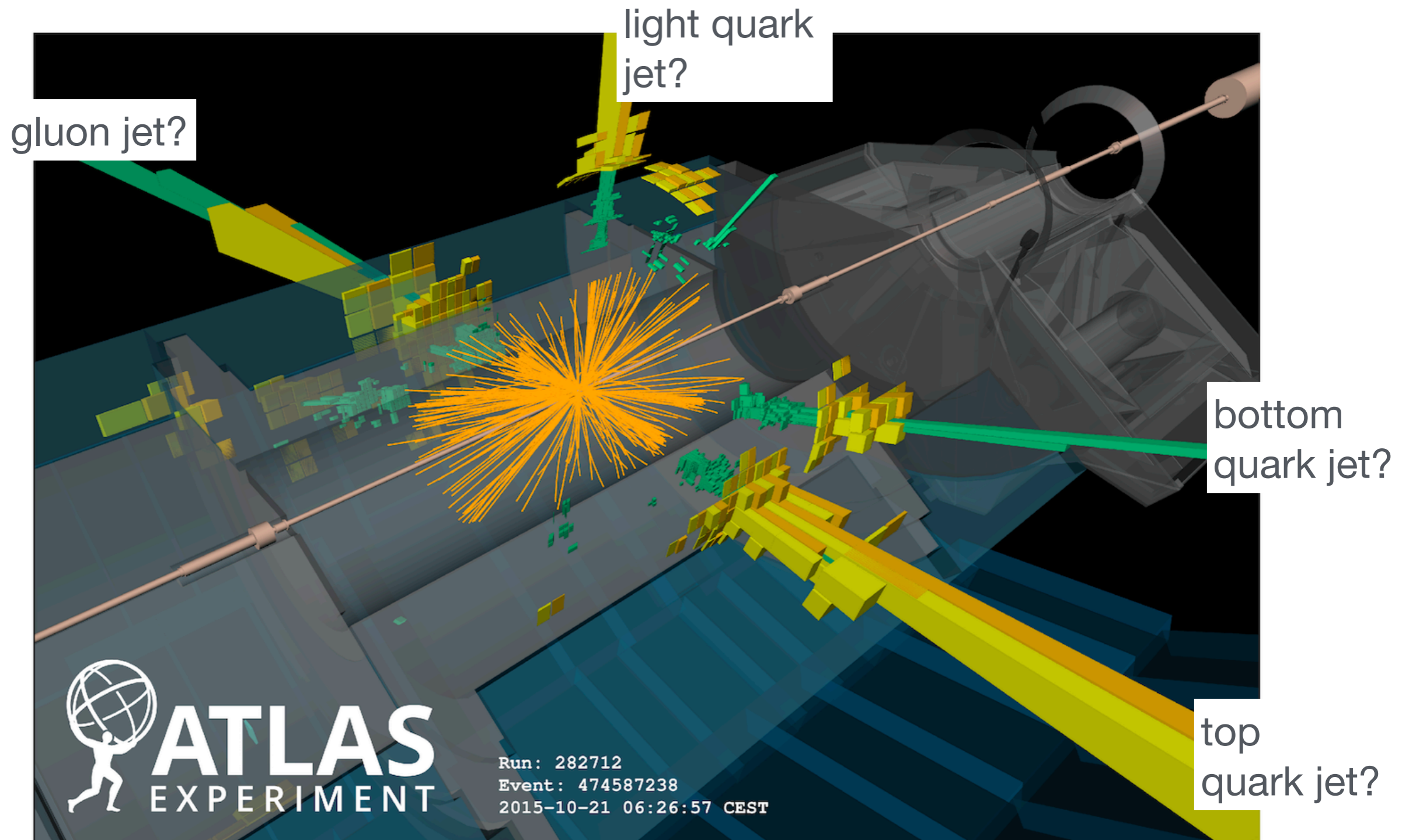
Tagging
Reconstruction

Unfolding
Anomaly Detection

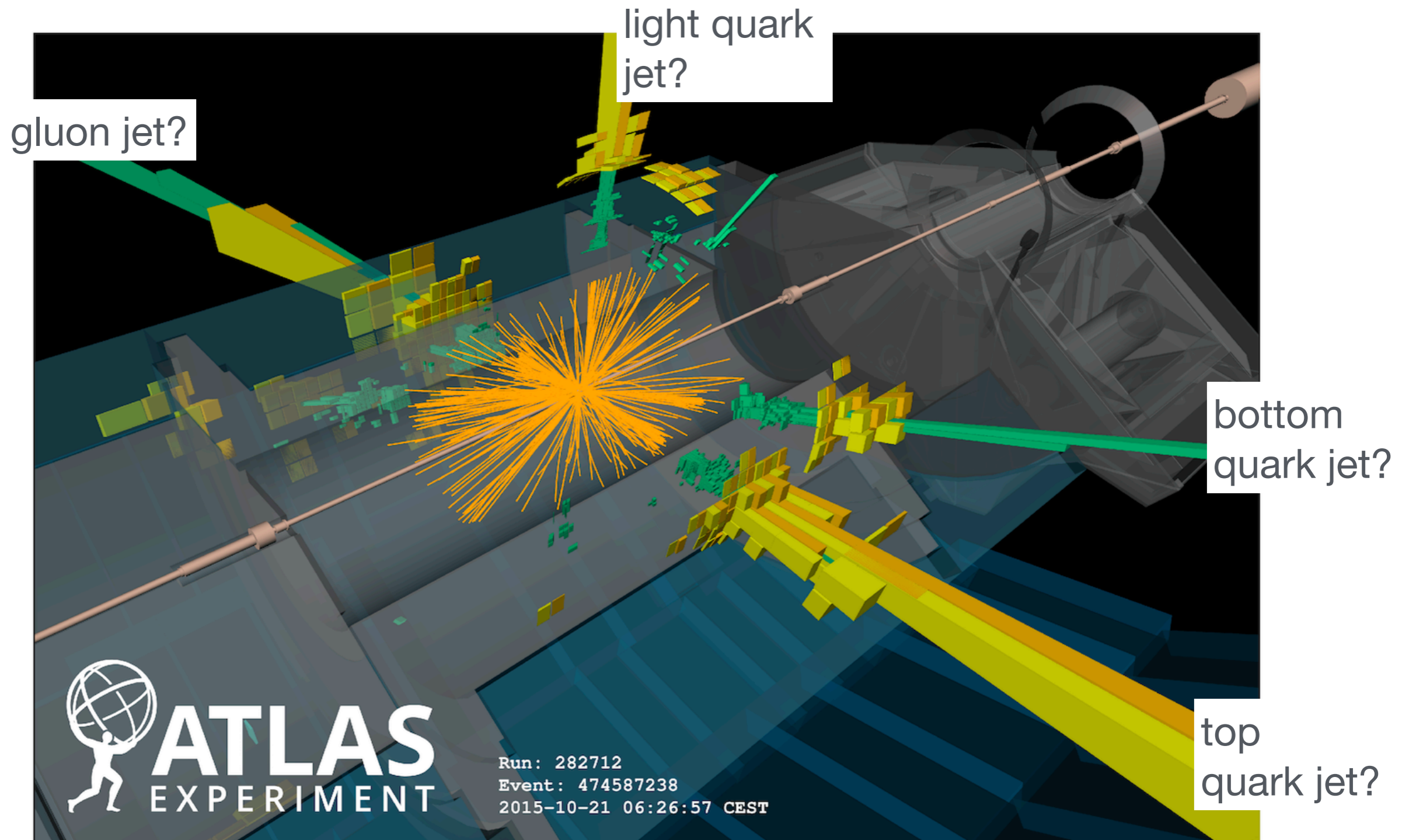




A jet is a
collimated shower of particles in the detector

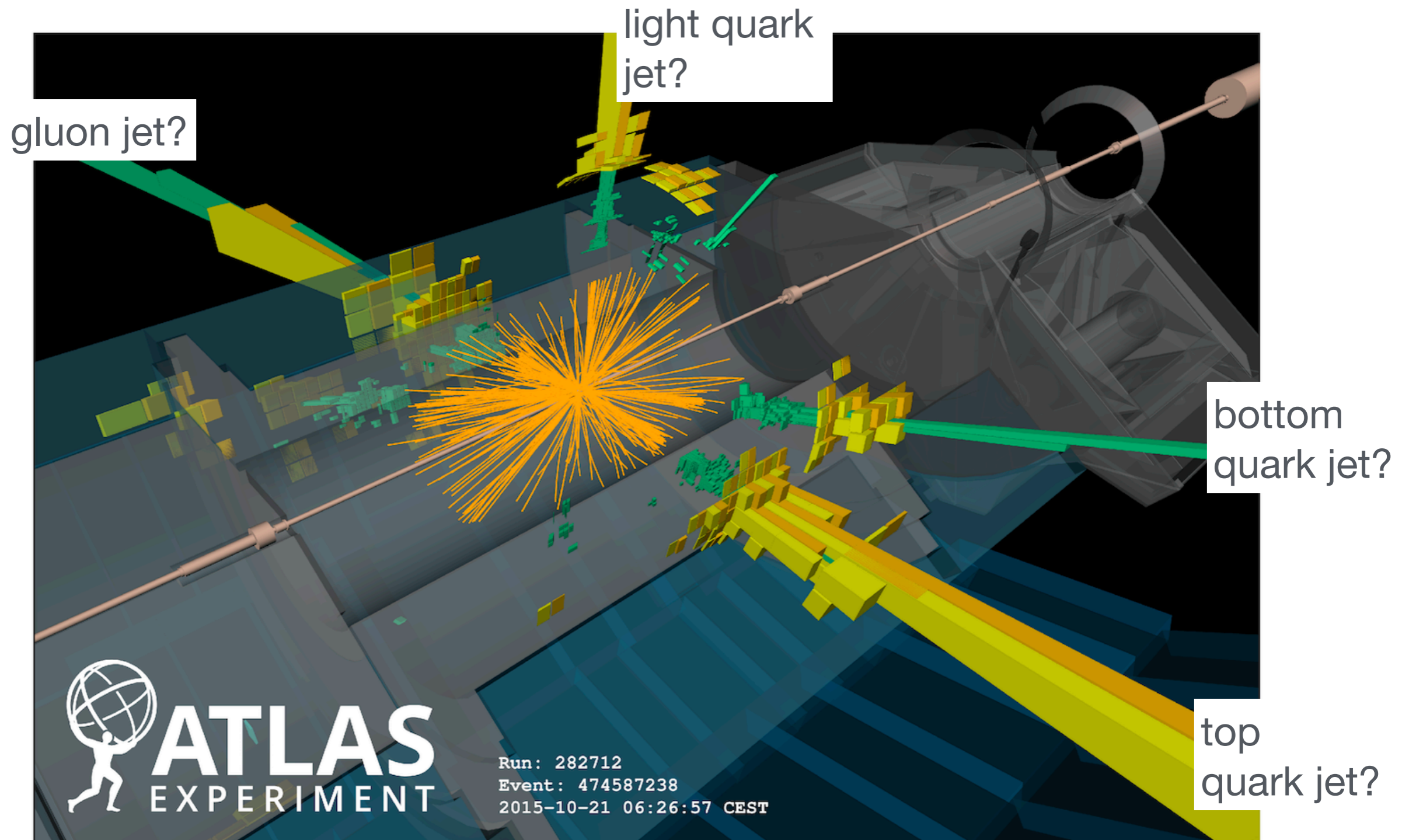


We want to know
which particle produced a jet

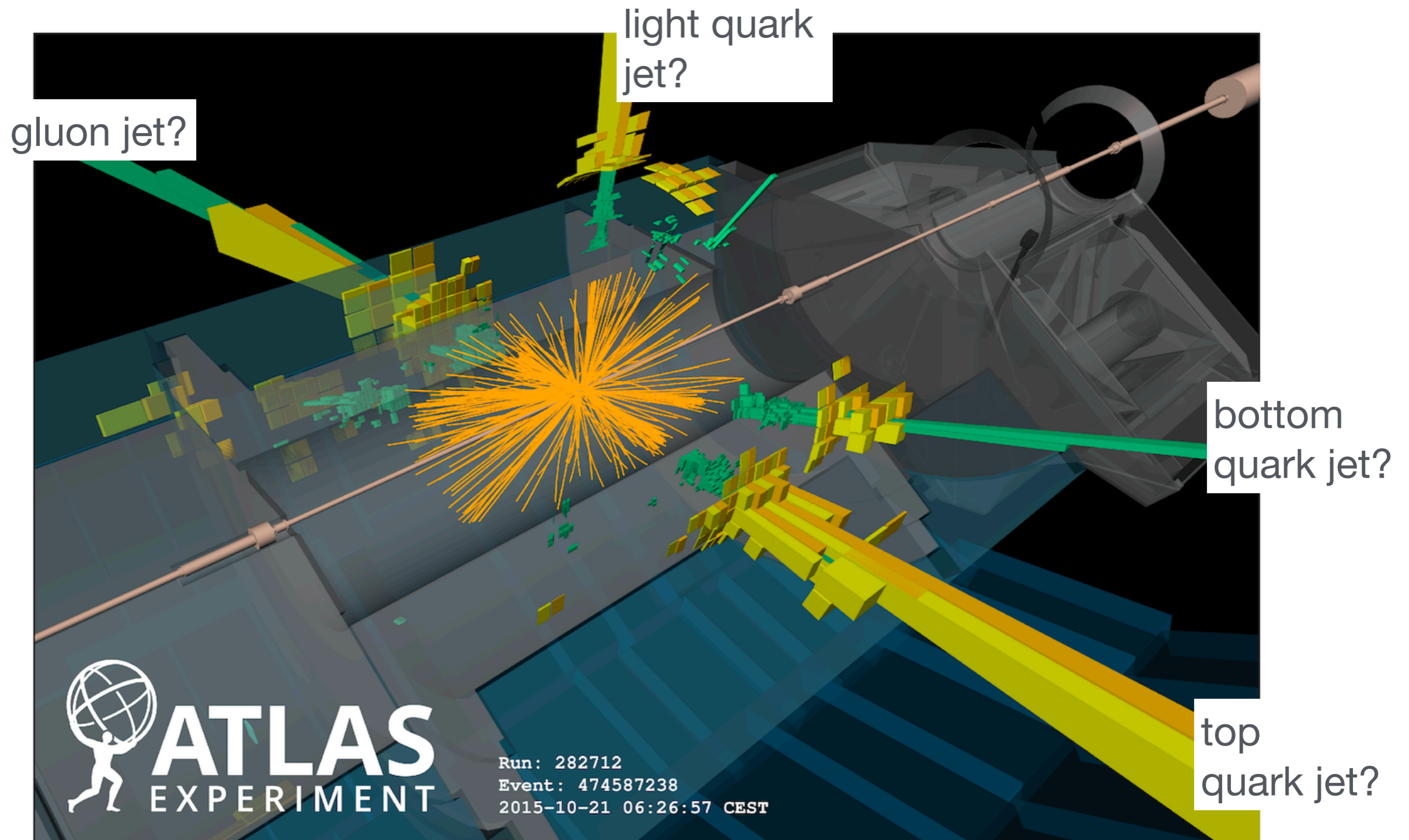


Why?

- Discover new particles
- Measure the Standard Model



Let's focus on **top quarks**
(Modern taggers are multi-class)



How to build ML algorithms for **complex, heterogenous** data?

Data most naturally viewed as **point cloud**:

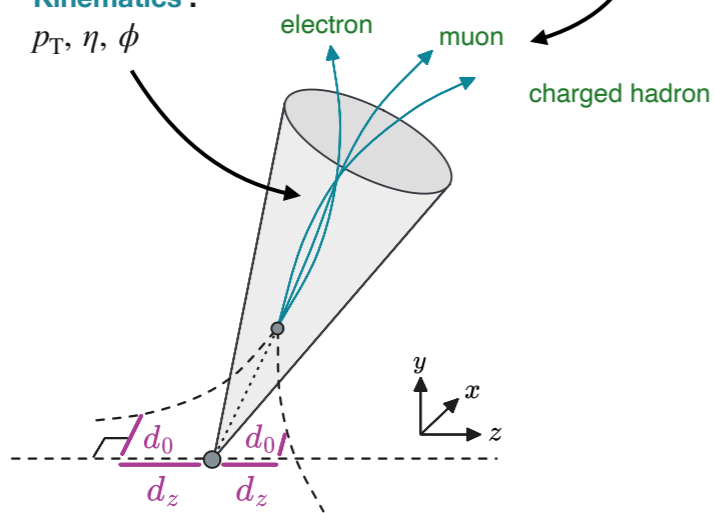
Each **input** (e.g. jet, event, ..) is a **set of k-dimensional vectors** (individual particles, hits, ..)

$$J_i = \{ \vec{p}_1, \dots, \vec{p}_n \}$$

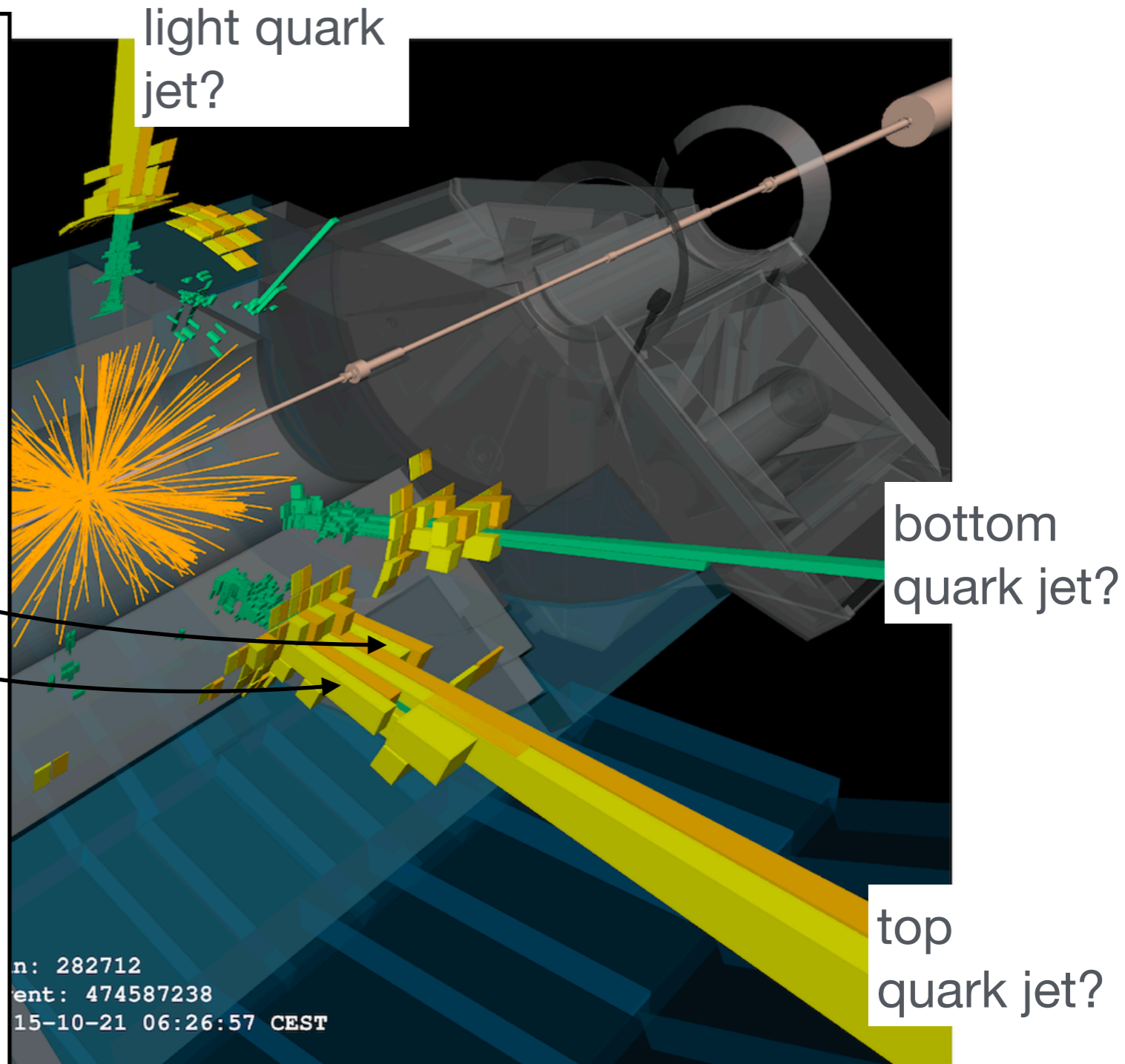
Particle-ID and charge :
isElectron, isMuon, ...

Kinematics :
 p_T, η, ϕ

Example per-particle features



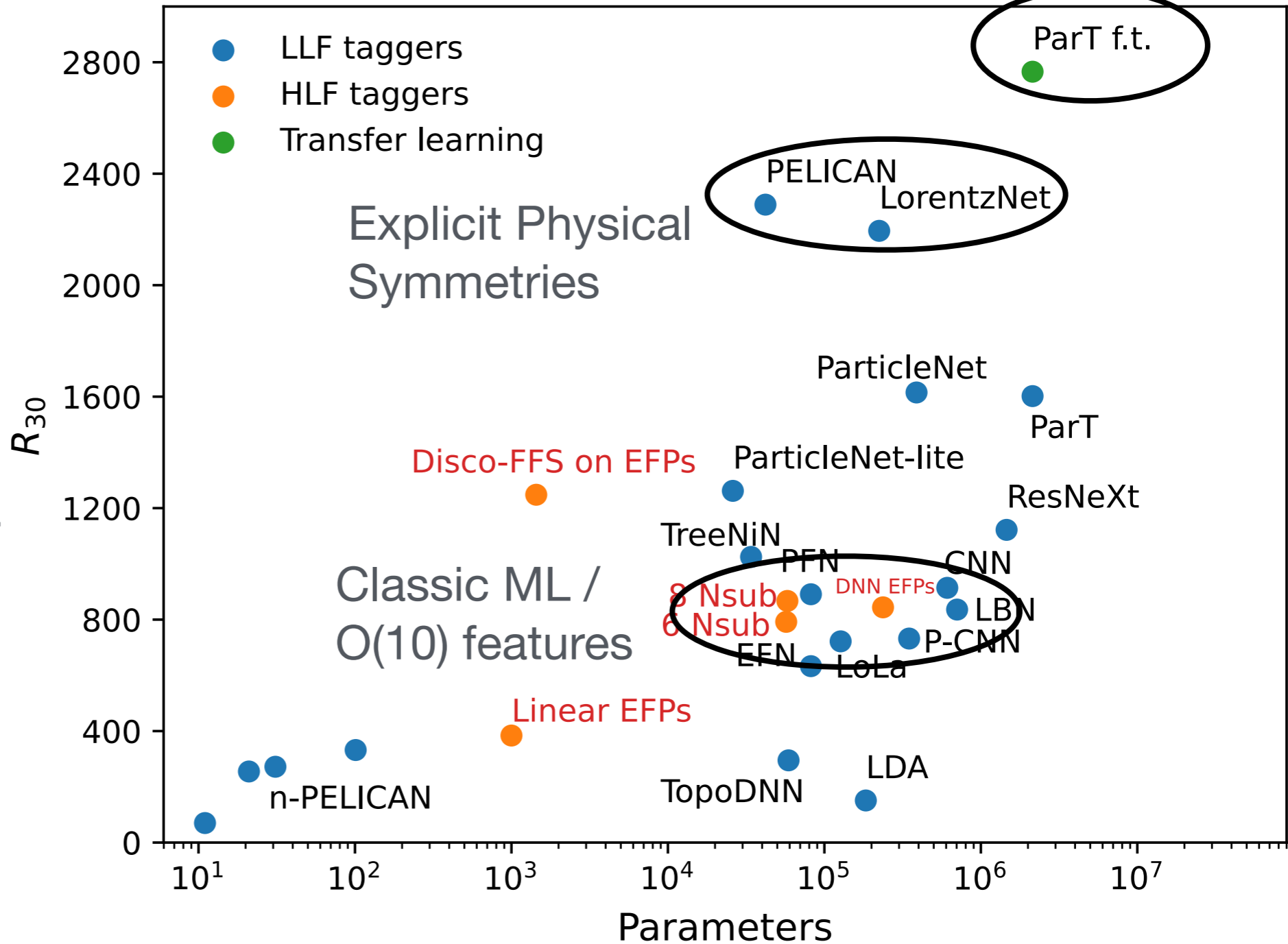
Trajectory displacement :
 d_0 : closest approach to PV in xy -plane
 d_z : z position where d_0 is evaluated



Status

Transfer learning from larger dataset

3x+ gain in background rejection by going from classical ML on few low level features to deep architectures that know physics (either built-in or transfer learned)

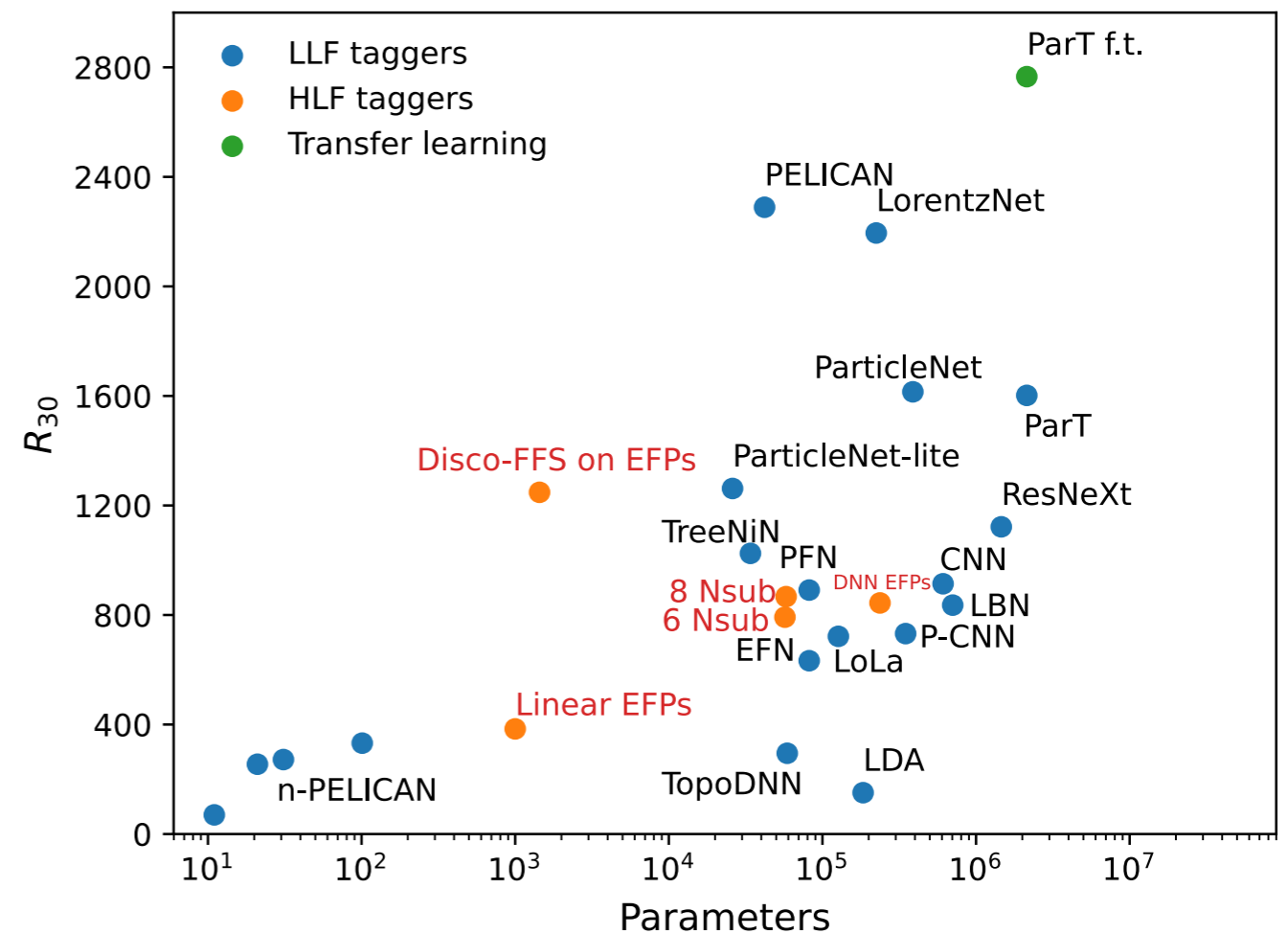


See talk by **Jonas**

(Some) Current challenges

- “Calibration”: Domain adaptation between simulation and collider data
- Local vs global optimisation
- Uncertainty aware training
- Interpretability

See talk by **Jesse, Oliver**



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

Inference

Experiment Design

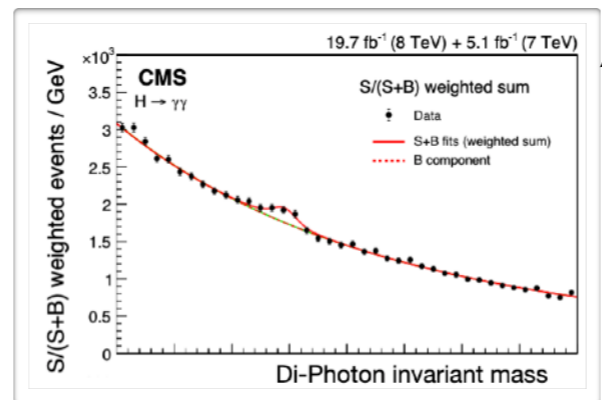
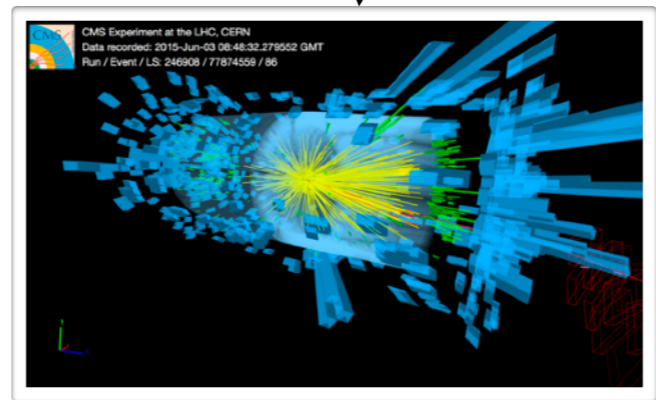
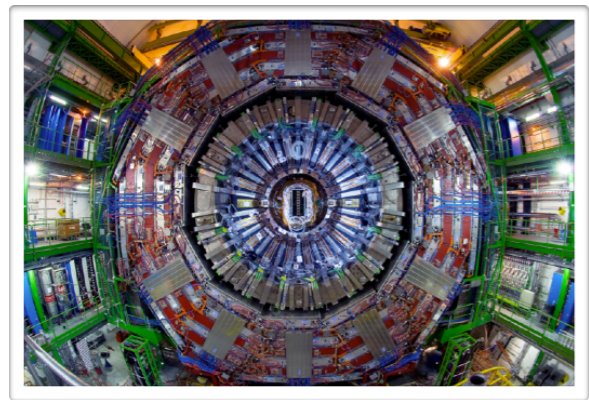
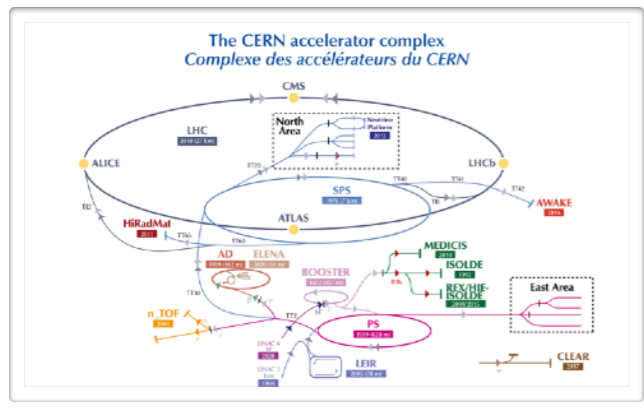
Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection

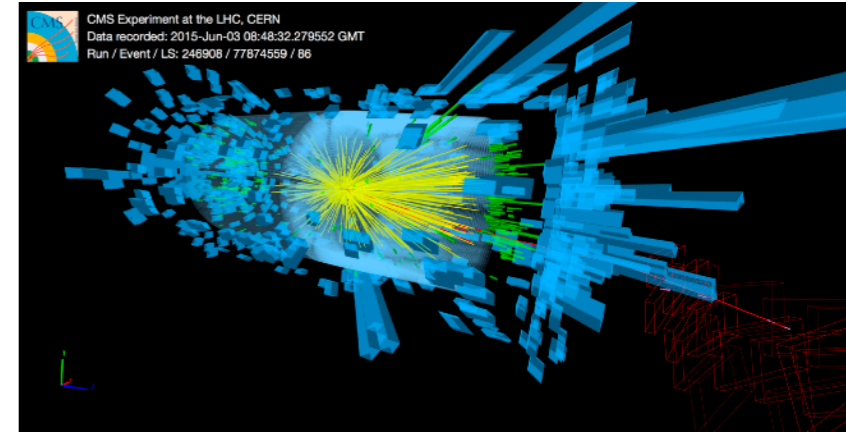
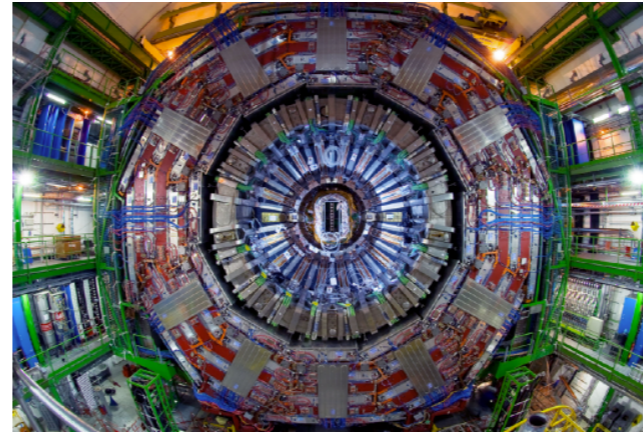
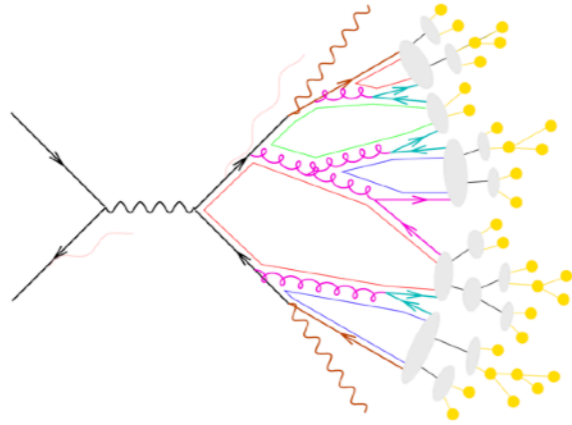
AI



Generative Models

This happens in the experiment

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi}\not{D}\psi + h.c. \\ & + \chi_i Y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu\phi|^2 - V(\phi) \end{aligned}$$



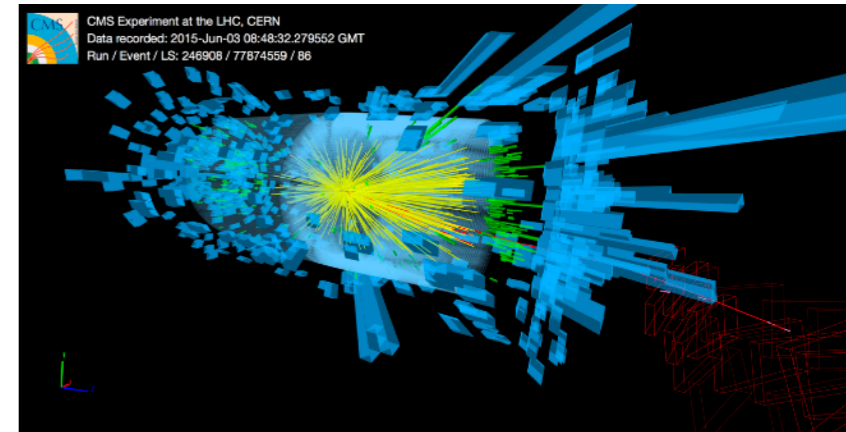
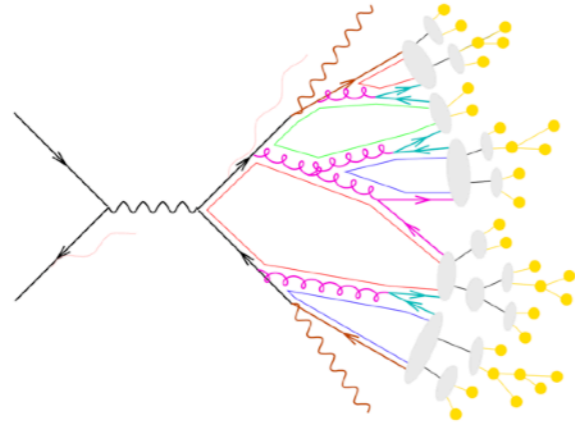
This is what we want to know

Simulation is crucial to connect
experimental data with theory
predictions

Generative Models

This happens in the experiment

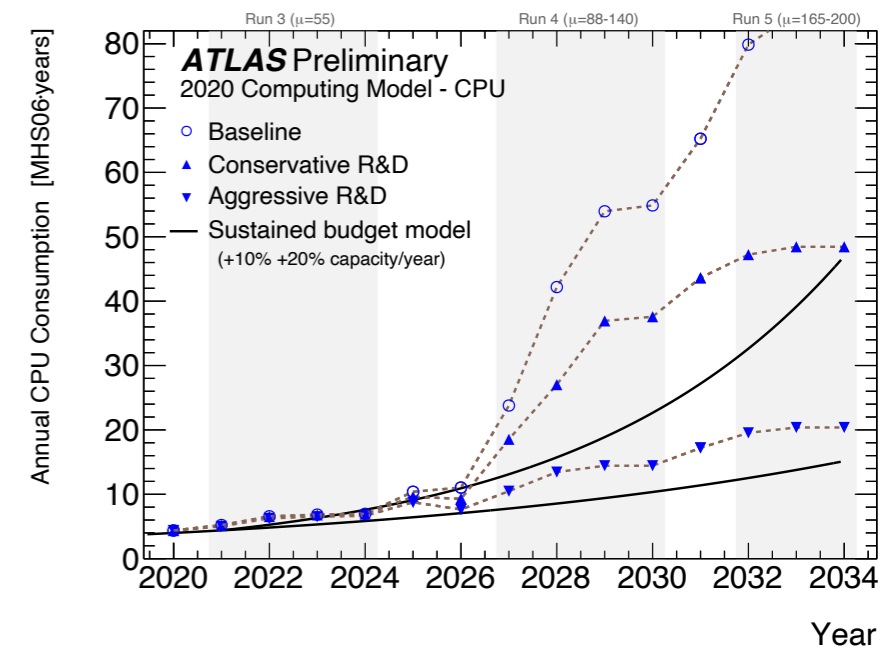
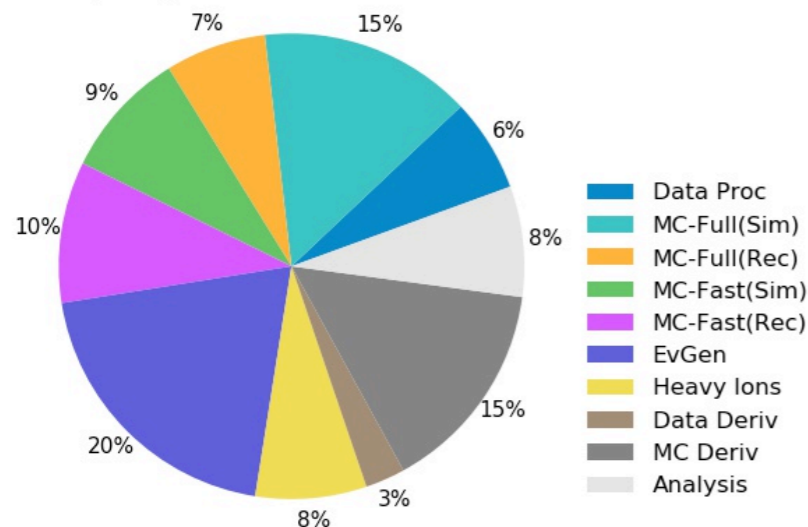
$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$



This is what we want to know

Simulation is crucial to connect experimental data with theory predictions, **but computationally very costly**

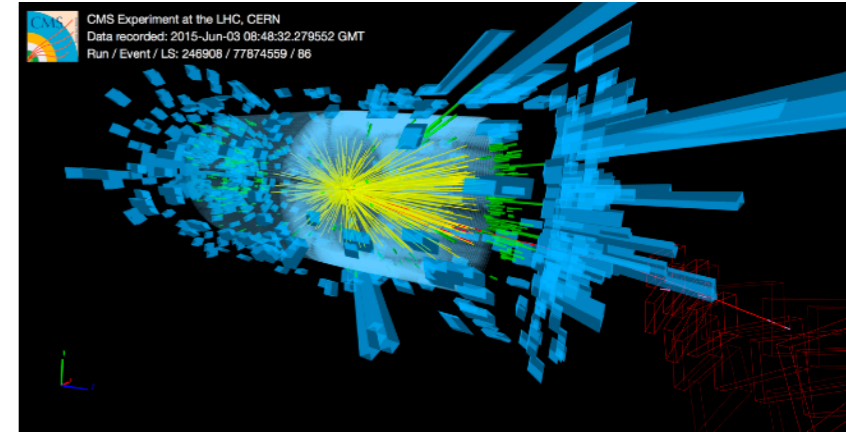
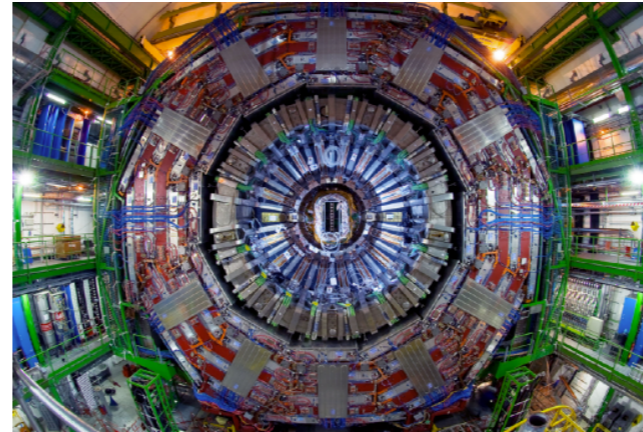
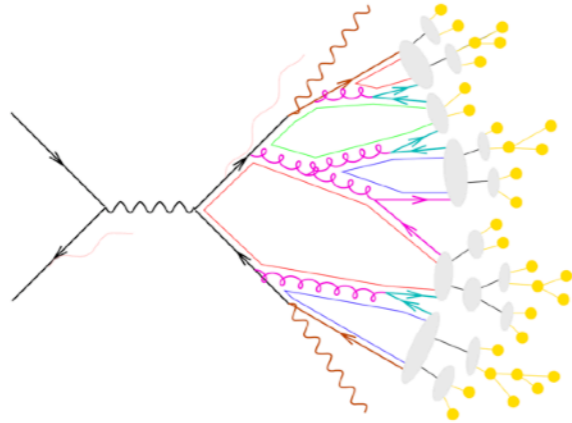
ATLAS Preliminary
2020 Computing Model - CPU: 2030: Baseline



Generative Models

This happens in the experiment

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + h.c. \\ & + \chi_i Y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu \phi|^2 - V(\phi) \end{aligned}$$



This is what we want to know

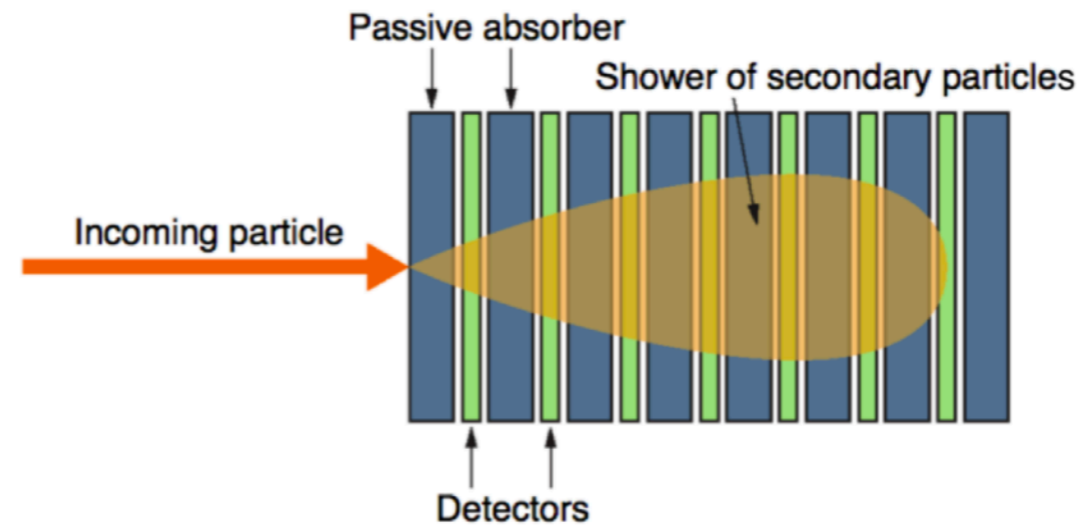
Simulation is crucial to connect experimental data with theory predictions, but computationally very costly

Use AI to **improve efficiency** of simulation codes or **learn surrogates**

Calorimeter Simulation

Interaction of particles with multi-layer detectors to determine their **initial energy** (and type)

Measurement of **energy, position, (and time)** of secondary particle hits



Calorimeter Simulation

Interaction of particles with multi-layer detectors to determine their **initial energy** (and type)

Measurement of **energy, position, (and time)** of secondary particle hits

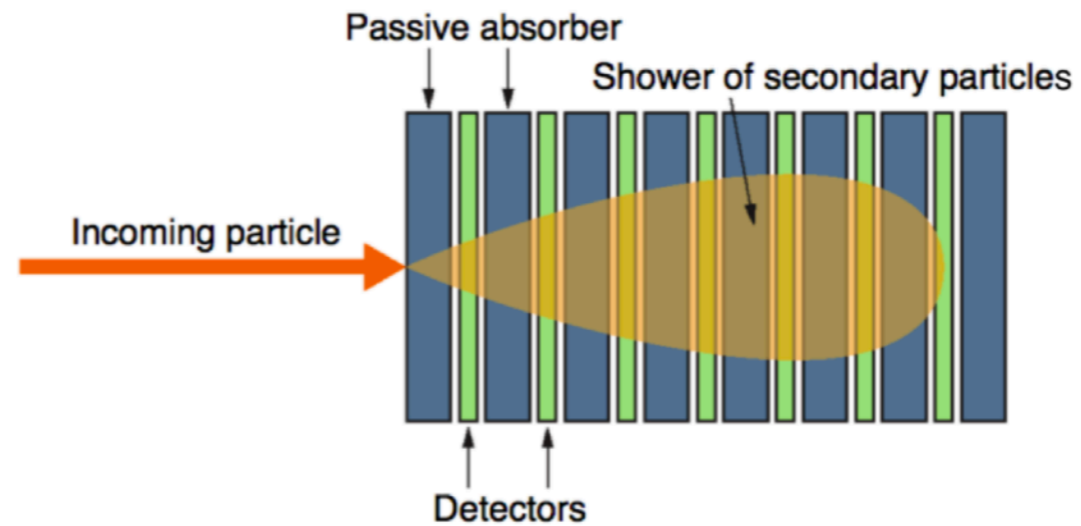
Represent data as

-**fixed grid**

(3d matrix of detector elements, value=energy)

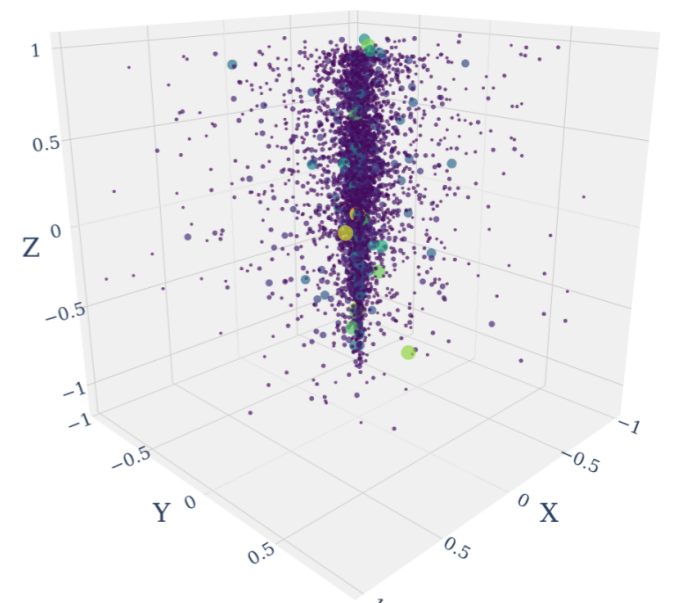
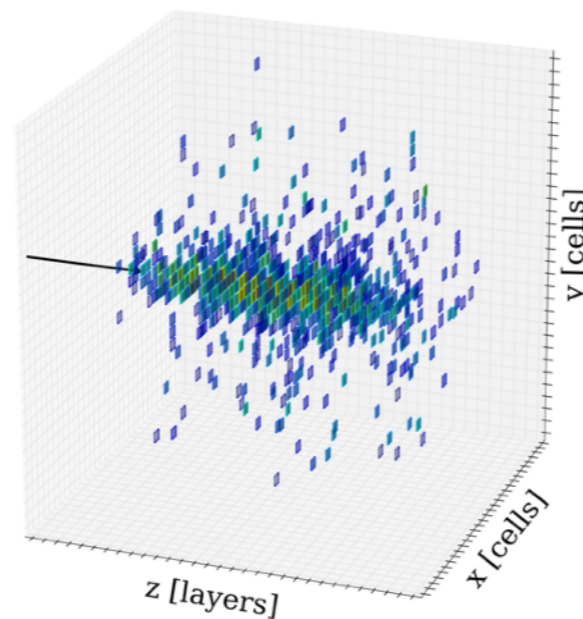
-**point cloud**

(set of hits, each hit is a 3d vector with position+energy)



as **fixed grid**

as **point cloud**

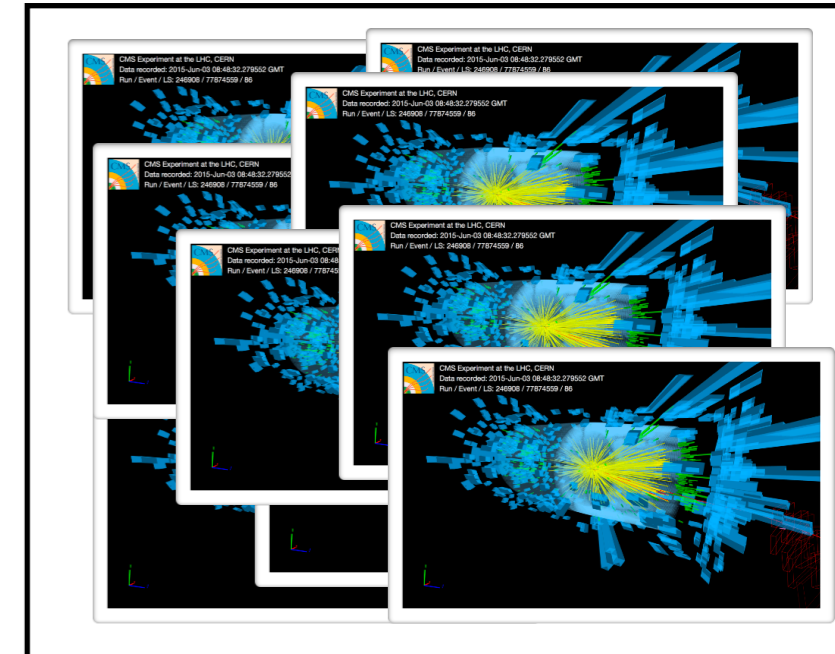
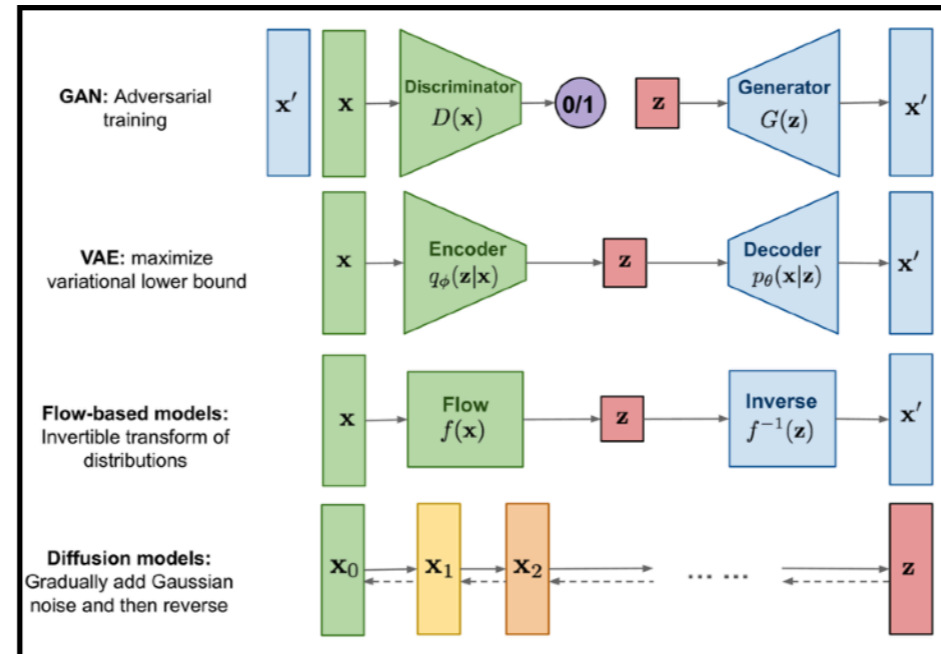
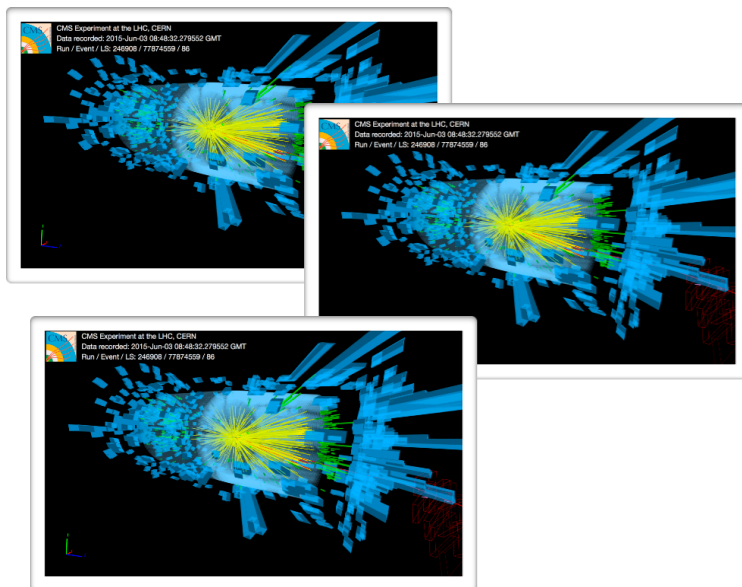


Strategy

1. Use classical simulation or collider data as input

2. Train generative surrogate

3. Oversample



See talk by **Ramon, Tobias**

Surrogate Models

Collider or
classical
simulation

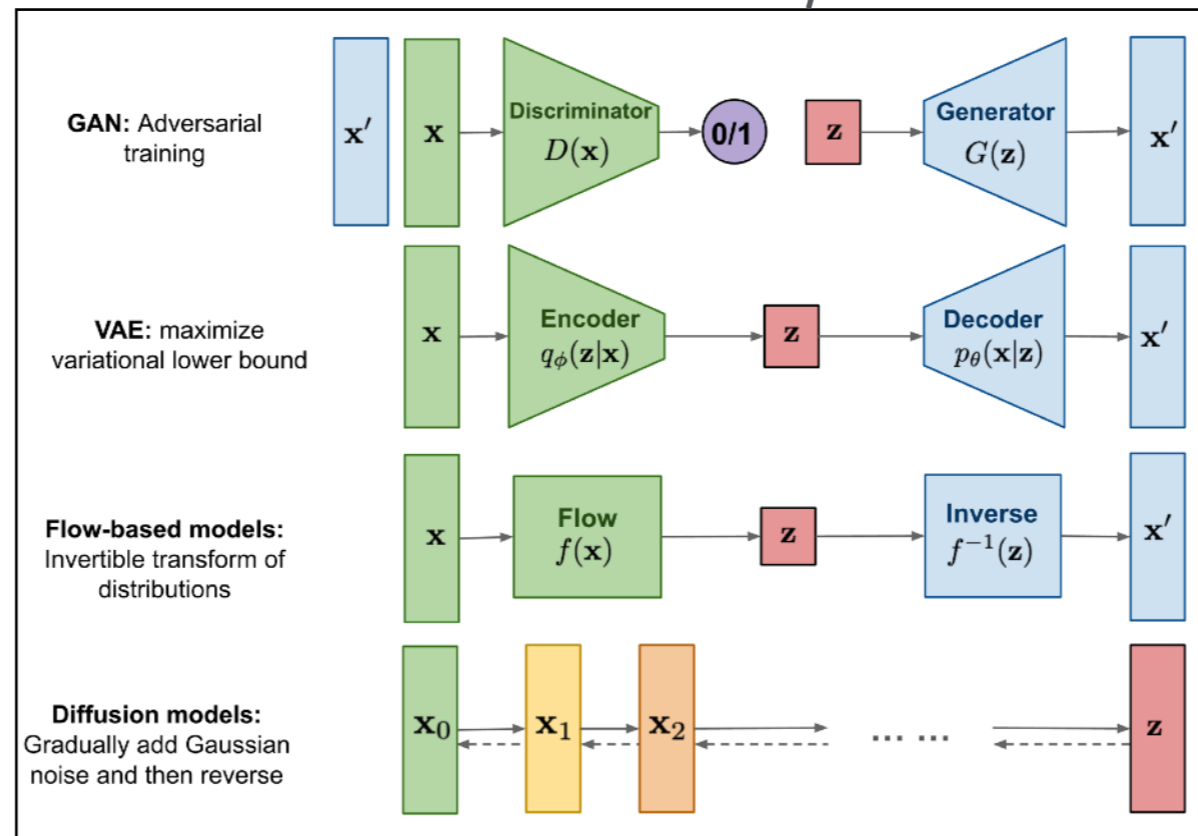
Slow

Training Data Set

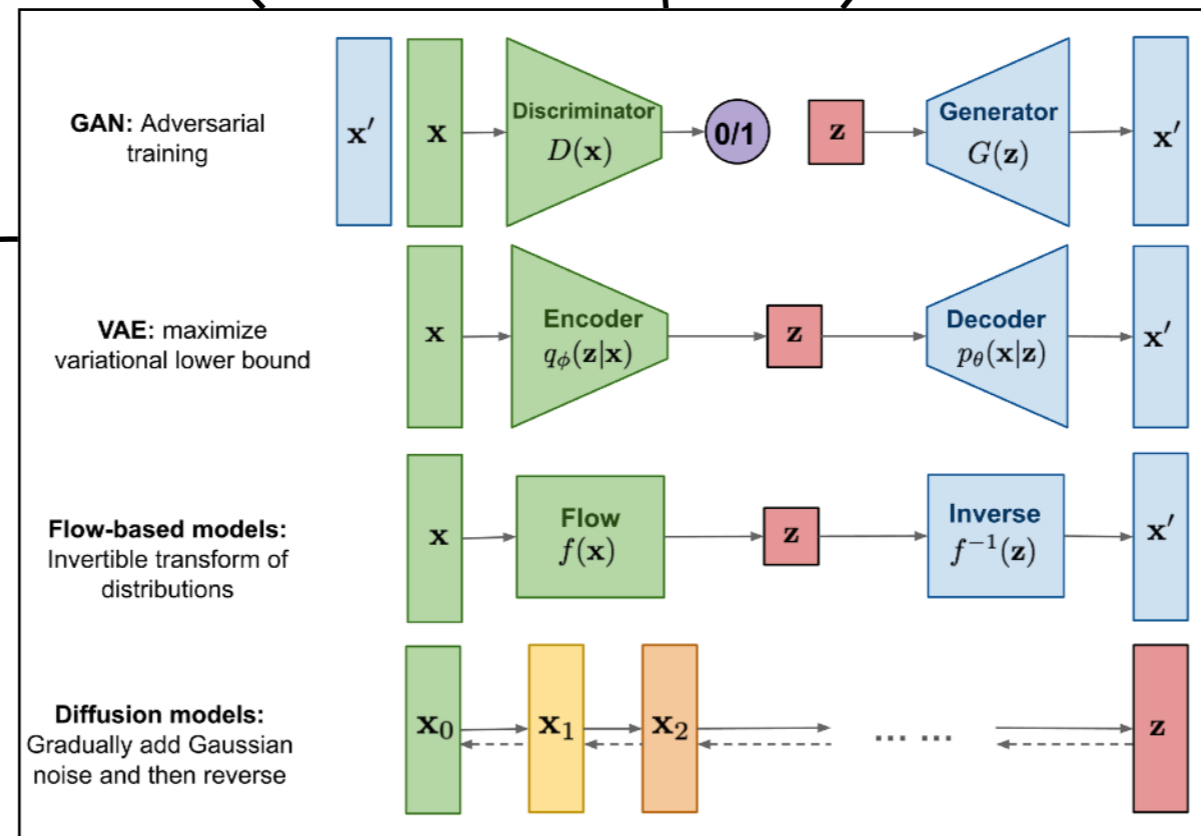
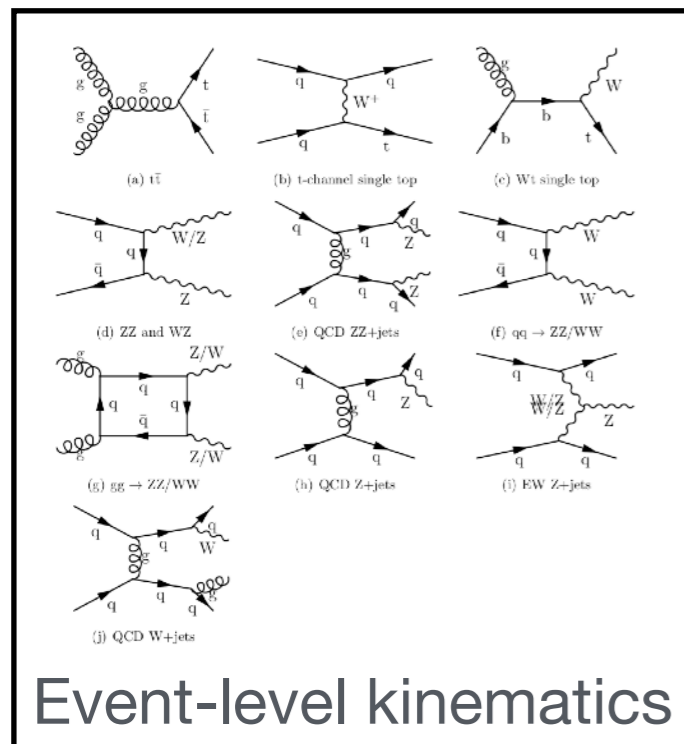
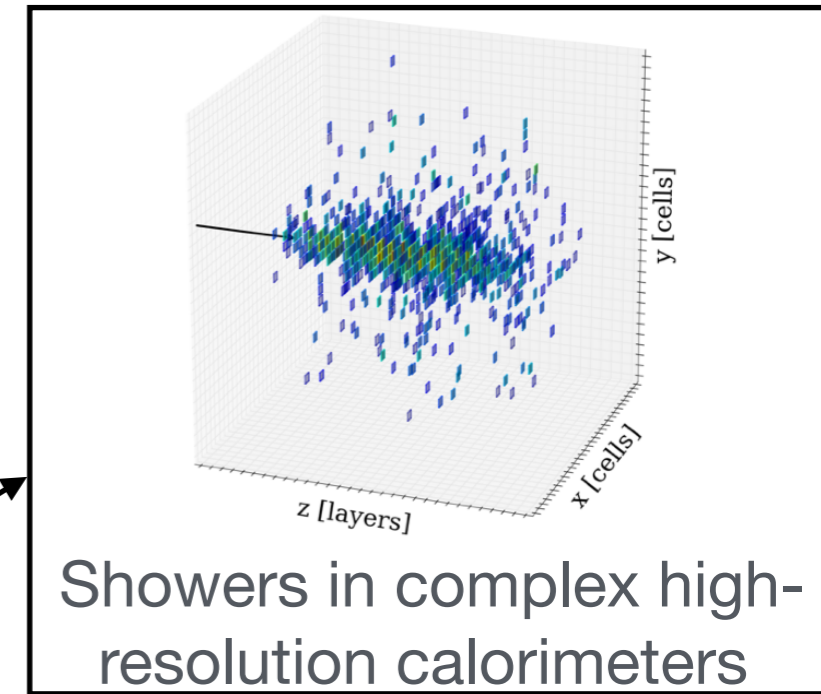
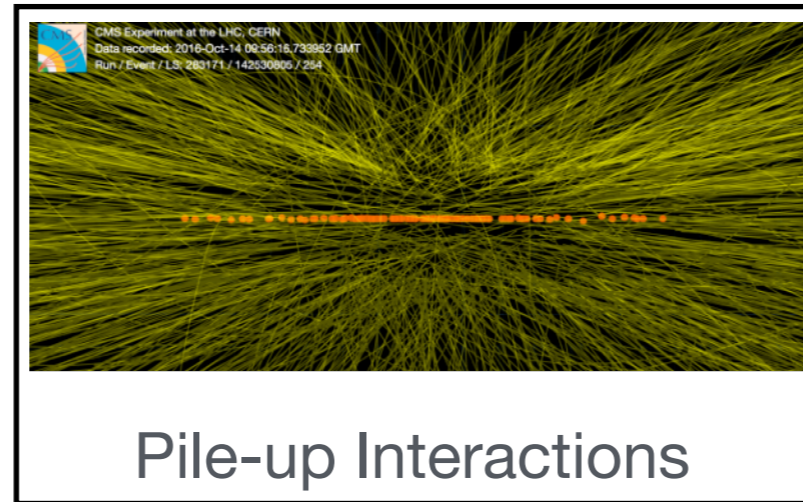
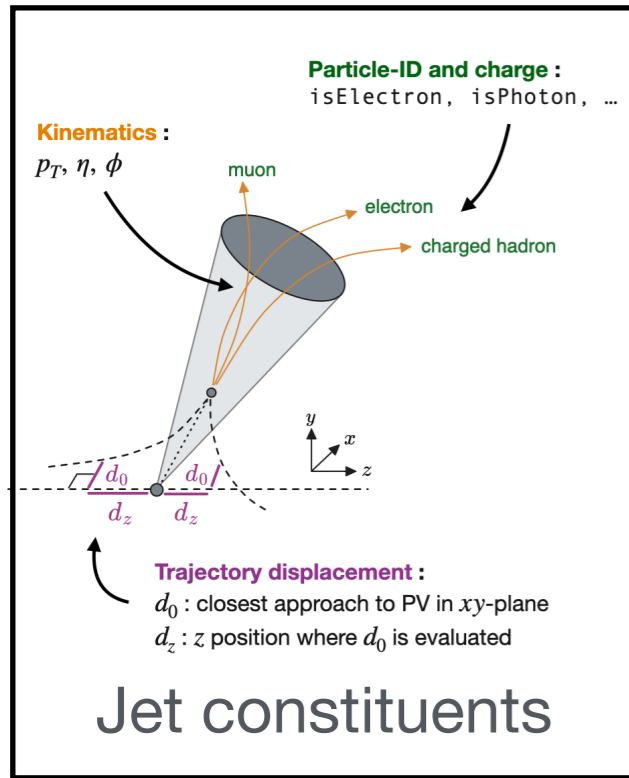
Surrogate Model

Fast

Synthetic data
used in analysis



Surrogate Models



Surrogate Models

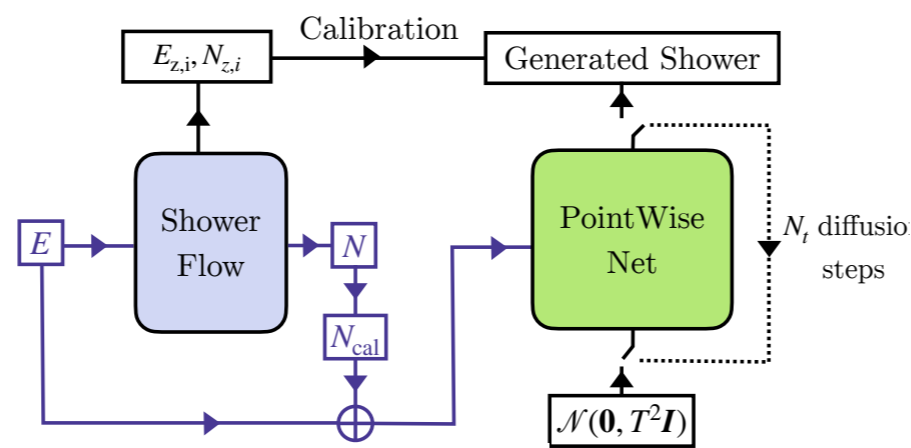
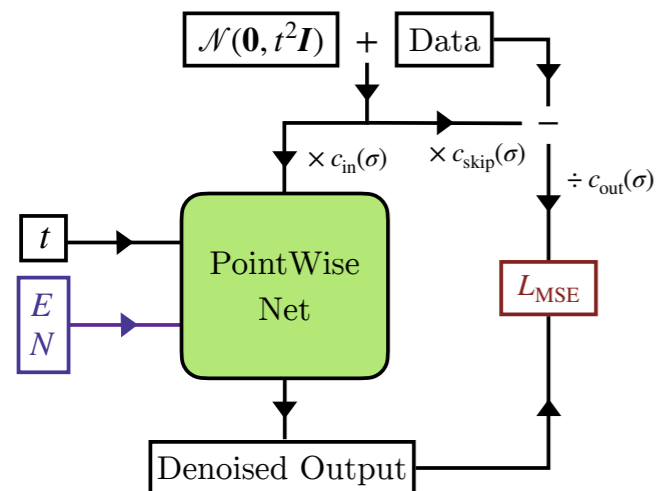
Collider or
classical
simulation

Training Data Set

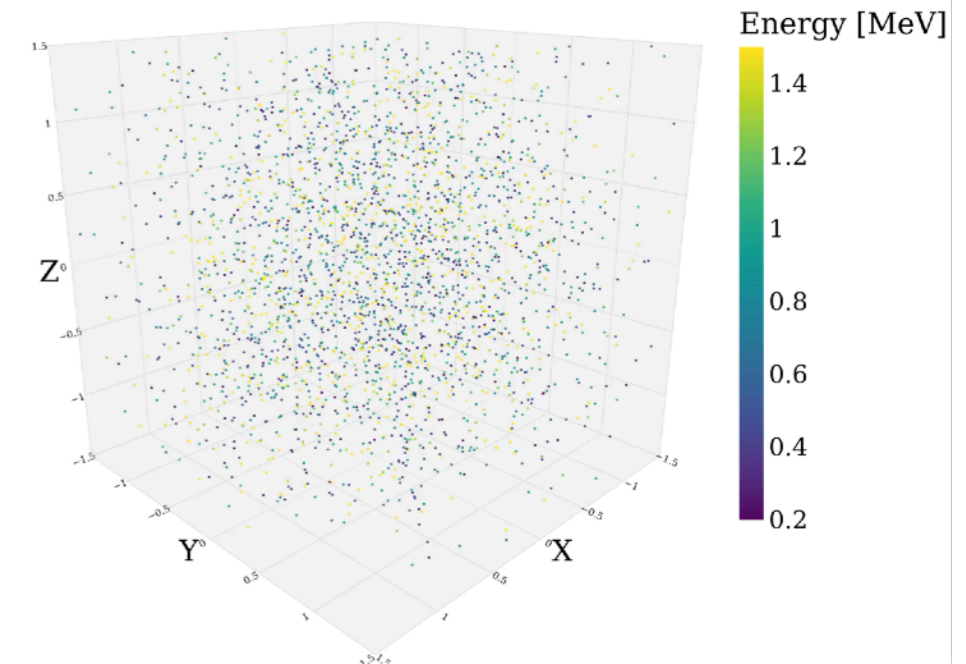
Surrogate Model

Synthetic data
used in analysis

Example



CaloCloud, time stamp: t_{99}



Surrogate Models

Collider or
classical
simulation

Training Data Set

Surrogate Model

Synthetic data
used in analysis

How to assess quality?

Is one surrogate **better** than the
other?

Is the synthetic data **good enough** for
usage?

What **additional uncertainties** to take
into account?

Surrogate Models

Collider or
classical
simulation

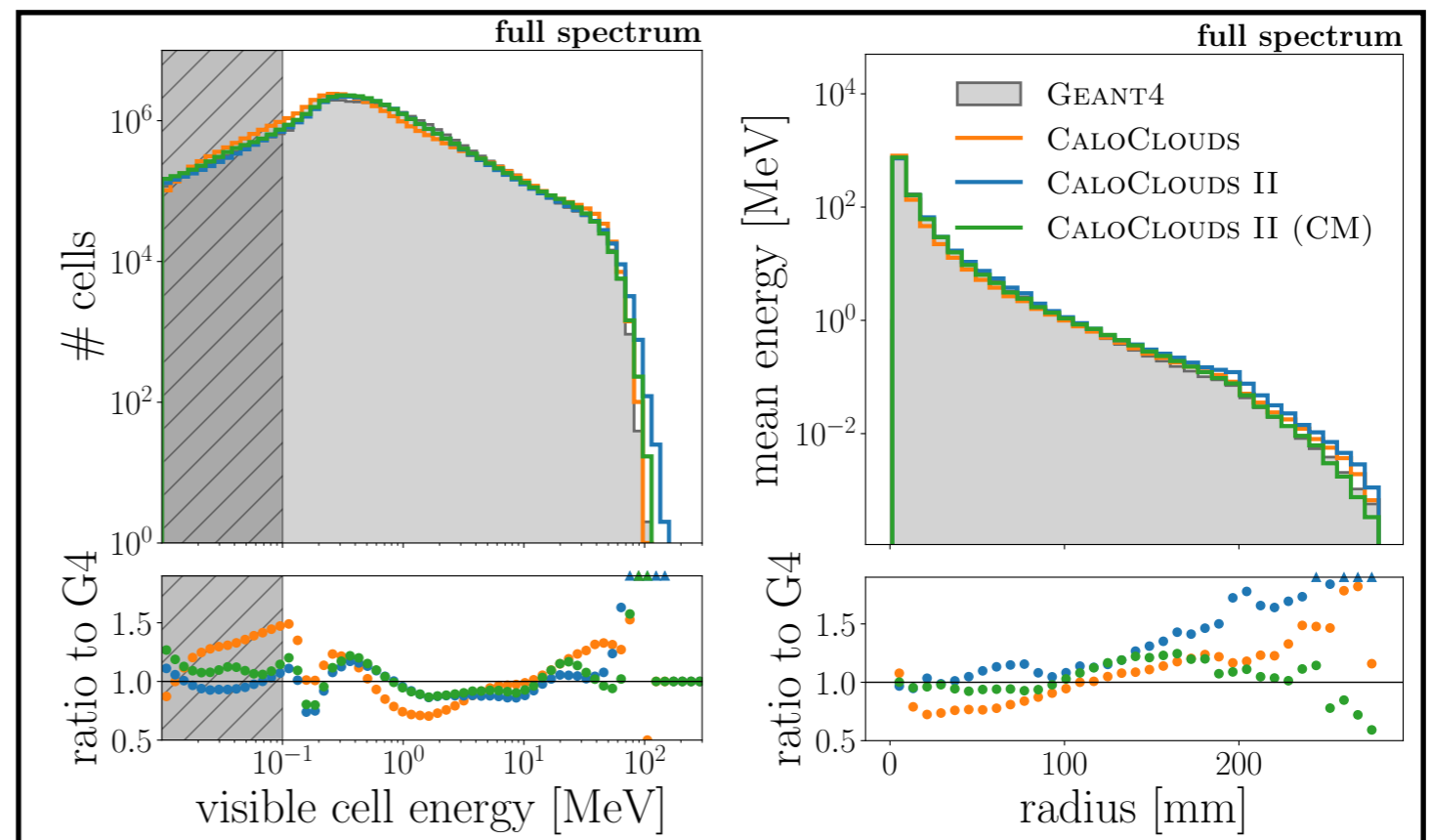
Training Data Set

Surrogate Model

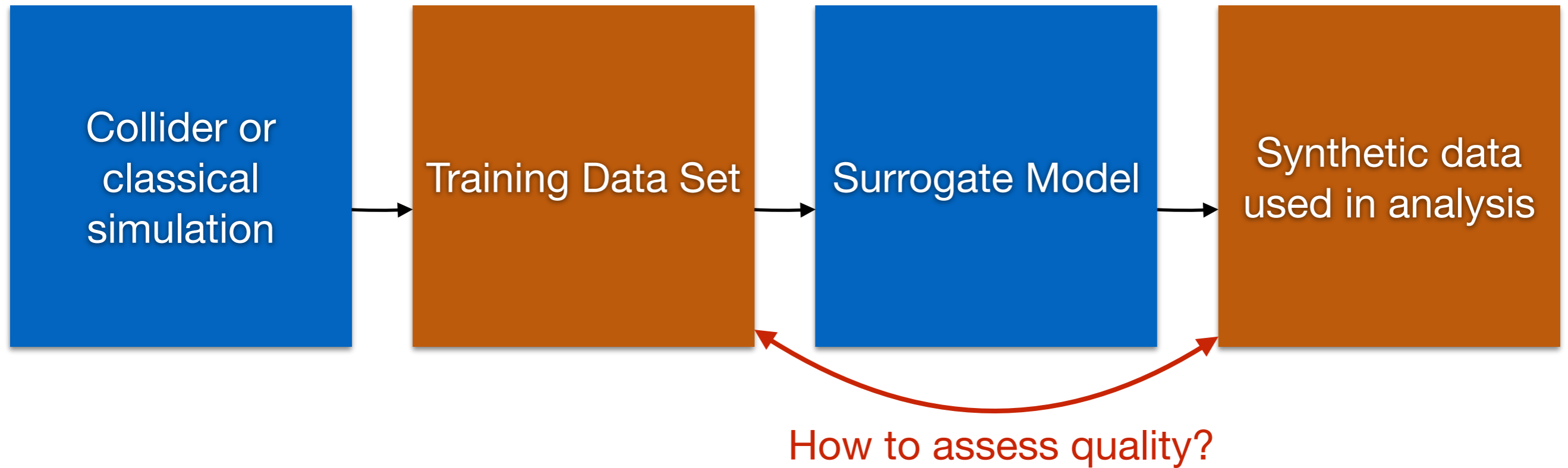
Synthetic data
used in analysis

How to assess quality?

Define and manually inspect
relevant distributions



Surrogate Models



Simulator	$W_1^{N_{\text{hits}}}$ ($\times 10^{-3}$)	$W_1^{E_{\text{vis}}/E_{\text{inc}}}$ ($\times 10^{-3}$)	$W_1^{E_{\text{cell}}}$ ($\times 10^{-3}$)	$W_1^{E_{\text{long}}}$ ($\times 10^{-3}$)	$W_1^{E_{\text{radial}}}$ ($\times 10^{-3}$)	$W_1^{m_{1,X}}$ ($\times 10^{-3}$)	$W_1^{m_{1,Y}}$ ($\times 10^{-3}$)	$W_1^{m_{1,Z}}$ ($\times 10^{-3}$)
GEANT4	0.7 ± 0.2	0.8 ± 0.2	0.9 ± 0.4	0.7 ± 0.8	0.7 ± 0.1	0.9 ± 0.1	1.1 ± 0.3	0.9 ± 0.3
CALOCLOUDS	2.5 ± 0.3	11.4 ± 0.4	15.9 ± 0.7	2.0 ± 1.3	38.8 ± 1.4	4.0 ± 0.4	8.7 ± 0.3	1.4 ± 0.5
CALOCLOUDS II	3.6 ± 0.5	26.4 ± 0.4	15.3 ± 0.6	3.7 ± 1.6	11.6 ± 1.5	2.4 ± 0.4	7.6 ± 0.2	3.9 ± 0.4
CALOCLOUDS II (CM)	6.1 ± 0.7	9.8 ± 0.5	16.0 ± 0.7	2.0 ± 1.4	8.3 ± 1.9	3.0 ± 0.4	9.5 ± 0.6	1.2 ± 0.5

Define distributions and calculate 1D Wasserstein distance or Kullback-Leibler divergence

Surrogate Models

Collider or
classical
simulation

Training Data Set

Surrogate Model

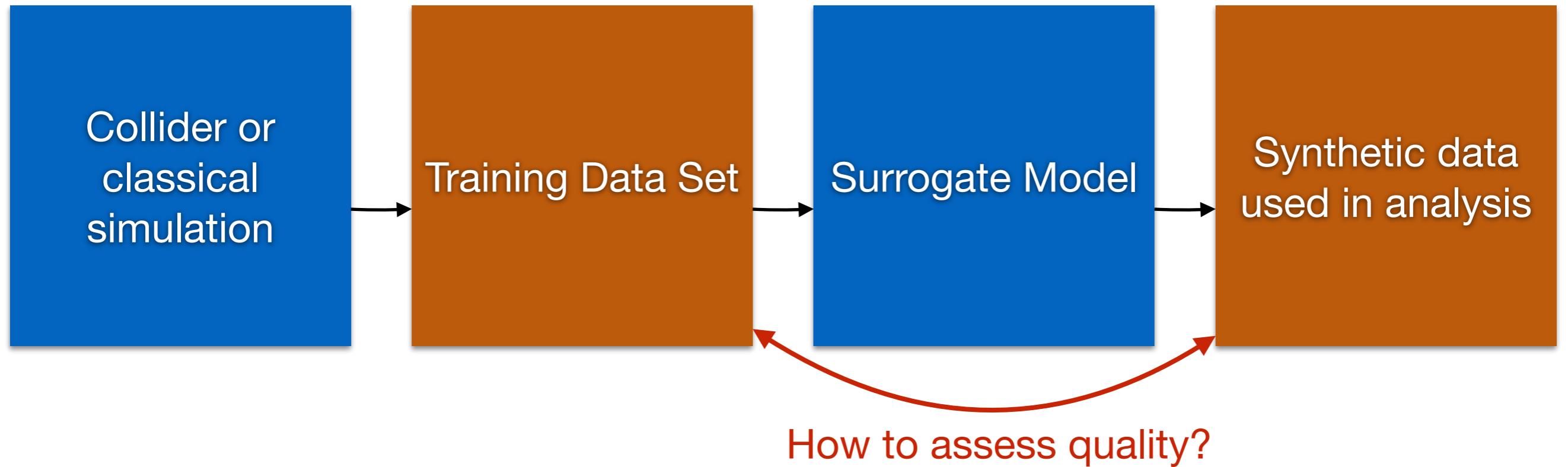
Synthetic data
used in analysis

How to assess quality?

Train a classifier and
look at area under
curve/JSD

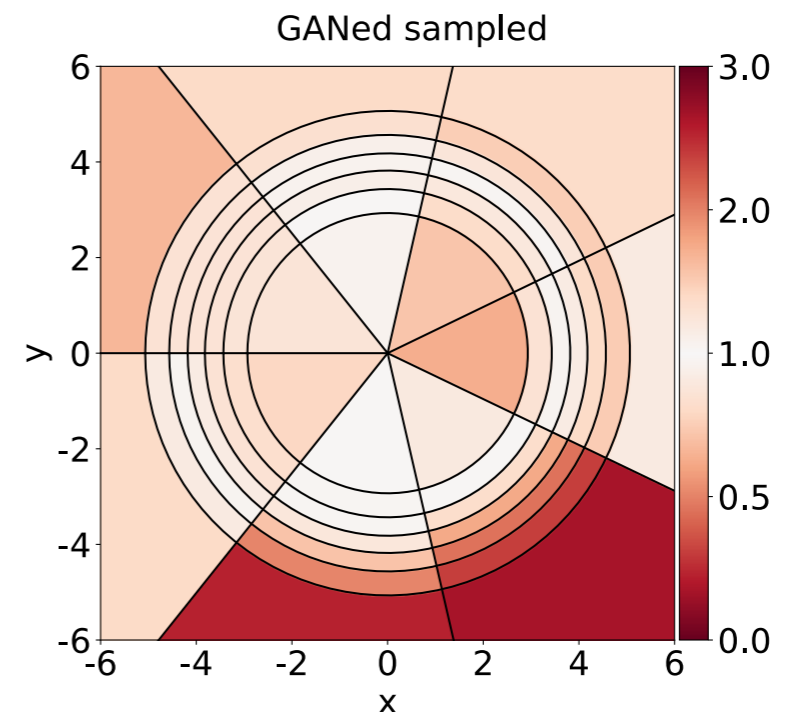
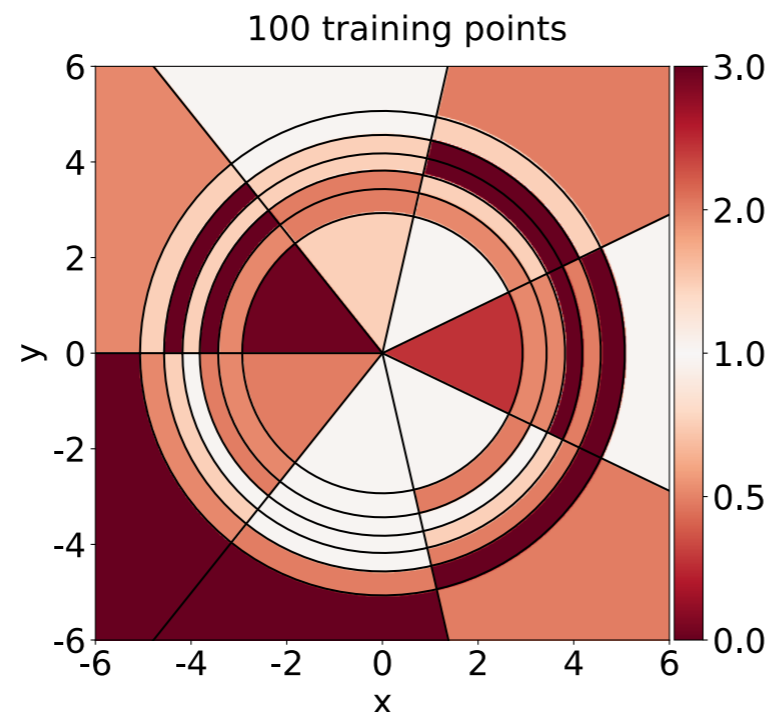
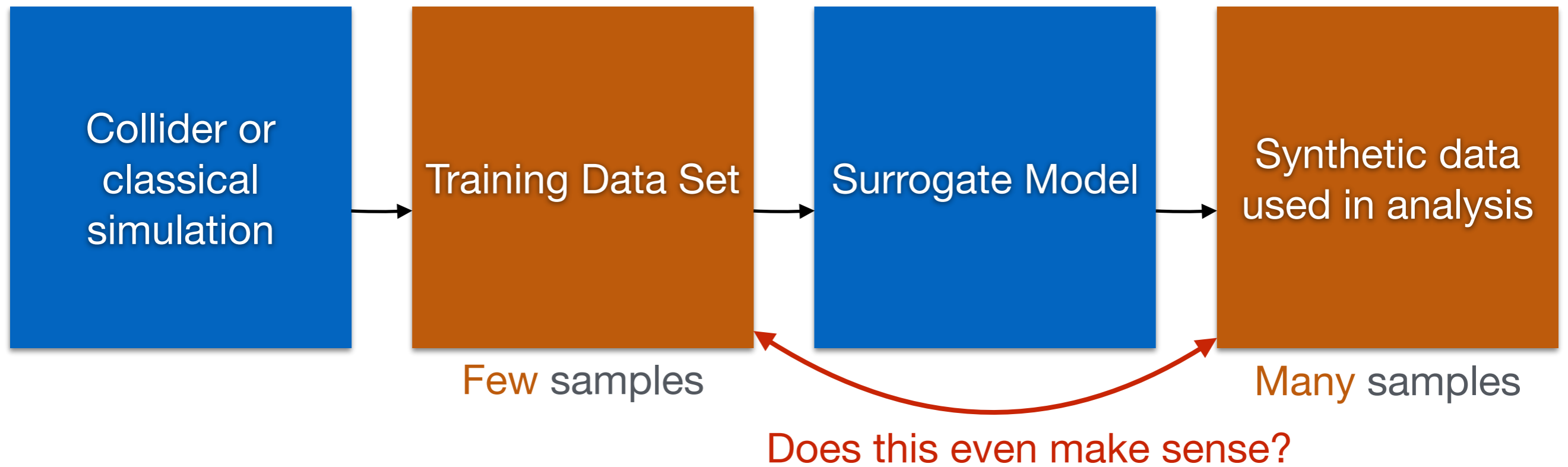
Dataset	Simulator	high level classifier		low level classifier	
		AUC	JSD	AUC	JSD
GETTINGHIGH	L2LFlows	$.634 \pm .002$	$.047 \pm .002$	$.905 \pm .003$	$.438 \pm .009$
	BIB-AE	$.903 \pm .002$	$.436 \pm .005$	$\gg .999$	$.985 \pm .001$
CALOCHALLENGE 3	L2LFlows	$.686 \pm .002$	$.084 \pm .001$	$.983 \pm .002$	$.760 \pm .013$

Surrogate Models

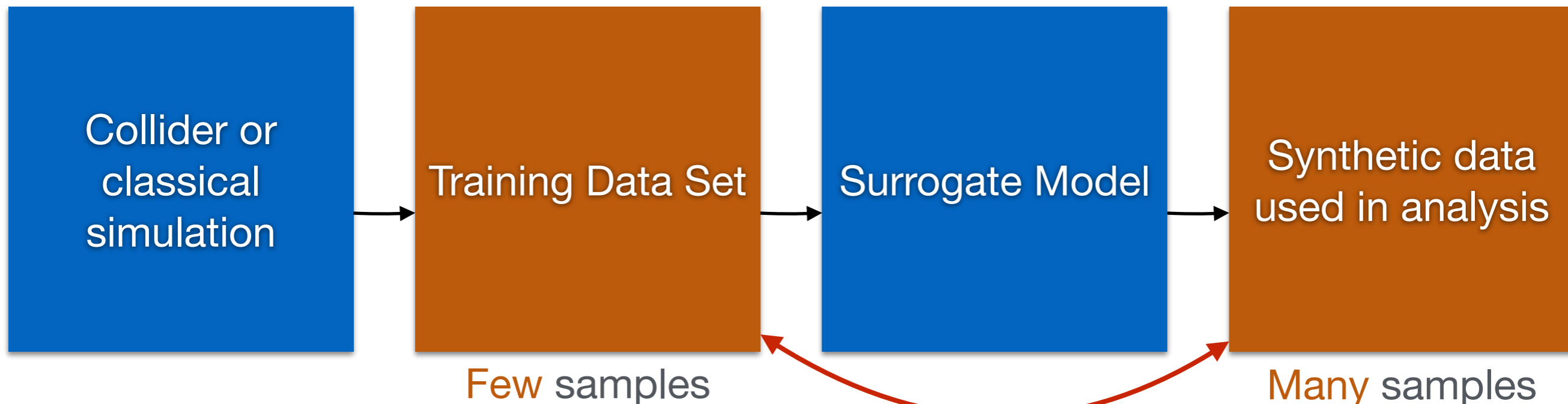


Room for a principled, holistic (for high-D data) quality measure that works for low amounts of reference data

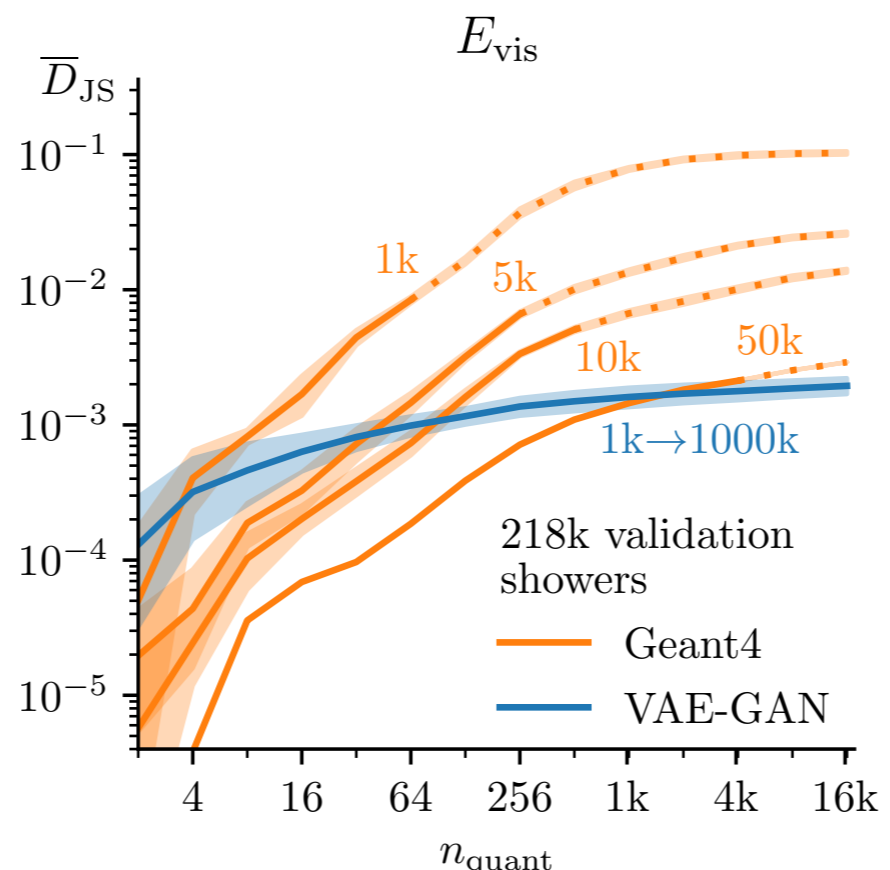
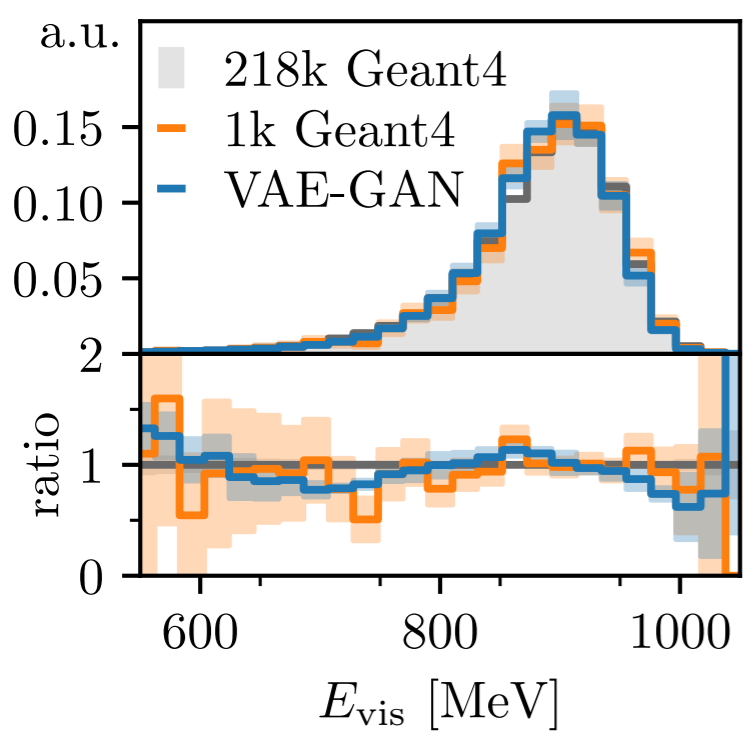
Surrogate Models



Surrogate Models

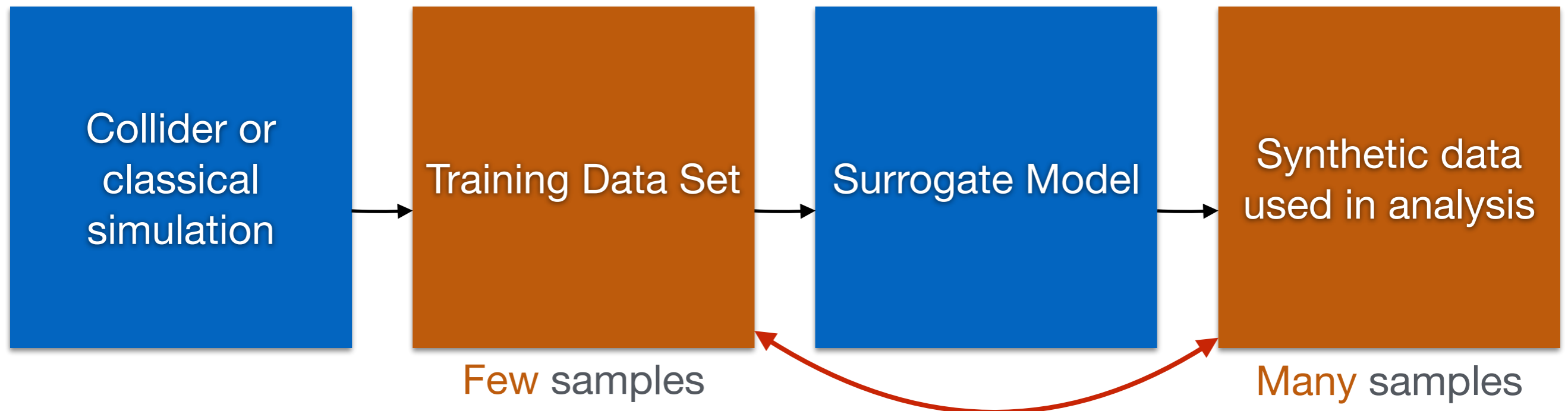


Does this even make sense?



Scaling of difference to ground truth with resolution again better for the generative model.

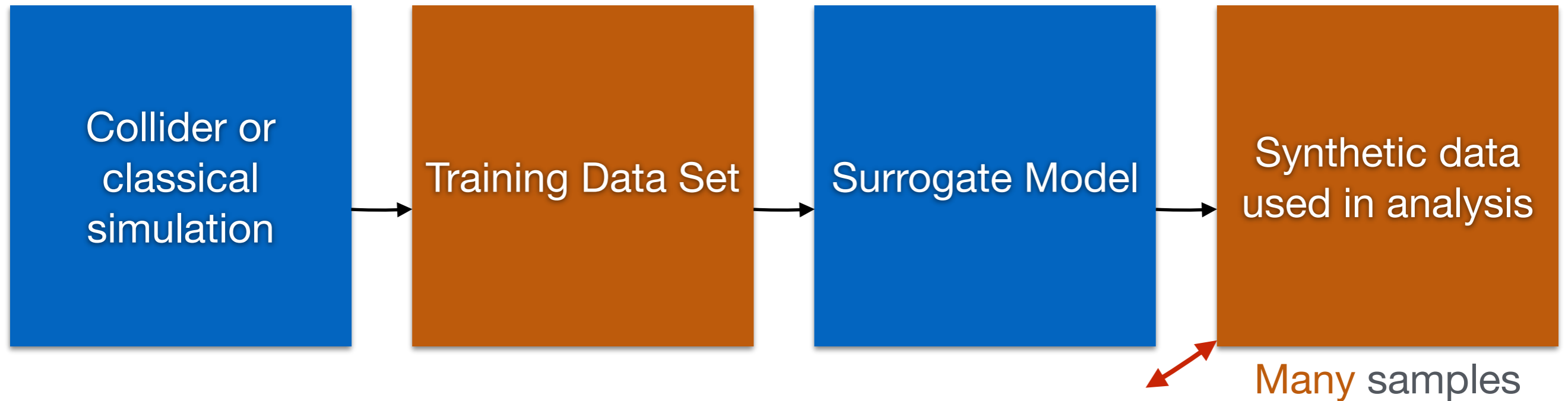
Surrogate Models



Does this even make sense?

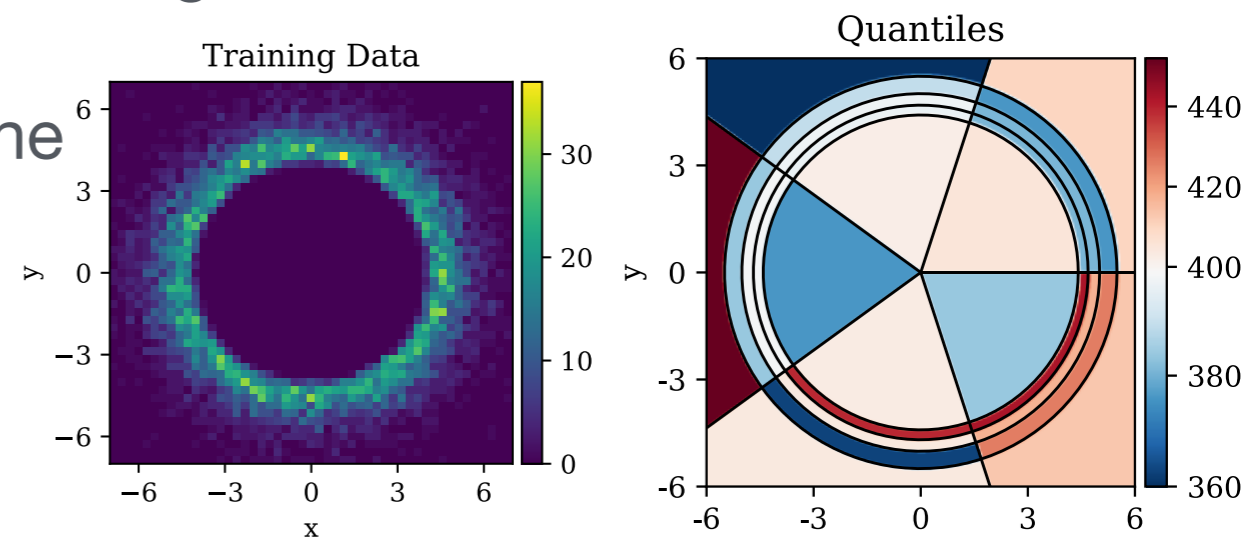
Seems so, especially if we include mixing (multiple showers/event) and interpolation

Surrogate Models



Can we determine statistical power of a sample without truth knowledge/ large reference?

- Train a **generative Bayesian** (e.g. Bayes-by-backprop or AdamMCMC) network (e.g. continuous normalising flow)
- **Sample weights** (i.e. individual models) from the Bayes model
- **Sample examples** from the individual models
- Compare **predicted uncertainty** to truth



Surrogate Models

Collider or
classical
simulation

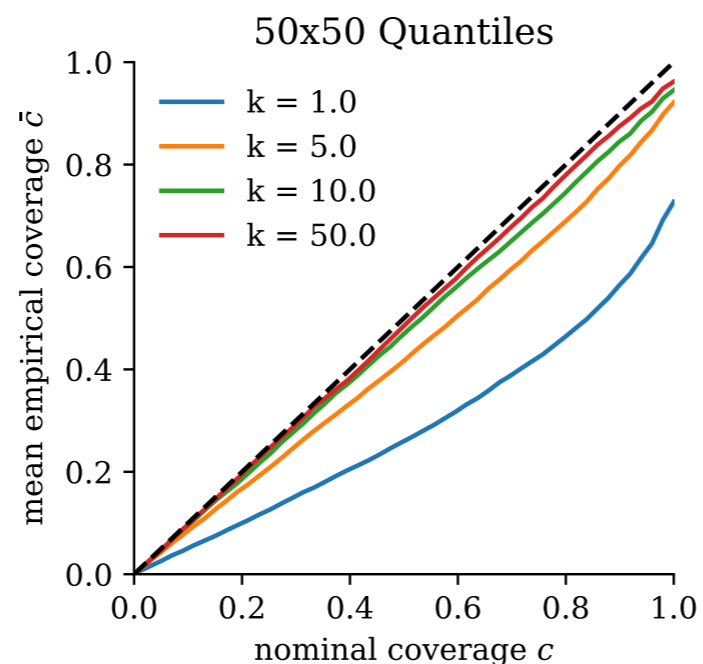
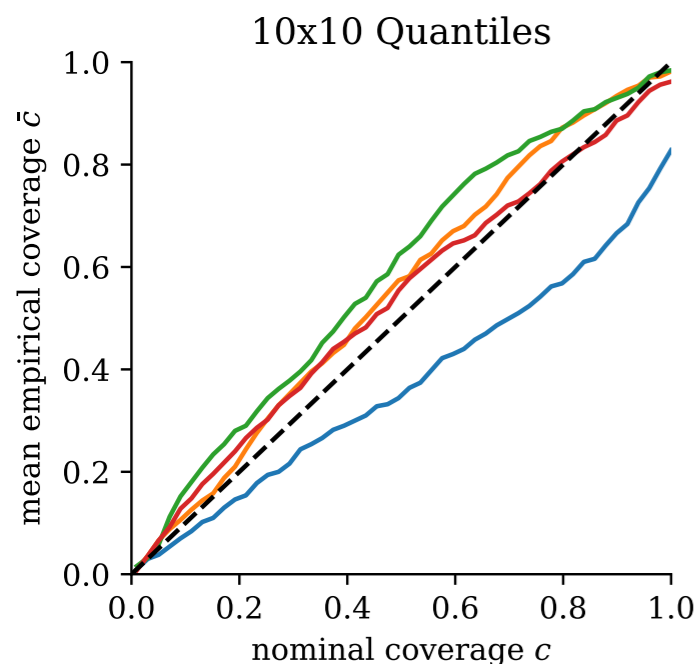
Training Data Set

Surrogate Model

Synthetic data
used in analysis

Many samples

Can we determine statistical power of
a sample without truth knowledge/
large reference?



Bayesian model is
well calibrated

Surrogate Models

Collider or
classical
simulation

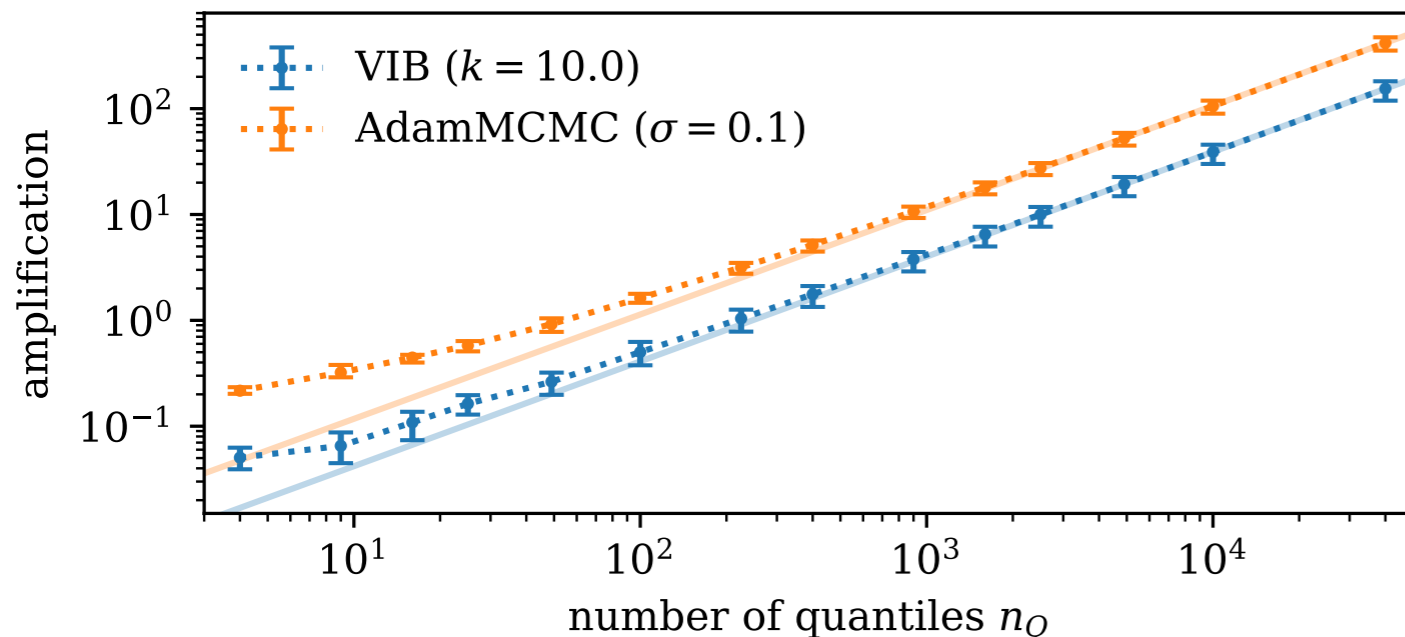
Training Data Set

Surrogate Model

Synthetic data
used in analysis

Many samples

Can we determine statistical power of
a sample without truth knowledge/
large reference?



Equate Bayesian uncertainty
to Poisson error to effective
sample size

Surrogate Models

Collider or
classical
simulation

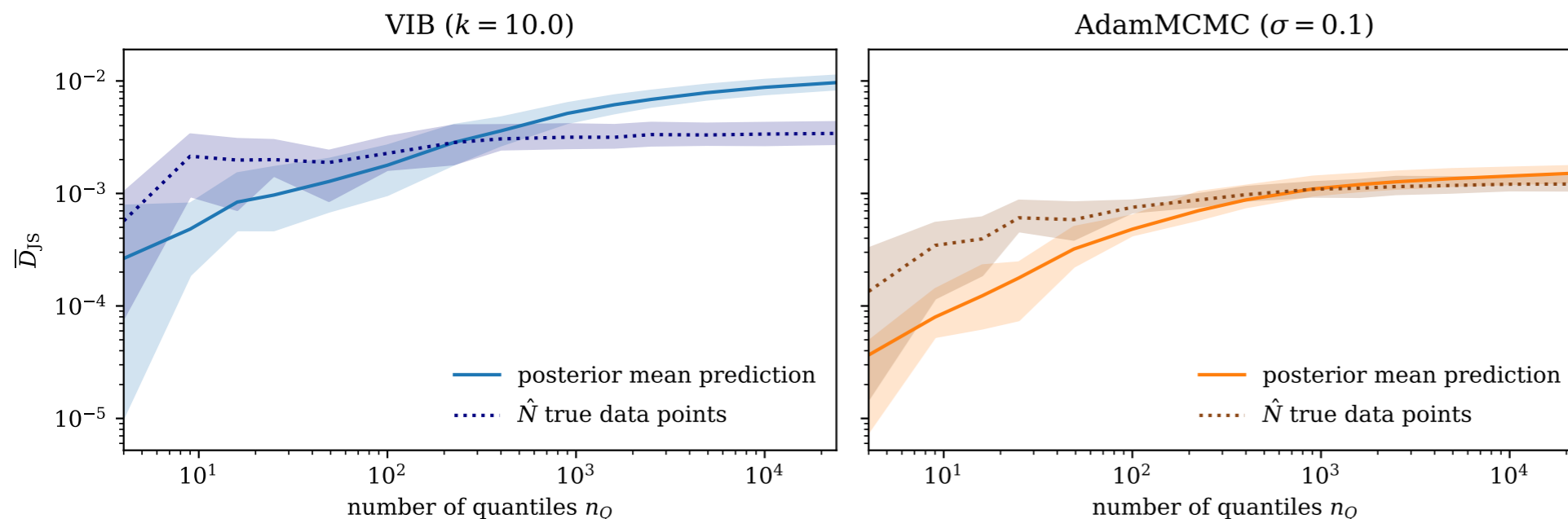
Training Data Set

Surrogate Model

Synthetic data
used in analysis

Many samples

Can we determine statistical power of
a sample without truth knowledge/
large reference?



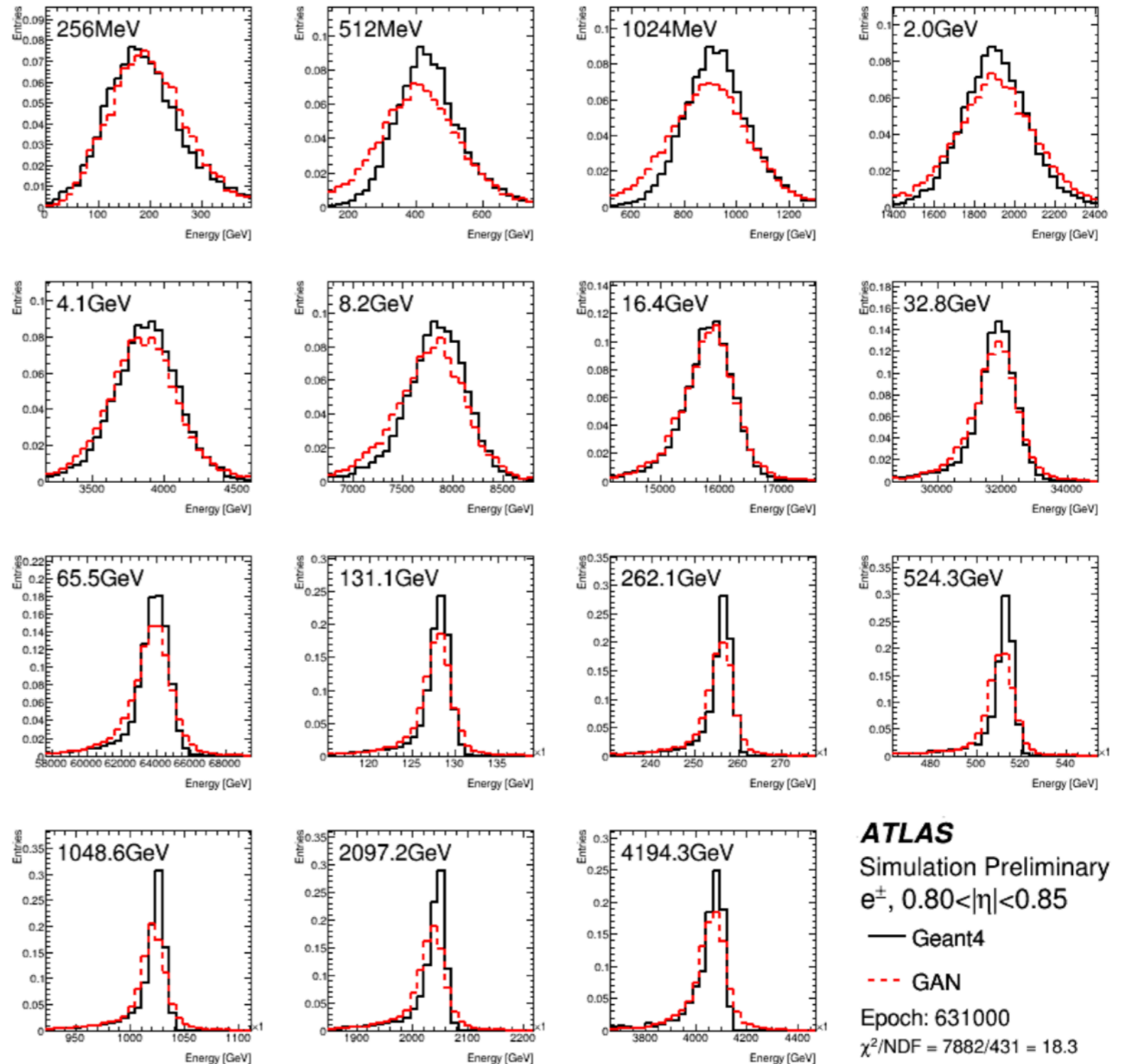
Agrees with JSD from
independent dataset

Application

Not only theoretical development: e.g. ATLAS includes **FastCaloGAN** in ATLFAST3

100 networks (slices in η)

$O(500)$ voxels



Moving forward

- 3 **Public datasets** to compare simulation techniques
 - Simplest: ATLAS dataset (see prev. page)
 - Most complex: Future detector with 40k voxels
 - Write-up currently ongoing

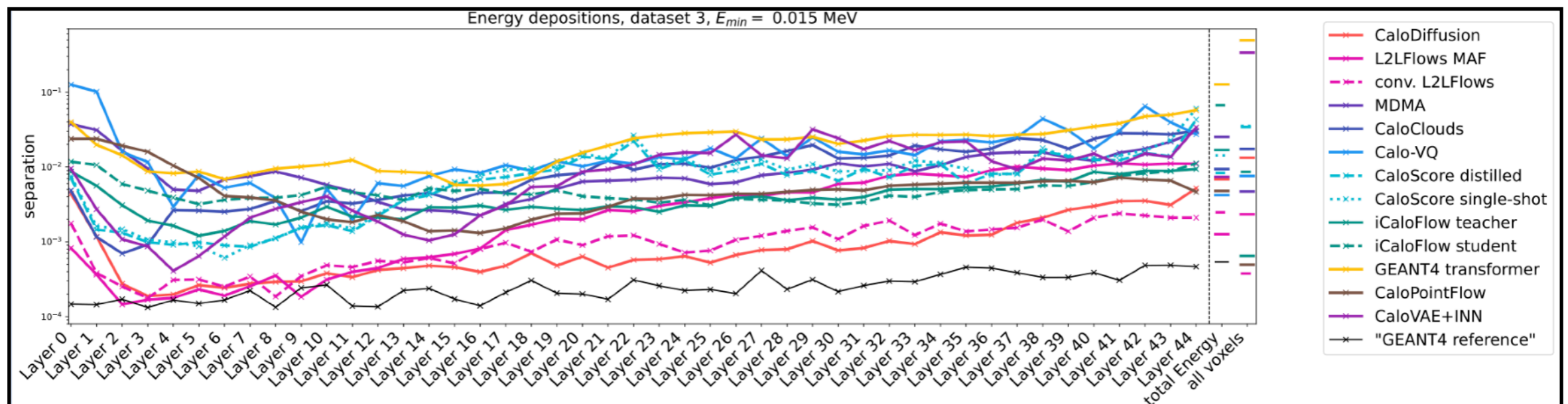
Fast Calorimeter Simulation Challenge 2022

[View on GitHub](#)

Welcome to the home of the first-ever Fast Calorimeter Simulation Challenge!

The purpose of this challenge is to spur the development and benchmarking of fast and high-fidelity calorimeter shower generation using deep learning methods. Currently, generating calorimeter showers of interacting particles (electrons, photons, pions, ...) using GEANT4 is a major computational bottleneck at the LHC, and it is forecast to overwhelm the computing budget of the LHC experiments in the near future. Therefore there is an urgent need to develop GEANT4 emulators that are both fast (computationally lightweight) and accurate. The LHC collaborations have been developing fast simulation methods for some time, and the hope of this challenge is to directly compare new deep learning approaches on common benchmarks. It is expected that participants will make use of cutting-edge techniques in generative modeling with deep learning, e.g. GANs, VAEs and normalizing flows.

This challenge is modeled after two previous, highly successful data challenges in HEP – the [top tagging community challenge](#) and the [LHC Olympics 2020 anomaly detection challenge](#).



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

AI

Inference

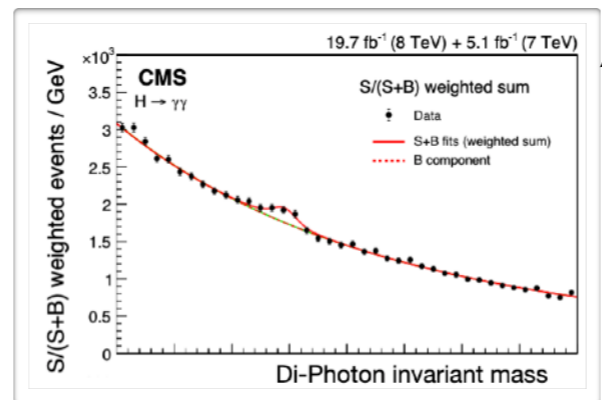
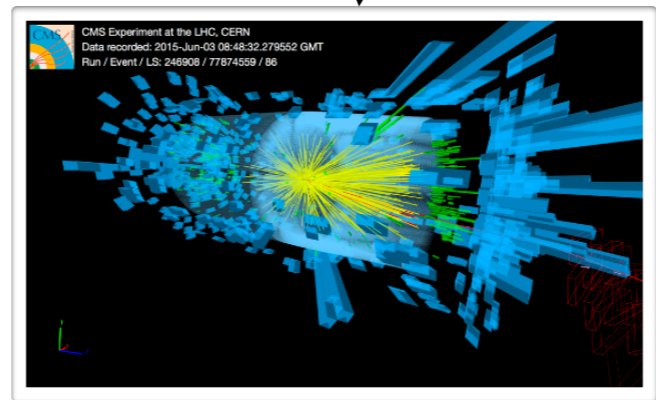
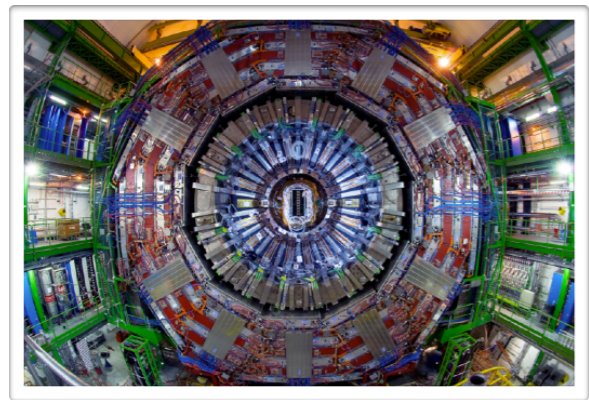
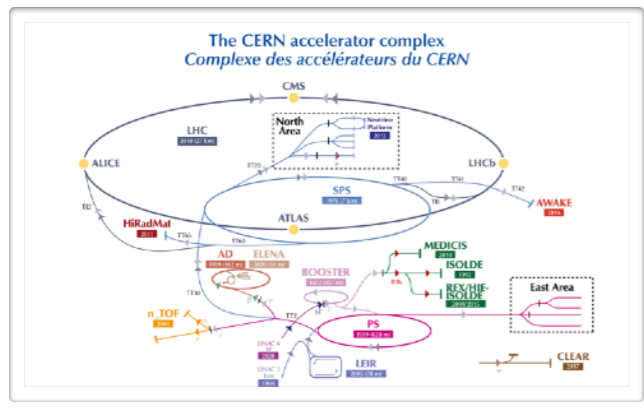
Experiment Design

Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection



See talk by **Vinicius**

Unfolding

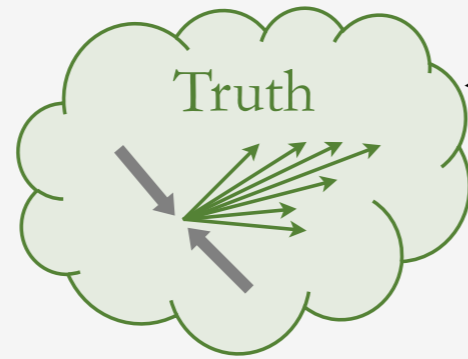
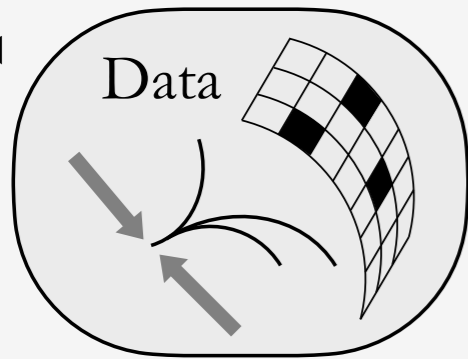
Observe

Want to know

Detector-level

Particle-level

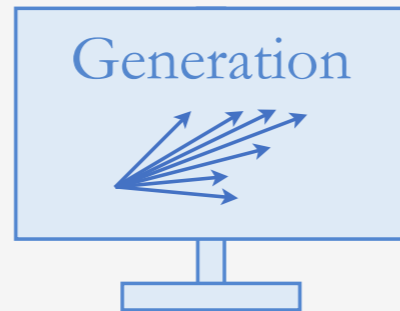
Natural



(and relate to fundamental theory)

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + \text{h.c.} \\ & + \chi_i Y_{ij} \chi_j \phi + \text{h.c.} \\ & + |D_\mu \phi|^2 - V(\phi) \end{aligned}$$

Synthetic



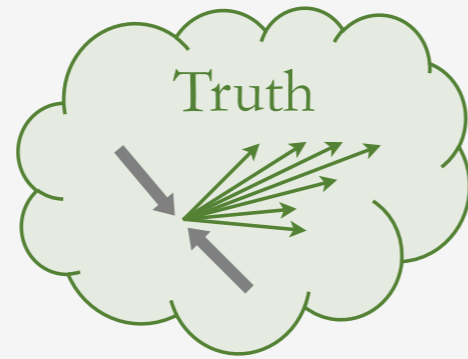
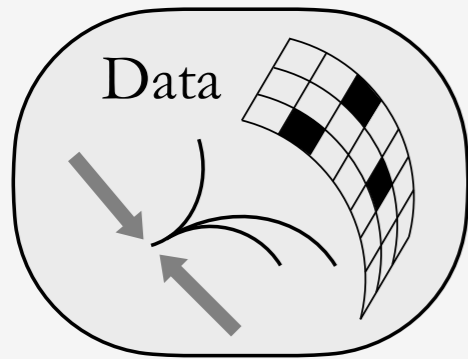
Synthetic data provides both views: How to use?

Unfolding

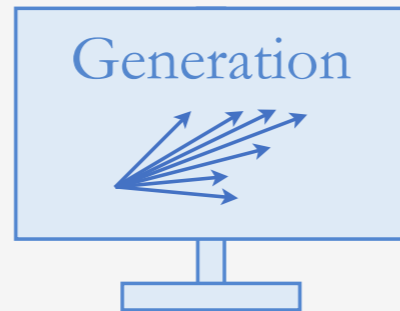
Detector-level

Particle-level

Natural



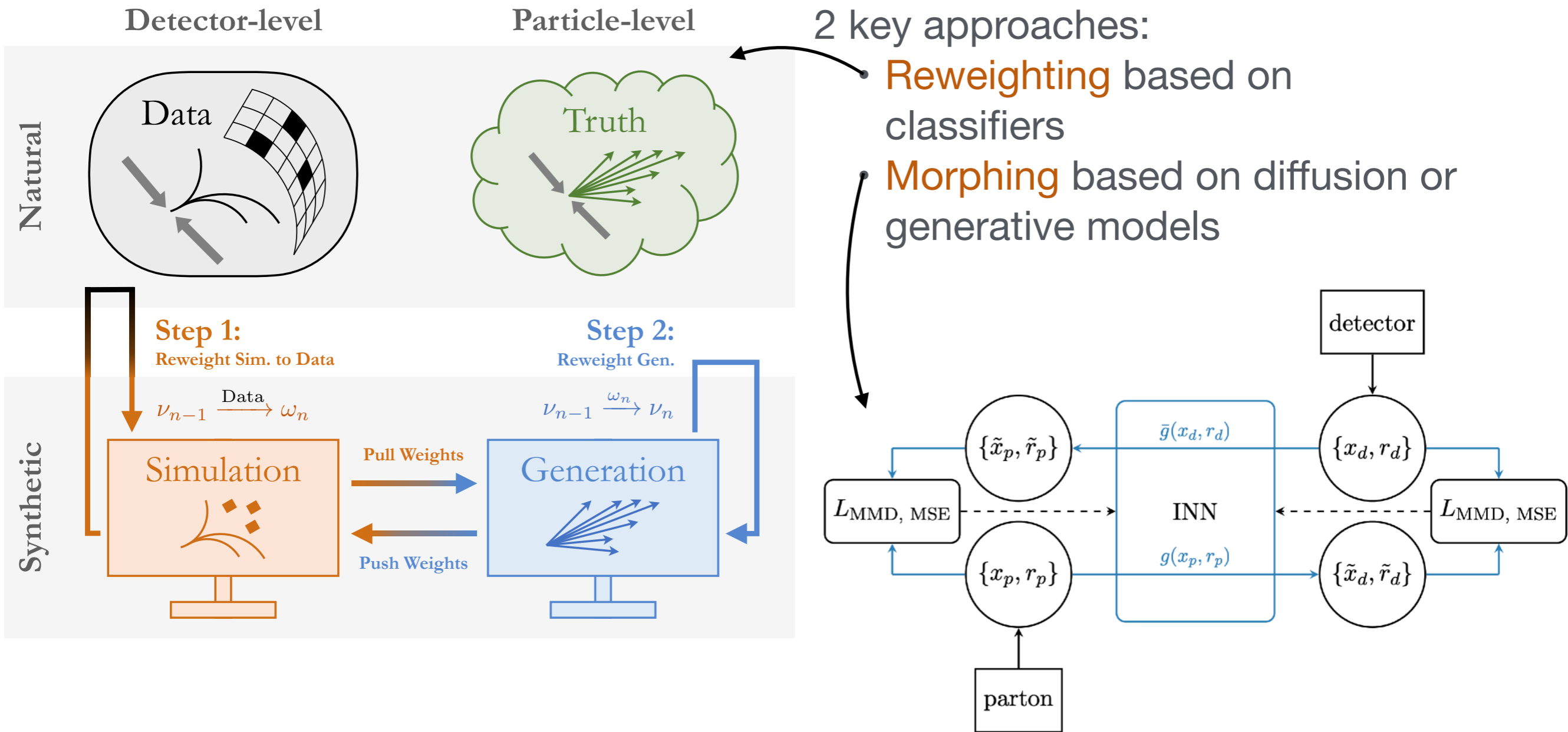
Synthetic



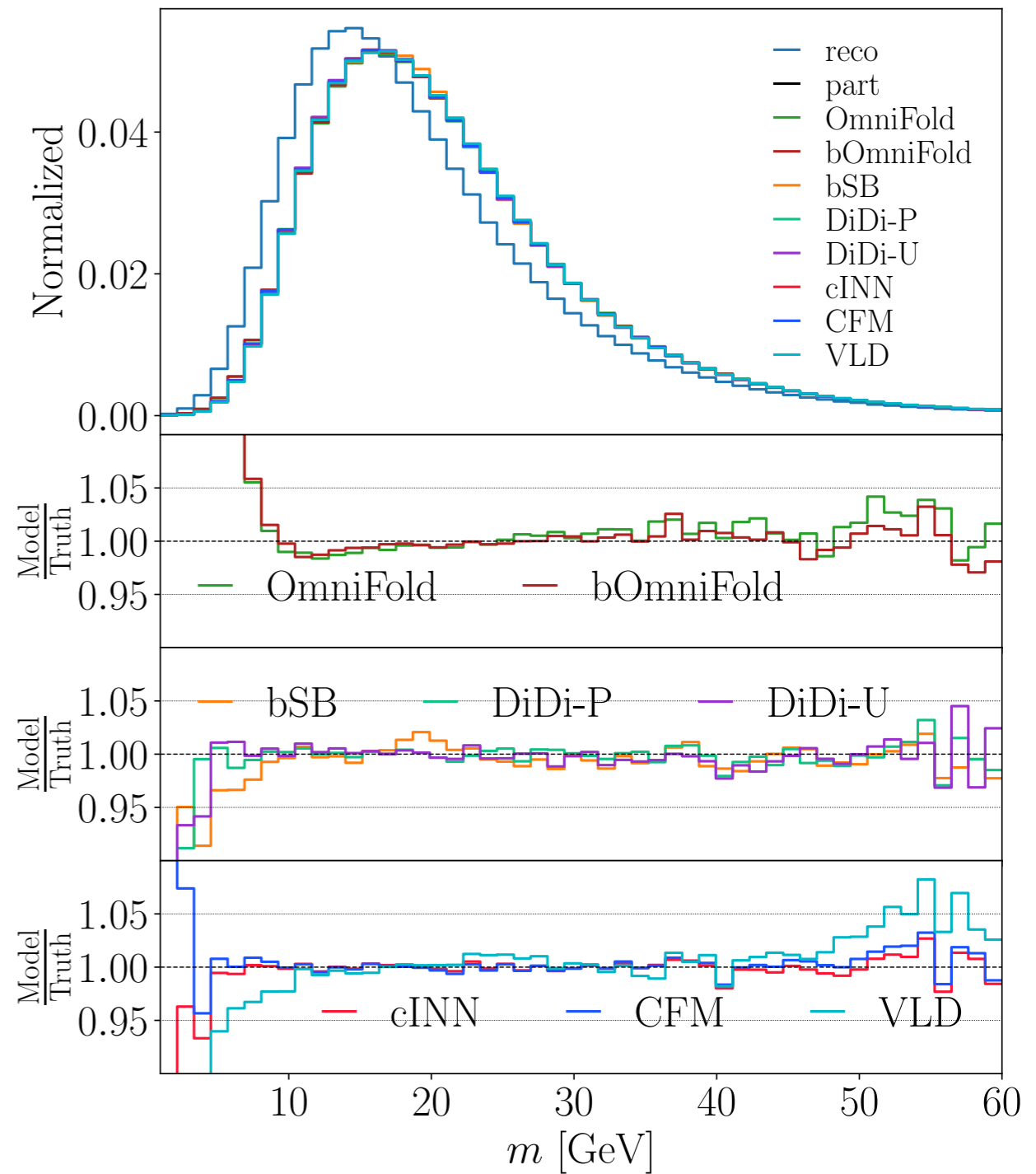
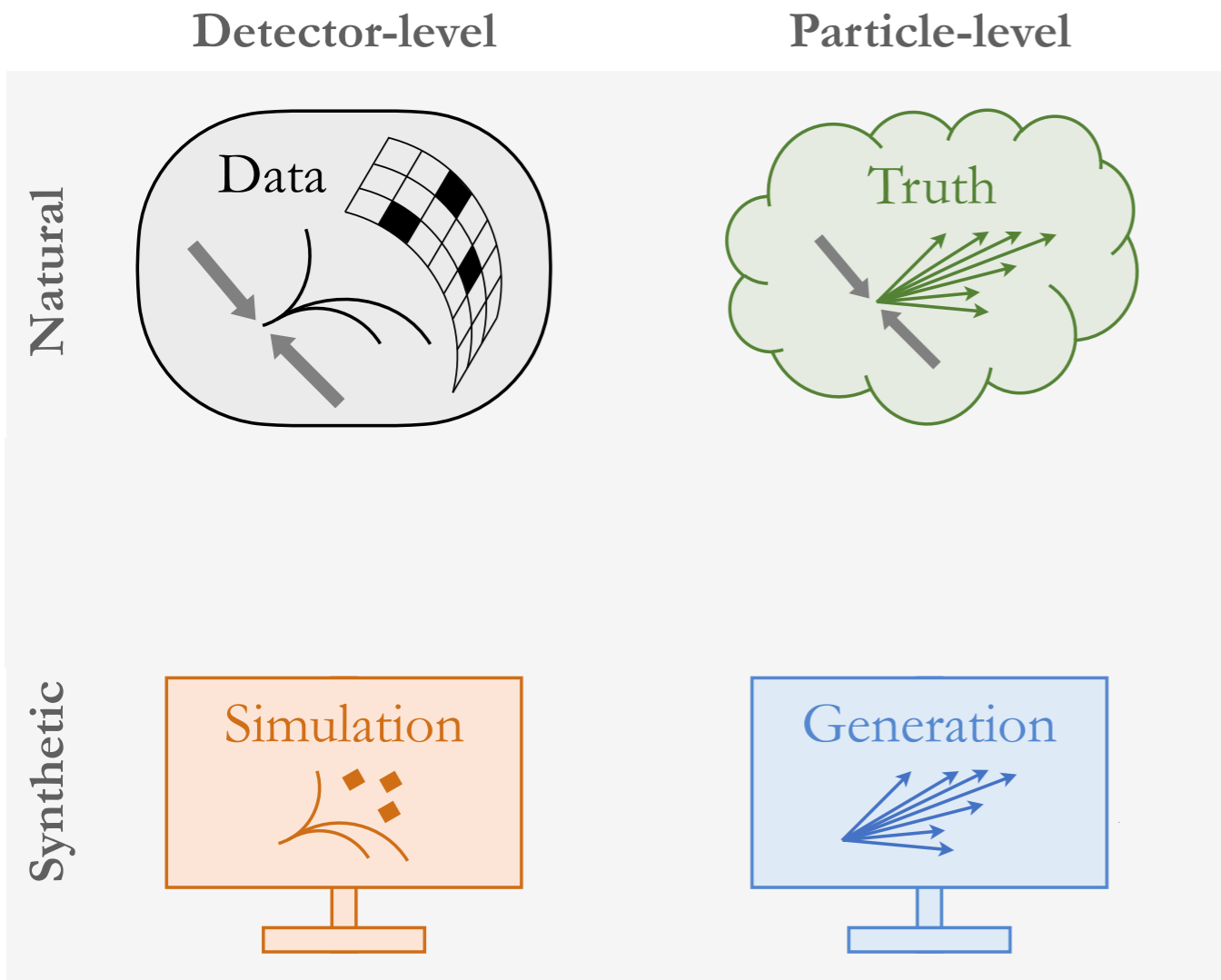
2 key approaches:

- **Reweighting** based on classifiers
- **Morphing** based on diffusion or generative models

Unfolding



Unfoldina



Example: Unfold Z+jets distributions in six dimensions

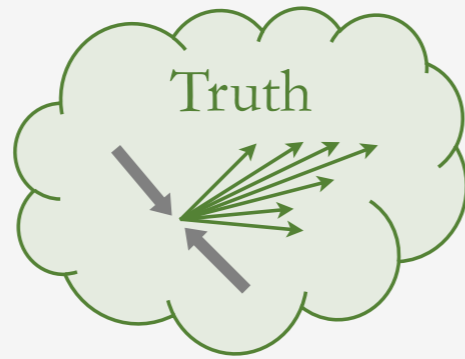
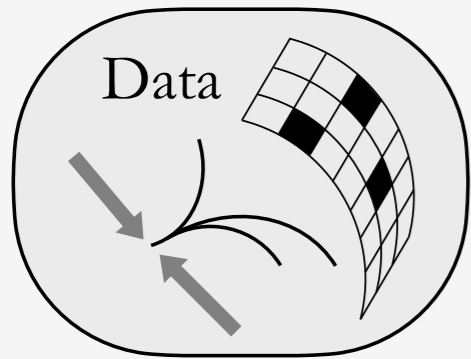
See talk by **Tilman** and **Vinicius**

Unfolding

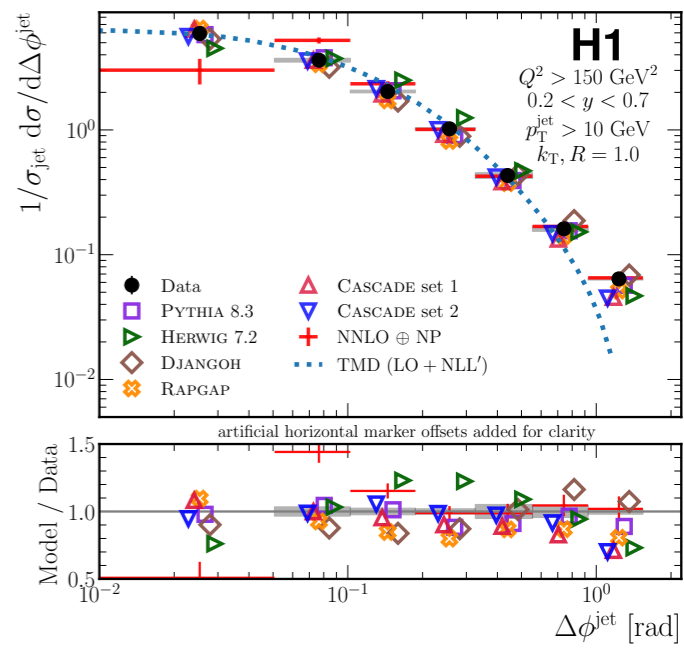
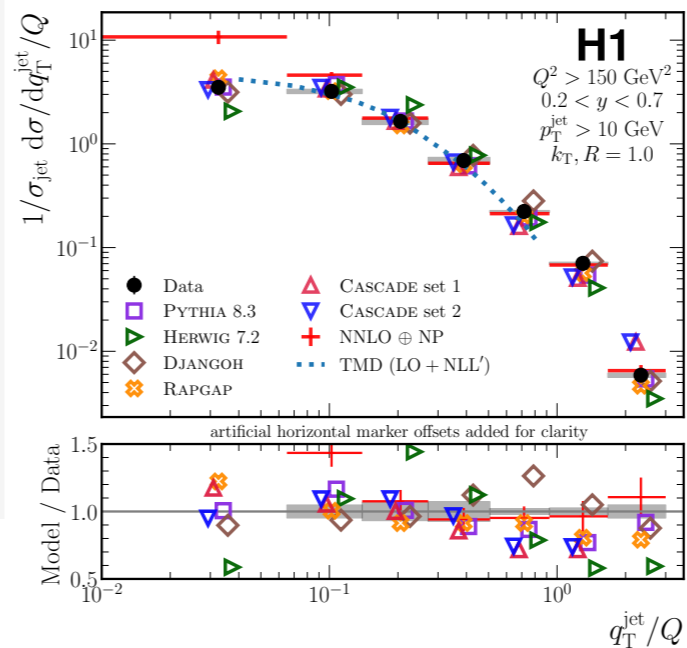
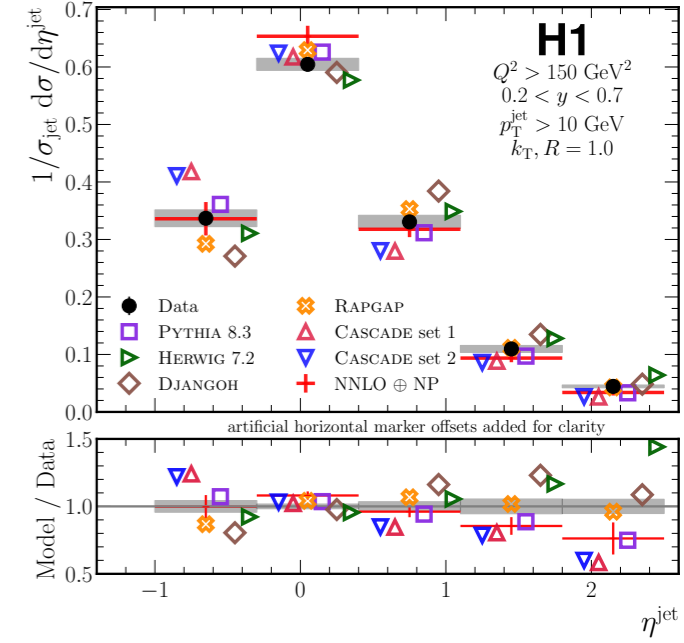
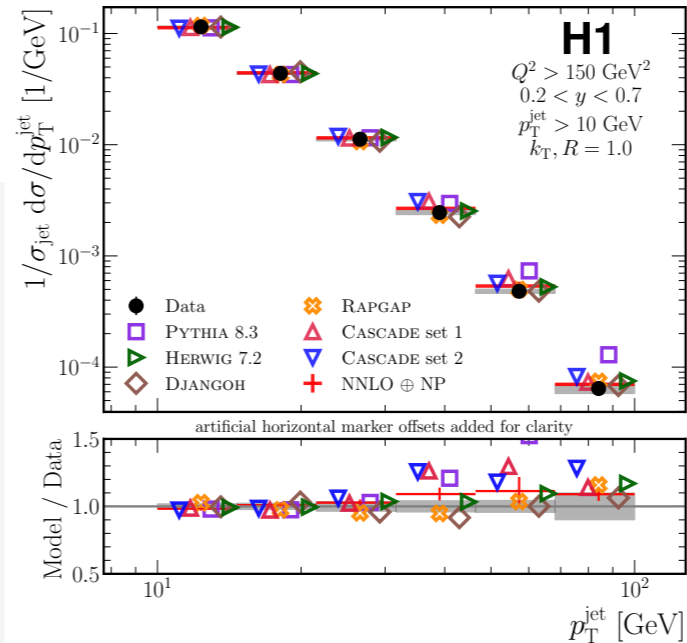
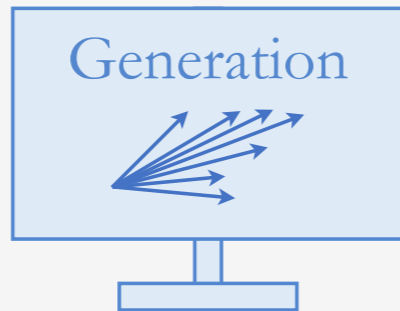
Detector-level

Particle-level

Natural



Synthetic



Already applied to collider data:
Multifold on lepton/jet events at H1

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

AI

Inference

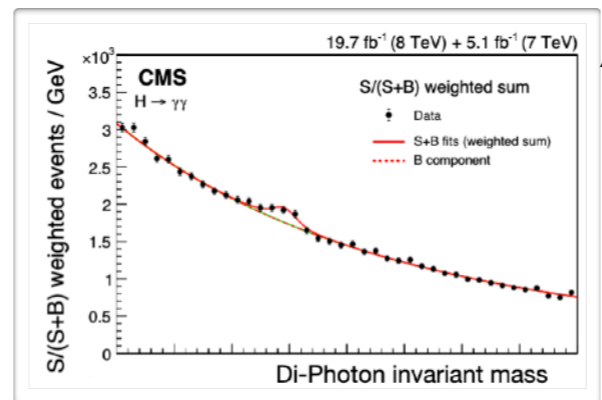
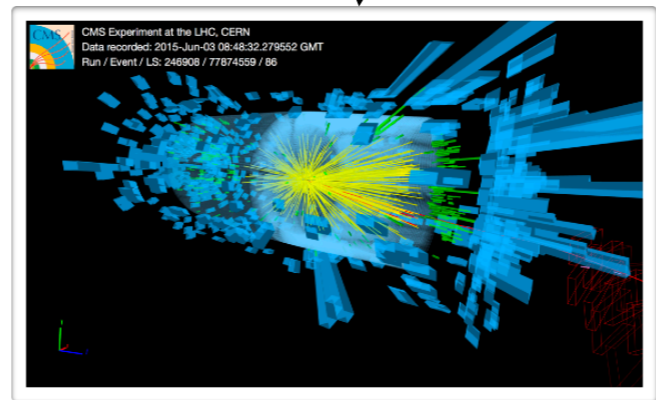
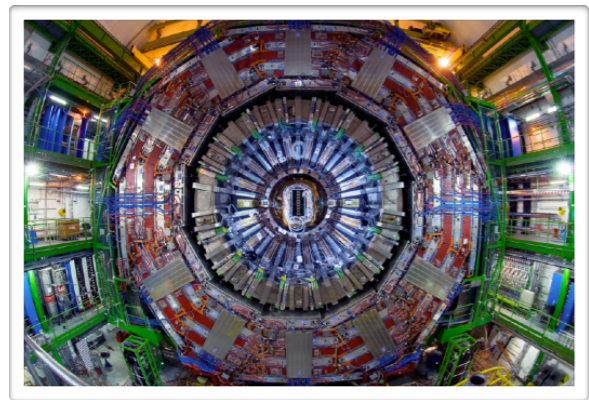
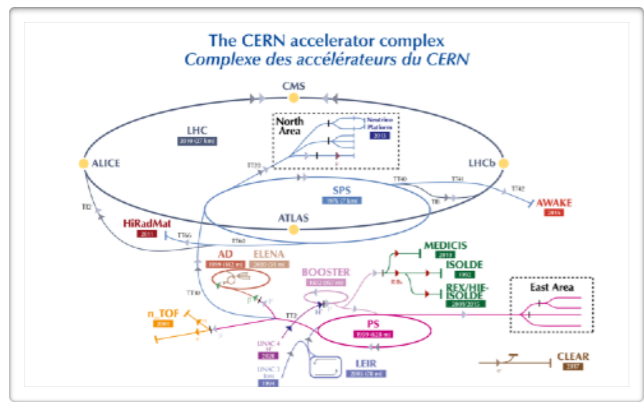
Experiment Design

Simulation

Triggers

Tagging Reconstruction

Unfolding Anomaly Detection

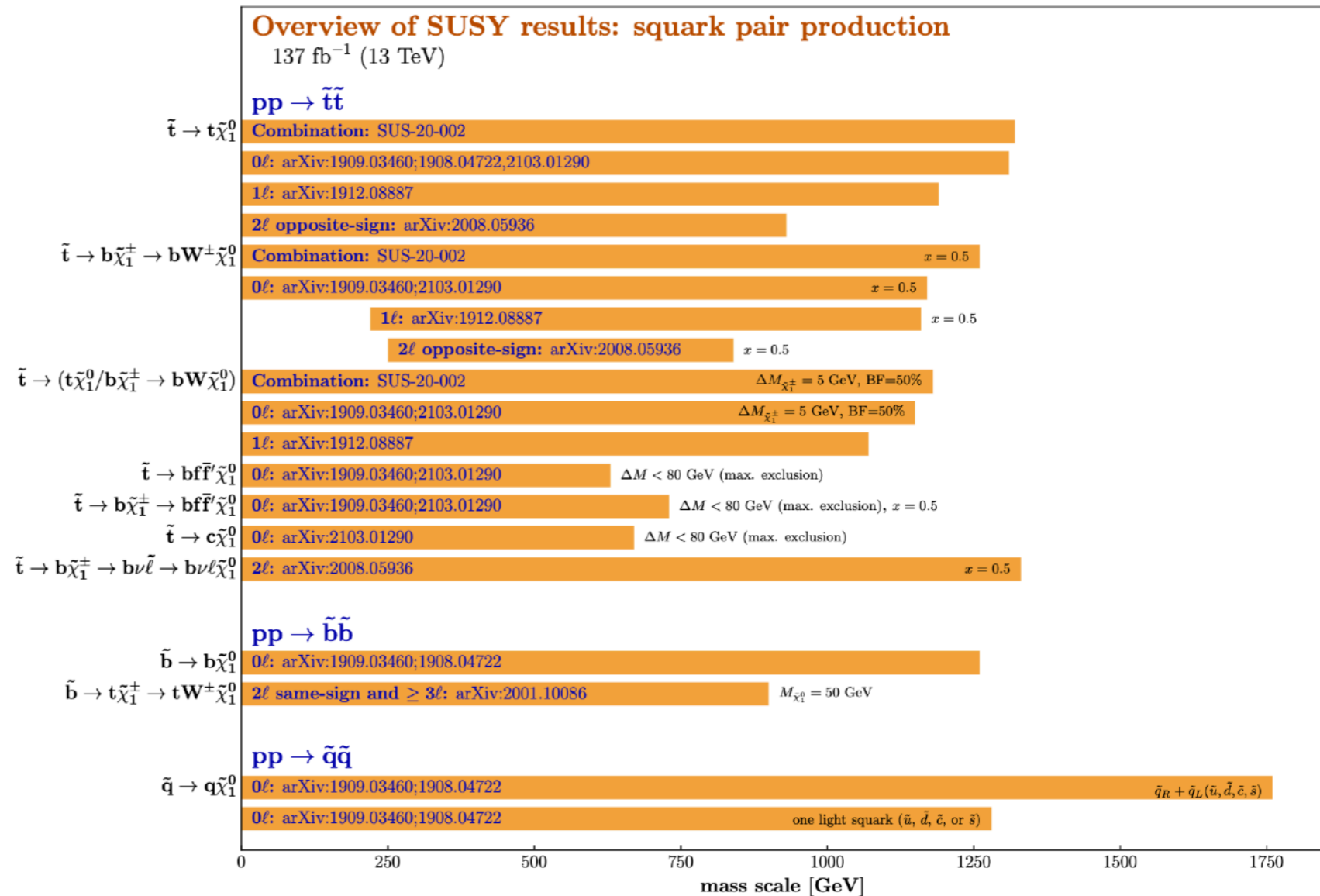


Motivation

- Expect physics beyond the Standard Model
- Only negative results in searches
- Two discovery strategies:
 - Model-specific
 - **Model independent**
- Trade off: Sensitivity to specific model vs broad coverage

CMS (preliminary)

Moriond 2021

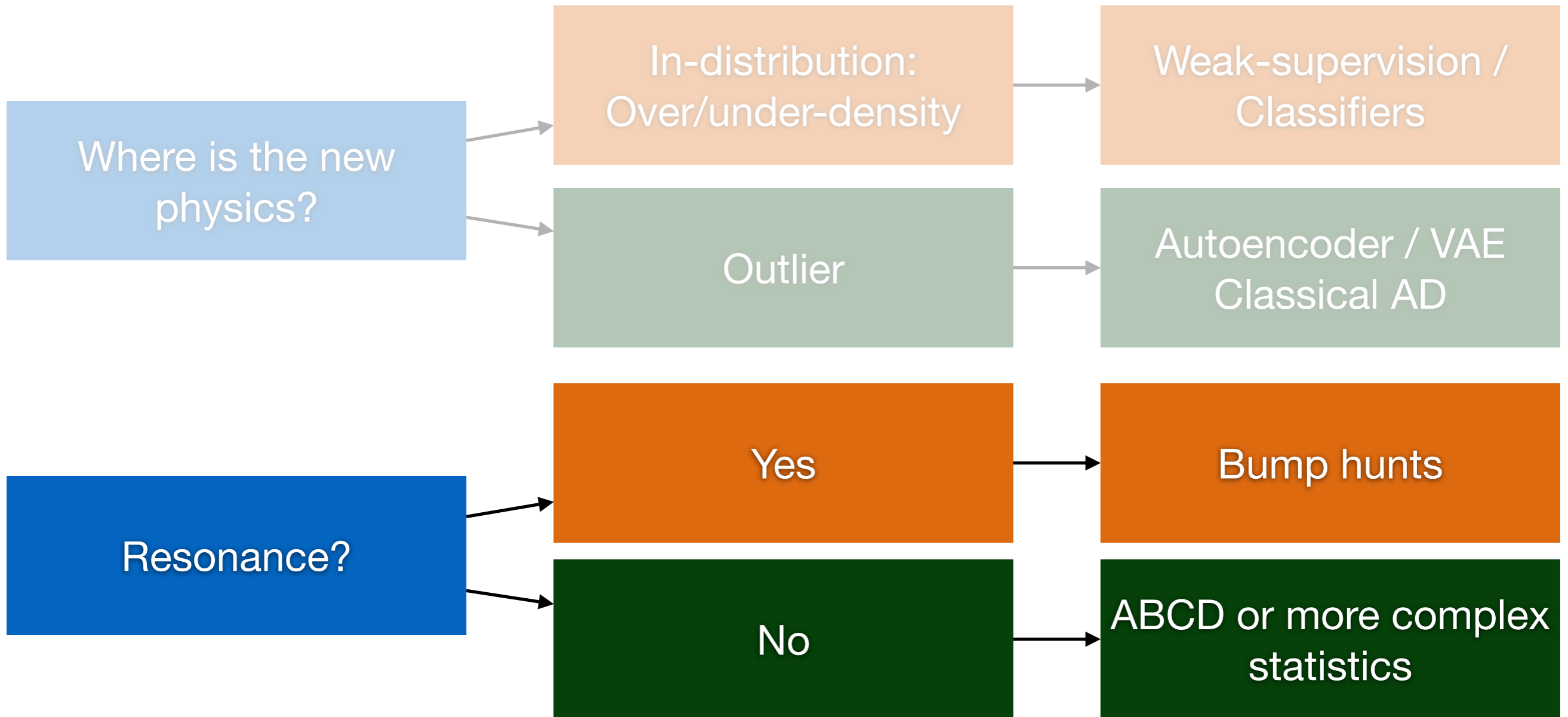


Selection of observed limits at 95% C.L. (theory uncertainties are not included). Probe up to the quoted mass limit for light LSPs unless stated otherwise. The quantities ΔM and x represent the absolute mass difference between the primary sparticle and the LSP, and the difference between the intermediate sparticle and the LSP relative to ΔM , respectively, unless indicated otherwise.

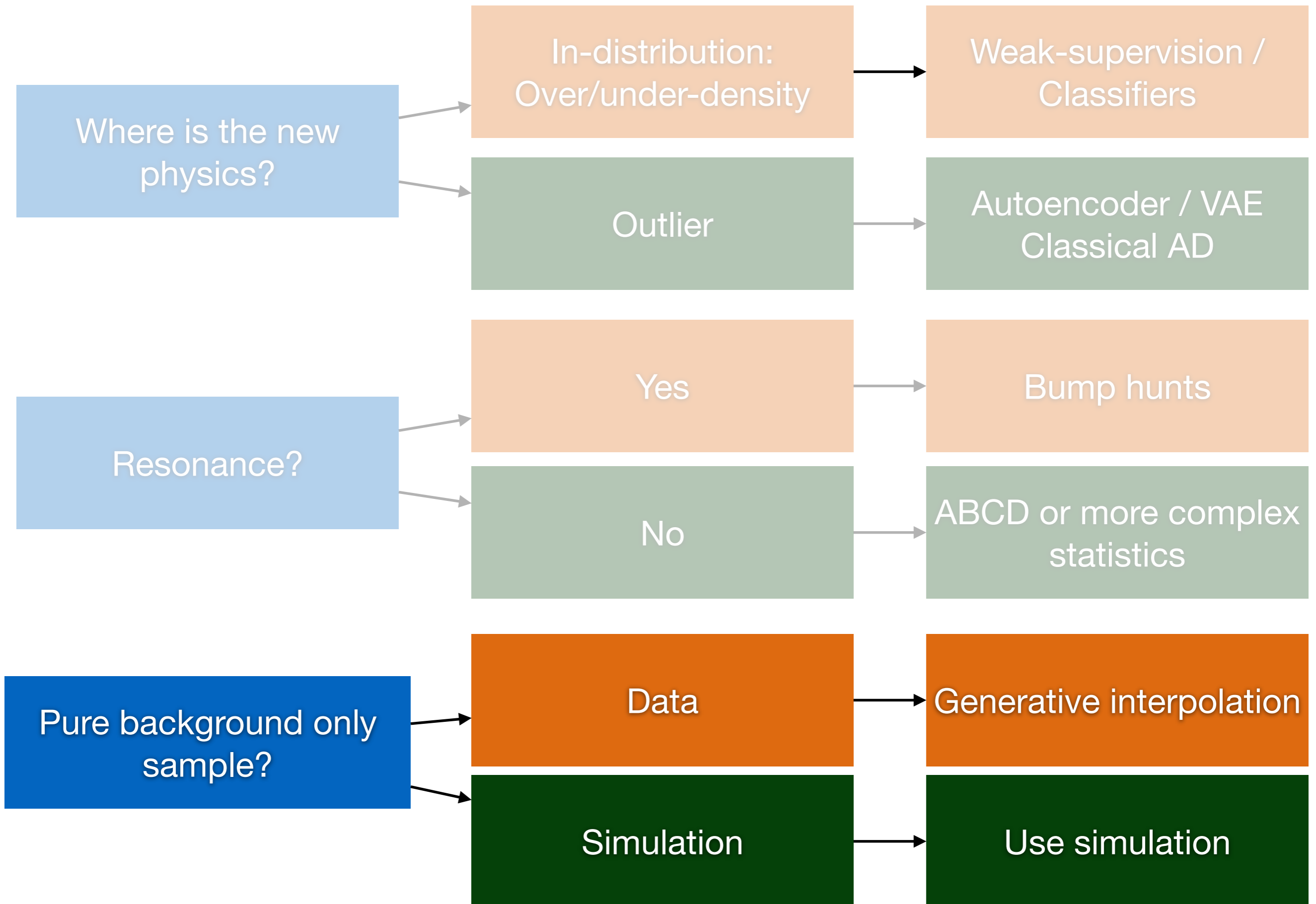
Choices



Choices



Choices



More Choices

Tails?

Feature Dimension?

Interpolation approach?

...

Choices

Where is the new physics?

In-distribution:
Over/under-density

Weak-supervision /
Classifiers

Outlier

Autoencoder / VAE
Classical AD

Resonance?

Yes

Bump hunts

No

ABCD or more complex
statistics

Pure background only
sample?

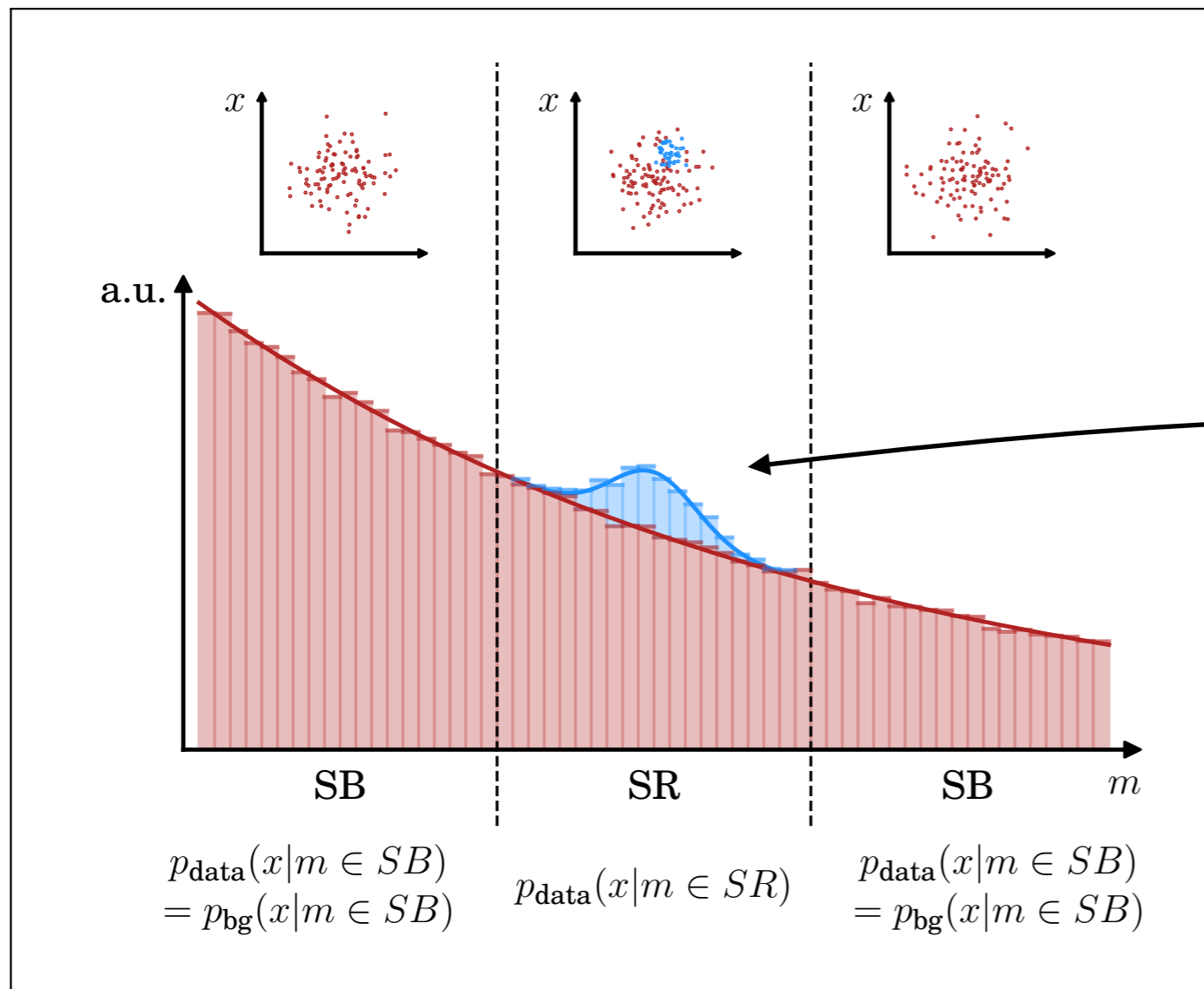
Data

Generative
interpolation

Simulation

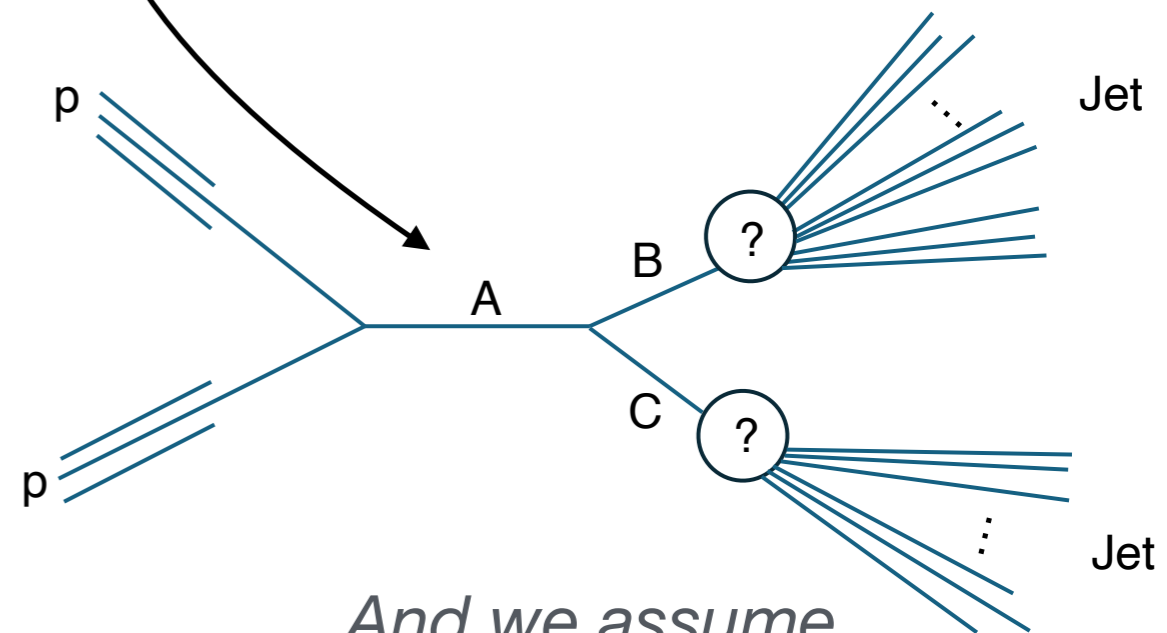
Use simulation

CATHODE



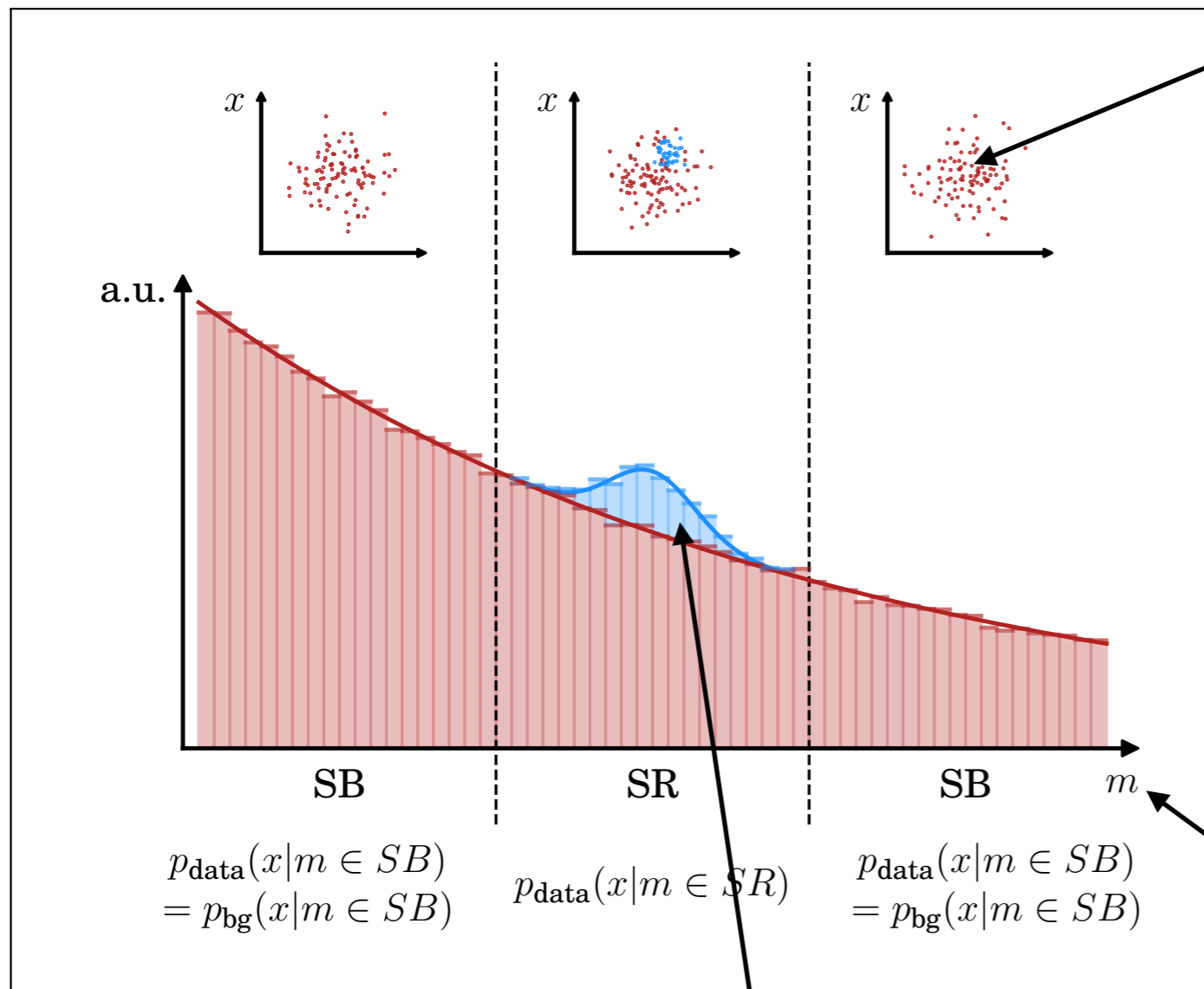
Consider resonant anomalies:
fully data-based construction of
anomaly detection score

*We don't assume
the **mass and type**
of the resonant
particle*

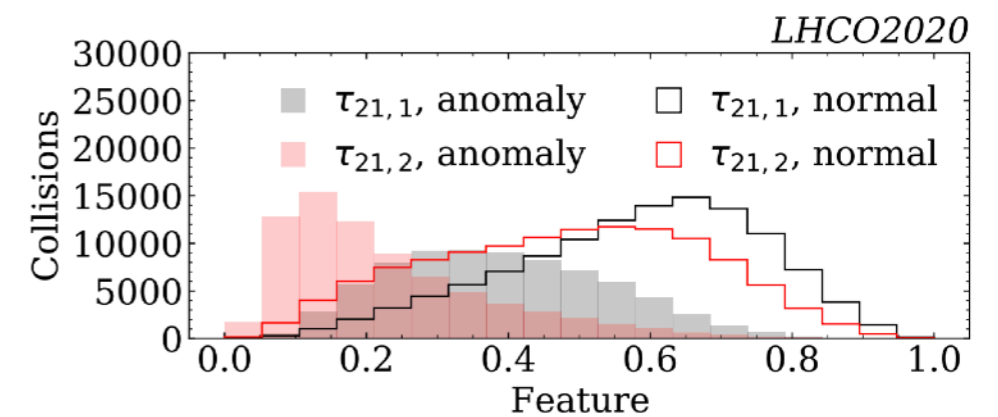
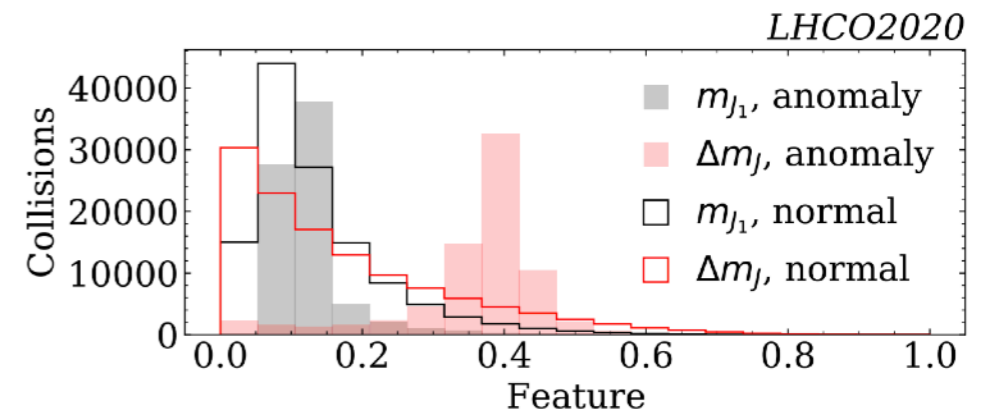


GK, Nachmann, Shih et al 2101.08320; Hallin, .., **GK** et al 2109.00546; Many similar approaches — see e.g. Golling, **GK** et al 2307.11157 for an overview

CATHODE



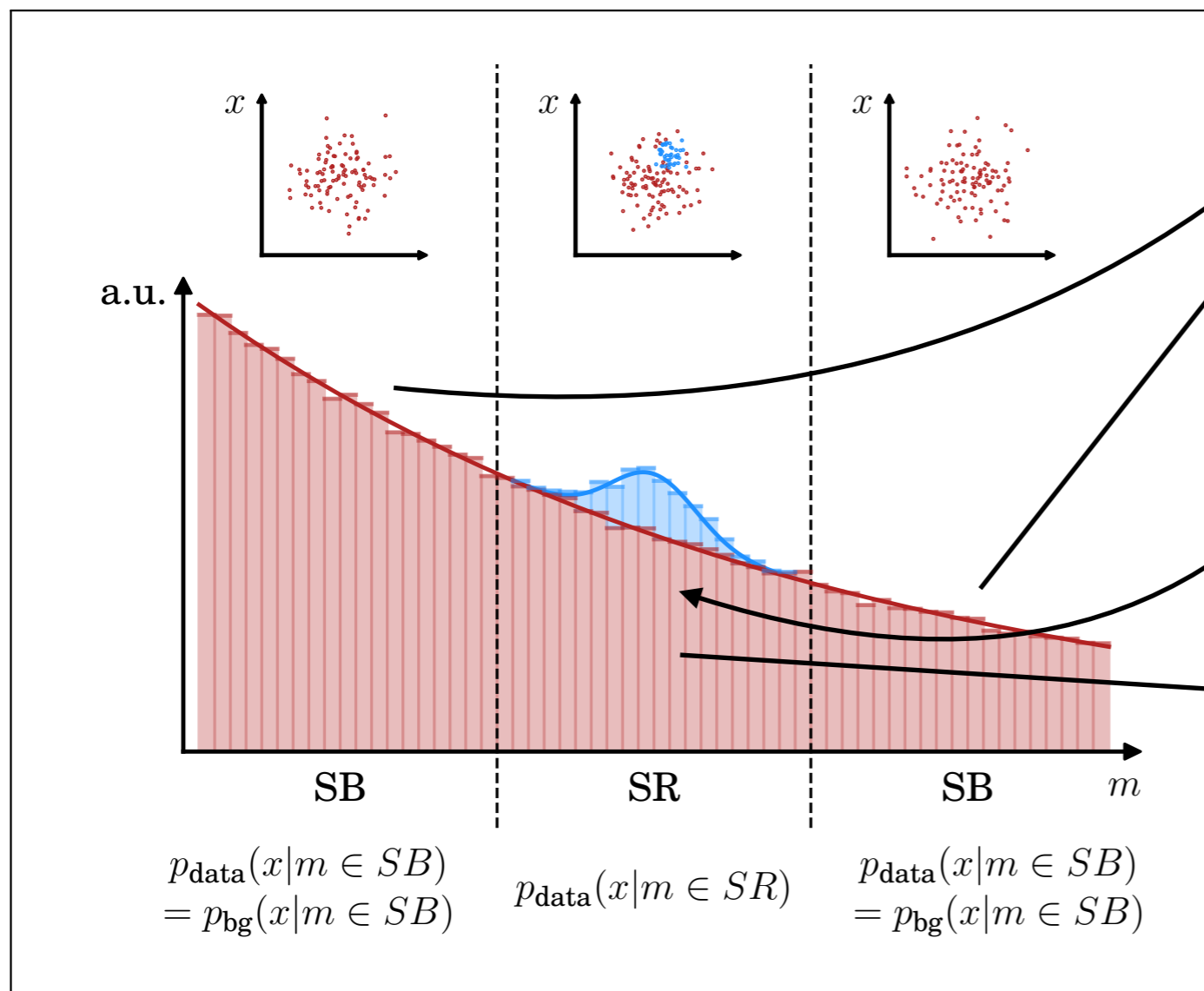
4 additional features



Signal too small to be visible in inclusive distribution

one resonant feature

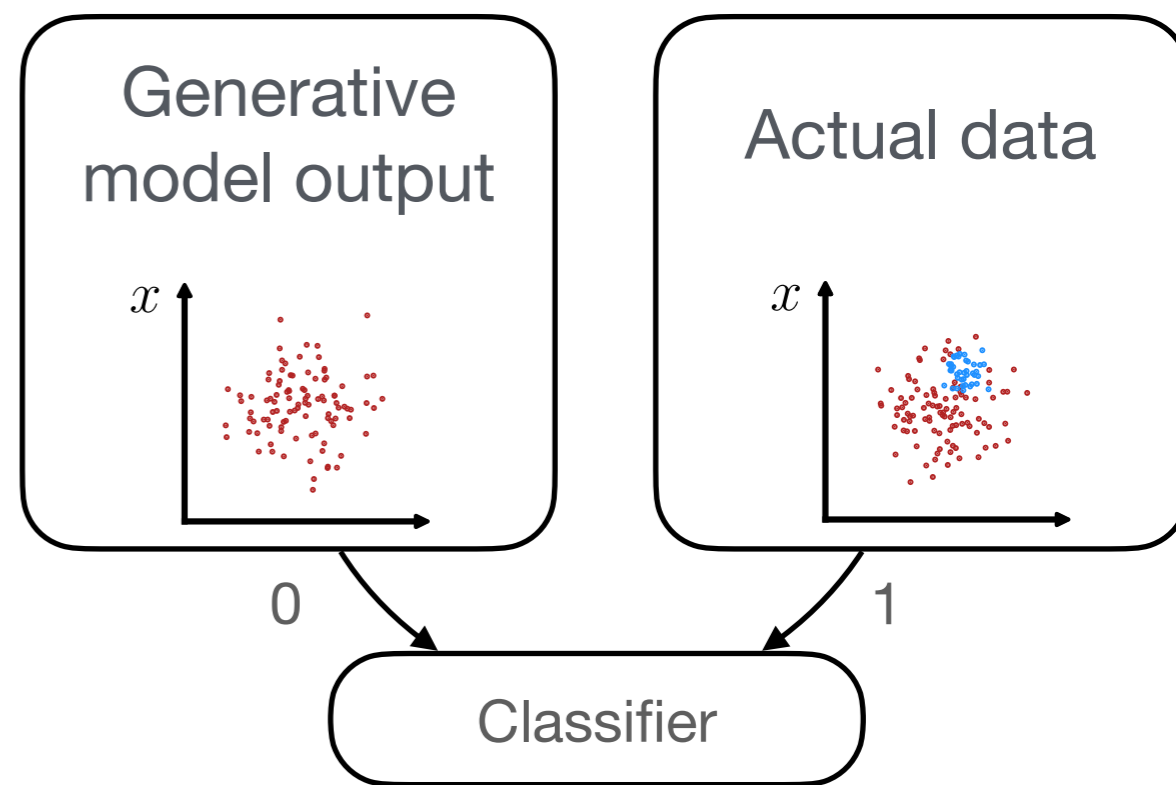
CATHODE



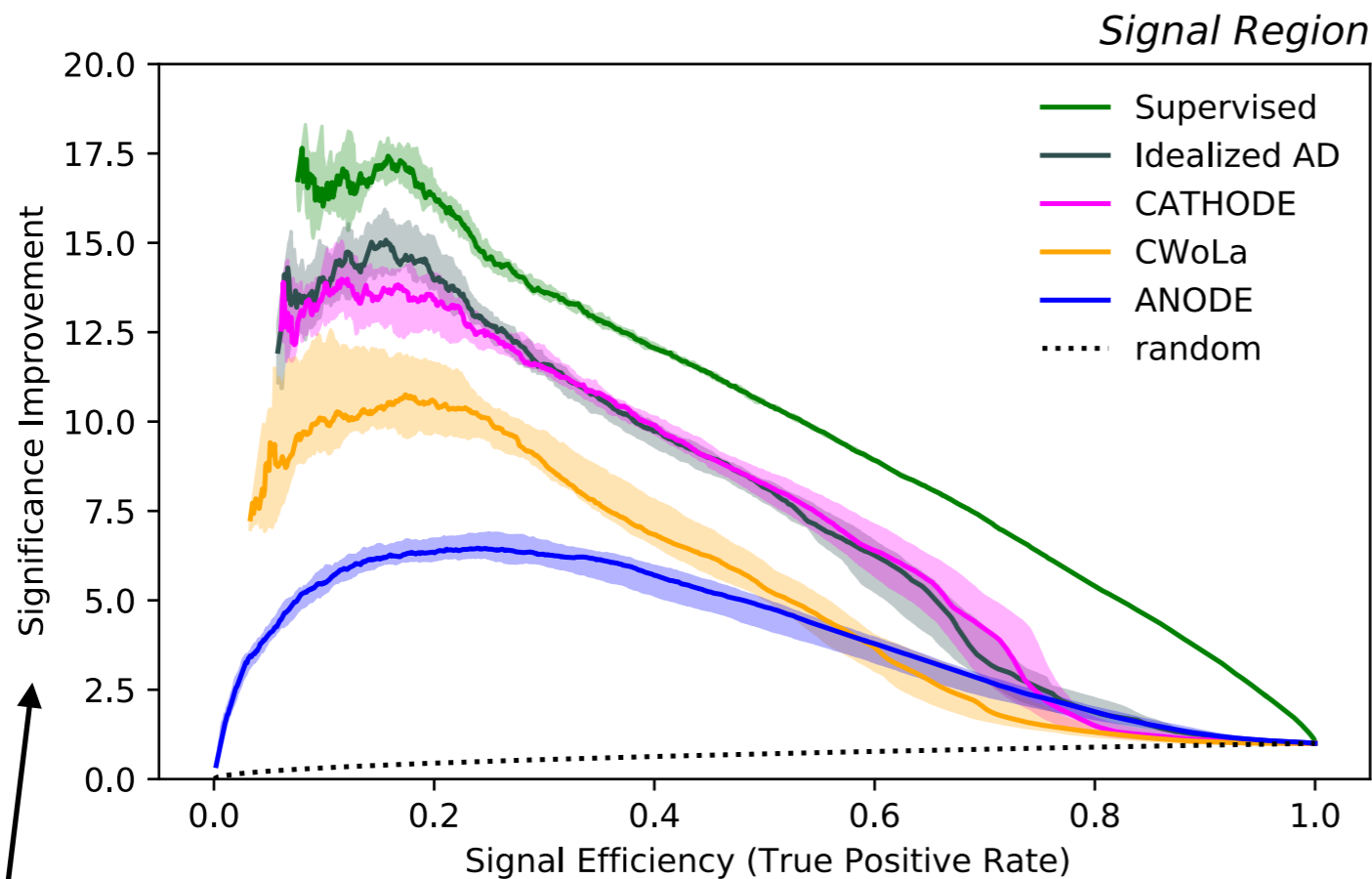
Train **generative** model conditional on m

Interpolate & and **sample** here

Train a classifier between **prediction vs data**



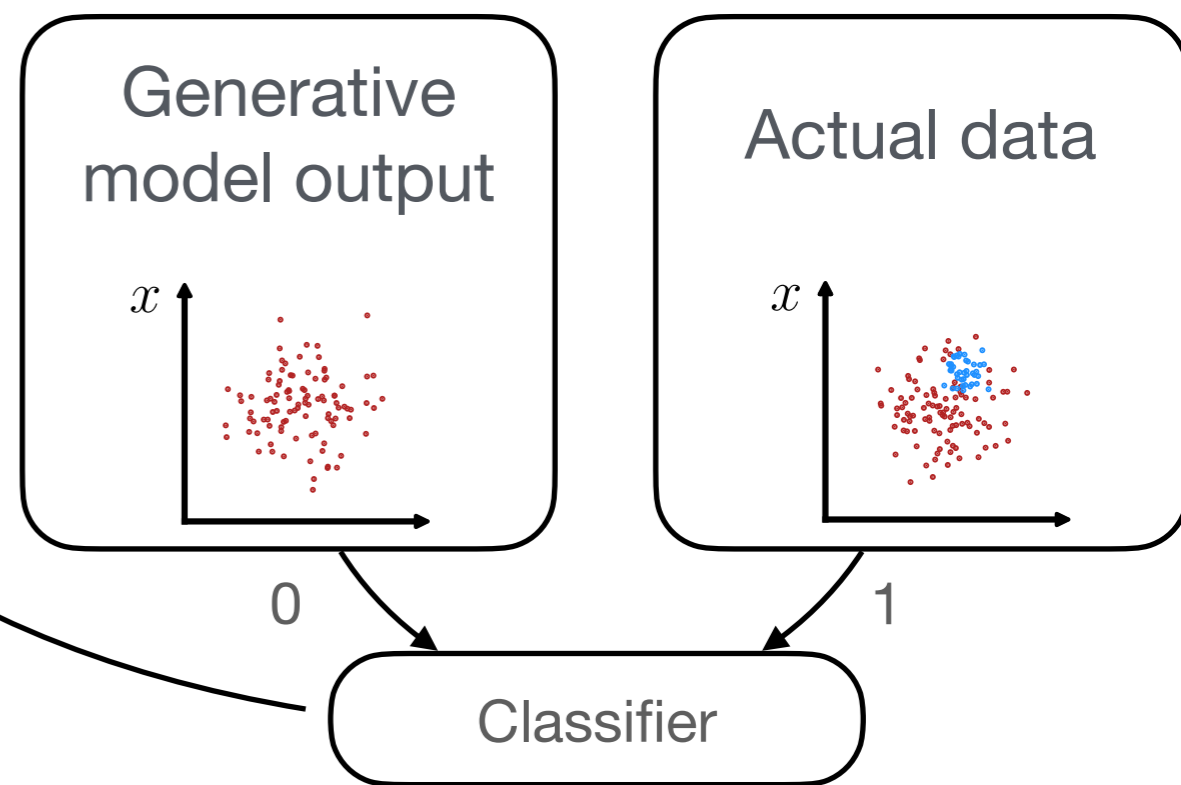
CATHODE



Use classifier to **identify anomalies**

Promising, but does this work on data?

$$\text{SIC} = \frac{\epsilon_S}{\sqrt{\epsilon_B}}$$



CASE

Available on the CERN CDS information server

CMS PAS EXO-22-026

CMS Physics Analysis Summary

Contact: cms-pag-conveners-exotica@cern.ch

2024/03/20

Model-agnostic search for dijet resonances with anomalous jet substructure in proton-proton collisions at $\sqrt{s} = 13$ TeV

The CMS Collaboration

Abstract

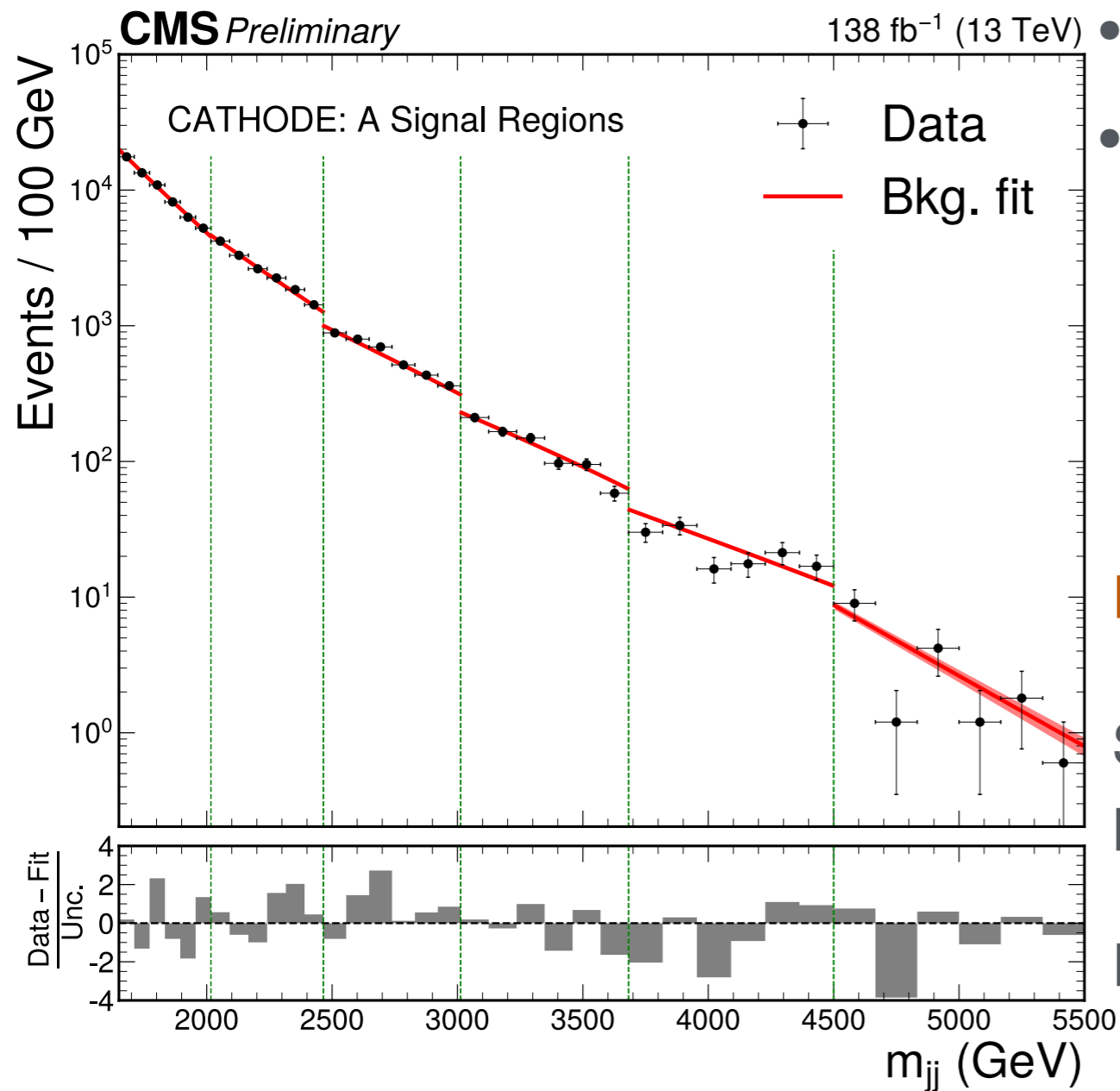
This note introduces a model-agnostic search for new physics in the dijet final state. Other than the requirement of a narrow dijet resonance with a mass in the range of 1800-6000 GeV, minimal additional assumptions are placed on the signal hypothesis. Search regions are obtained by utilizing multivariate machine learning methods to select jets with anomalous substructure. A collection of complementary anomaly detection methods – based on unsupervised, weakly-supervised and semi-supervised algorithms – are used in order to maximize the sensitivity to unknown new physics signatures. These algorithms are applied to data corresponding to an integrated luminosity of 138 fb^{-1} , recorded in the years 2016 to 2018 by the CMS experiment at the LHC, at a centre-of-mass energy of 13 TeV. No significant excesses above background expectation are seen, and exclusion limits are derived on the production cross section of benchmark signal models varying in resonance mass, jet mass and jet substructure. Many of these signatures have not previously been searched for at the LHC, making the limits reported on the corresponding benchmark models the first ever and the most stringent to date.

© 2024 CERN for the benefit of the CMS Collaboration. CC-BY-4.0 license

- **New result** by the CMS collaboration: CMS Anomaly Search Effort (CASE)
- Full Run 2 dataset
- **6 anomaly** detectors in parallel

CASE

- **New result** by the CMS collaboration: CMS Anomaly Search Effort (CASE)
- Full Run 2 dataset
- **6 anomaly** detectors in parallel



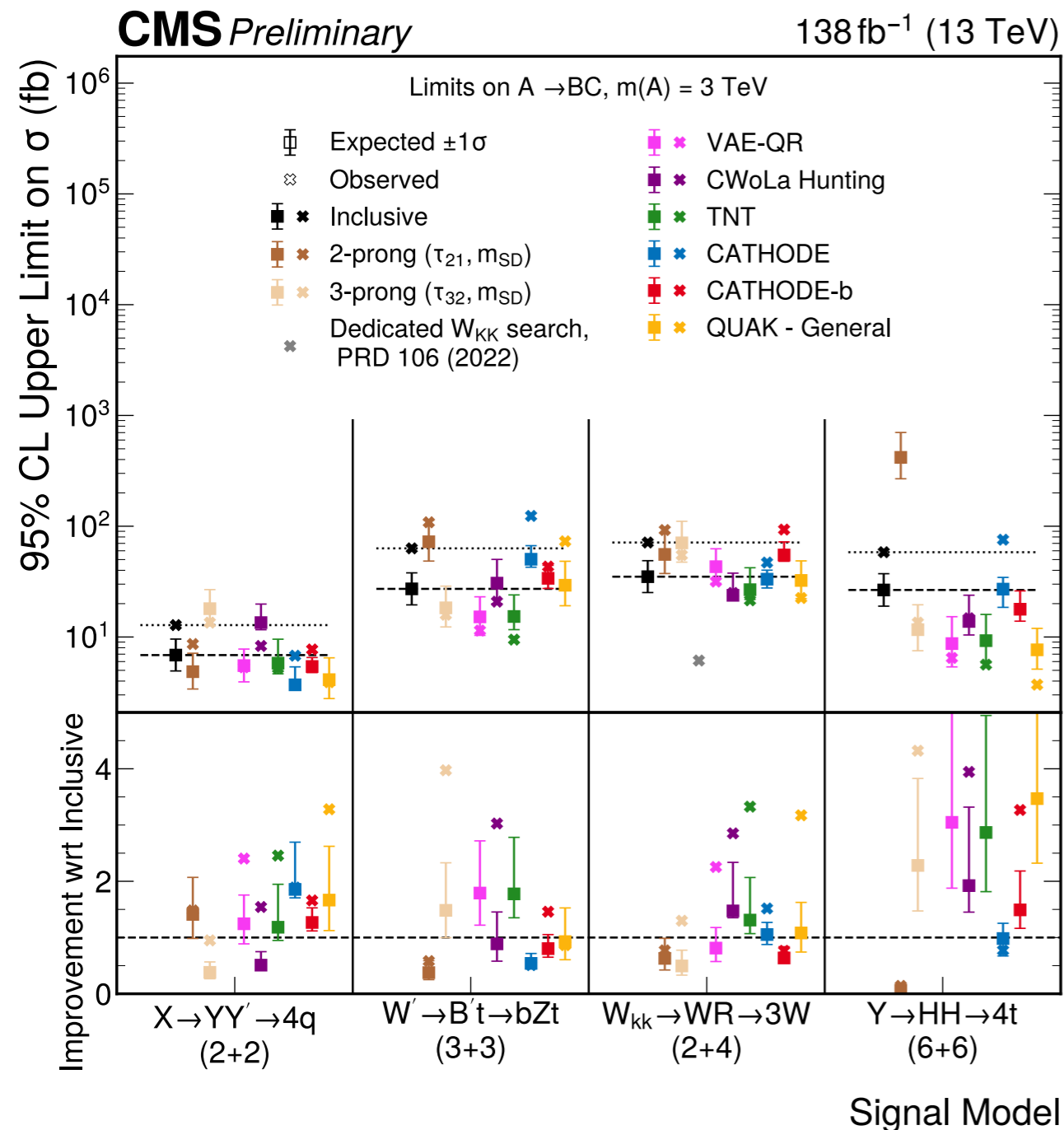
Fully train CATHODE on **data**

Select **top 1%** most anomalous events, perform **bump-hunt**

No signal-like outlier: set limits

CASE

- **New result** by the CMS collaboration: CMS Anomaly Search Effort (CASE)
- Full Run 2 dataset
- **6 anomaly** detectors in parallel



For limits: **inject potential signals**

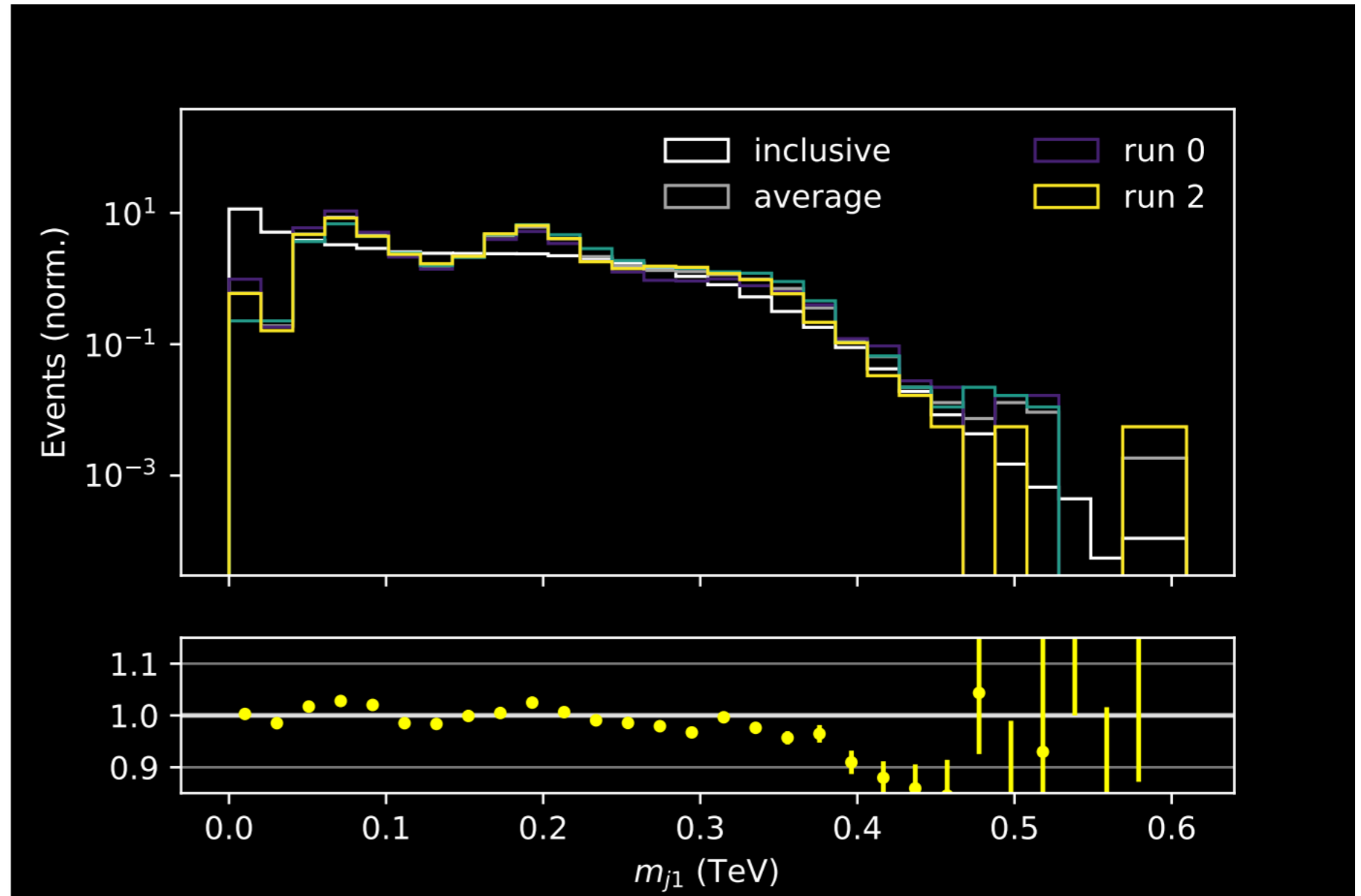
Includes **uncertainties**, e.g. multi-prong jets modelling

Altogether set limits for **43 different signal scenarios**

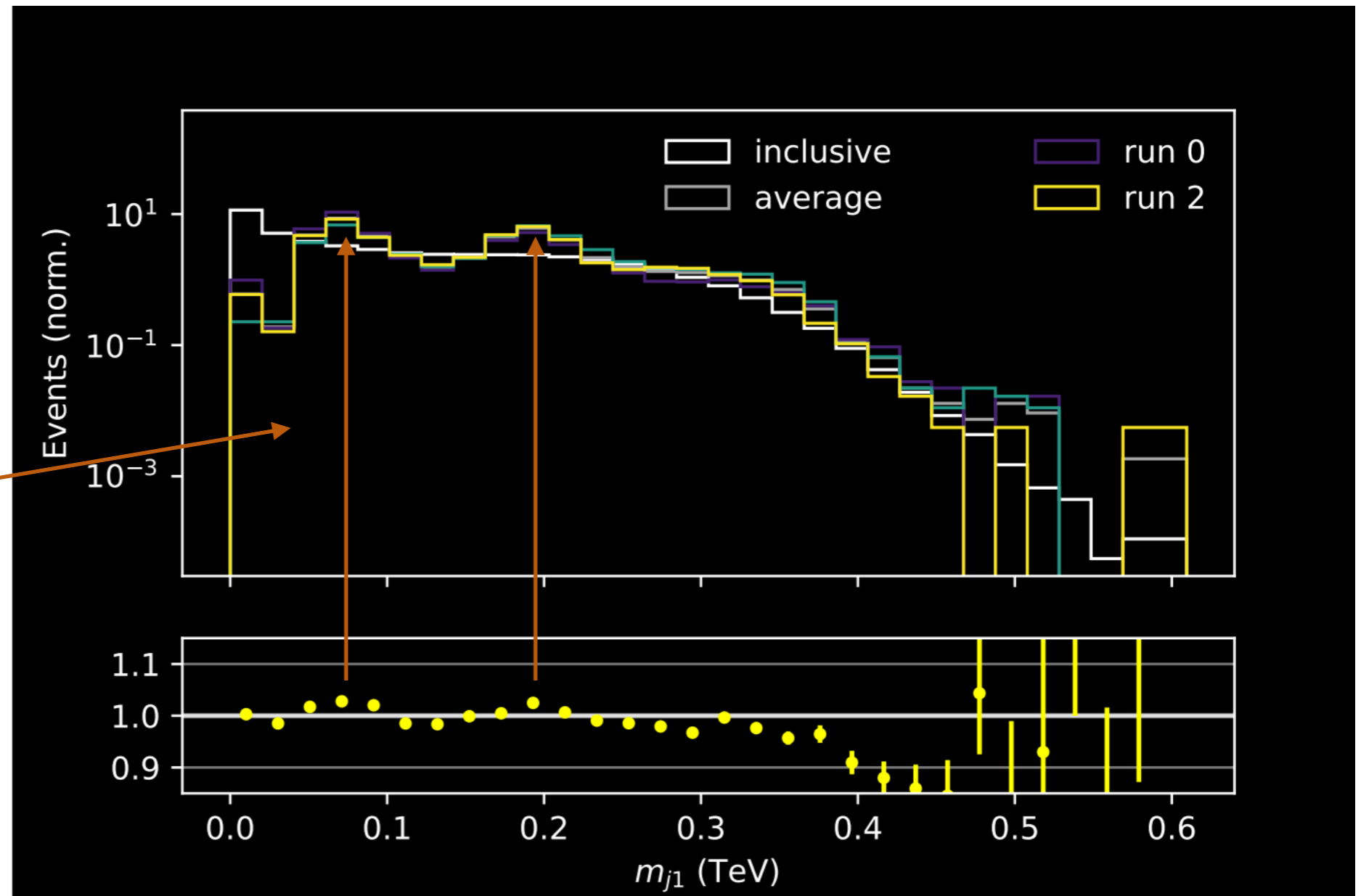
Generative non-closure

Inclusive is sideband;
other distributions
after classifier
cut

True sideband/
Generated sideband



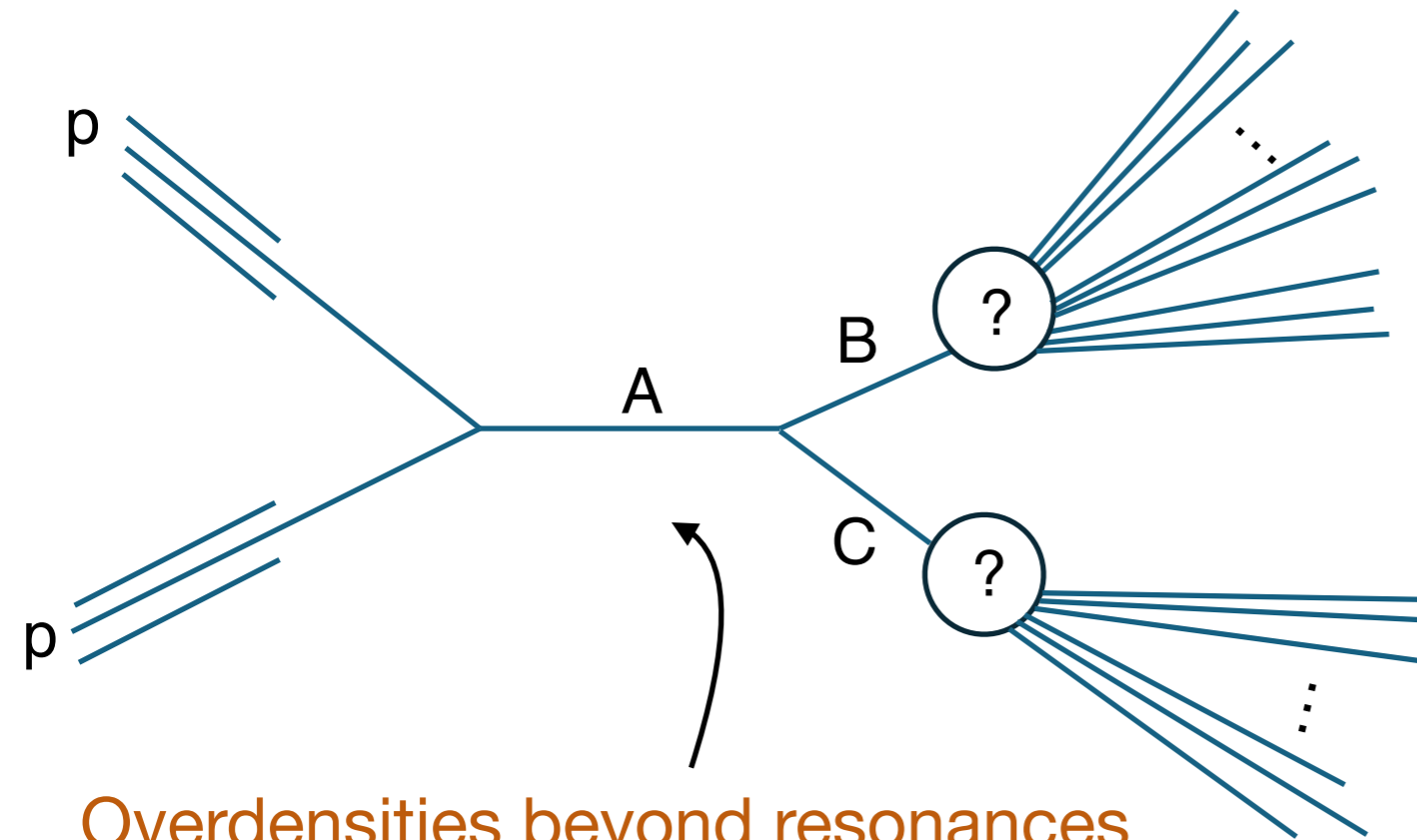
Generative non-closure



Sensitive to **percent-level** differences

Might benefit (highly) from **clever uncertainty** ideas

Other developments & issues



More features per jet
(e.g. 2309.13111)

Low-level input data
(e.g. 2310.06897)

Overdensities beyond resonances
(e.g. 2404.07258, 2311.12924)

Better sensitivity for weak
signals (e.g. 2312.11629)

Reduce shaping of
distributions

More topologies

Anomalies as outliers (e.g.
substantial literature on auto
encoder based methods)

Robust statistical treatment beyond
bump-hunts (e.g. 2111.13633)

Treatment of uncertainties

Applications to data
monitoring

Sharing of results

See talks by **Thea, Lily, Gaia, and Mikael**

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

Inference

Experiment Design

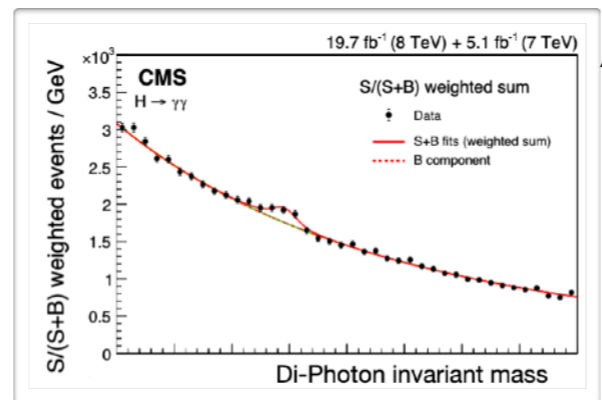
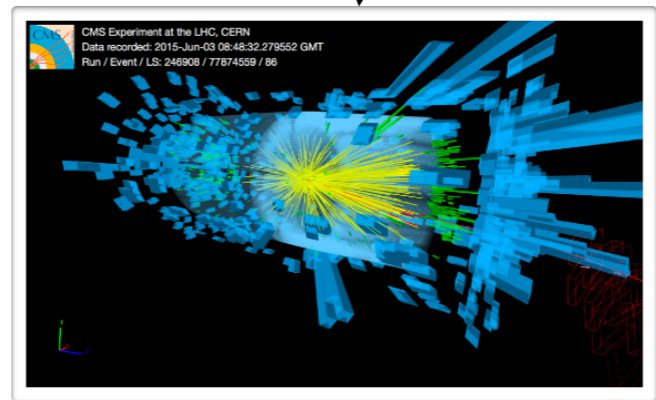
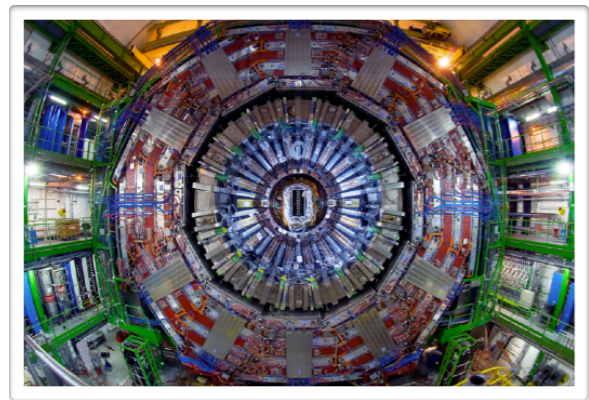
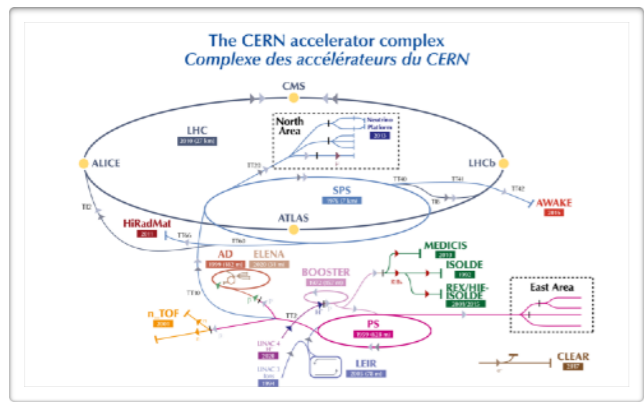
Simulation

Triggers

Tagging Reconstruction

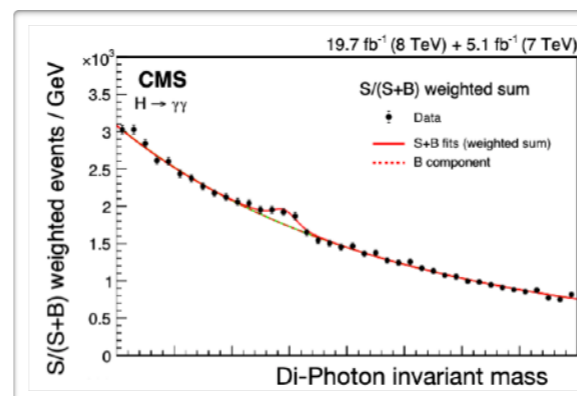
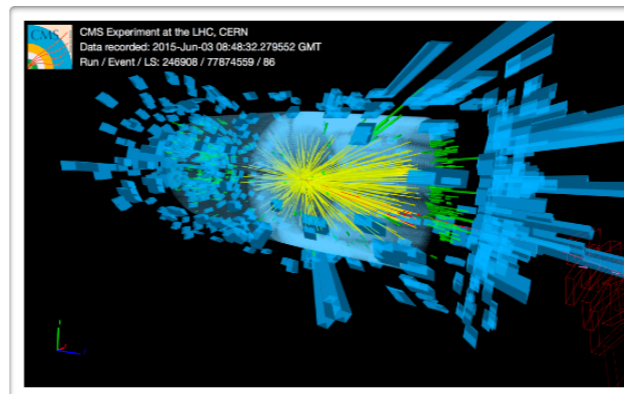
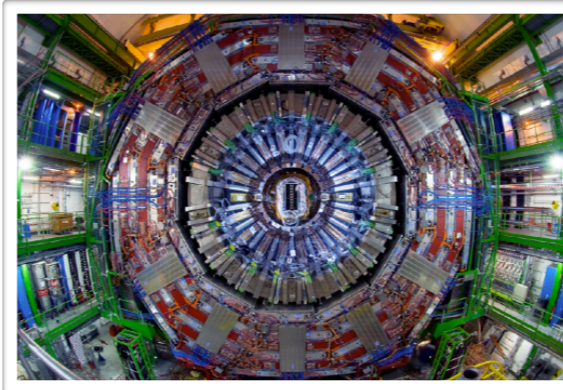
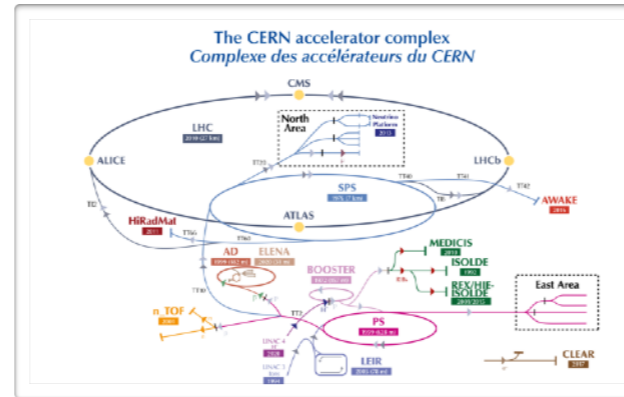
Unfolding Anomaly Detection

AI



Differentiable versions
of **all steps** in the particle
physics processing chain

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + h.c. \\ & + \chi_i Y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu \phi|^2 - V(\phi) \end{aligned}$$

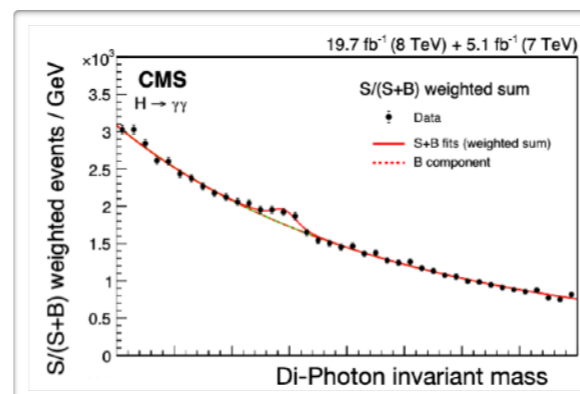
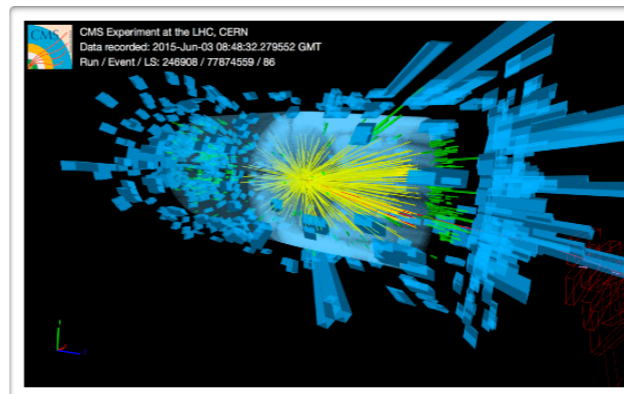
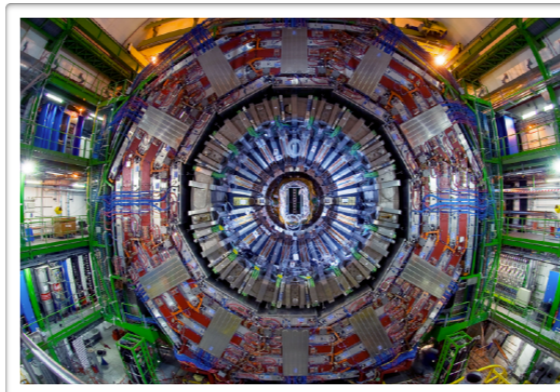
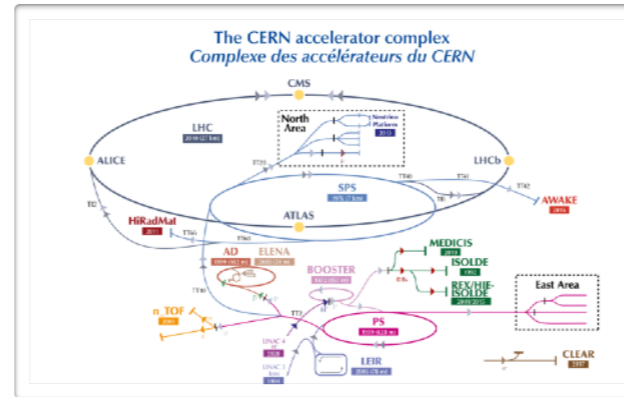


Differentiable versions
of **all steps** in the particle
physics processing chain

Either as ML-based
surrogate models

Or via e.g. **differentiable
programming**

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + h.c. \\ & + \chi_i Y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu \phi|^2 - V(\phi) \end{aligned}$$



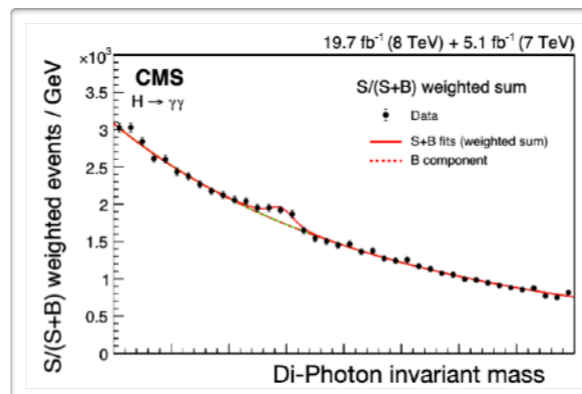
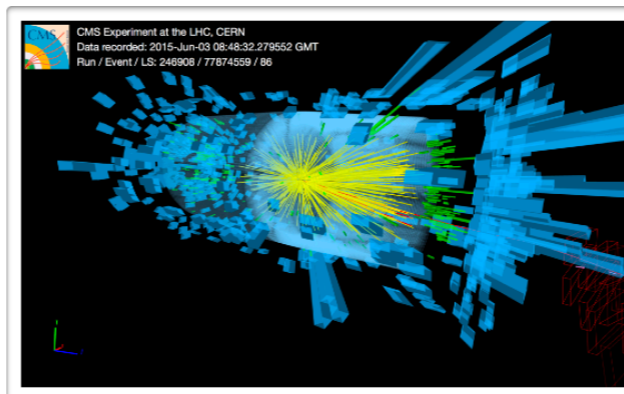
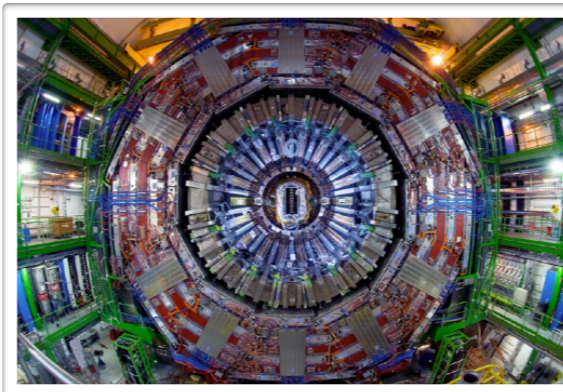
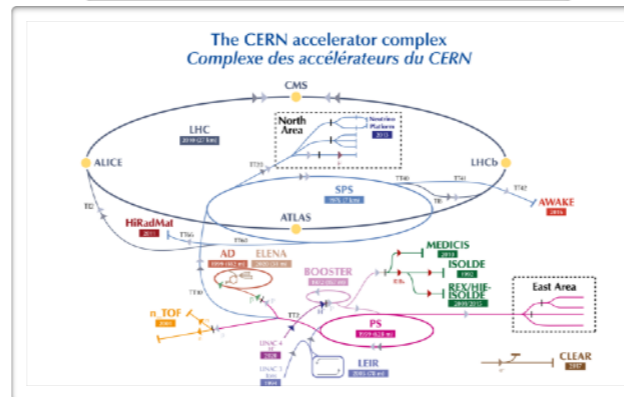
Differentiable versions
of **all steps** in the particle
physics processing chain

Either as ML-based
surrogate models

Or via e.g. **differentiable
programming**

What can we do with this?

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + h.c. \\ & + \chi_i Y_{ij} \chi_j \phi + h.c. \\ & + |D_\mu \phi|^2 - V(\phi) \end{aligned}$$



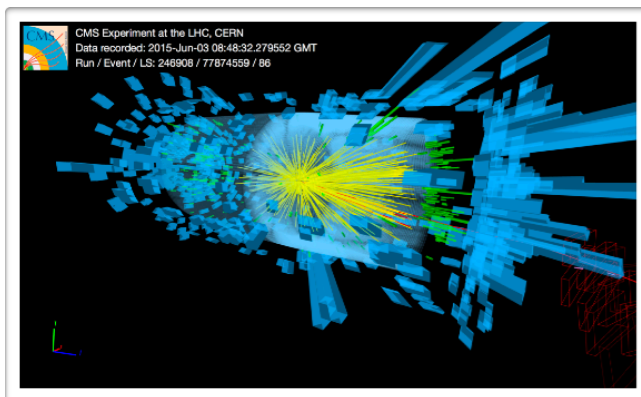
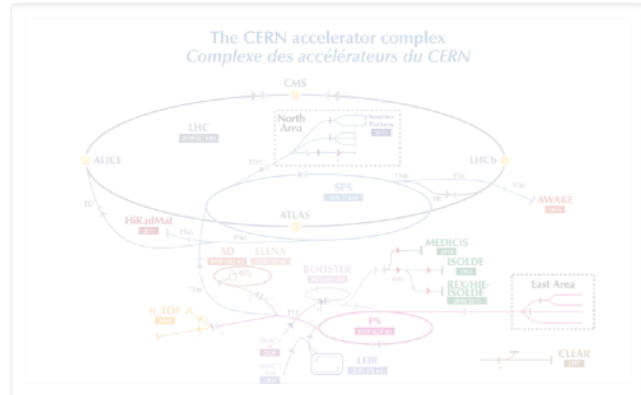
Inference

$$\begin{aligned} \mathcal{L} = & -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} \\ & + i\bar{\psi} \not{D} \psi + \text{h.c.} \\ & + \chi_i y_{ij} \chi_j \phi + \text{h.c.} \\ & + |D_\mu \phi|^2 - V(\phi) \end{aligned}$$

Goal: Learn parameters of theory (e.g. couplings) directly from high-dimensional data

No exact likelihood, but forward simulations available: likelihood-free / **simulation based inference**

Inference



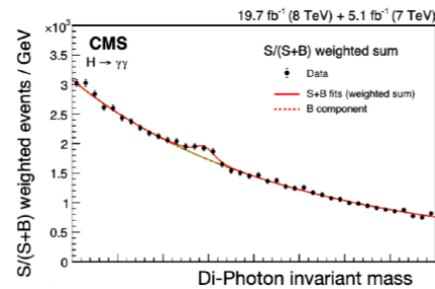
Inference

$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

Goal: Learn parameters of theory (e.g. couplings) directly from high-dimensional data

No exact likelihood, but forward simulations available: likelihood-free / **simulation based inference**

Inference



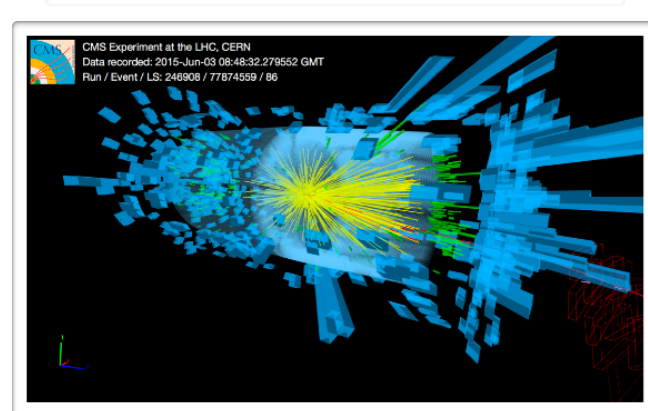
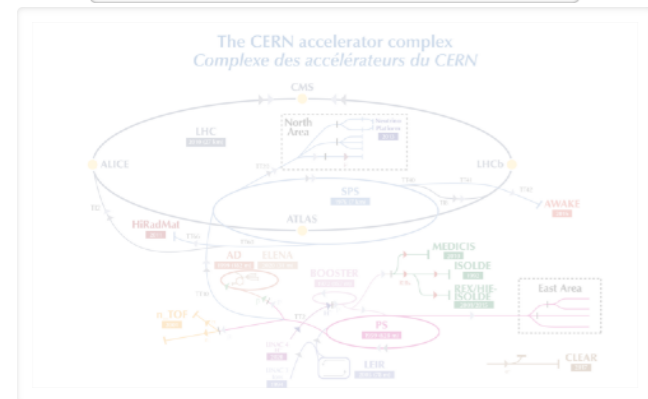
Summary Statistics

Likelihood Learning (e.g. flows or cINNs)

Likelihood ratio trick (e.g. CARL, swyft)

Integration (e.g. MadMiner)

See talk by **Aishik, Kyle, Artur**



$$\mathcal{L} = -\frac{1}{4} F_{\mu\nu} F^{\mu\nu} + i\bar{\psi}\not{D}\psi + h.c. + \chi_i Y_{ij} \chi_j \phi + h.c. + |D_\mu \phi|^2 - V(\phi)$$

Foundation Model

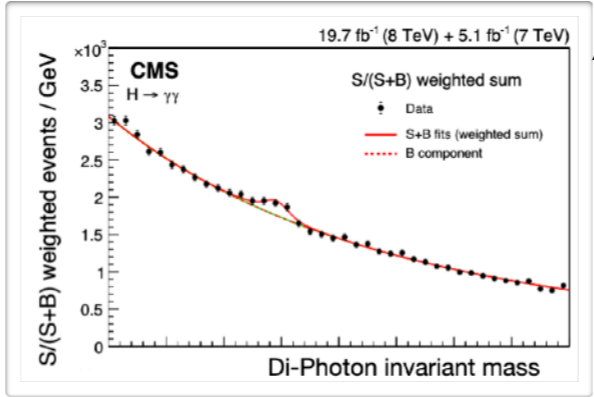
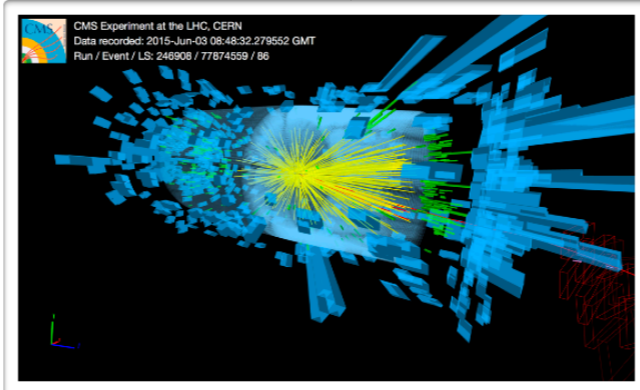
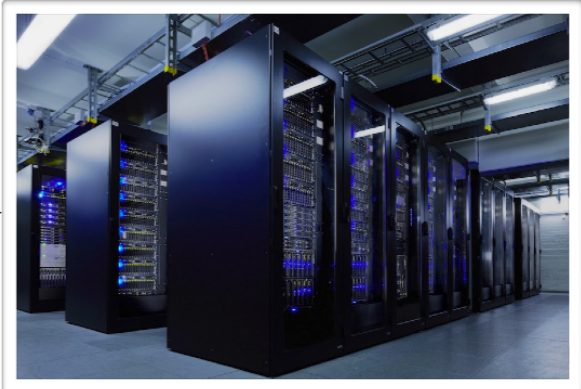
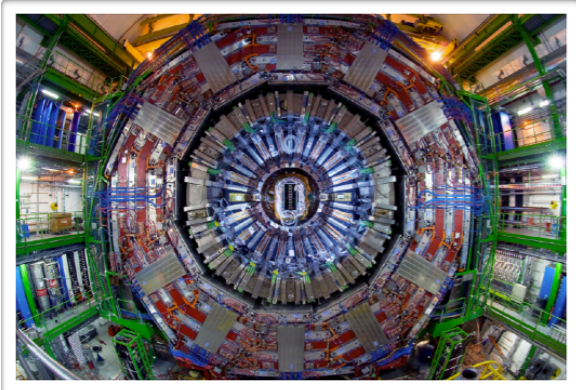
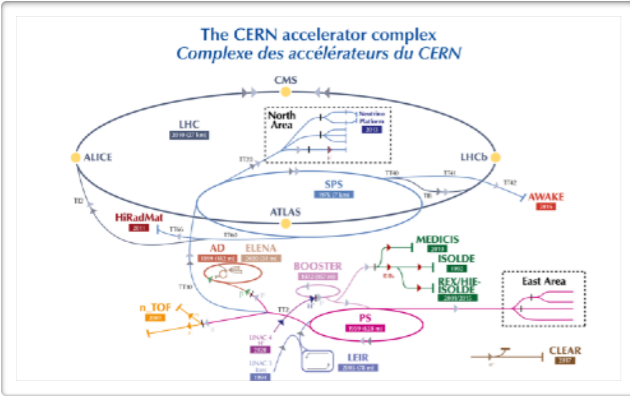
Foundation Model

Foundation Model

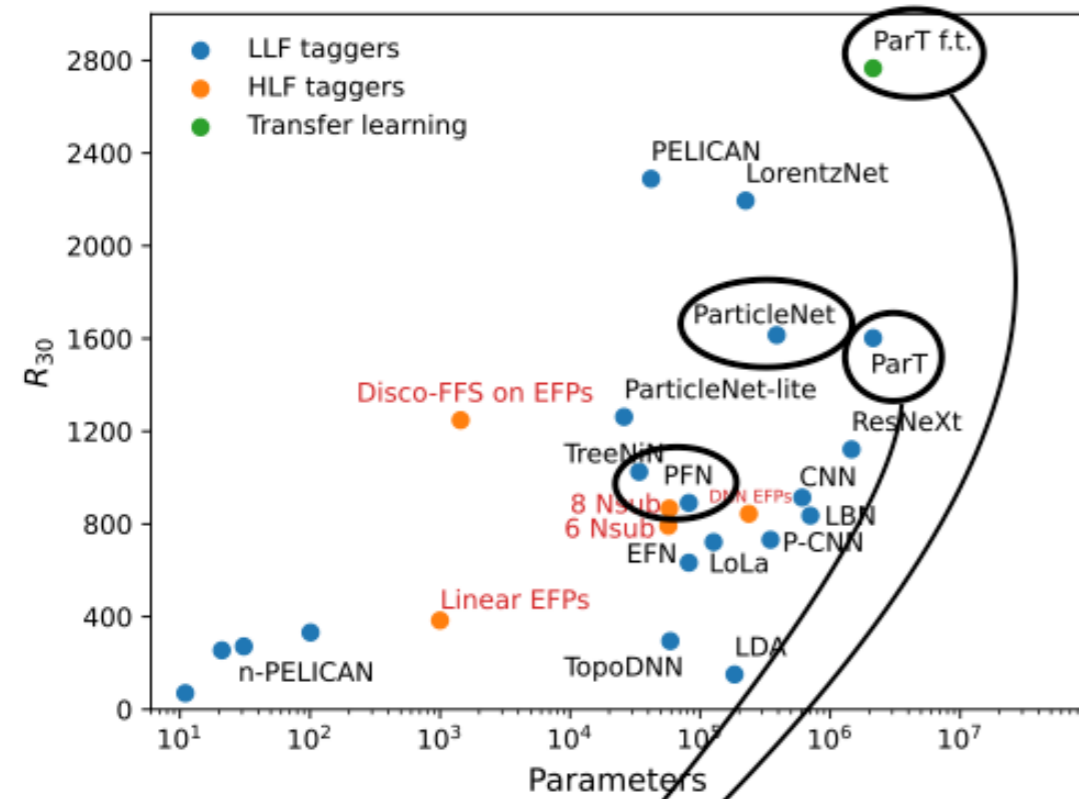
Foundation Model

Foundation Model

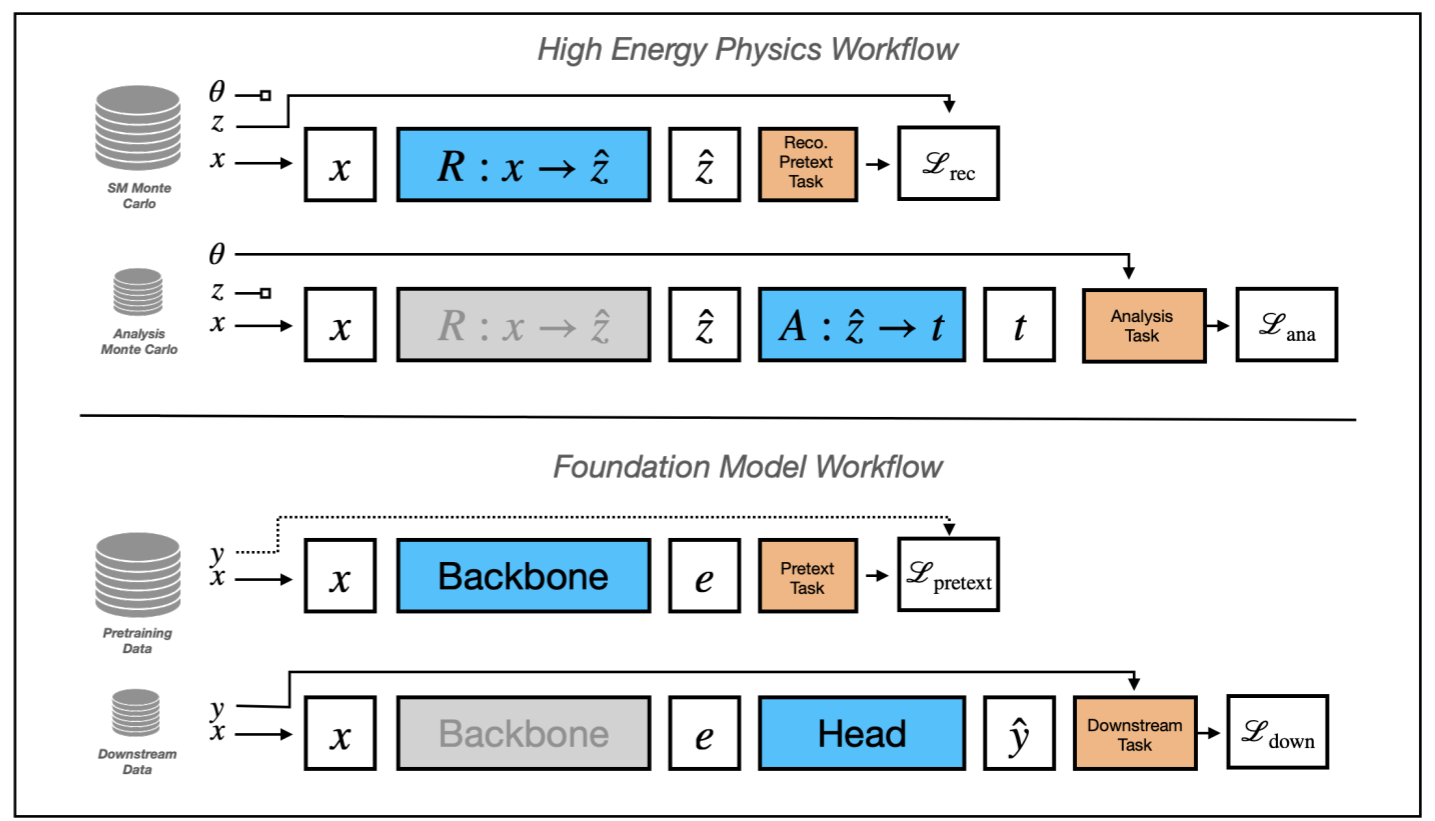
Foundation Model



Foundation models for physics data

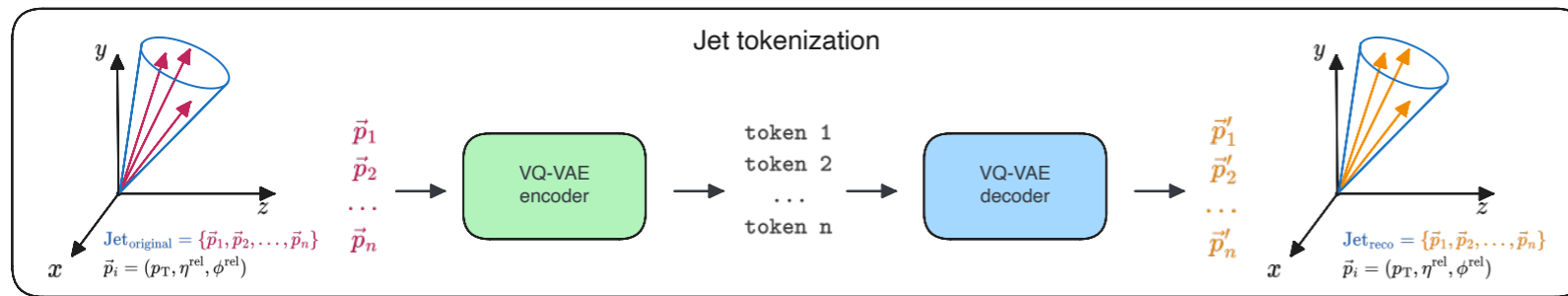


Already observed best performance in supervised classification by **transfer learning**

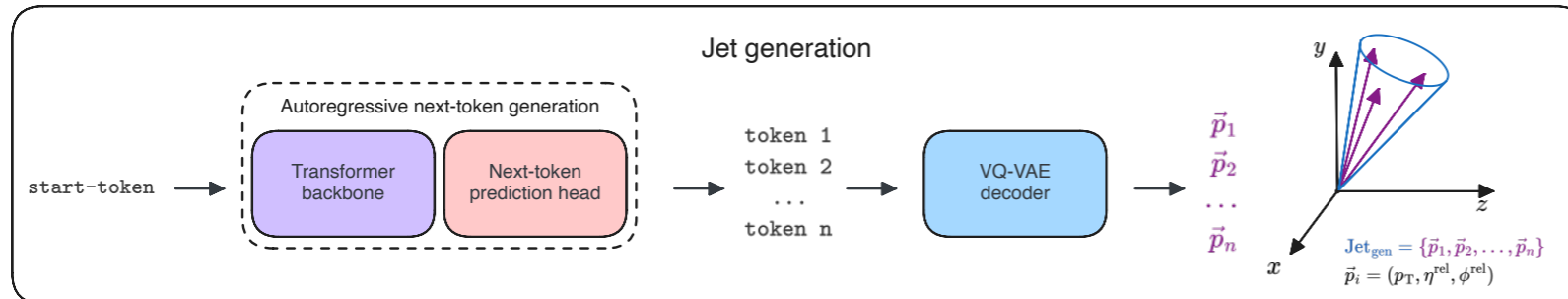


Foundation models extend transfer more broadly and **centralise and re-use training**

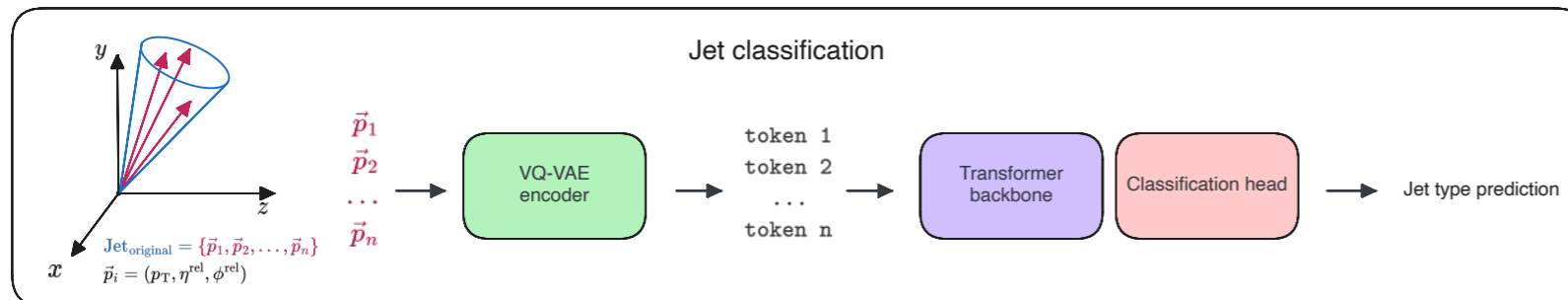
OmniJet-a



GPT for jets
using tokenised inputs



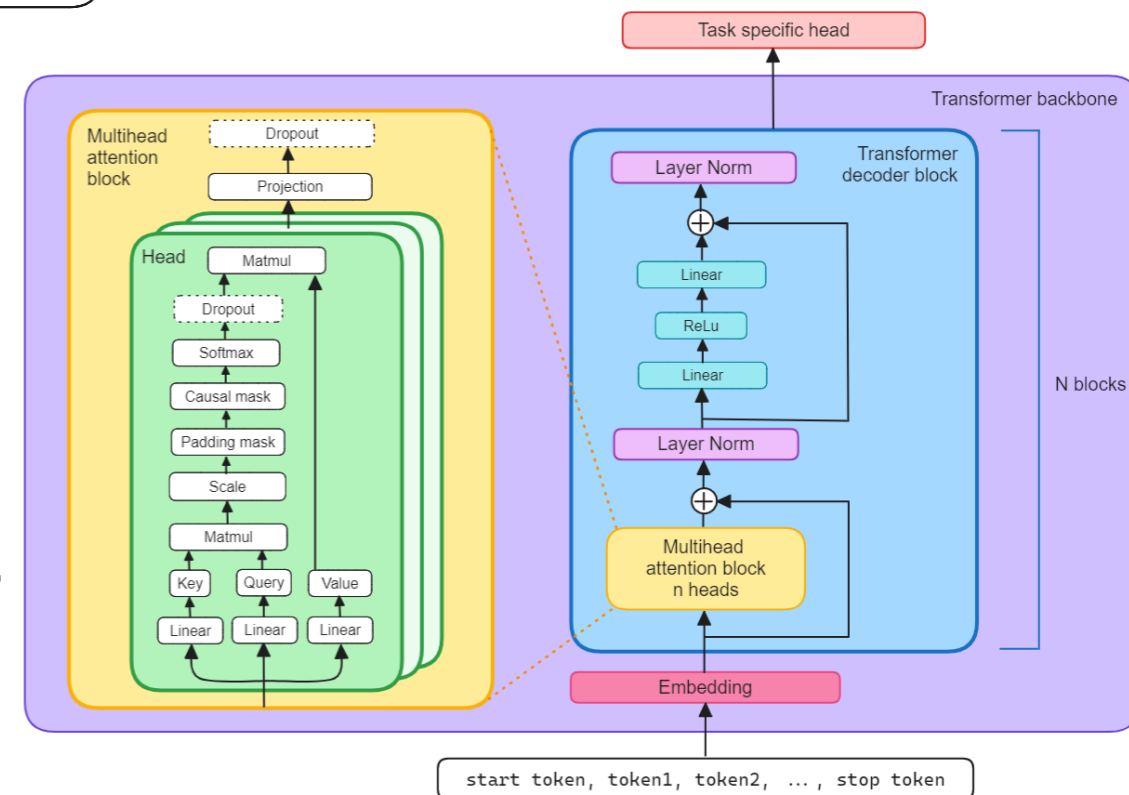
Train on
unsupervised generation



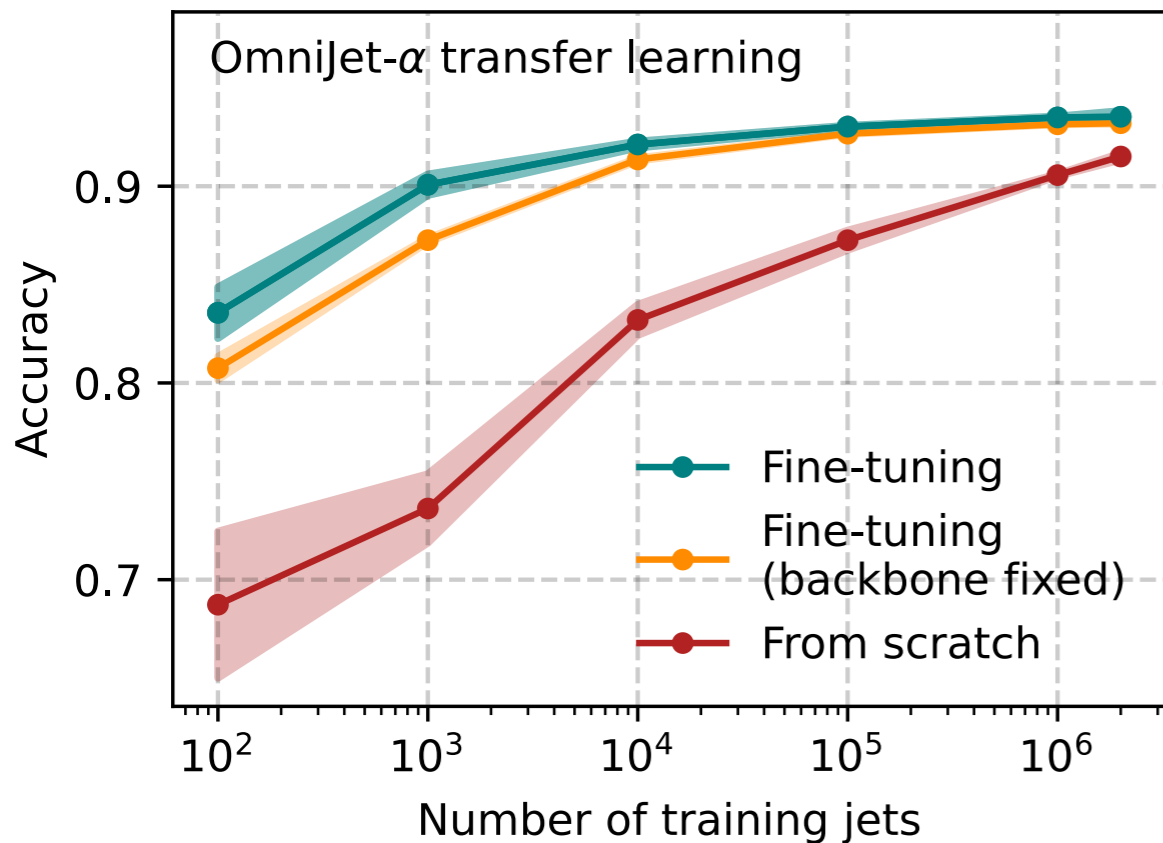
Evaluate for
supervised classification

Birk, Hallin, **GK** 2403.05618; Butter et al 2305.10475; Finke et al 2303.07364; Vigl et al 2401.13536; Heinrich et al 2401.13537; Mikuni, Nachman 2404.16091

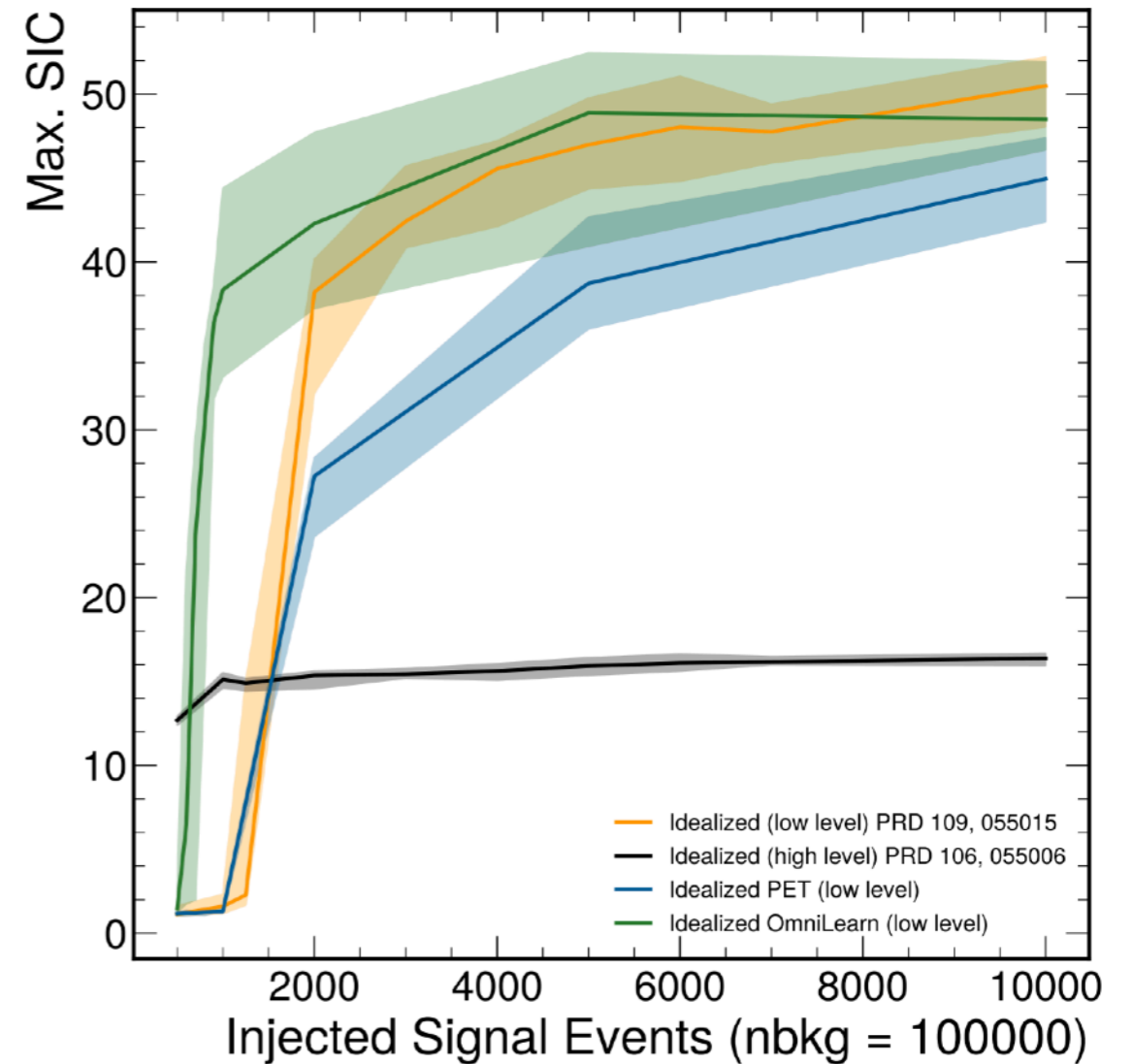
Transformer backbone



Generalisation

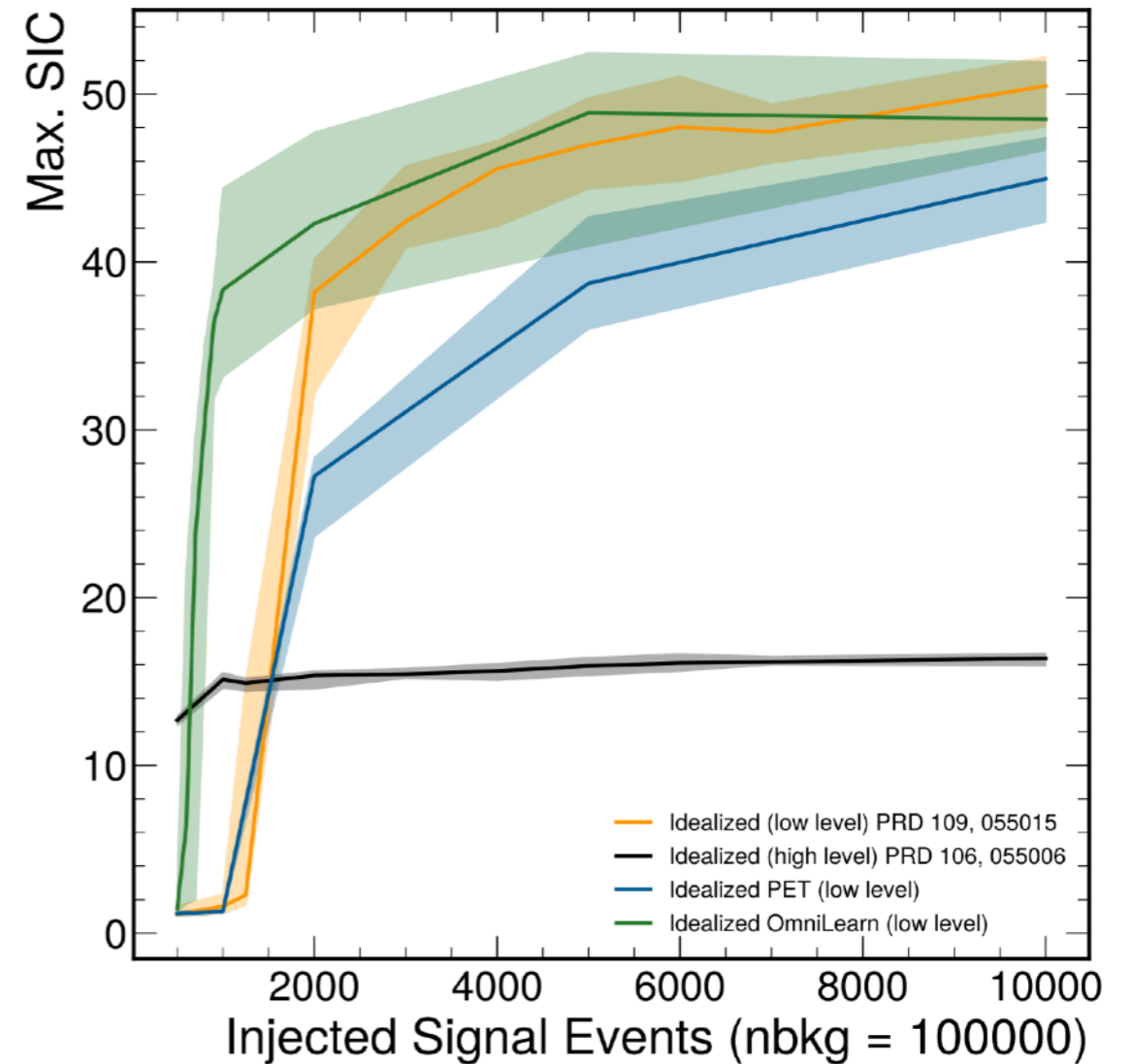
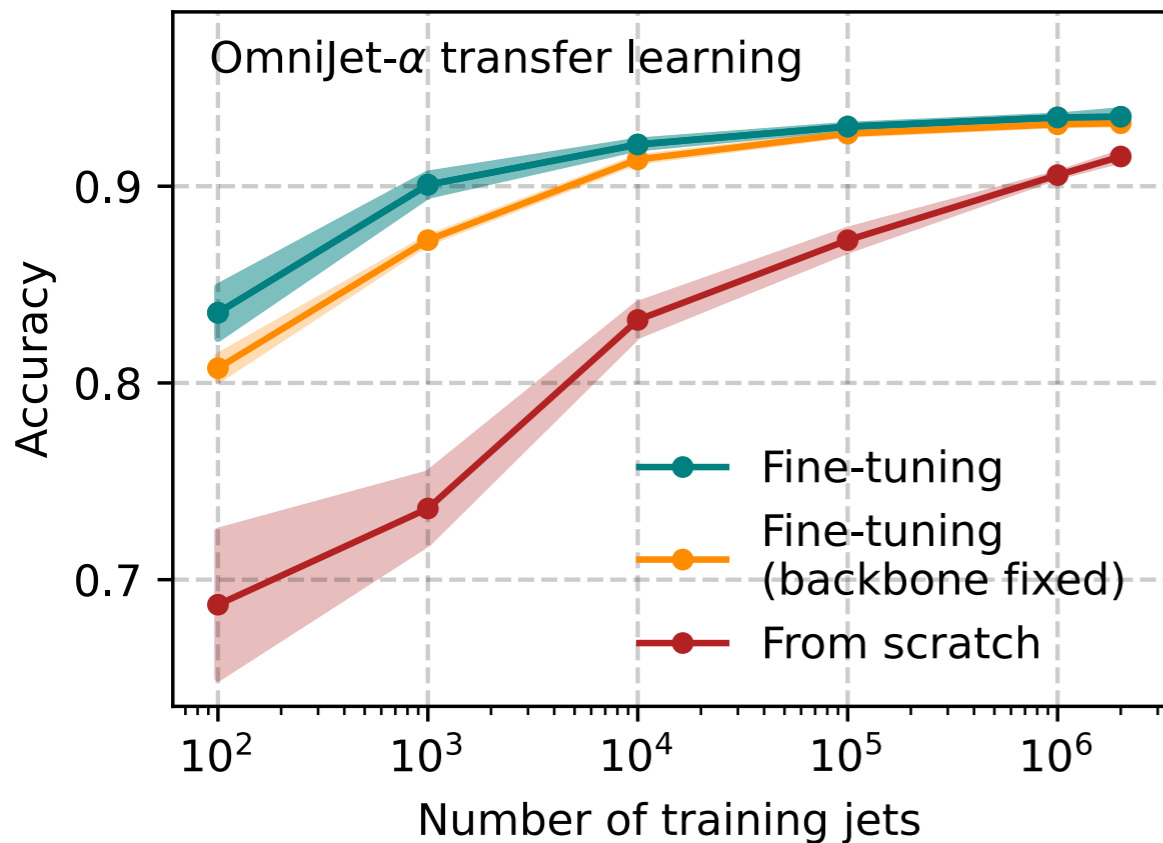


Pre-training on “cheap” unlabelled examples improves supervised classification data efficiency up to 100-1000x



Recent OmniLearn generalises across broad range of tasks including anomaly detection

Open questions



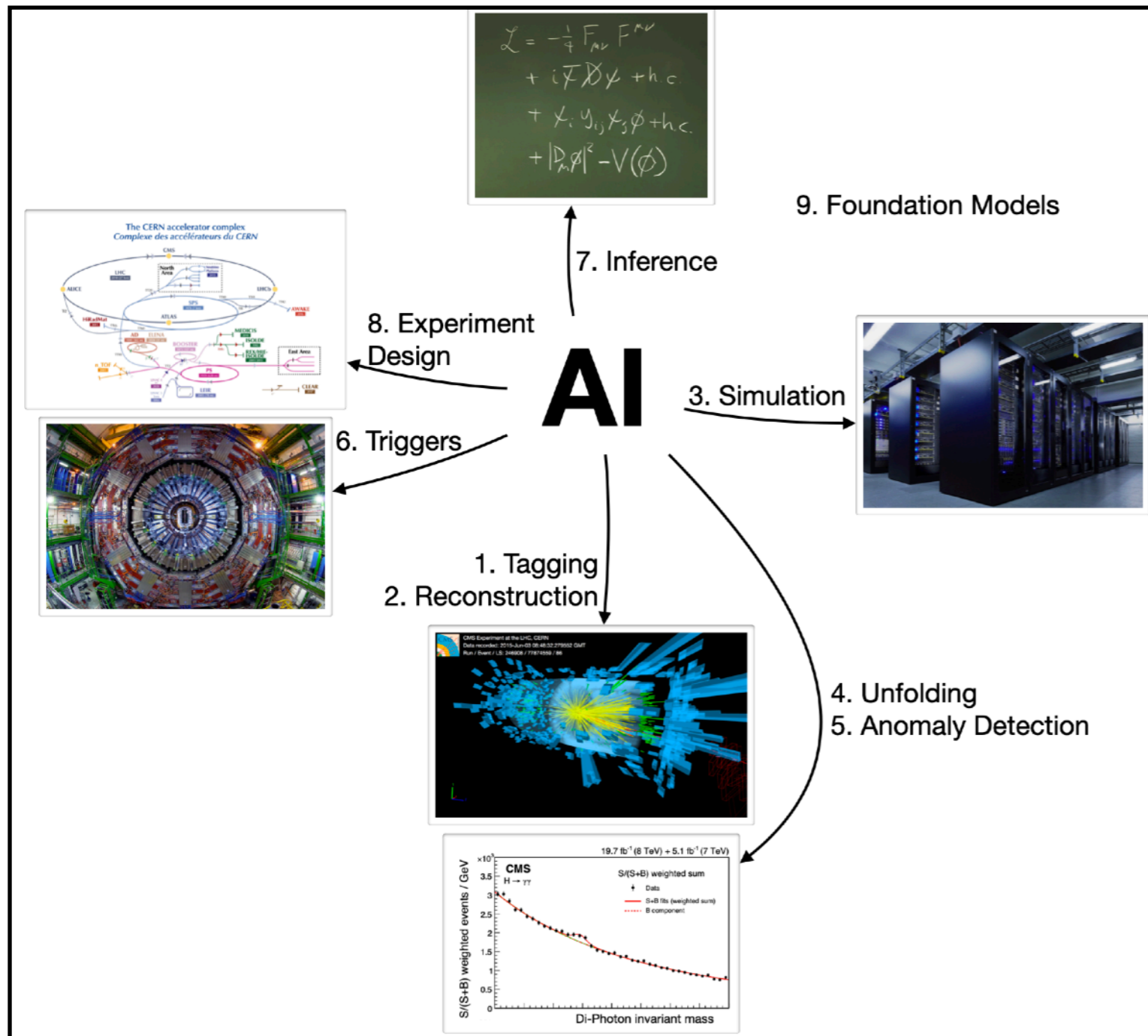
How far can transfer go

New issues from a widely shared model
(correlations across experiment?)

How to re-using training data in analysis

Closing

Conclusions



Extremely **broad** range of **application** for AI in particle physics

Way beyond concept studies: Modern tools are making a **real impact in data analysis**

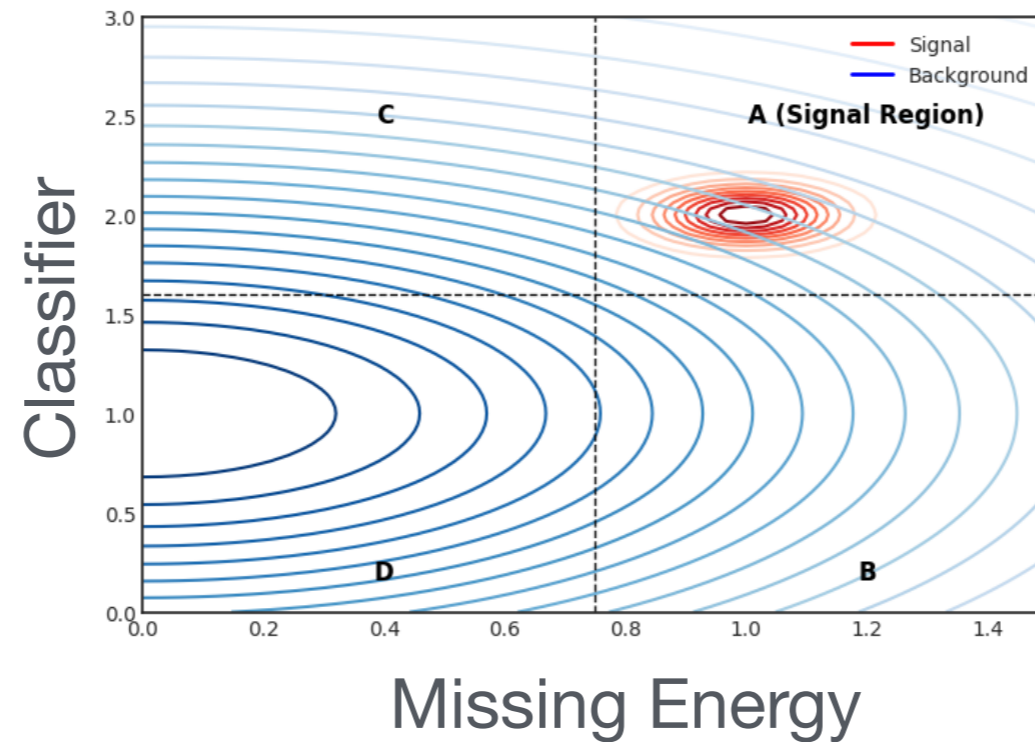
Start to realise **fully AI-based** processing chains

Significant compute effort: **Efficient models** and sharing with **foundation models** matter

Thank you!

Backup

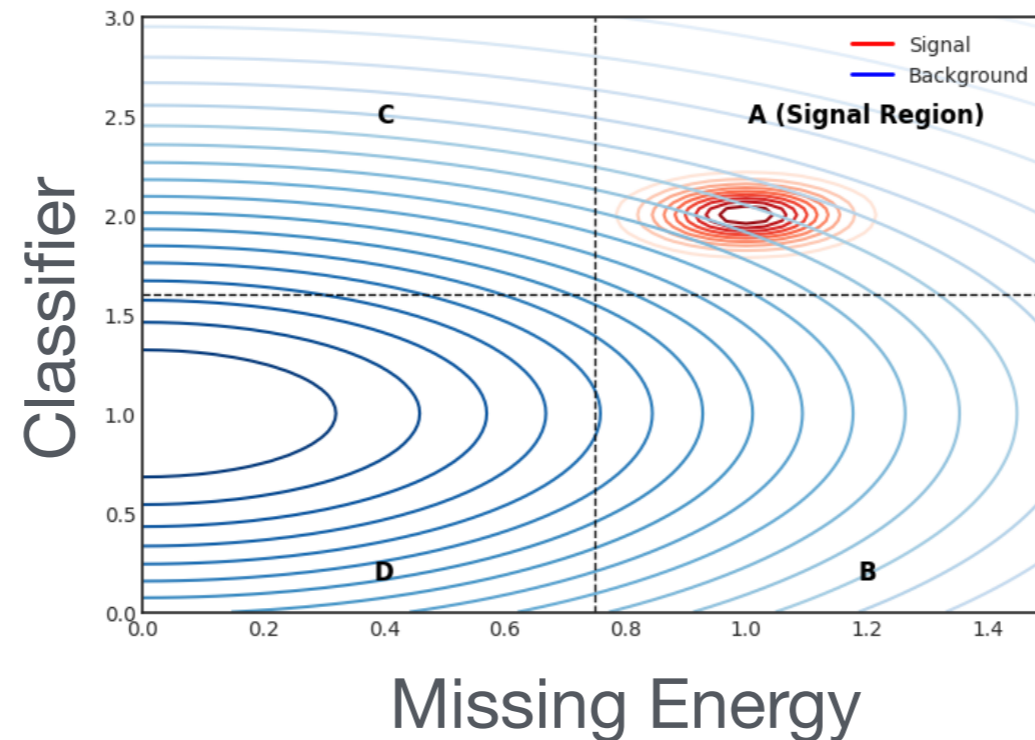
CONRAD



Given a classifier
independent of
missing energy, could
use **ABCD** method

$$N_{A,bg}^{pred} = \frac{N_{B,bg} \cdot N_{C,bg}}{N_{D,bg}}$$

CONRAD



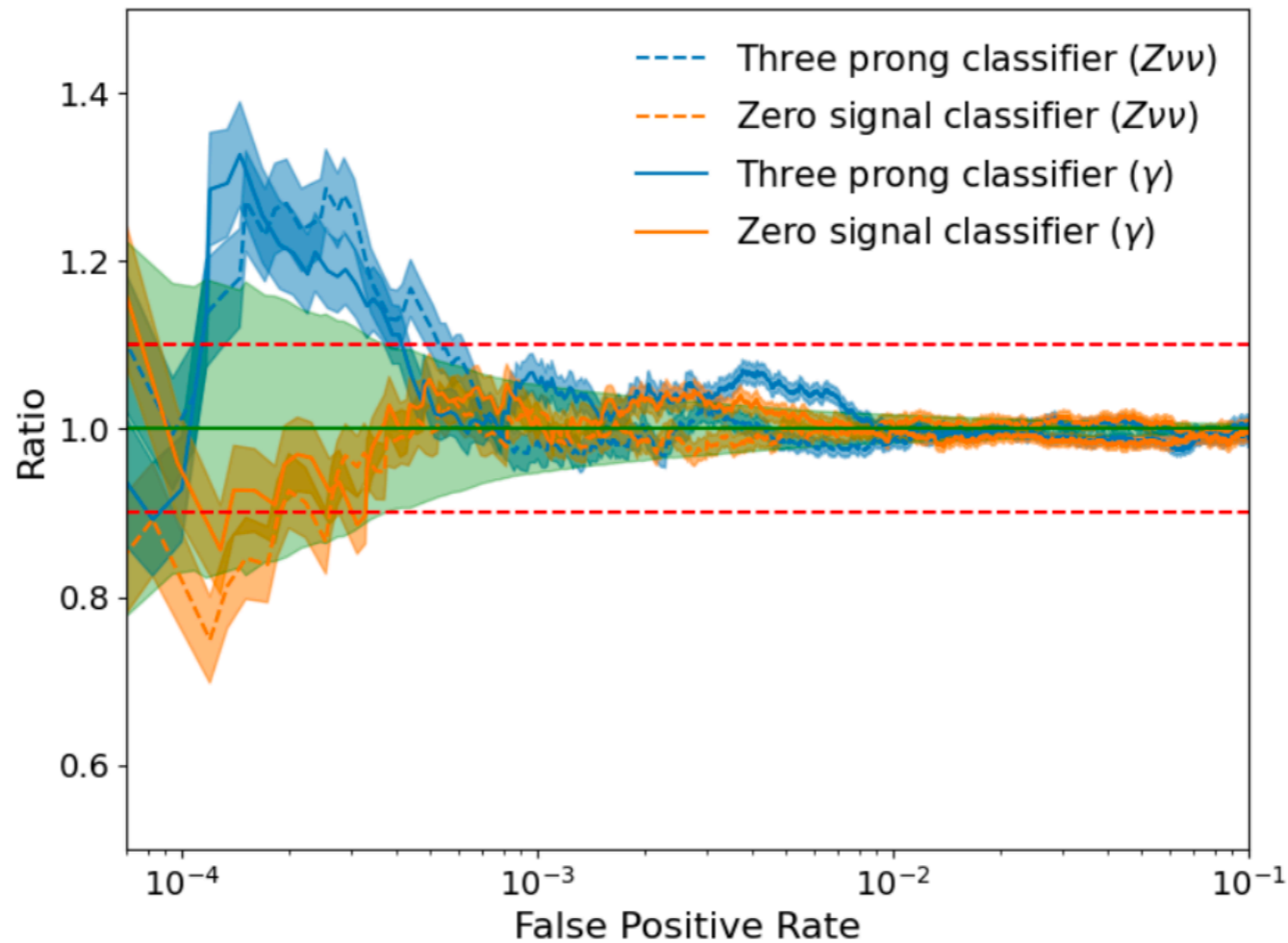
1. Train NF:
conditional mapping
for background-only
sample to latent-
space

2. Train classifier:
Map data to latent
space & train
classifier vs normal

3. Evaluate:
Construct ABCD
plane and analyse

CONRAD

Background
predicted/true

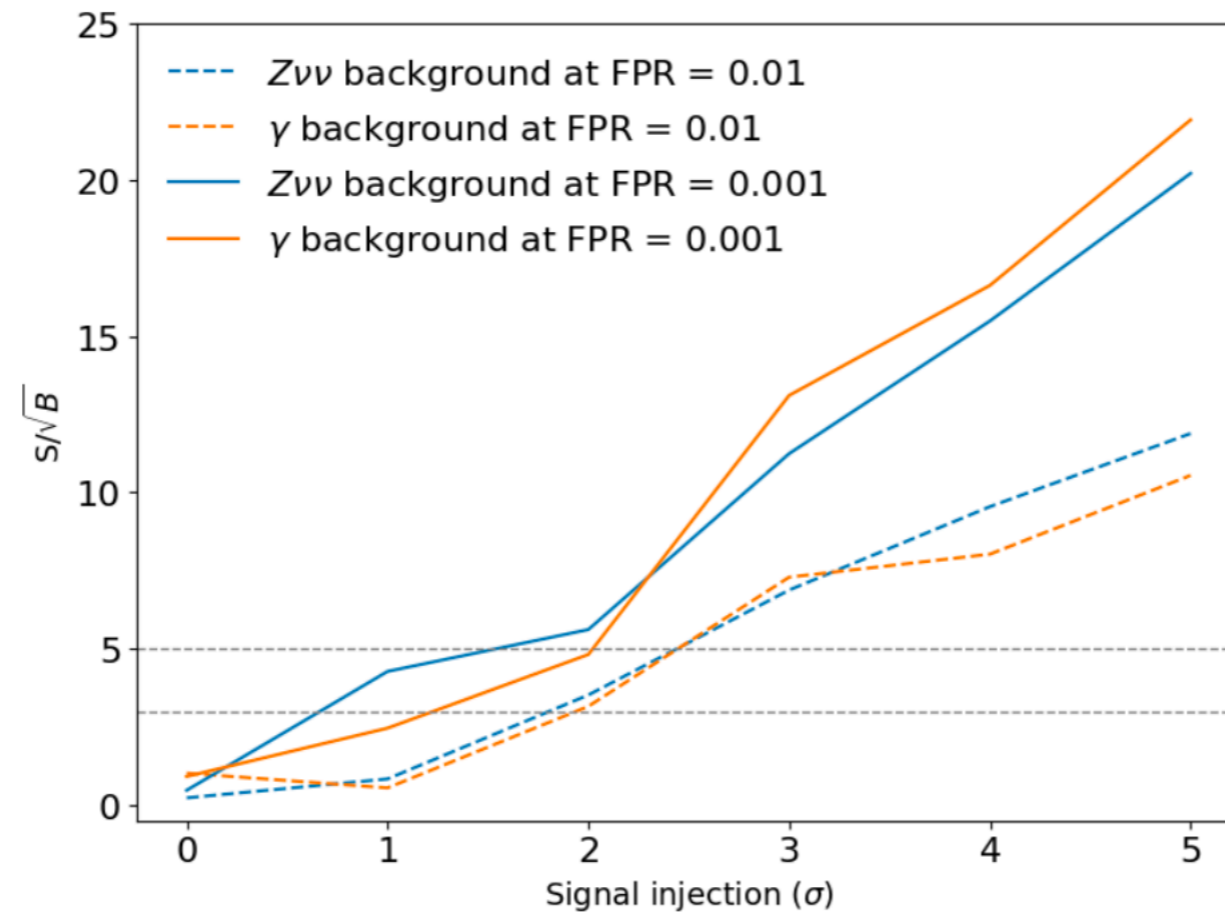


1. Train NF:
conditional mapping
for background-only
sample to latent-
space

2. Train classifier:
Map data to latent
space & train
classifier vs normal

3. Evaluate:
Construct ABCD
plane and analyse

CONRAD



1. Train NF:
conditional mapping
for background-only
sample to latent-
space

2. Train classifier:
Map data to latent
space & train
classifier vs normal

3. Evaluate:
Construct ABCD
plane and analyse