Machine Learning for Fundamental Physics

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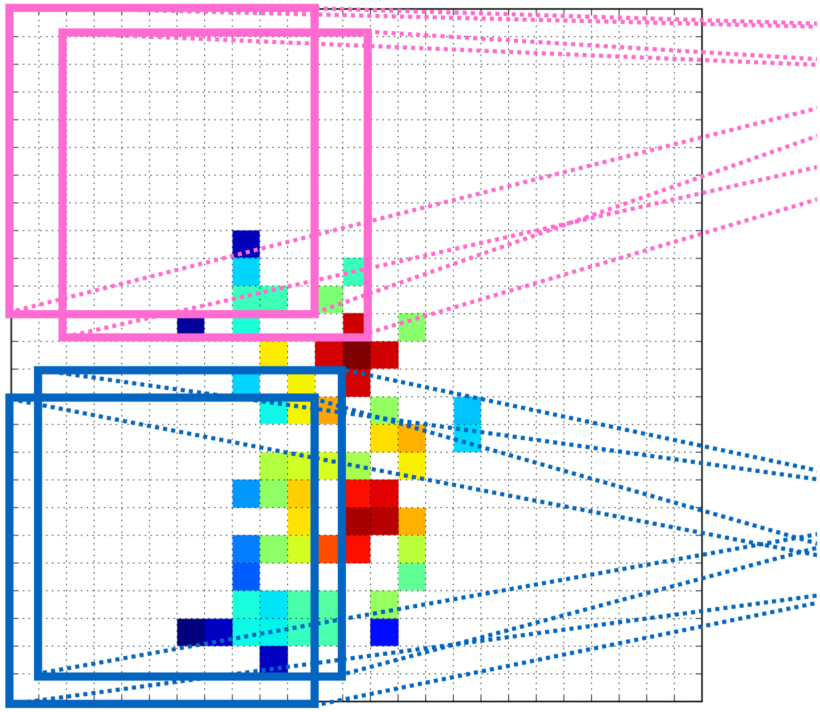
bnachman



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October 2022

Questions in fundamental physics

Theoretical and experimental questions motivate a deep exploration **of the fundamental structure of nature**

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Why is the Higgs boson so light?

Hierarchy problem

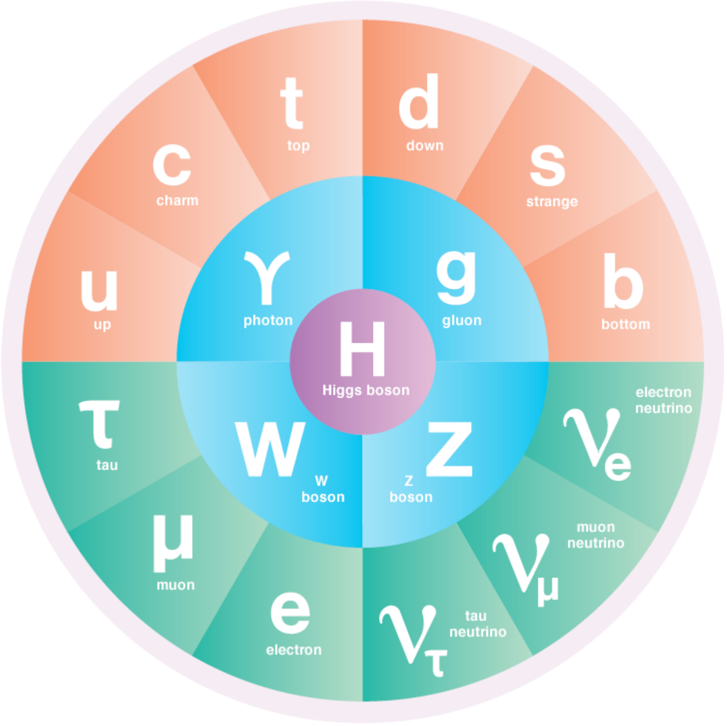

image source: symmetry magazine

See also: quantum gravity

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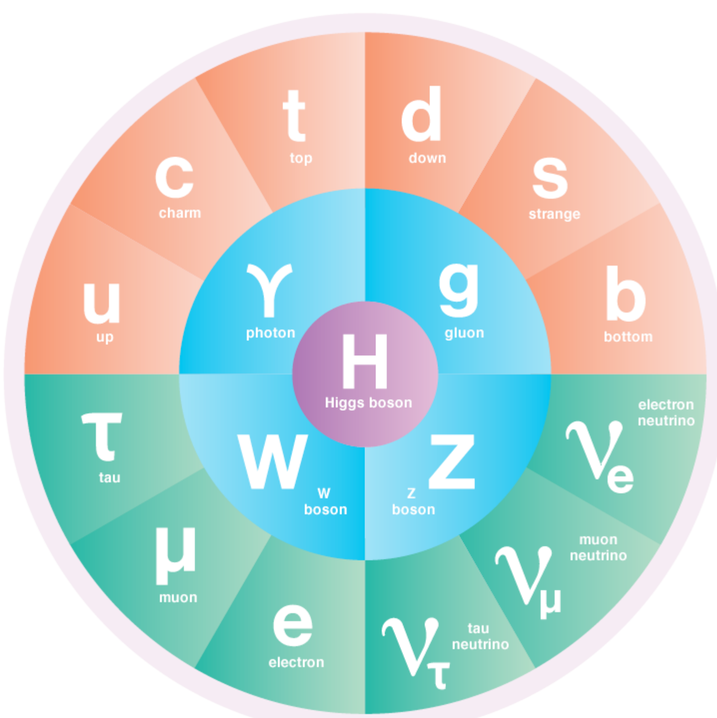

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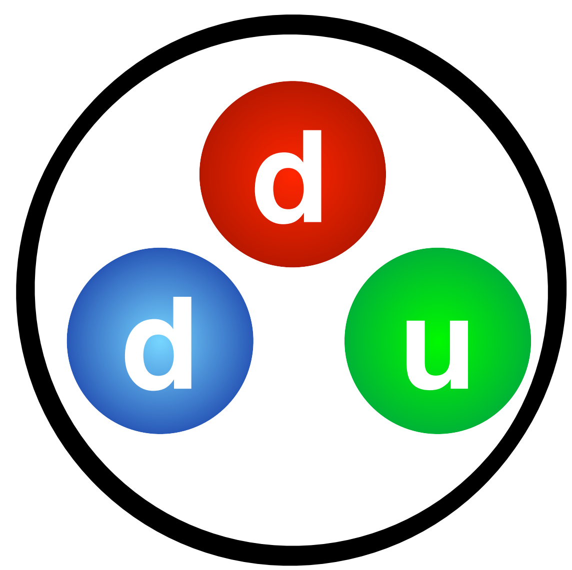
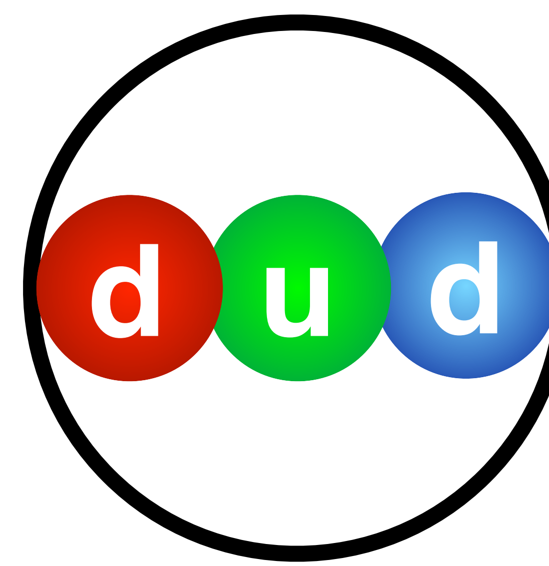
See also: quantum gravity

Why do neutrons have no dipole moment?

Strong CP



>99% of pictures on the internet



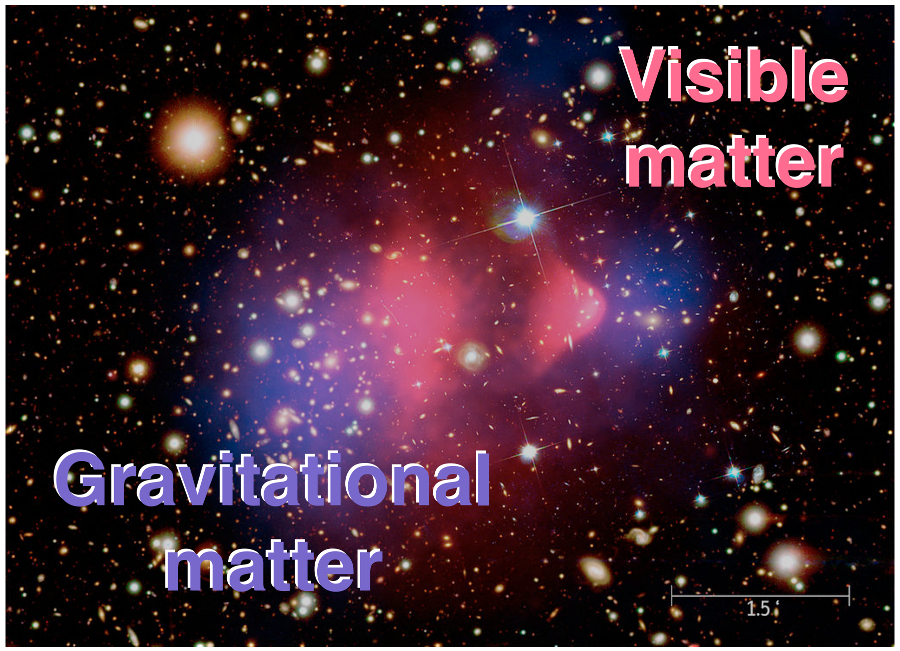
Reality

Questions in fundamental physics

Theoretical and **experimental** questions motivate a deep exploration **of the fundamental structure of nature**

What is the extra gravitational matter?

Dark Matter



NASA/CXC/M. Weiss - Chandra X-Ray Observatory: 1E 0657-56

See also: dark energy

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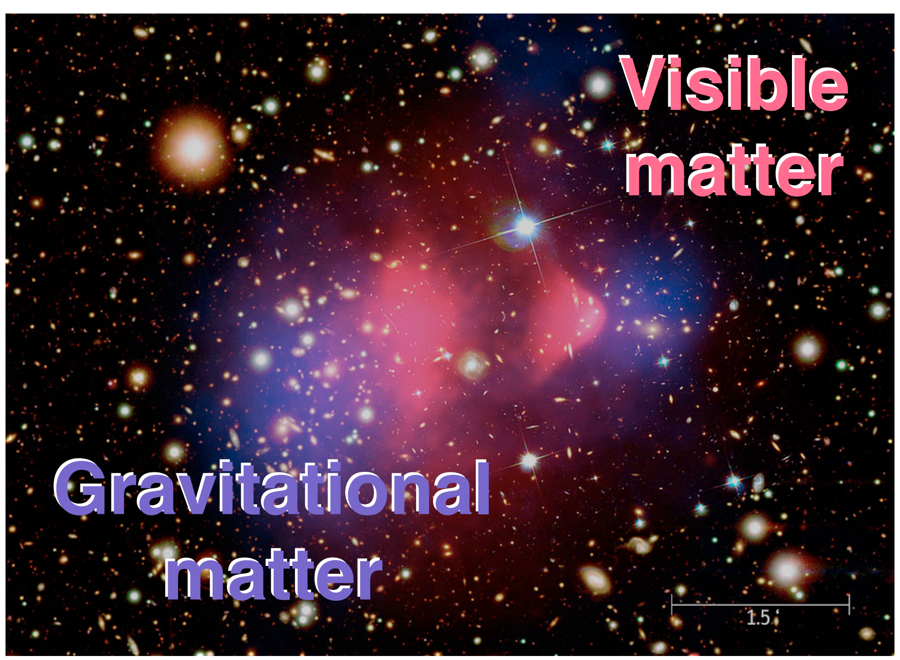
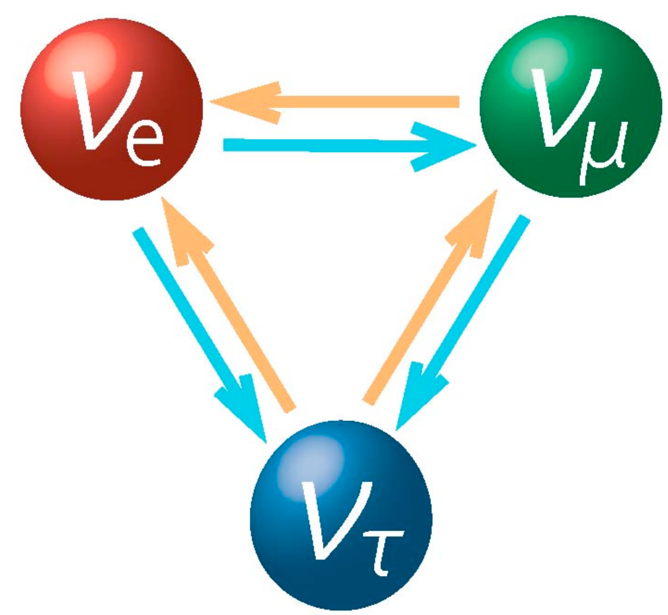


NASA/CXC/M. Weiss - Chandra X-Ray Observatory: 1E 0657-56

See also: dark energy

Why do neutrinos have a mass?

Flavor puzzles

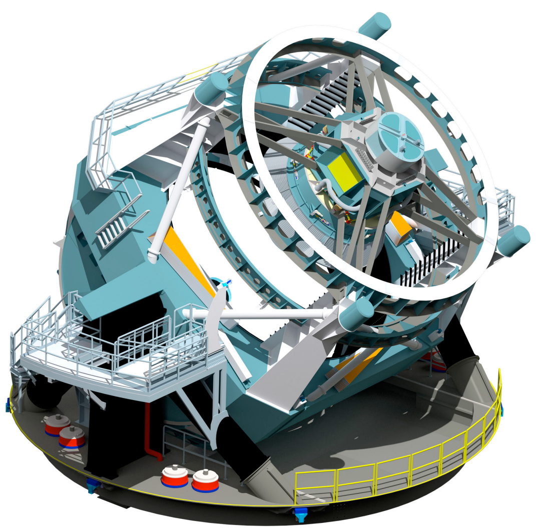


See also: Where did all the anti-particles go? (Baryogengesis)

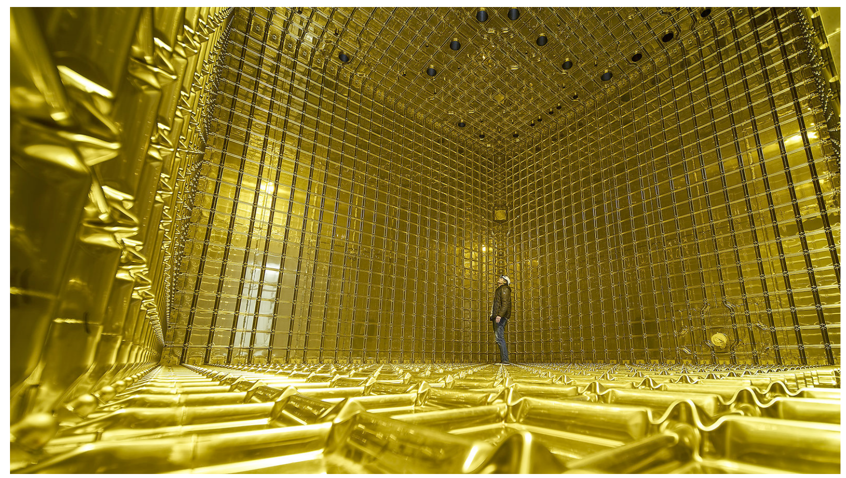
image source: T2K collaboration

Addressing the questions

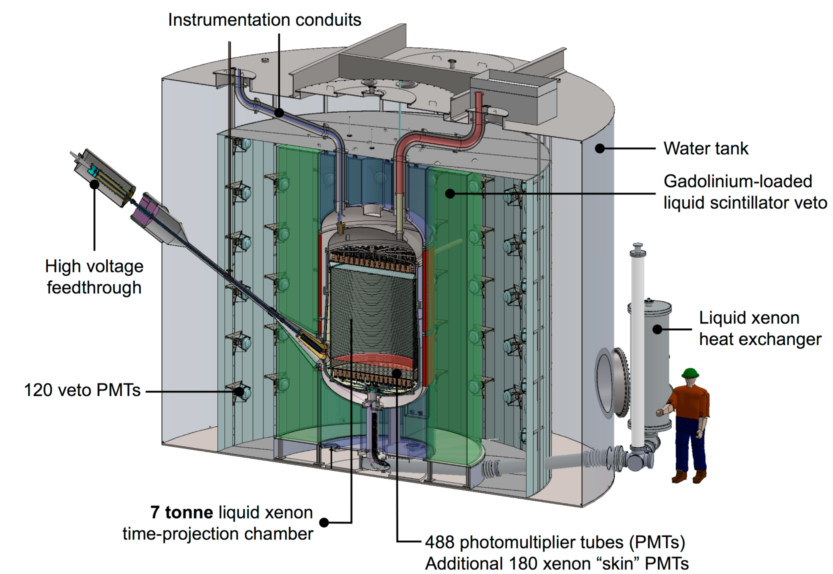
Dark matter/energy with Vera Rubin, CMB-S4, …



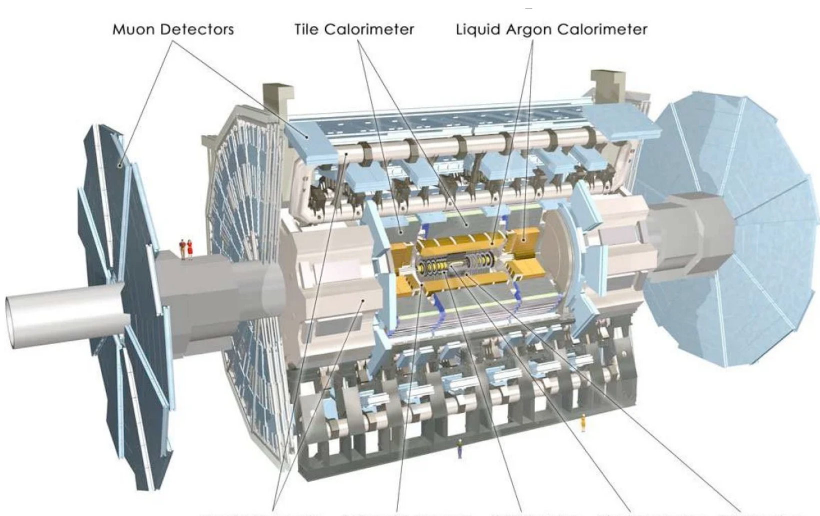
Fermilab, KEK neutrino experiments, …



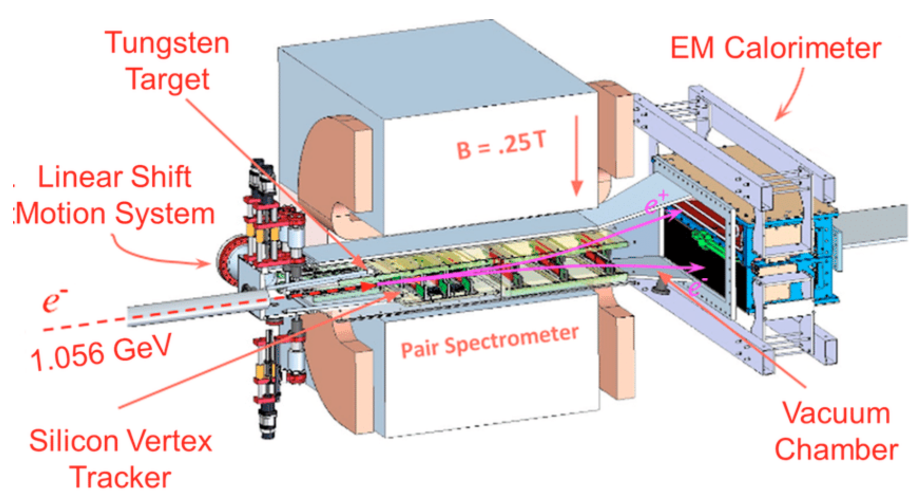
Dark Matter with LZ, XENON, …



Large Hadron Collider



Heavy Photon Search, …

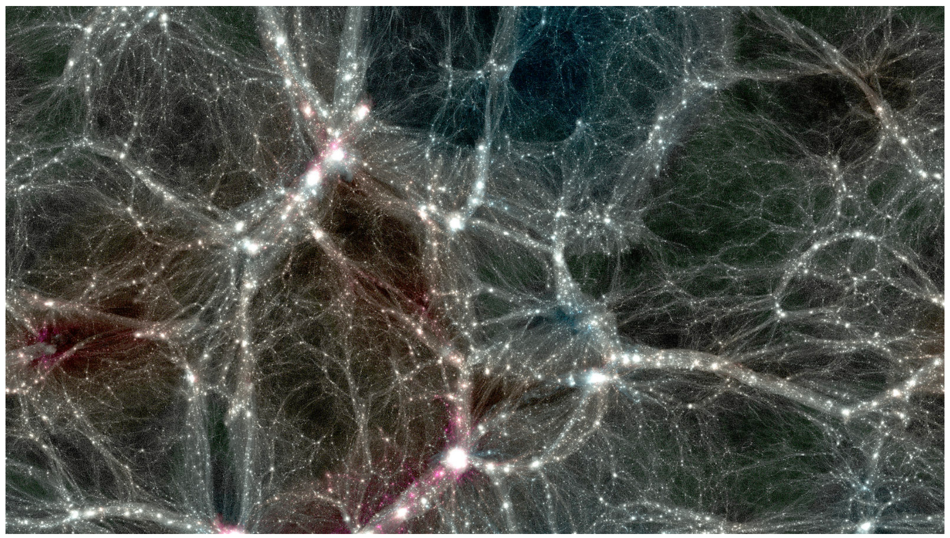


+ others !

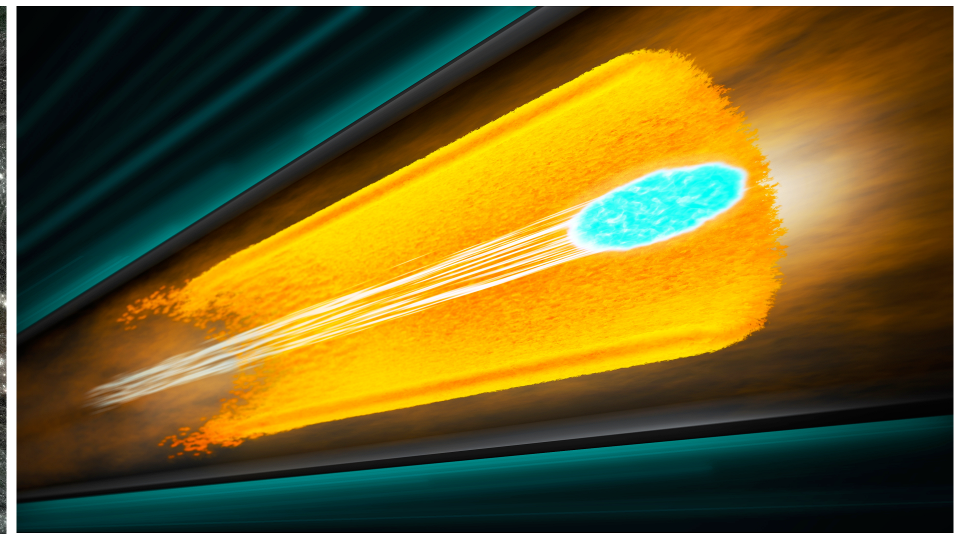
Image sources: LSST Corporation, CERN courier (CERN-201710-248-3), Berkeley Lab, CERN, HPS Collaboration

Addressing the questions

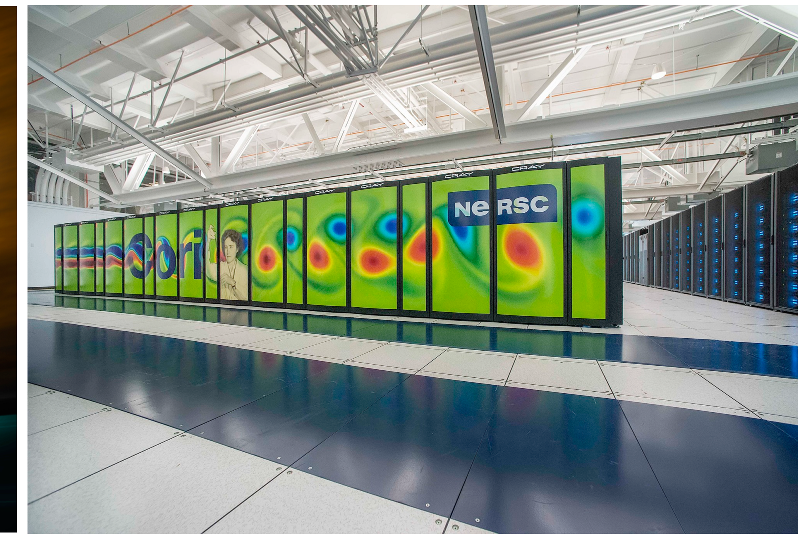
N-body simulations



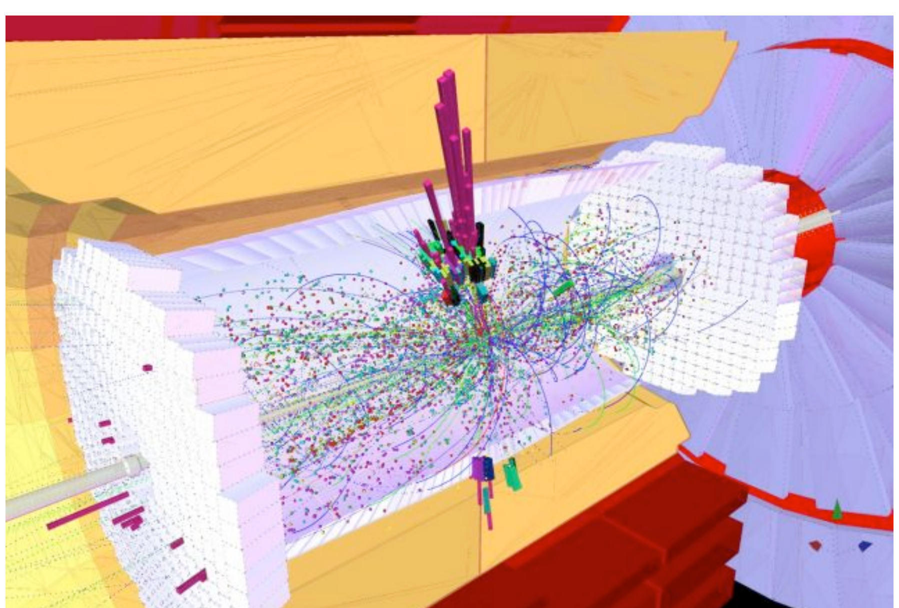
Advanced accelerators



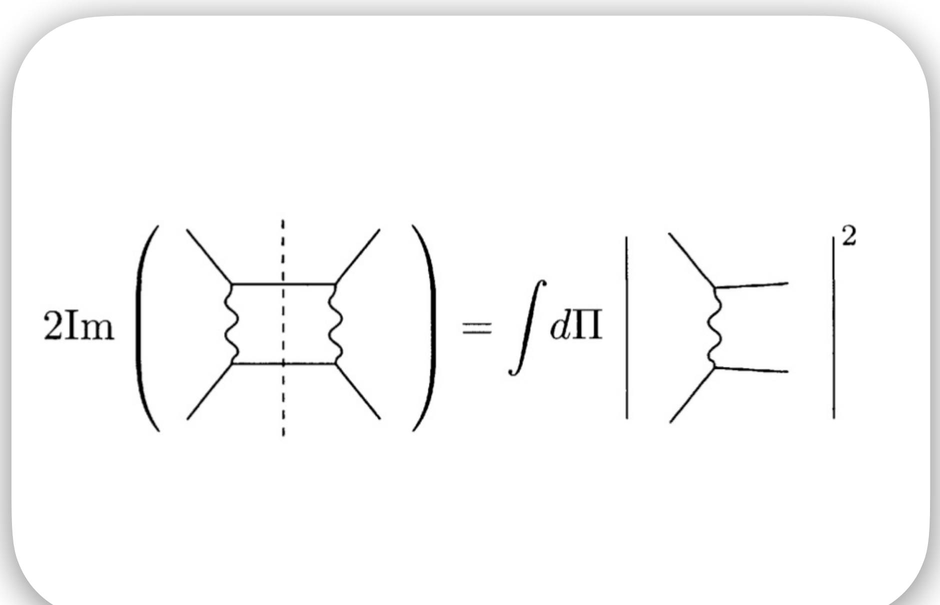
Supercomputers



Material interactions with Geant4



Theory Calculations

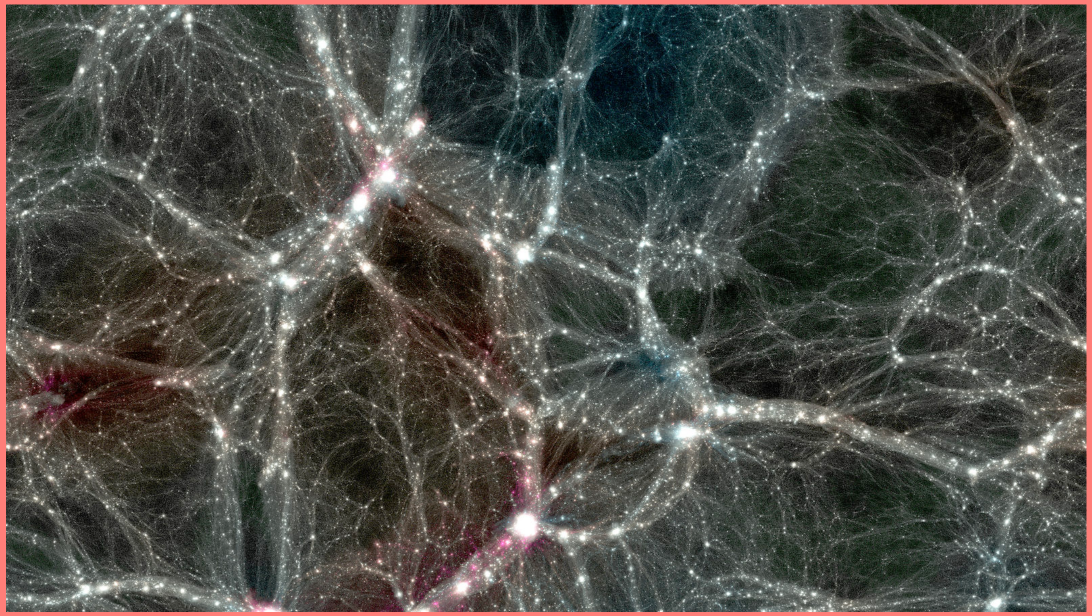


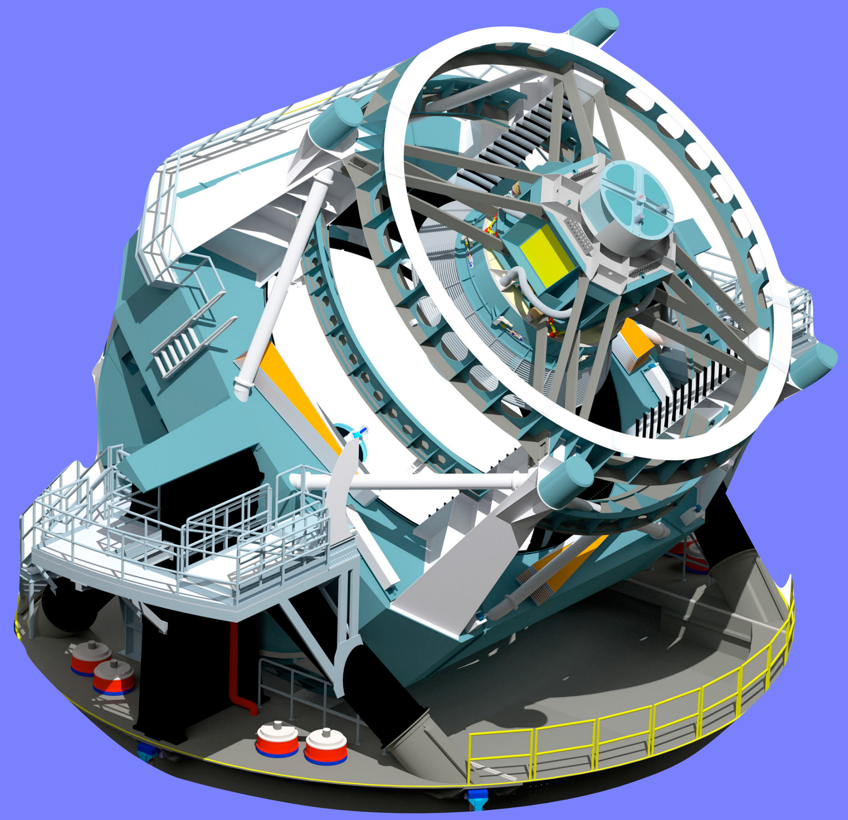
+ others !

Image sources: Dark Sky Simulations collaboration, SLAC, NERSC, Fermilab Today / Geant4, Peskin and Schroeder

A *hyper* challenge

Key **challenge** and **opportunity**: *hypervariate phase space* & *hyper spectral data*





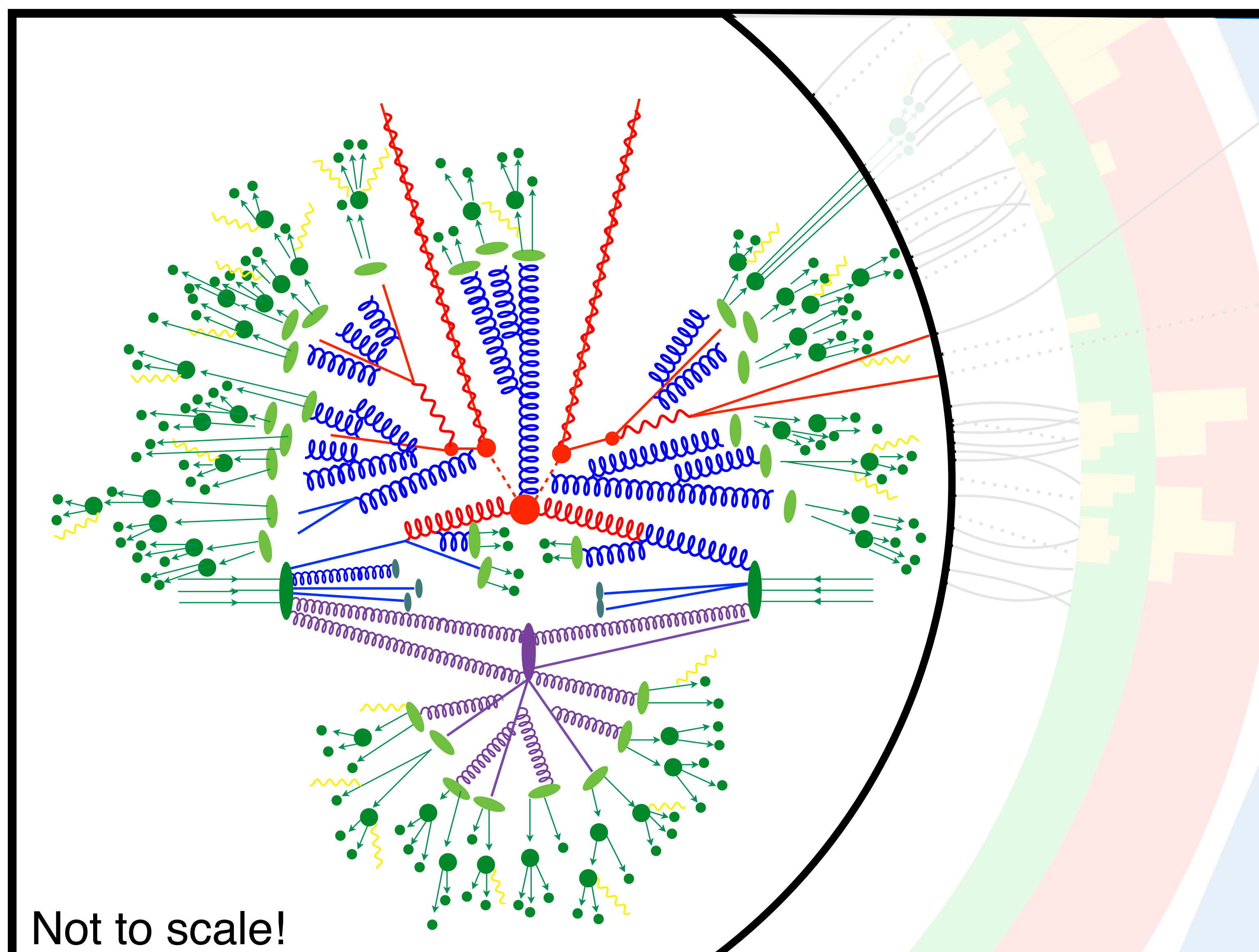
A *hyper* challenge

Key **challenge** and **opportunity**: *hypervariate phase space* & *hyper spectral data*

Typical collision events at the LHC produce **O(1000+)** particles

We detect these particles with **O(100 M)** readout channels

Image inspired by JHEP 02 (2009) 007



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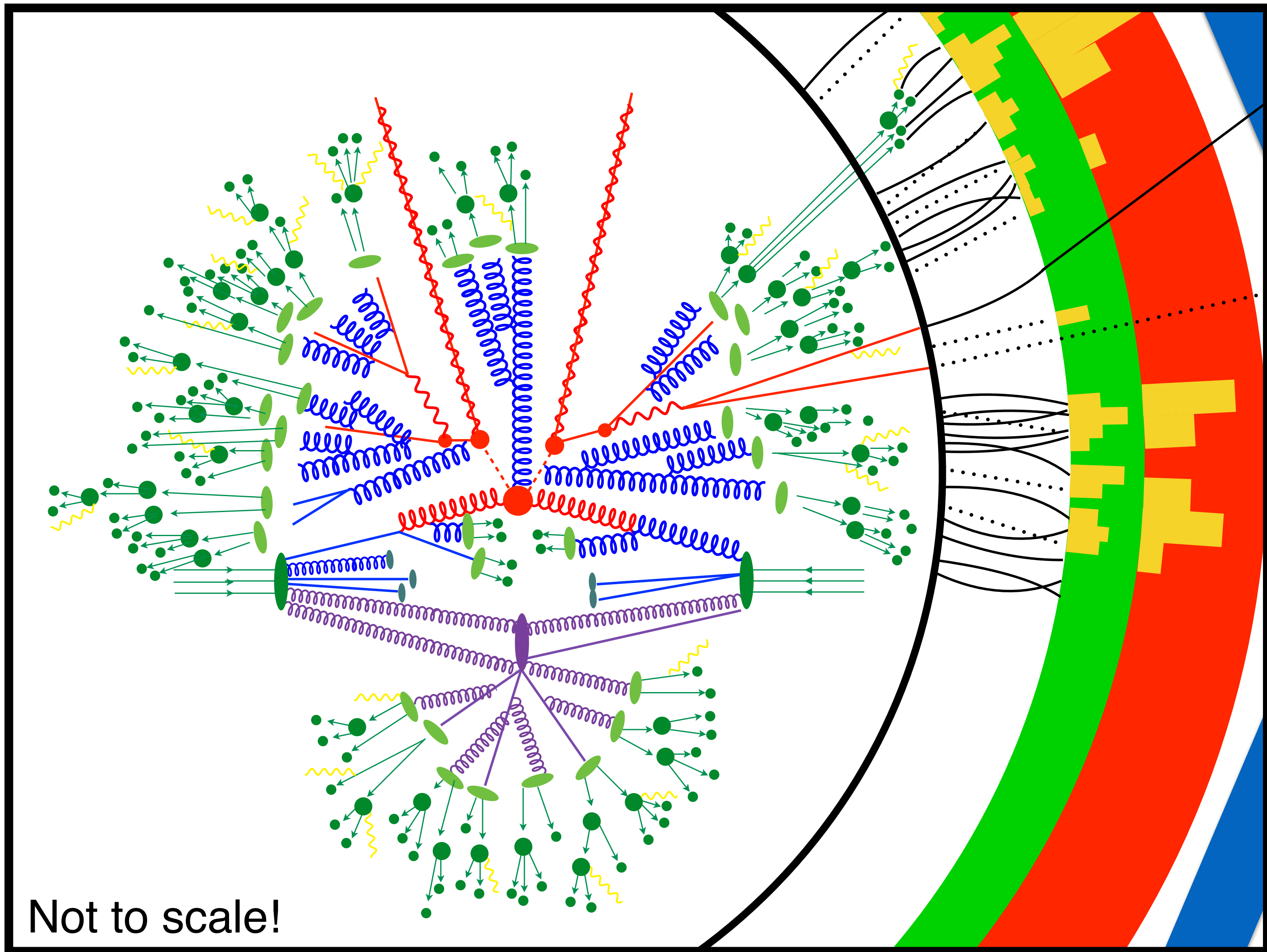

Hypervariate vision with deep learning

We have been conducting "multivariate" analysis of collision events for many years

Everyone is aware that there must be new physics, but maybe we need hypervariate vision to see it?

However, recent advances have opened up a **new way** of looking at our data. This **hypervariate vision** will lead to a deeper understanding of nature and perhaps surprises along the way…

Hypervariate vision with deep learning

We need innovative computational techniques to make the **data-driven discoveries of the future**.

This is not just about improving precision, it is about enabling new science!

Data analysis in fundamental physics

Theory of everything

↓

Physics simulators

↓

Detector-level observables

↓

Pattern recognition ⟷

Nature

↓

Experiment

↓

Detector-level observables

↓

Pattern recognition

Data analysis in fundamental physics

Theory of everything

↓

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↔

Nature

↓

Experiment

↓

Detector-level observables

↓

Pattern recognition

This is where most machine learning is being applied.

Data analysis in fundamental physics

Analysis
Observables

Calibration

Pattern
recognition

Noise
mitigation

Readout

Nature

↓

Experiment

↓

Detector-level observables

↓

Pattern recognition

This is where most machine learning is being applied.
I won't discuss this area at all for the remainder of the talk

Data analysis in fundamental physics

Lorentz Covariant Networks

S. Qiu, S. Han, X. Ju, **BN**, H. Wang
2203.05687

Algorithmic fairness
("decorrelation")

O. Kitouni, **BN**, C. Weisser, M. Williams
JHEP 04 (2021) 70, 2010.09745

Uncertainty-aware learning

A. Ghosh, **BN**, D. Whiteson
PRD 104 (2021) 056025, 2105.08742

Symmetry Discovery

K. Desai, **BN**, J. Thaler
PRD (2022), 2112.05722

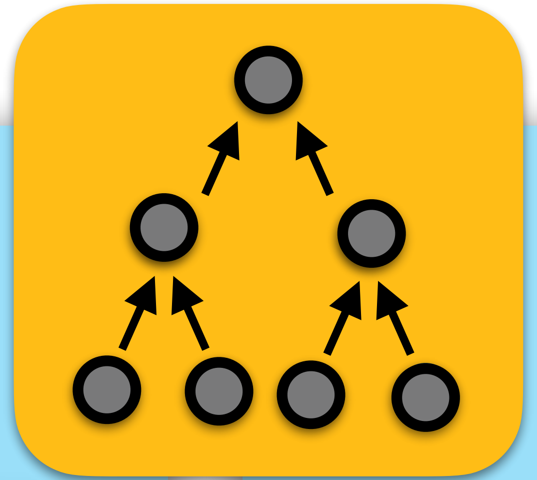
…many exciting topics I'd be happy to discuss later!

I won't discuss this area at all for the remainder of the talk

Data analysis in fundamental physics

Theory of everything	**Nature**
↓	↓
Physics simulators	Experiment
↓	↓
Detector-level observables	Detector-level observables
↓	↓
Pattern recognition ⟷	Pattern recognition

Data analysis in fundamental physics



Theory of everything

↓

Physics simulators

↓

Detector-level observables

↓

Pattern recognition ⟷ Pattern recognition

Nature

↓

Experiment

↓

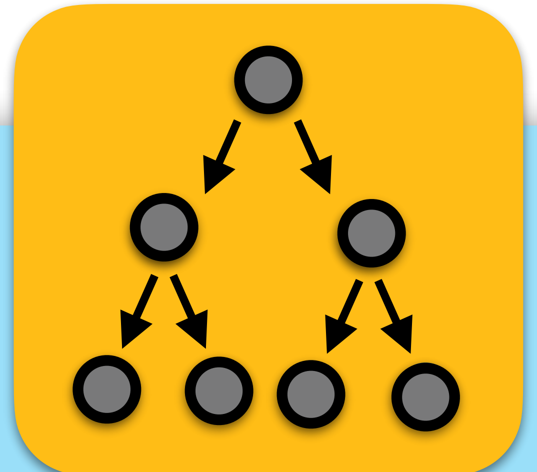
Detector-level observables

↓

Pattern recognition

A growing toolkit called “generative models” are being developed to accelerate or augment simulations.

Data analysis in fundamental physics



Theory of everything

↓

Physics simulators

↓

Detector-level observables

↓

Pattern recognition

Nature

↓

Experiment

↓

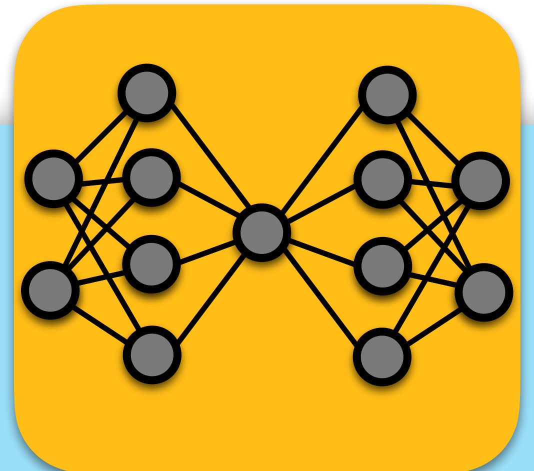
Detector-level observables

↓

Pattern recognition

This is the “inverse” direction, where we use simulations to infer properties of the fundamental theory.

Data analysis in fundamental physics



Theory of everything

↓

Physics simulators

↓

Detector-level observables

↓

Pattern recognition

↔

Nature

↓

Experiment

↓

Detector-level observables

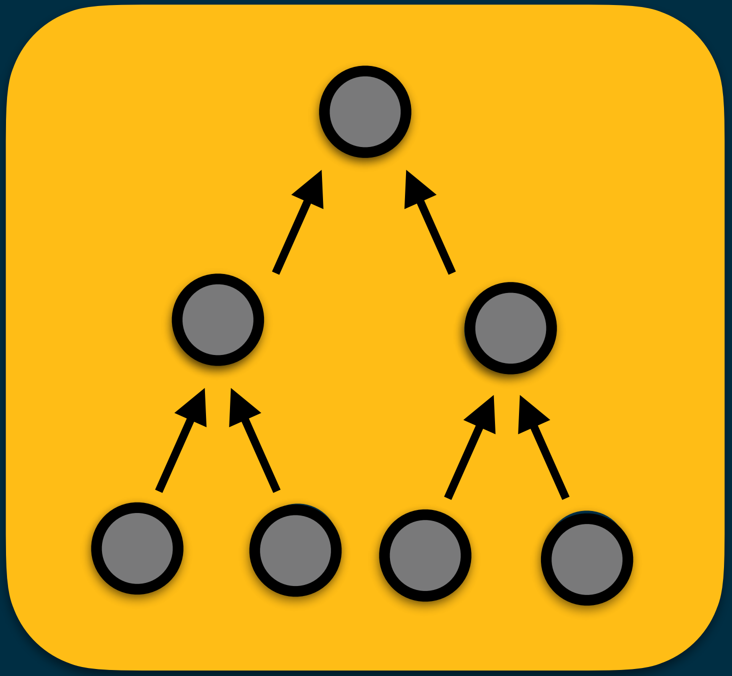
↓

Pattern recognition

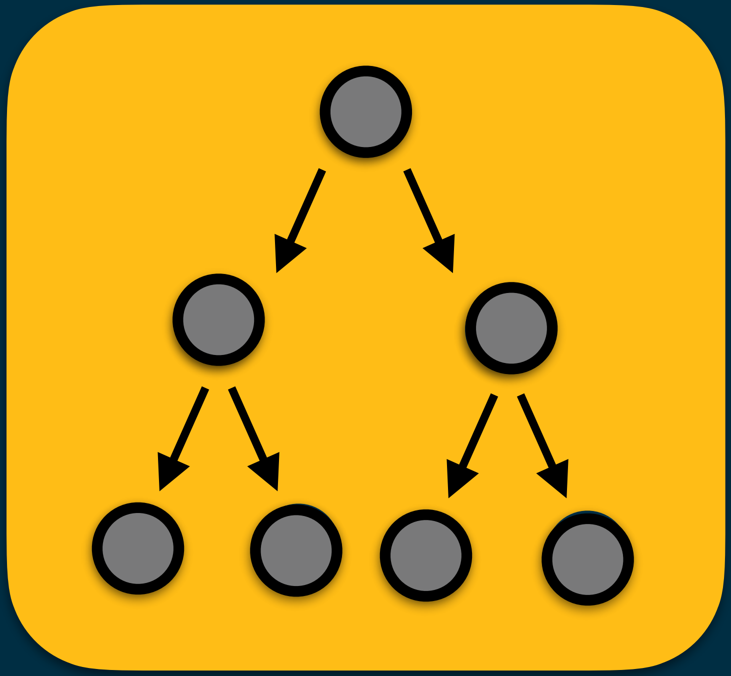
There is a growing need for simulation-independent methods that allow us to look for unanticipated scenarios.

Outline for today

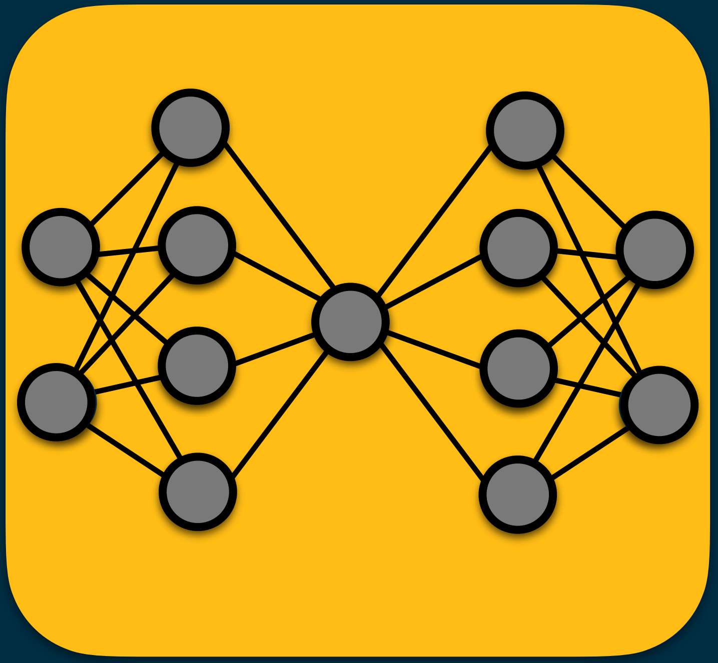
I'll focus on three core, cross-cutting areas of ML ∩ Physics



Forward Models



Inverse Models



Simulation-free

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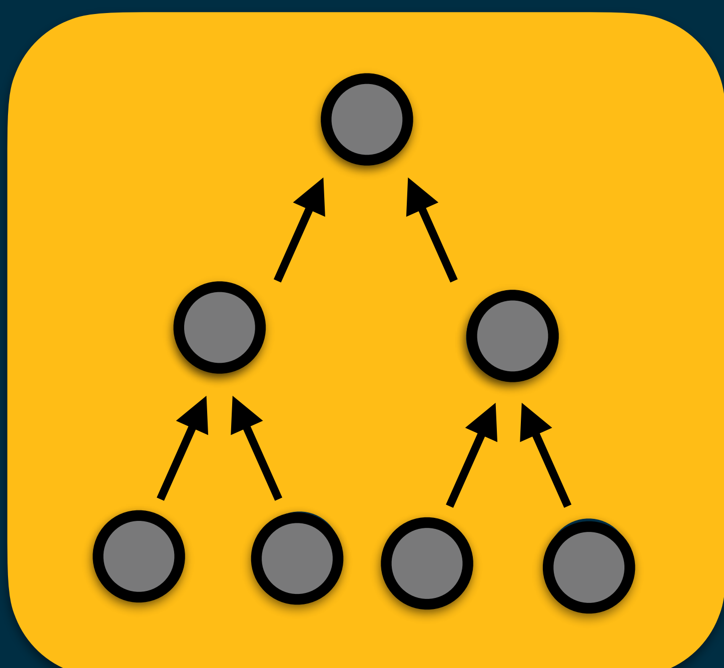
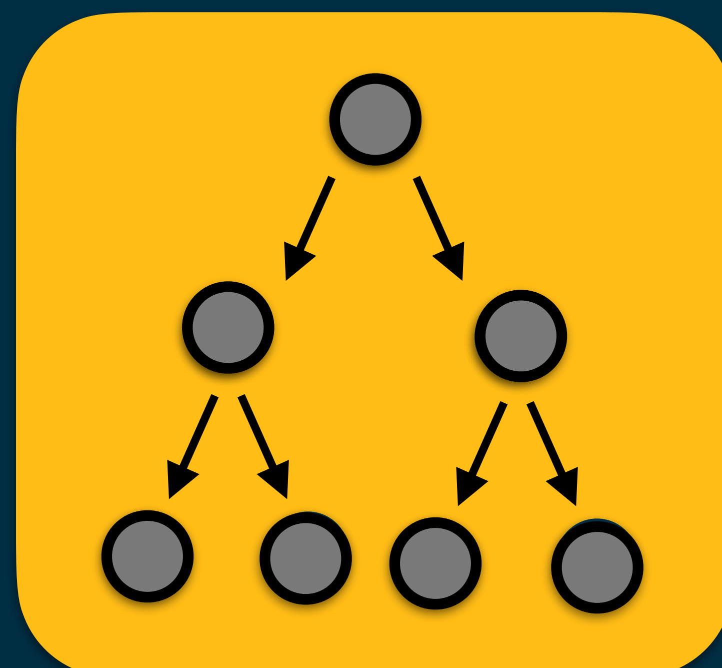
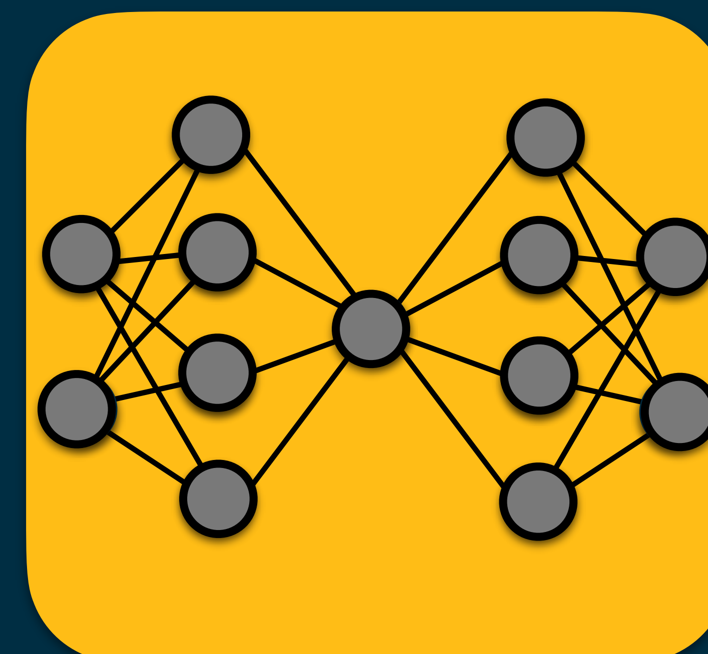


Forward Models
(fast simulation)



Inverse Models
(unfolding)



Simulation-free
(anomaly detection)

To illustrate these exciting topics, I'll give one vignette per area

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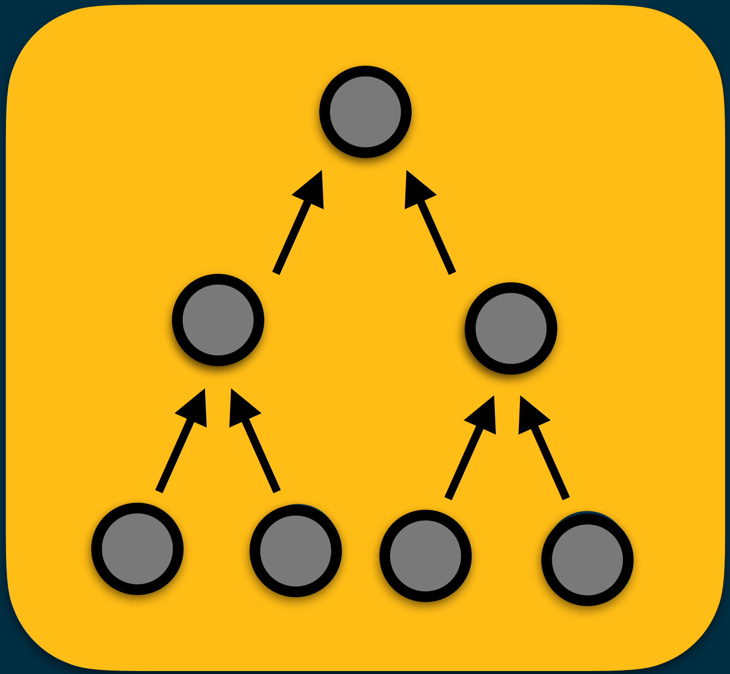

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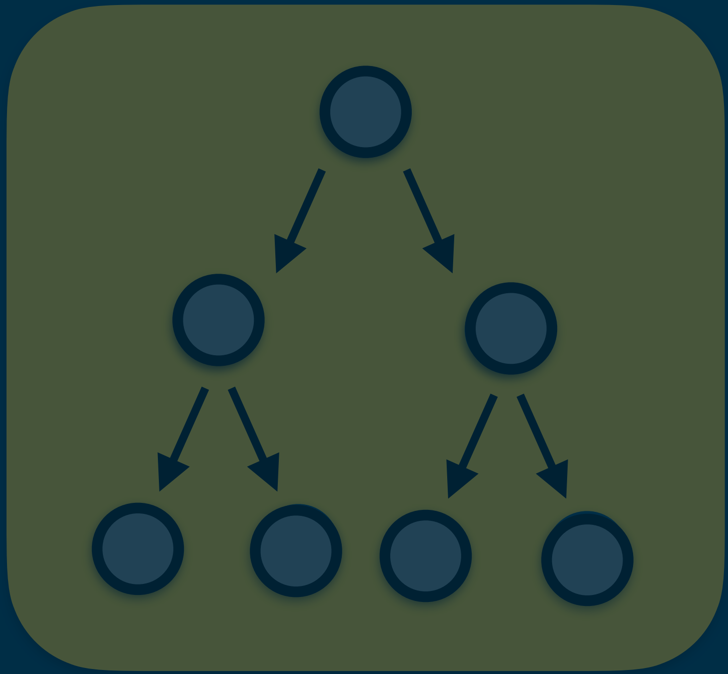

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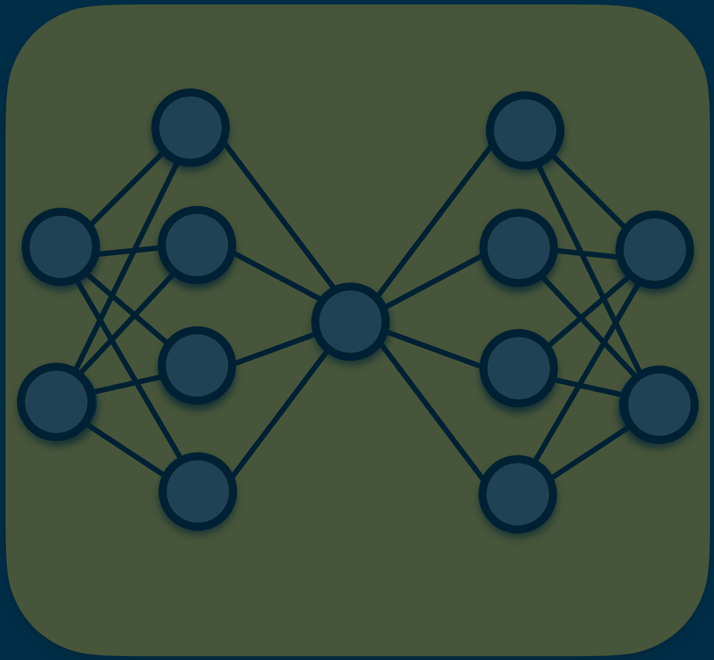

Simulation-free
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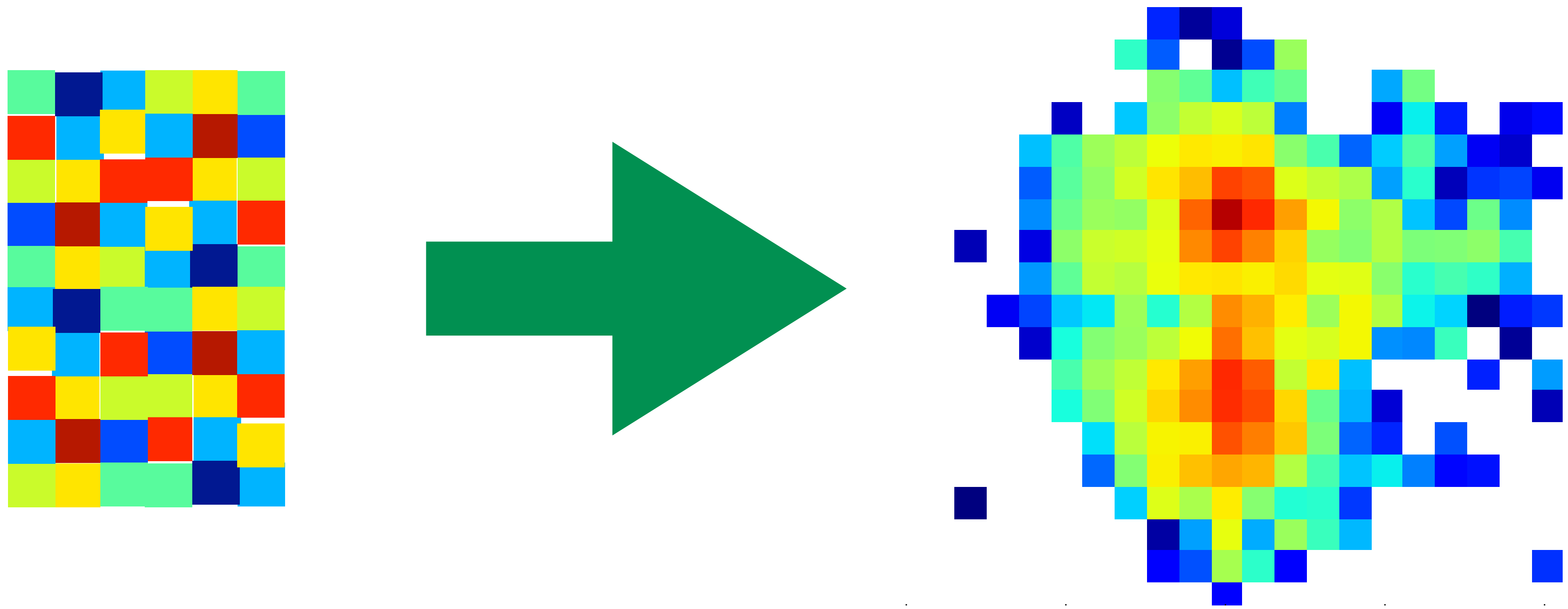
Introduction: generative models

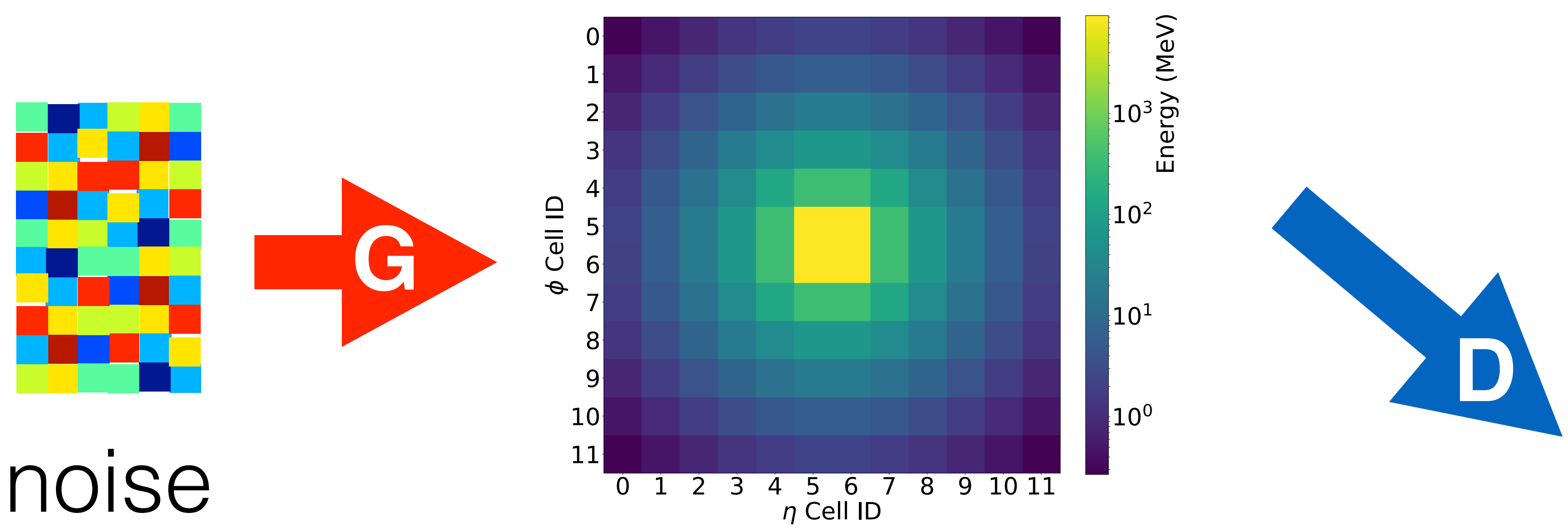
A **generator** is nothing other than a function that maps random numbers to structure.

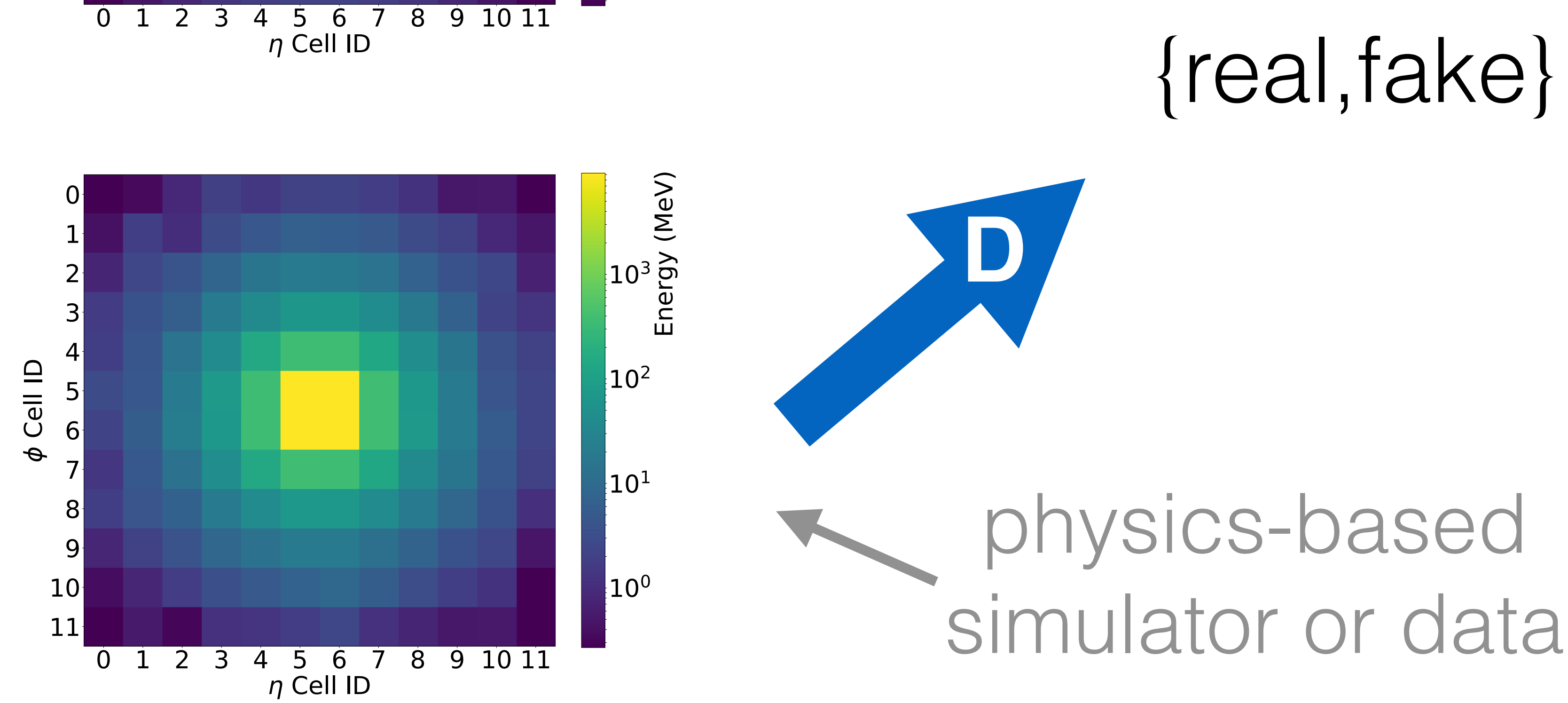


Deep generative models: the map is a deep neural network.

Introduction: GANs

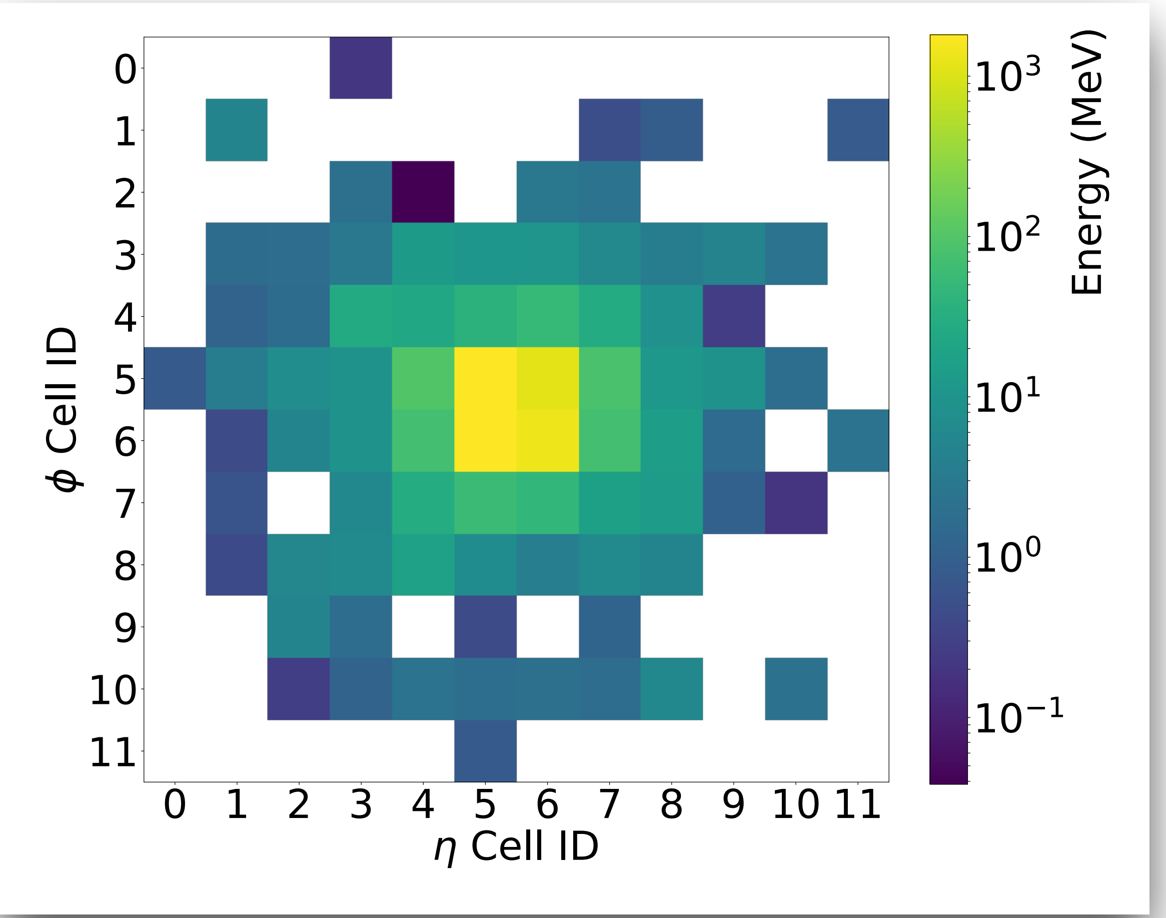
Generative Adversarial Networks (GANs):
A two-network game where one ***maps noise to structure*** *and one* ***classifies images as fake or real***.





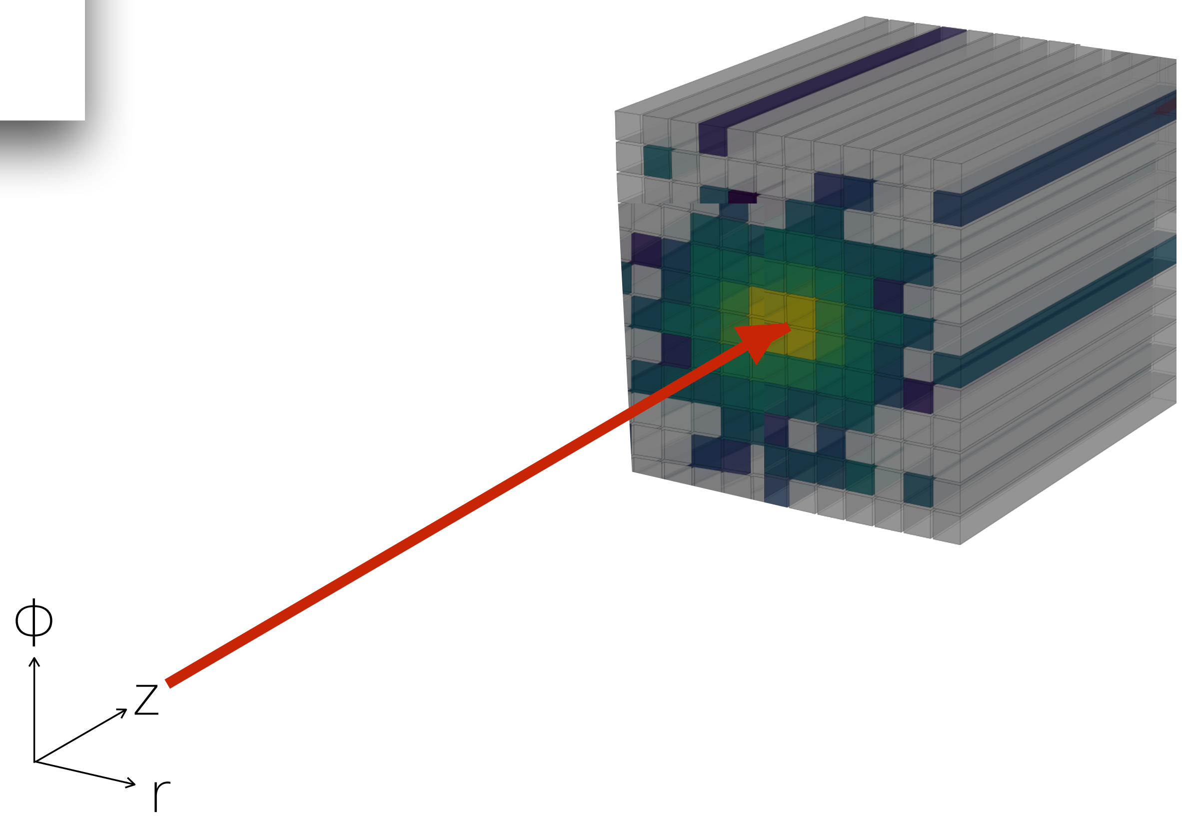
When **D** is maximally confused, **G** will be a good generator

Accelerating Detector Simulations



Calorimeters are often the slowest to simulate

stopping particles requires simulating interactions of all energies



Grayscale images: pixel intensity = energy deposited

Solution: CaloGAN

GANs and related deep generative models are promising tools for fast approximate simulations

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GANs and related deep generative models are promising tools for fast approximate simulations

These tools are automated, which enables portability

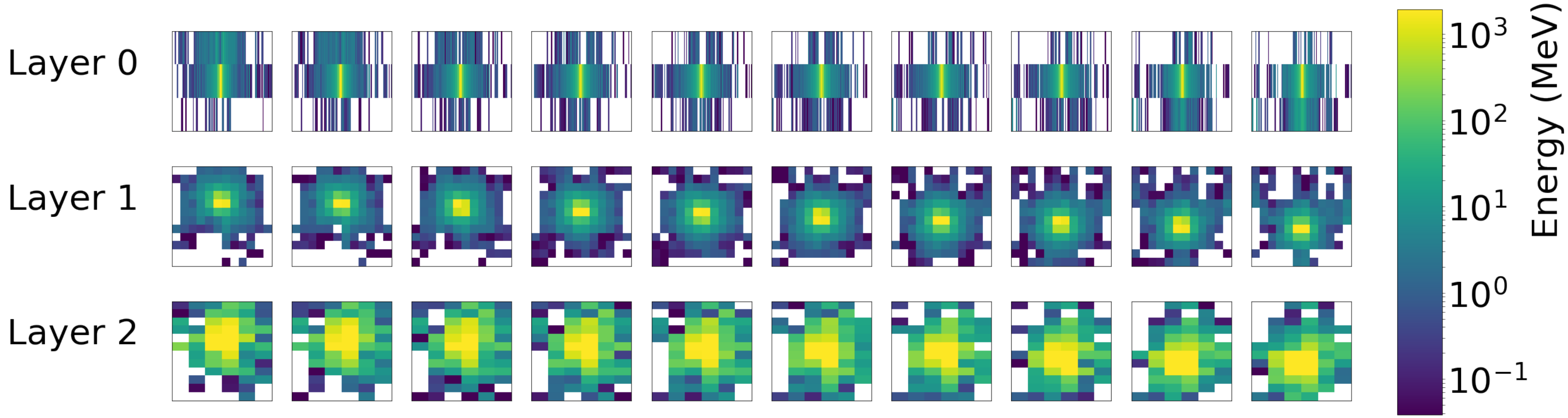
They are fast, can be readily retrained, and don't take much disk space

Solution: CaloGAN

GANs and related deep generative models are promising tools for fast approximate simulations

These tools are automated, which enables portability

We also have full control over the physics:

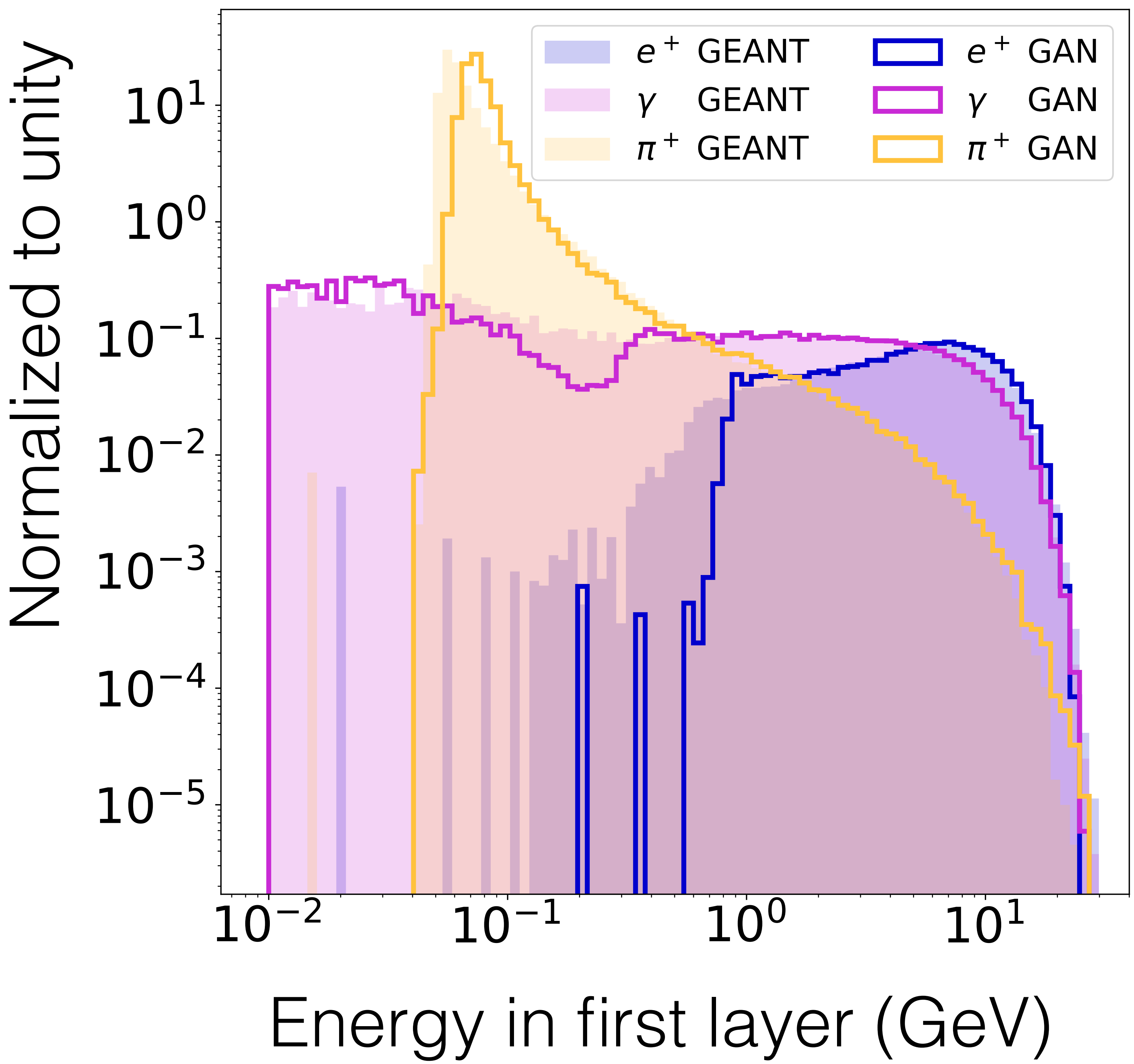


fix fluctuations, sweep shower location

M. Paganini, L. De Oliveira, **BN,** 1711.08813

Solution: CaloGAN

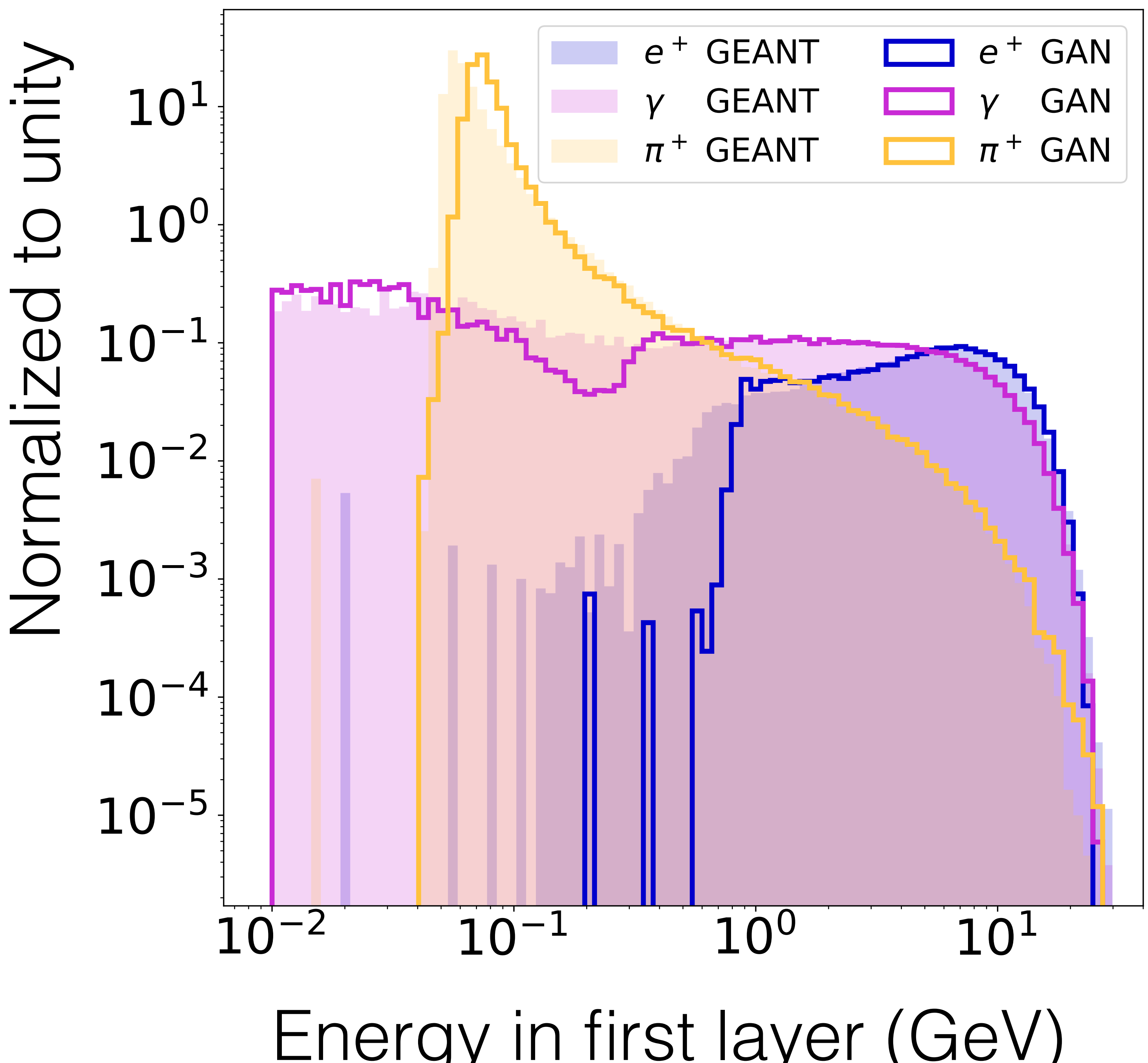
M. Paganini, L. De Oliveira, **BN**, PRL 120 (2018) 042003



Pions deposit much less energy in the first layers; leave the calorimeter with significant energy

Solution: CaloGAN

M. Paganini, L. De Oliveira, **BN**, PRL 120 (2018) 042003



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Time to generate an event is orders of magnitude faster than Geant4 and independent of energy

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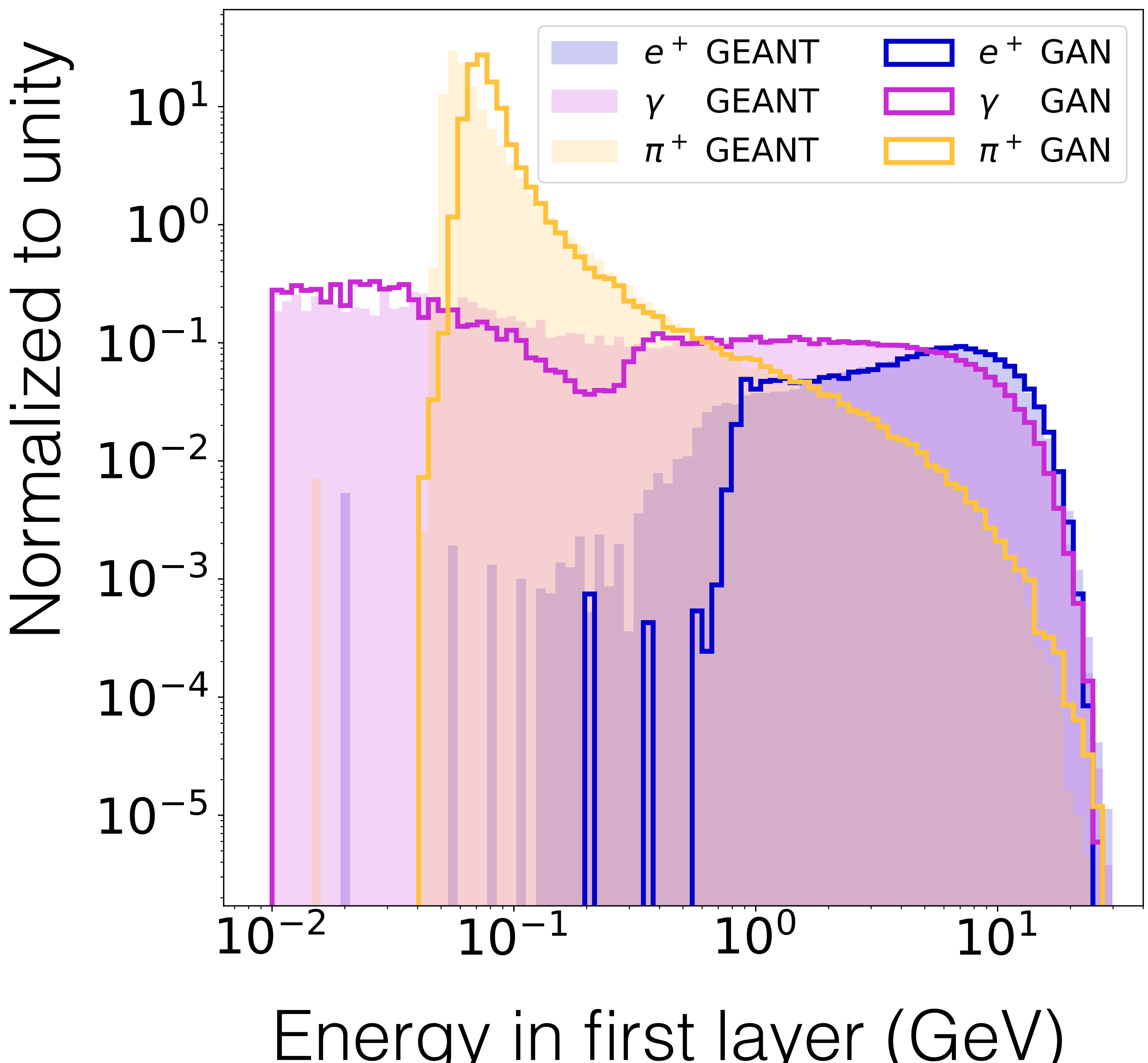
M. Paganini, L. De Oliveira, **BN**, PRL 120 (2018) 042003



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ATLAS now uses a CaloGAN-like approach and will use it to generate **billions of showers**!

ATLAS, 2109.02551

Future of Deep Generative Models

Goal: maintain speed, improve precision

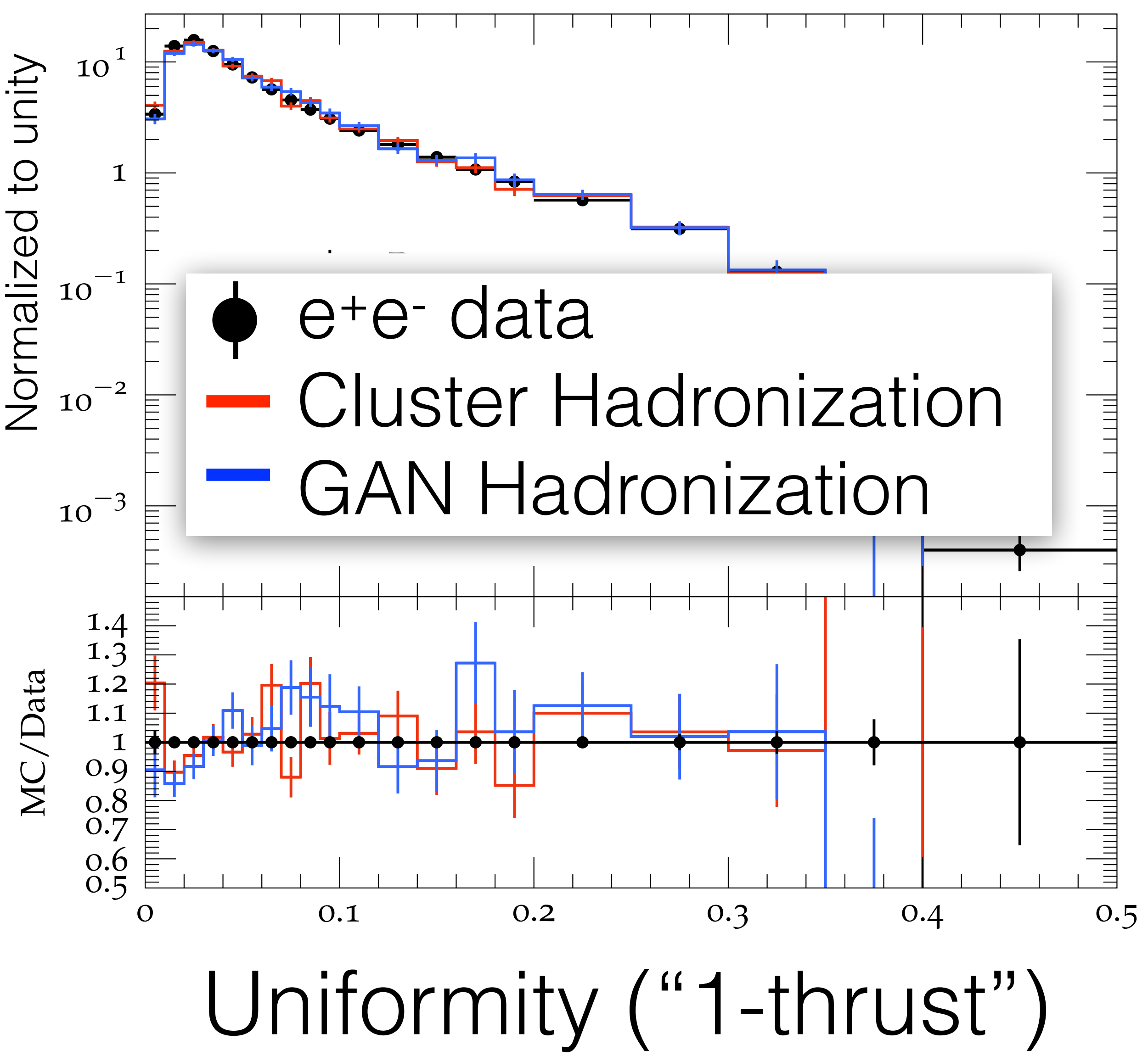
Methods

Next frontier: physics-informed generative models

Science

- Fast simulation for next-gen experiments
- Flexible, “non-parametric” functions for phenomenological models
  - Hadronization (quarks/gluons → hadrons)
  - Dark matter N-body → baryons

A. Ghosh, X. Ju, **BN**, A. Siodmok, 2203.12660



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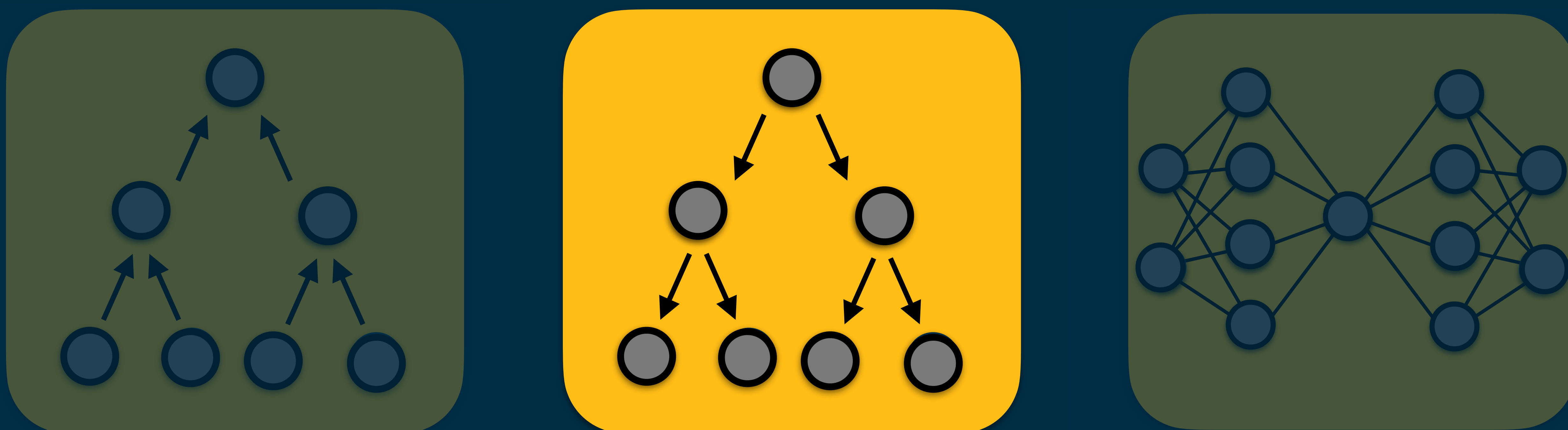


Forward Models (fast simulation)

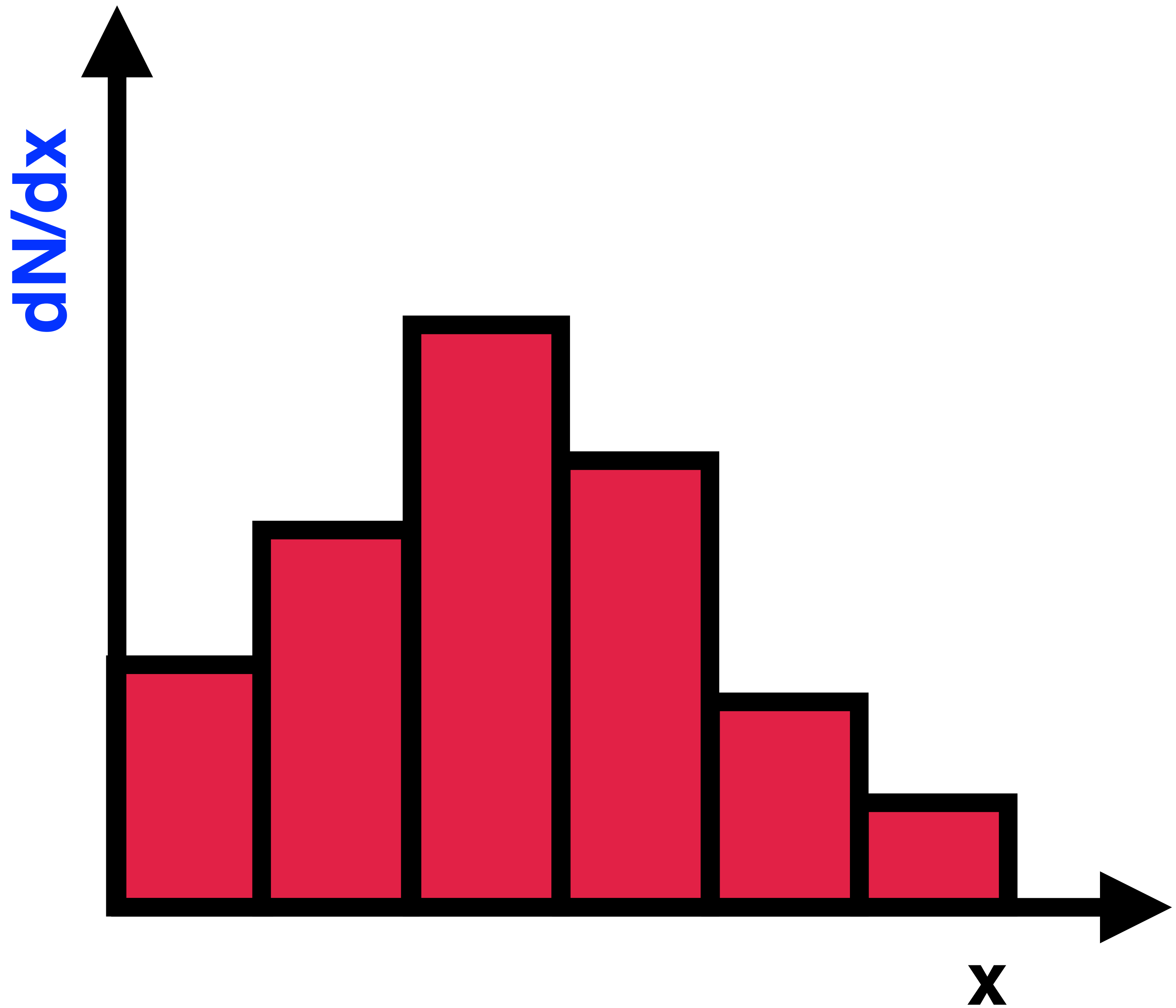
Inverse Models (unfolding)

Simulation-free (anomaly detection)

To illustrate these exciting topics, I'll give one vignette per area

Deconvolution/Unfolding

Differential cross section measurements are central to collider physics & are increasingly important in neutrino physics



Deconvolution/Unfolding

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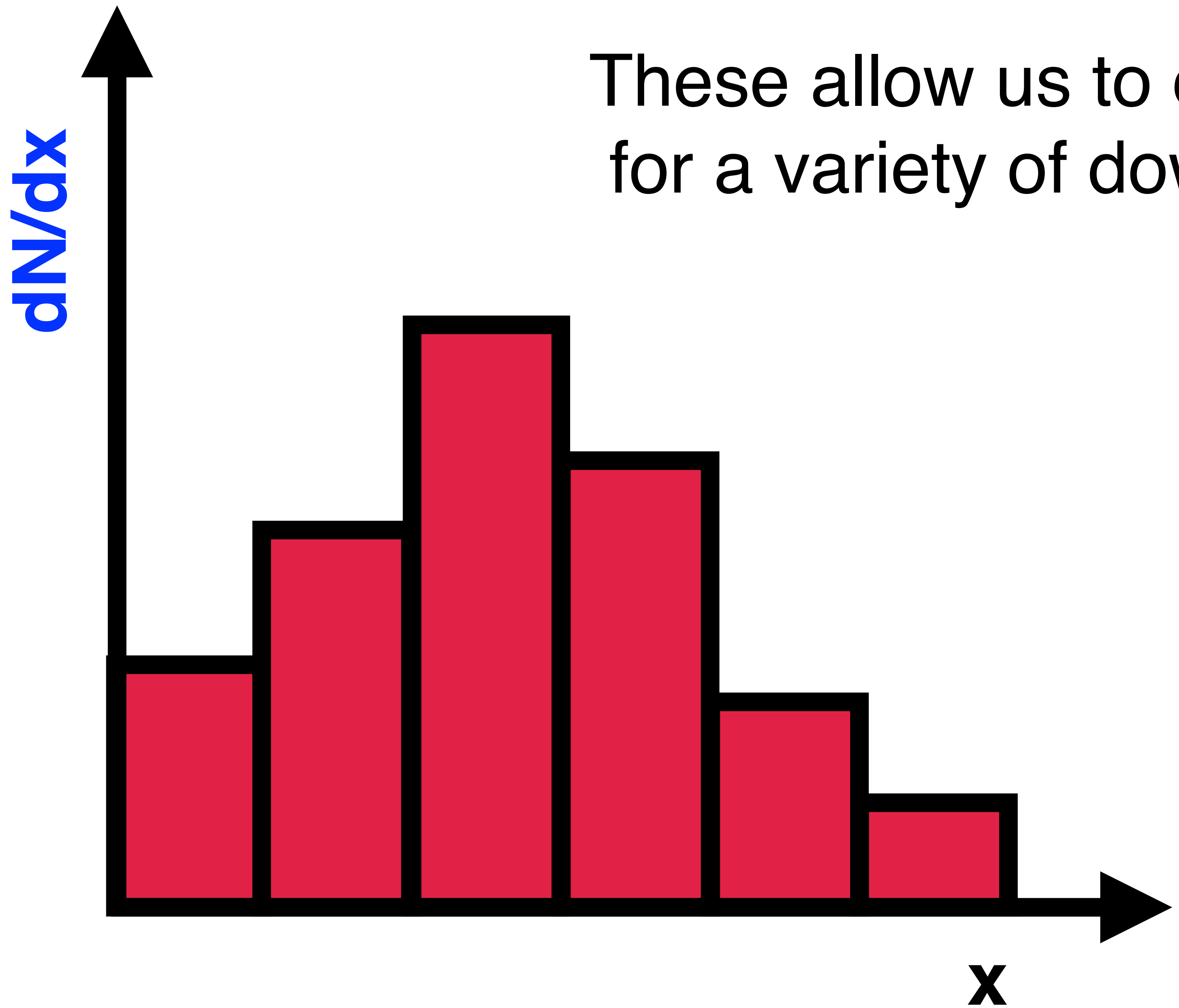
These allow us to compare data with theory for a variety of down-stream science goals



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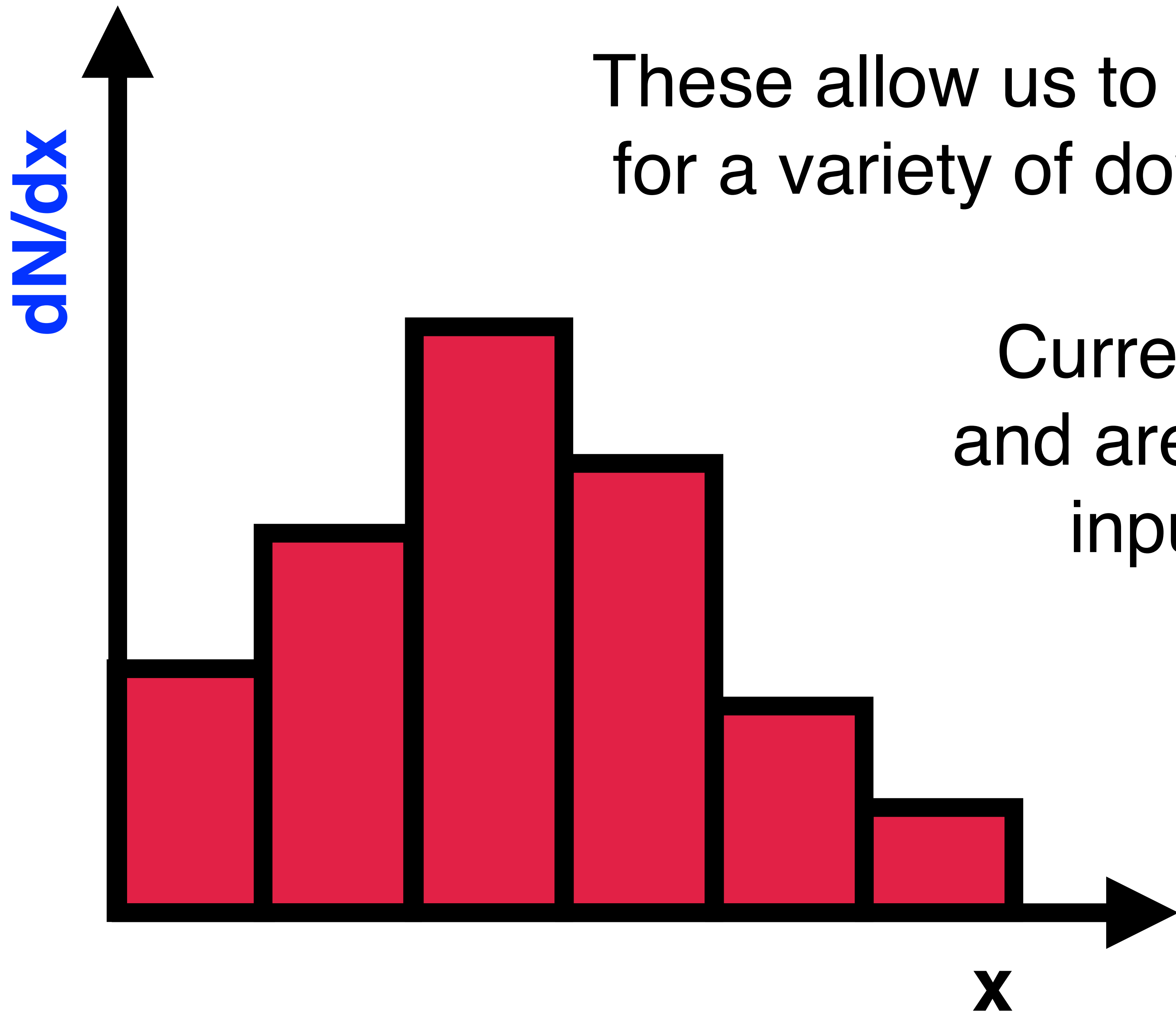

Current approaches use bins and are limited in the number of input/output dimensions.

Deconvolution/Unfolding

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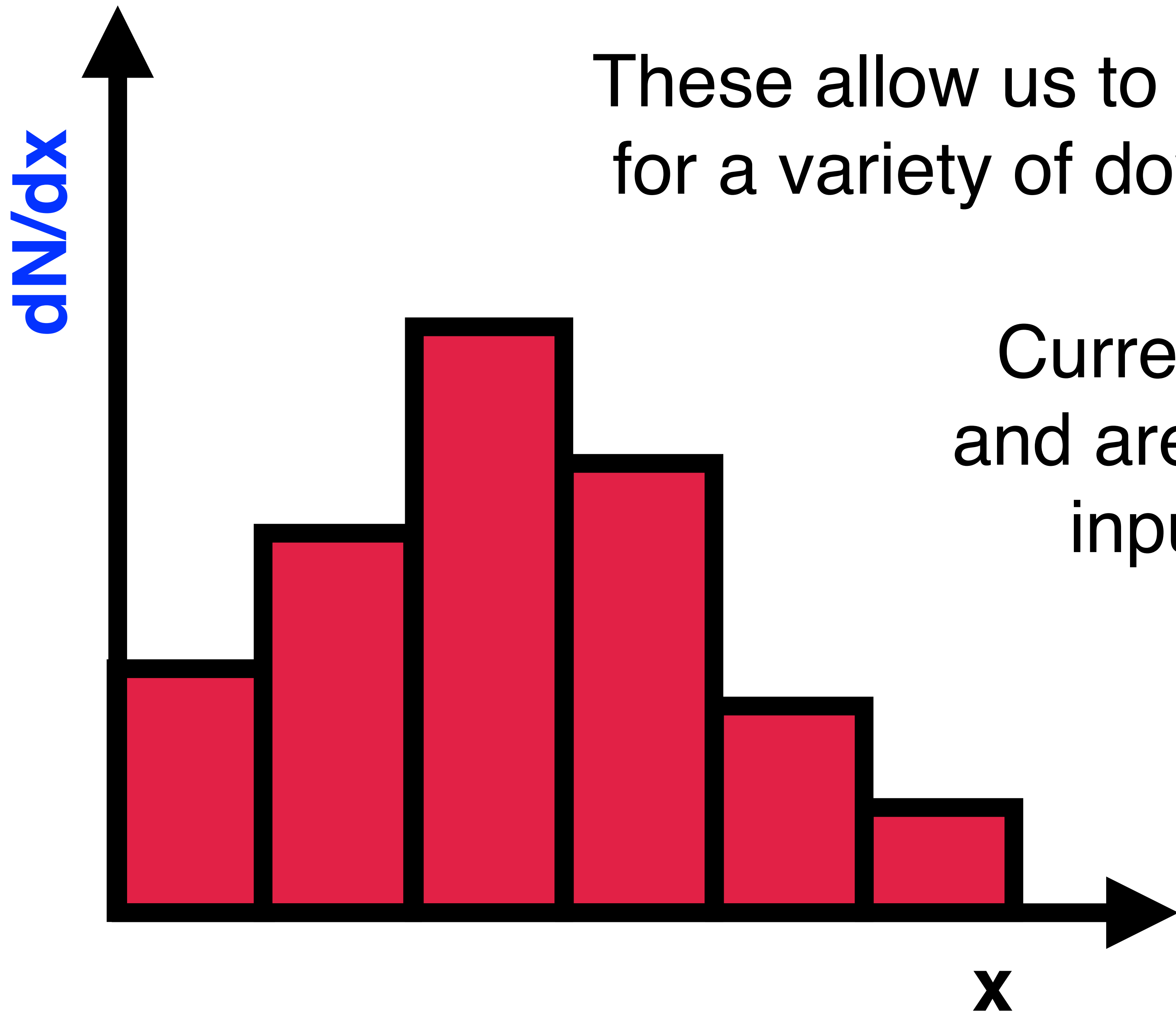

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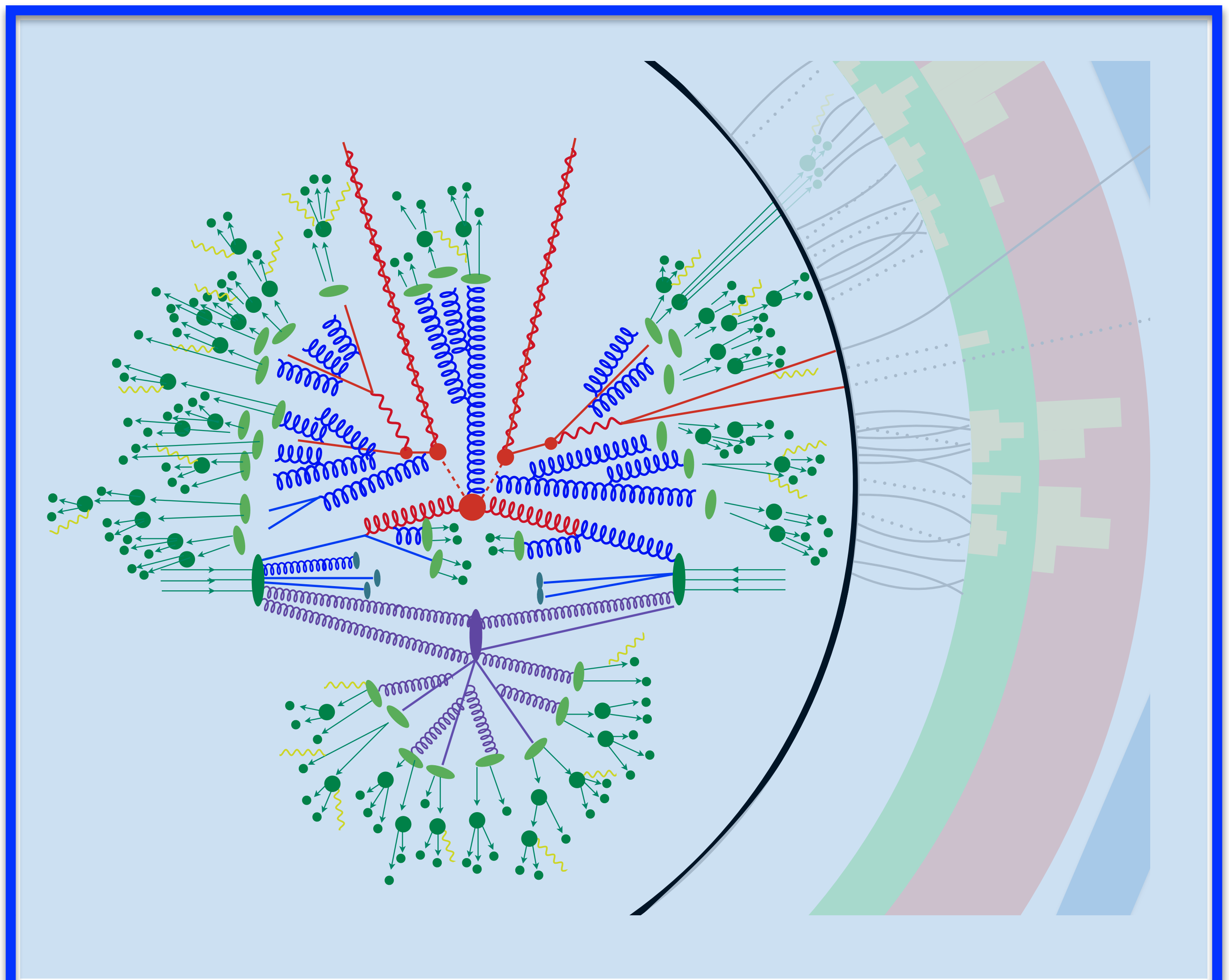
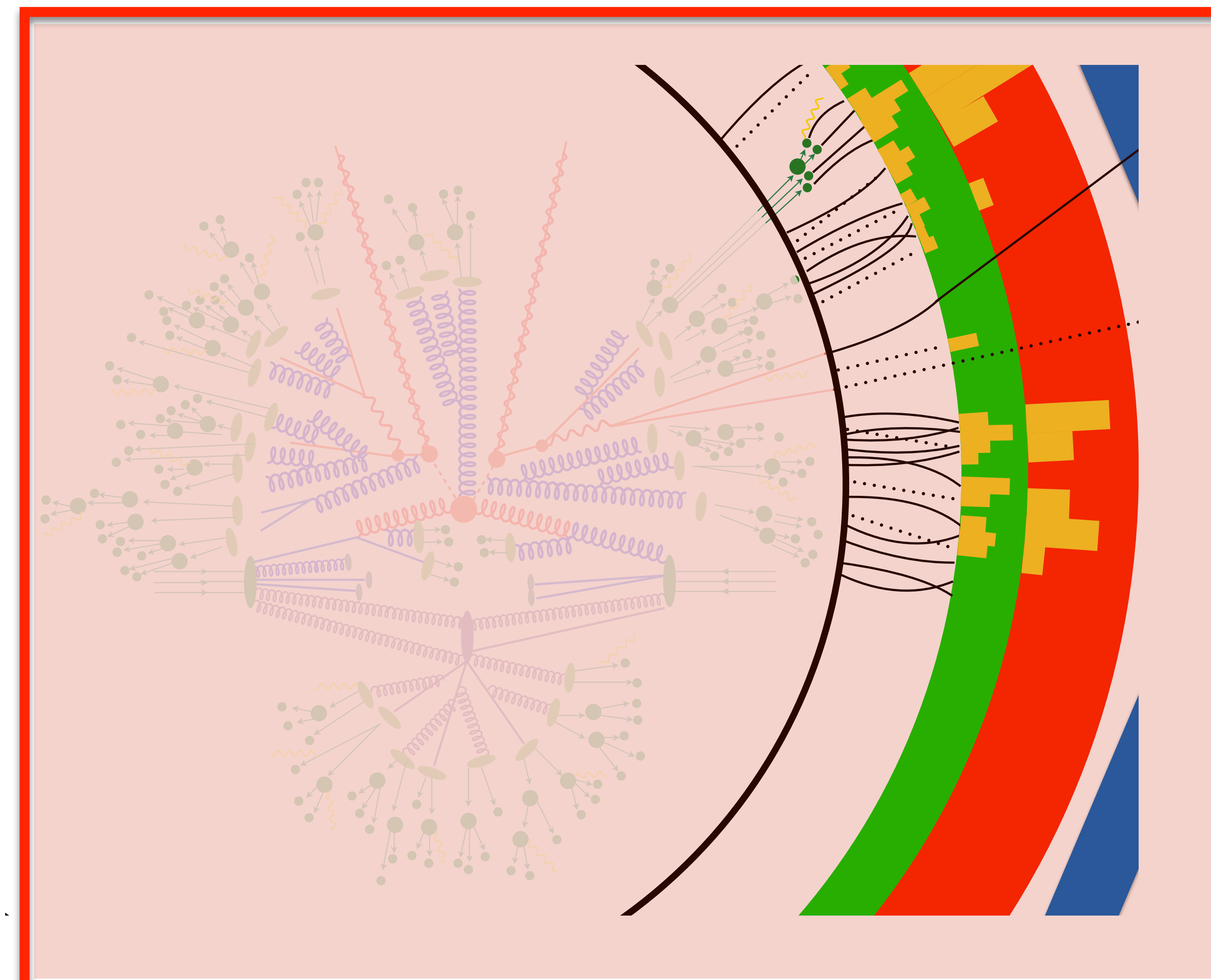
Current approaches use bins and are limited in the number of input/output dimensions.

Can we go unbinned and high-dimensional?

Deconvolution/Unfolding

Want this | **Measure this**



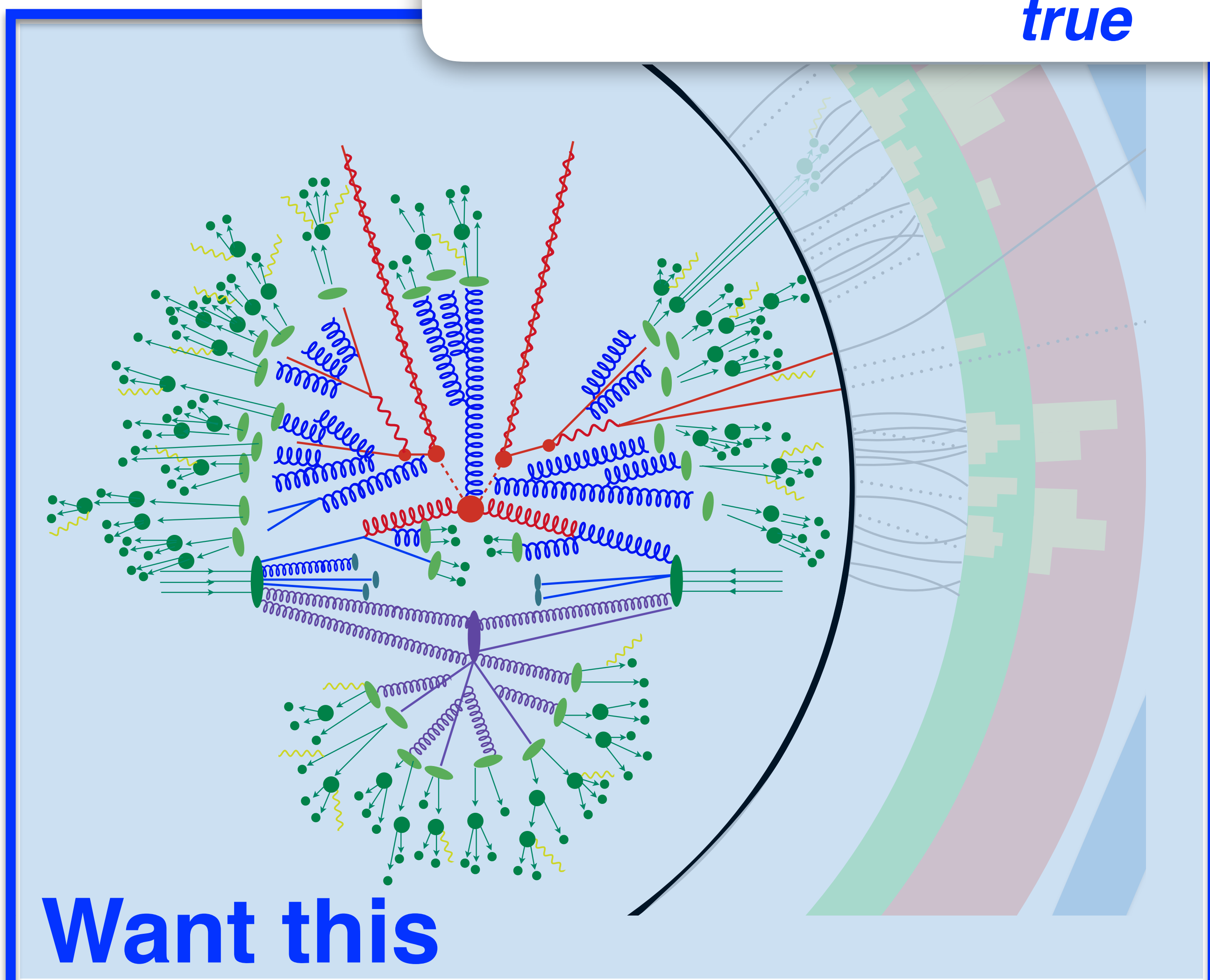


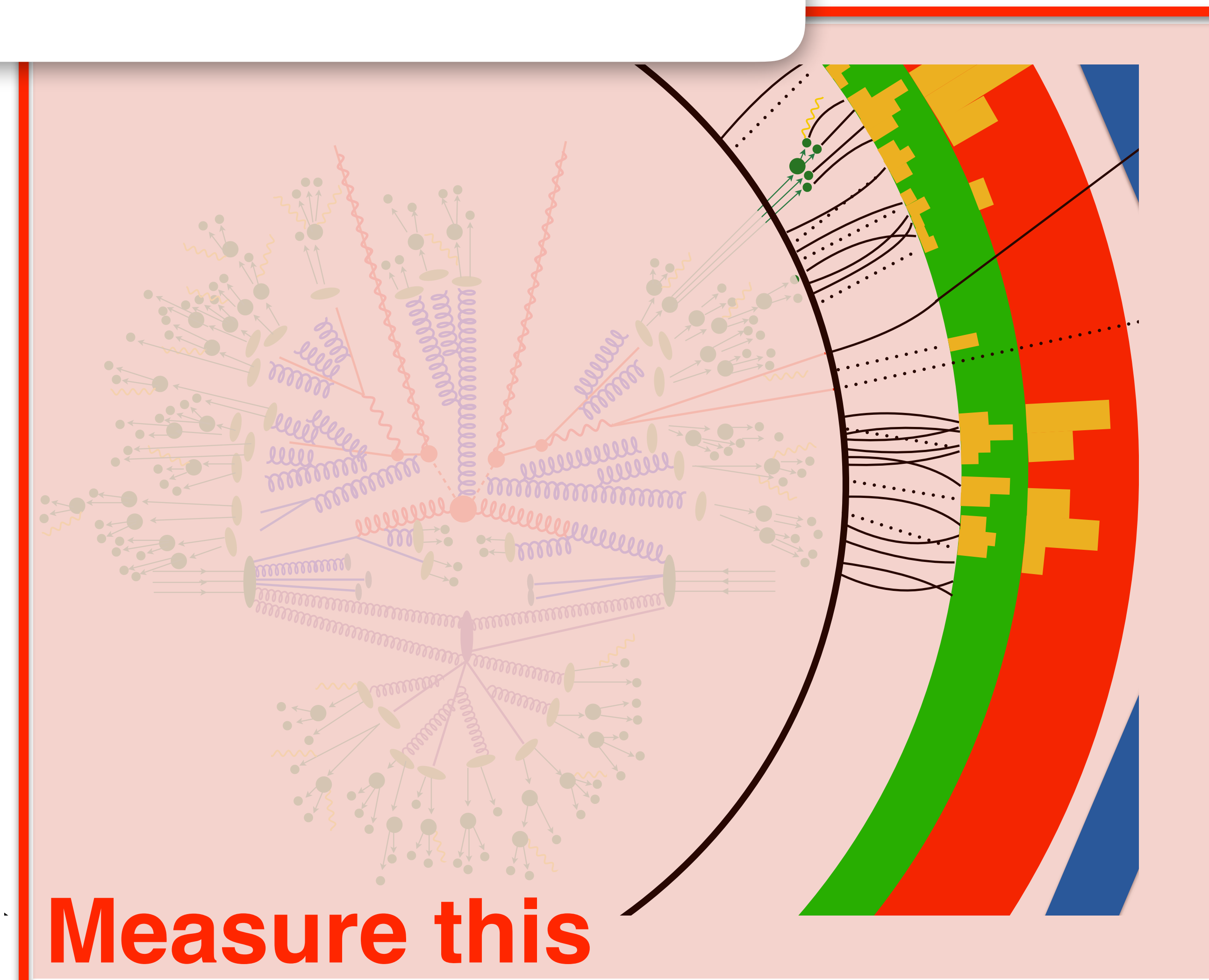
i.e. remove detector distortions

Deconvolution/Unfolding

If you know *p(meas. | true)*, could do maximum likelihood, i.e.

$$\textit{unfolded} = \underset{\textit{true}}{\operatorname{argmax}}\; p(\textit{measured} \mid \textit{true})$$





p(meas. | true) = “response matrix” or “point spread function”

Deconvolution/Unfolding

If you know *p(**meas.** / **true**)*, could do maximum likelihood, i.e.

$$\mathit{unfolded} = \underset{\mathit{true}}{\mathrm{argmax}}\; p(\mathit{measured} \,/\, \mathit{true})$$

Challenge: **measured** is hyperspectral and **true** is hypervariate … *p(**meas.** | **true**) is **intractable** !*

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Challenge: **measured** is hyperspectral and **true** is hypervariate … *p(**meas.** | **true**) is **intractable** !*

However: we have **simulators** that we can use to sample from *p(**meas.** | **true**)*

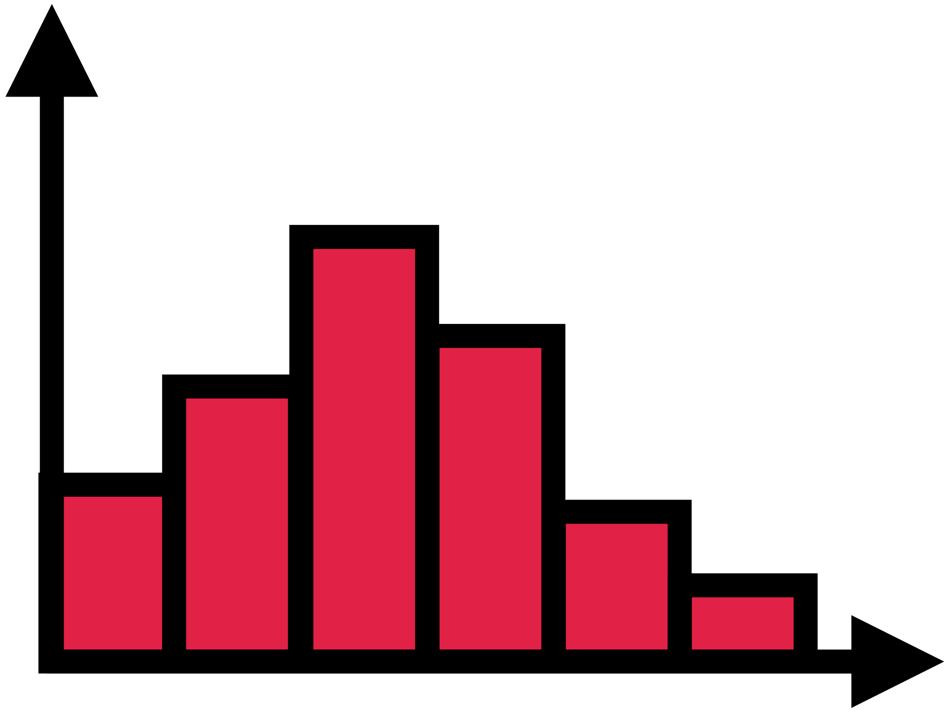
→ **Likelihood-free inference**

*p(**meas.** | **true**)* = “response matrix” or “point spread function”

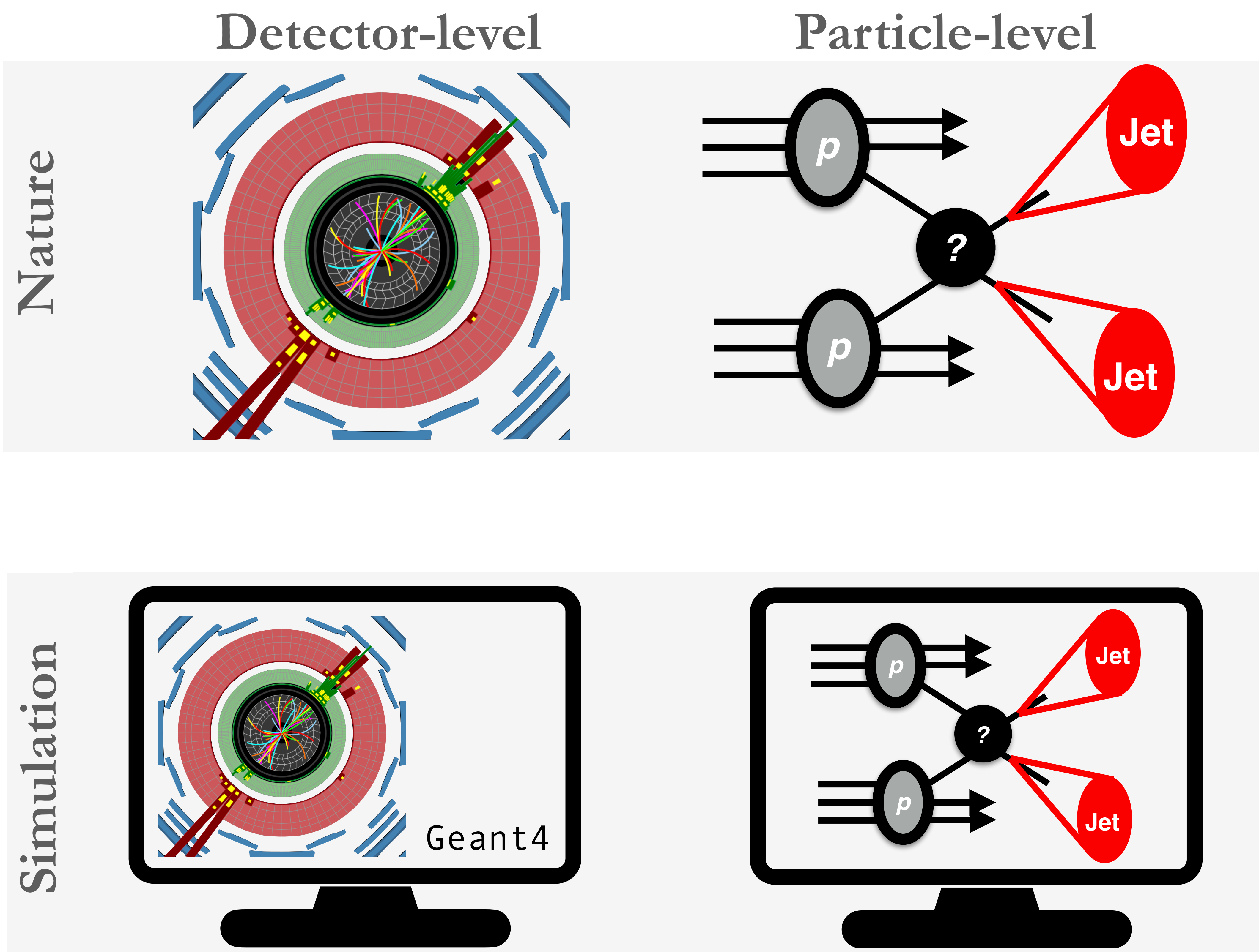
Solution: ML-based Unfolding

We have introduced new machine learning methods capable of **unbinned**, **high-dimensional** unfolding.

This will radically change the cross section measurement programs of collider and neutrino physics.



A brief introduction to OmniFold



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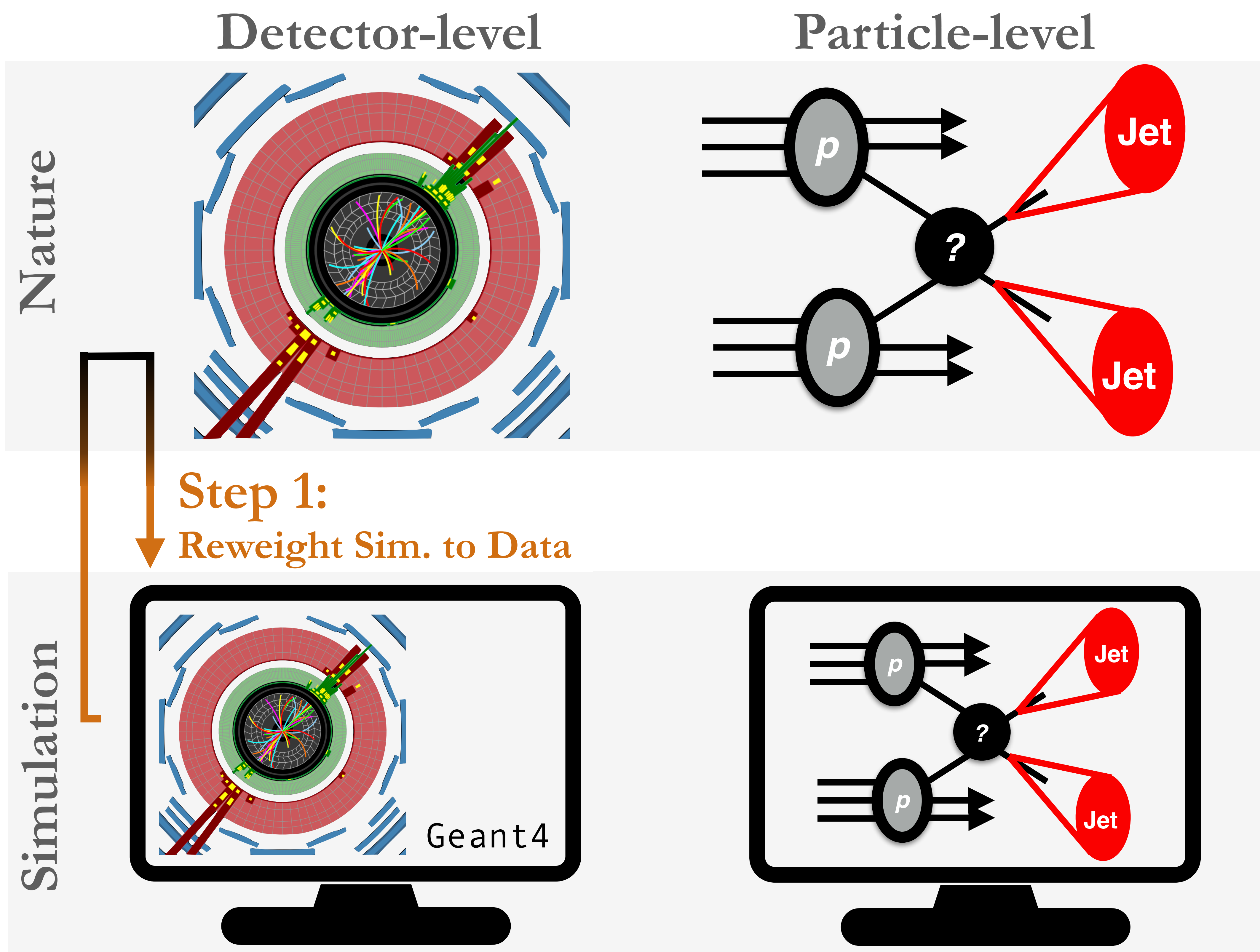

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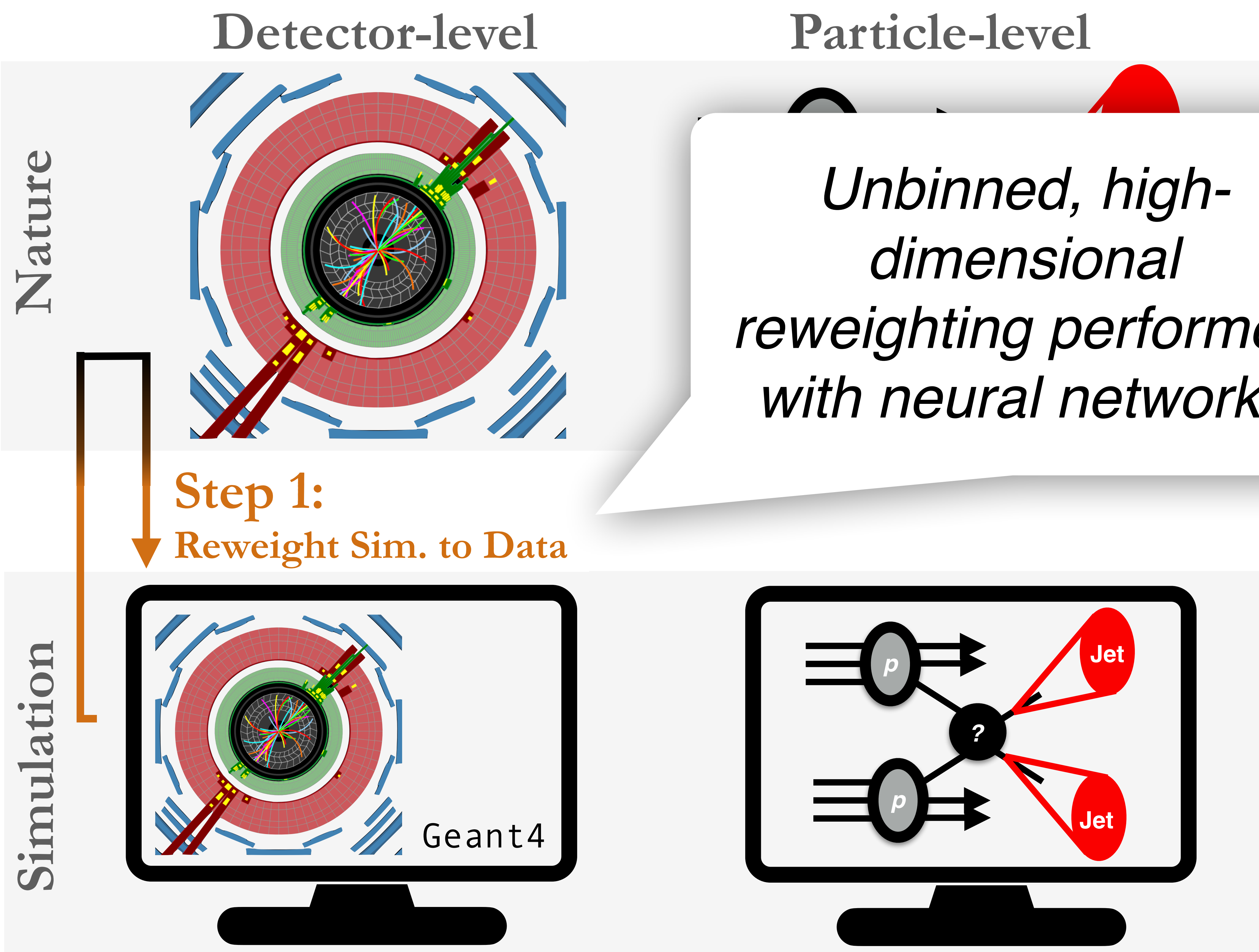
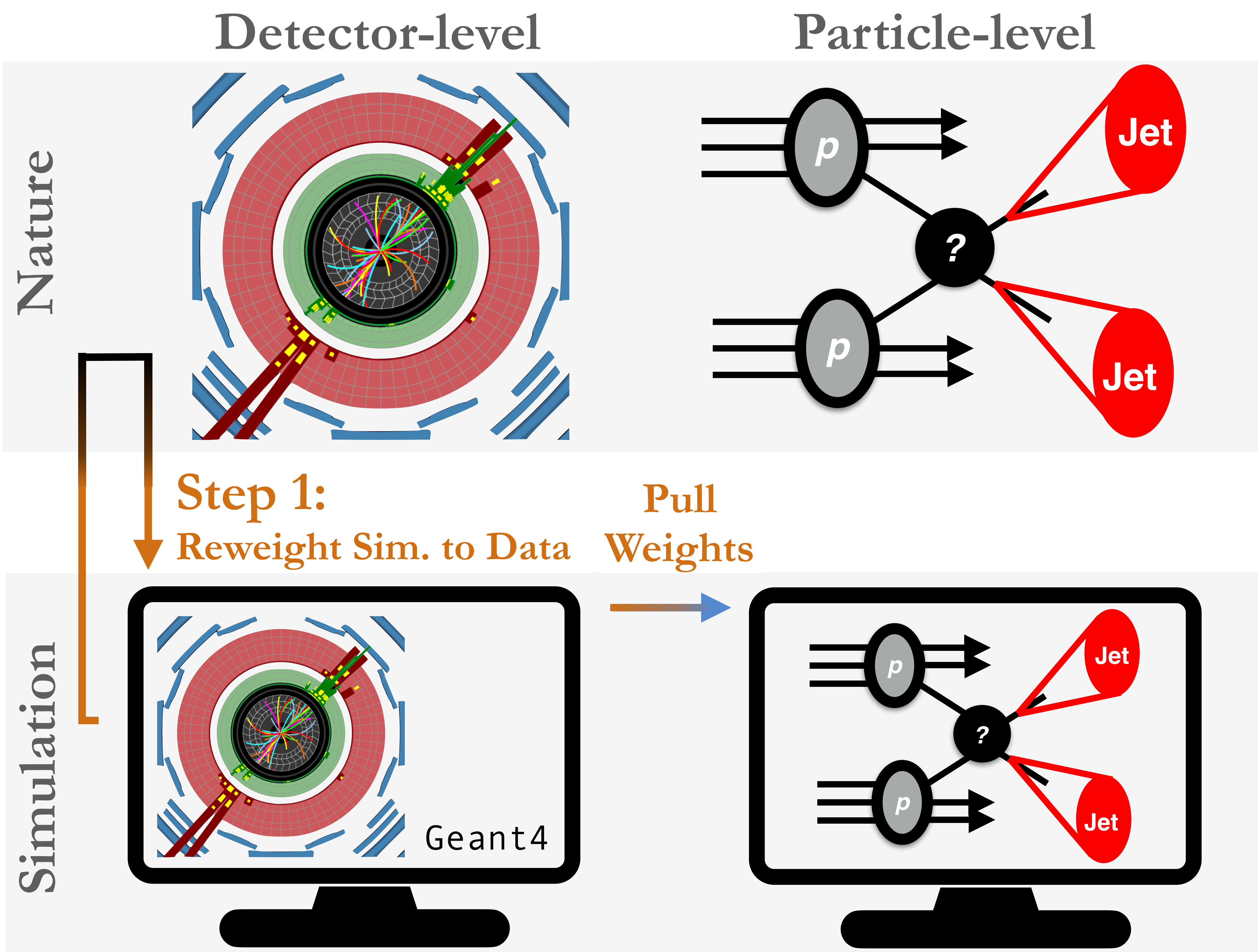


Unbinned, high-dimensional reweighting performed with neural networks

A brief introduction to OmniFold



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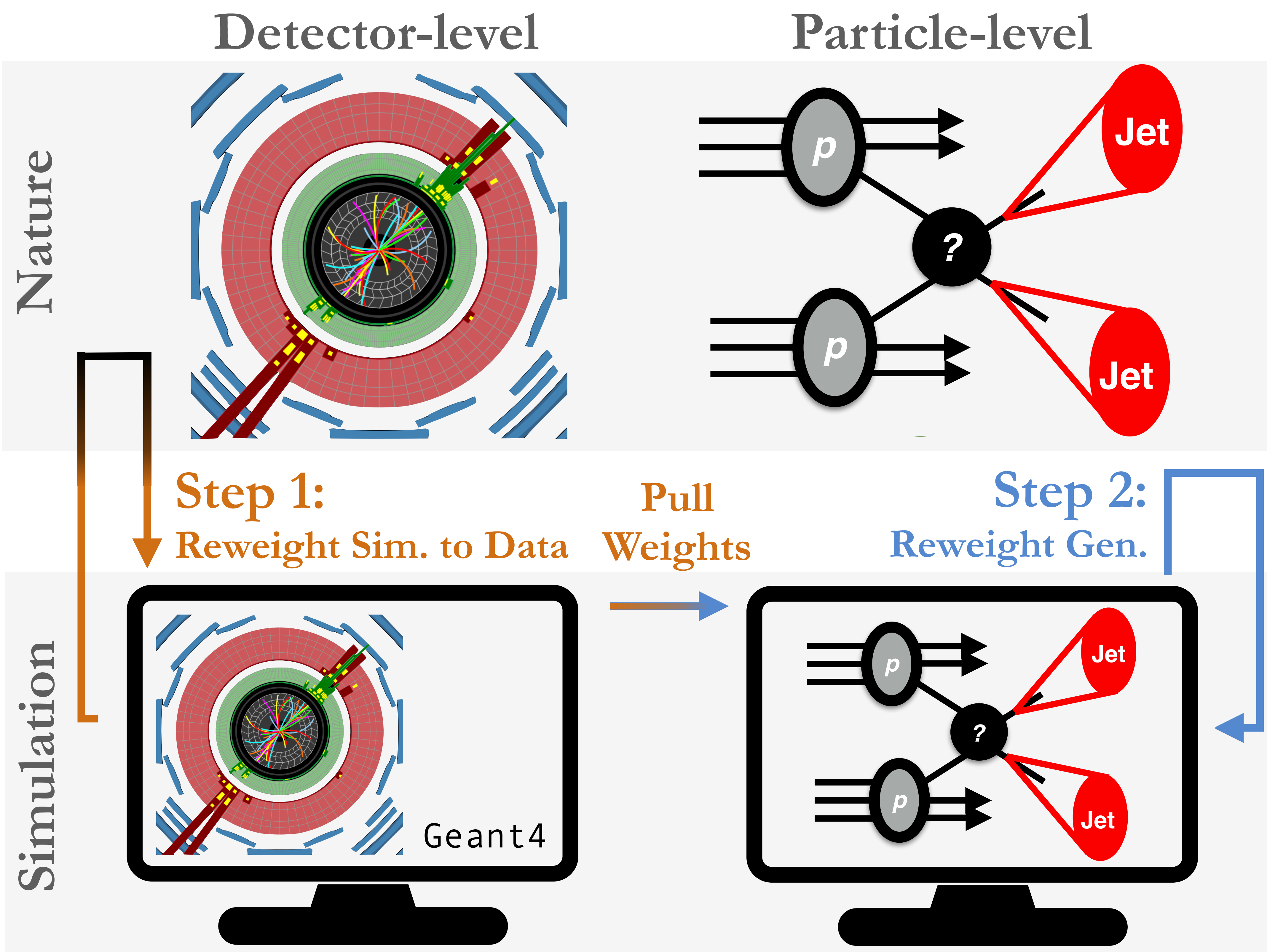

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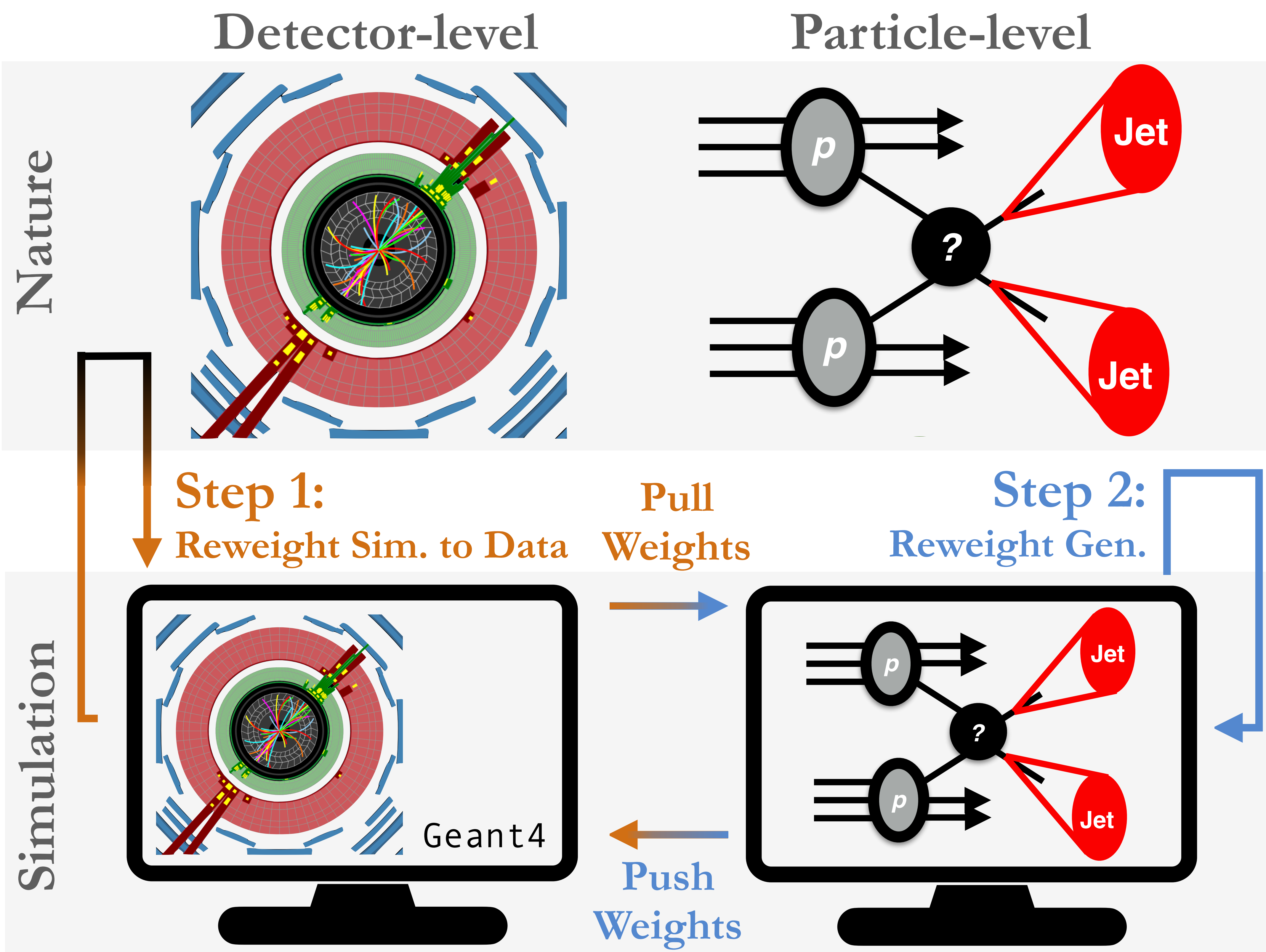

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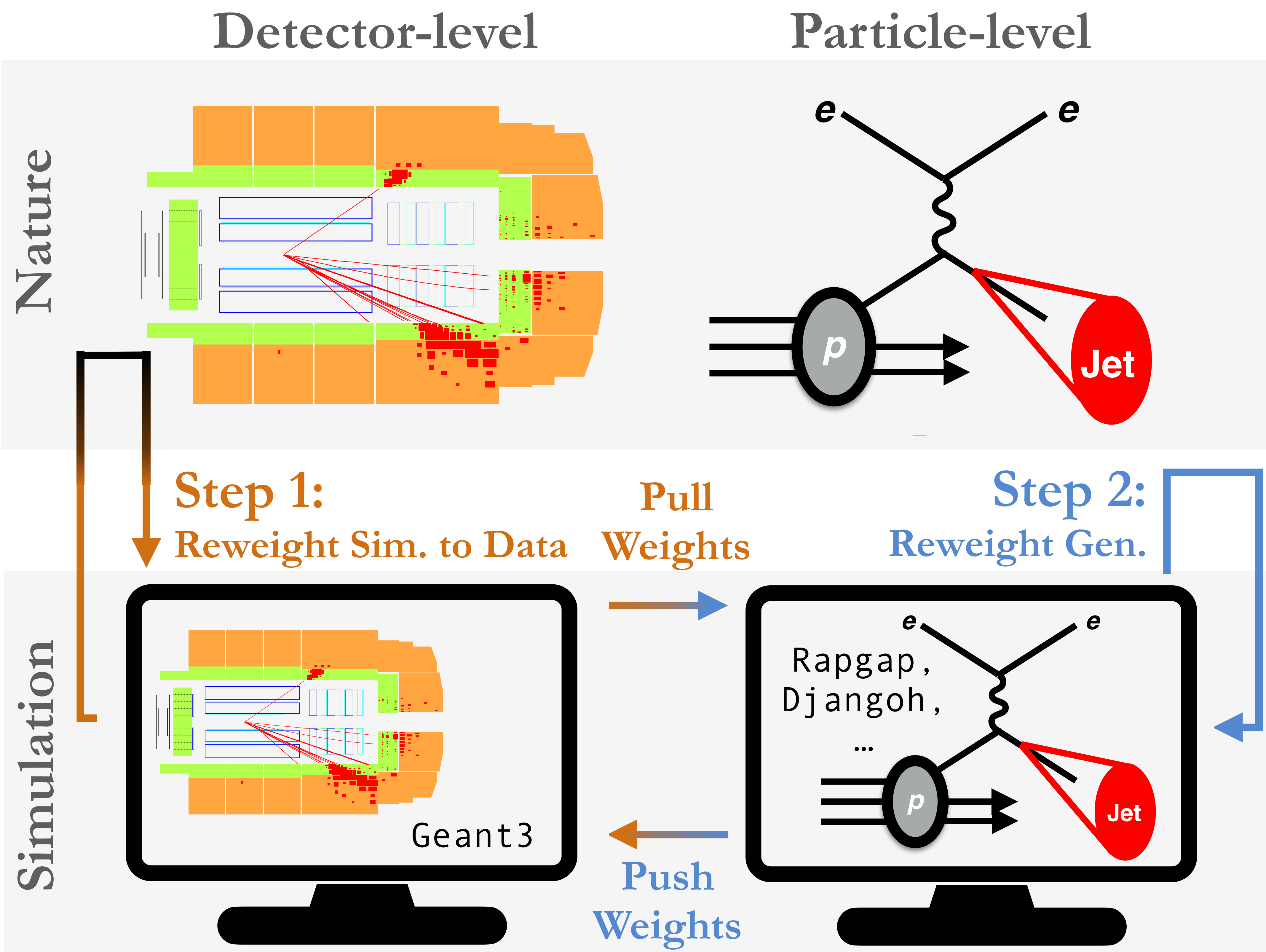
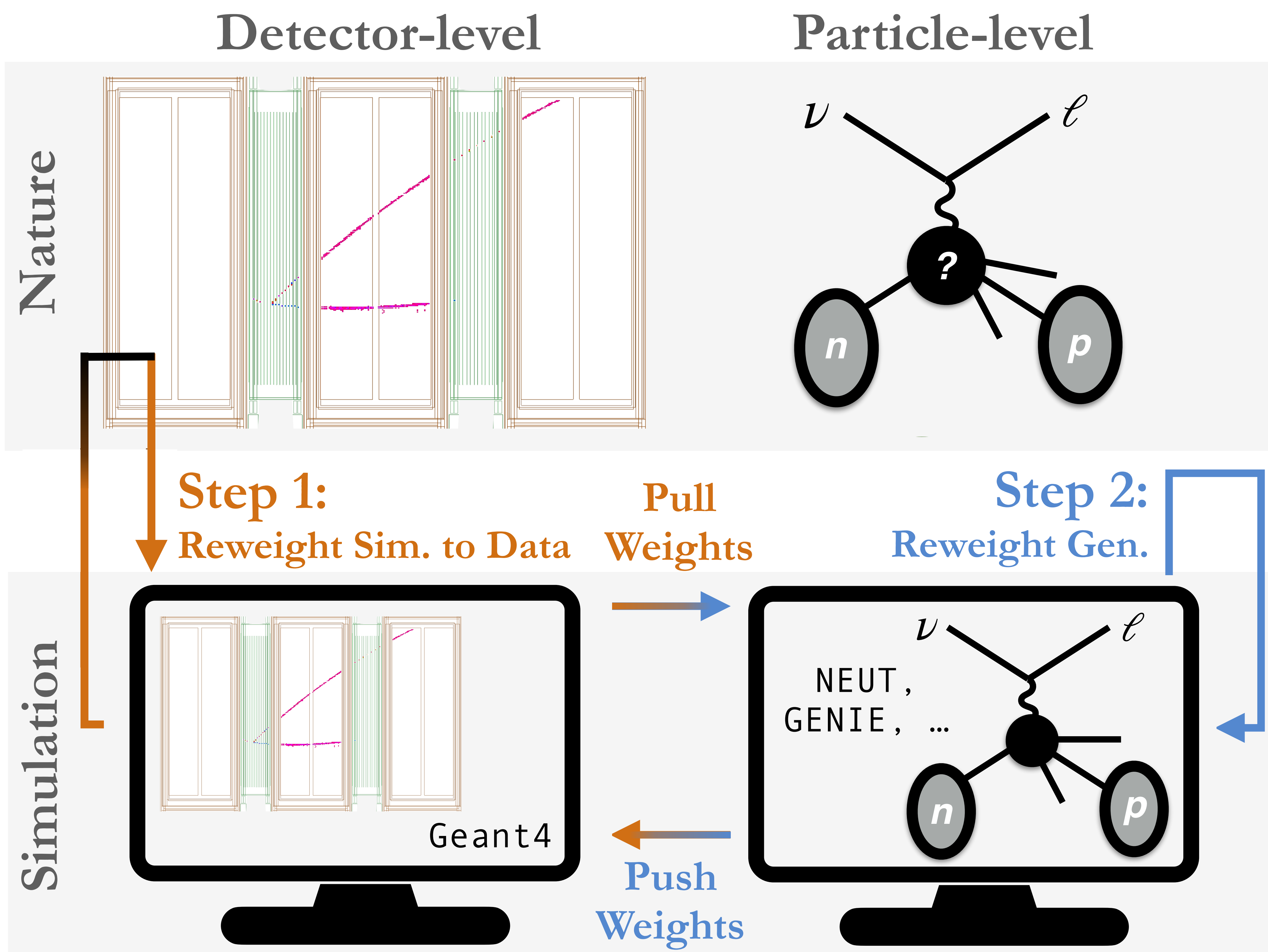


A brief introduction to OmniFold

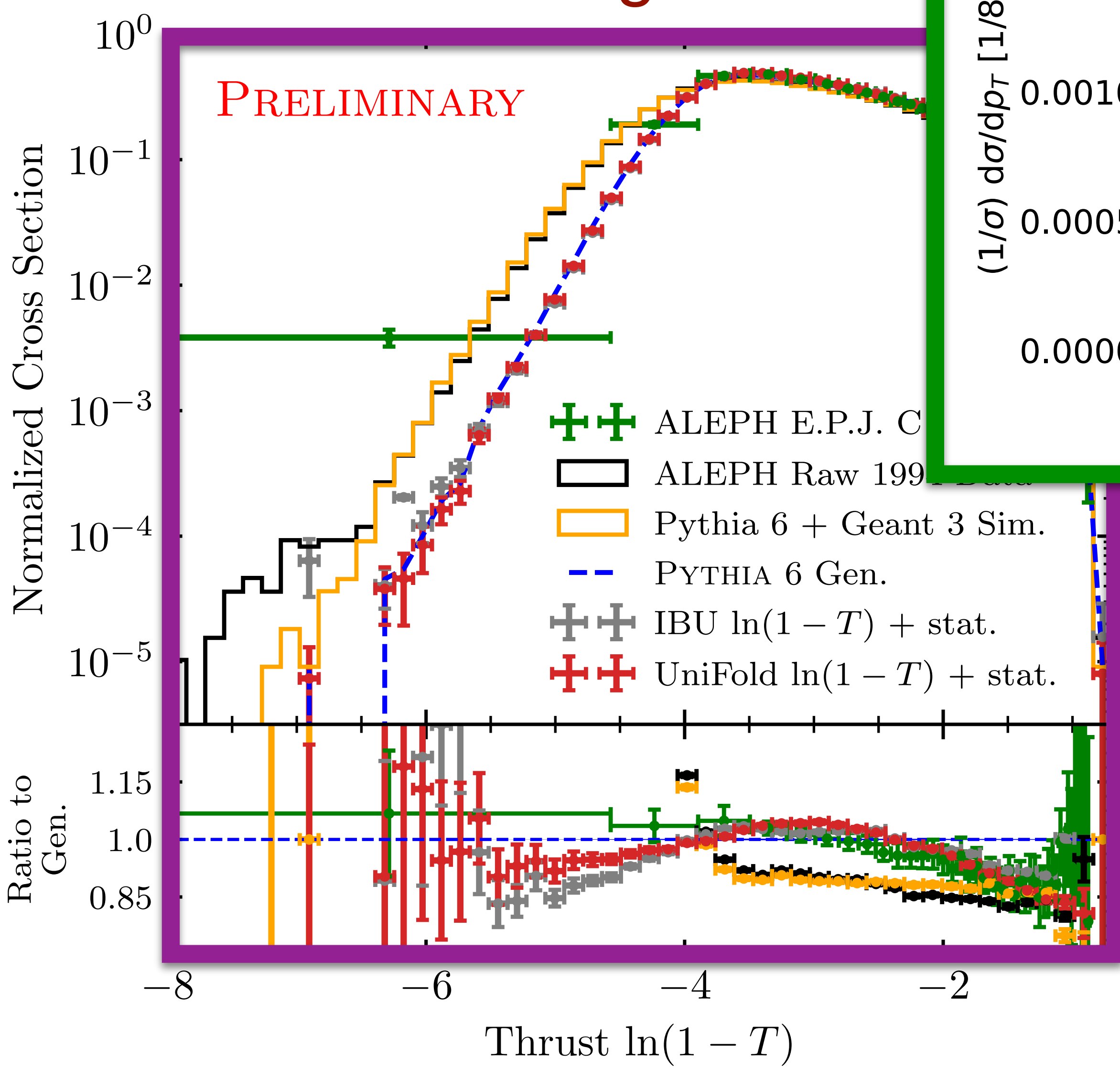


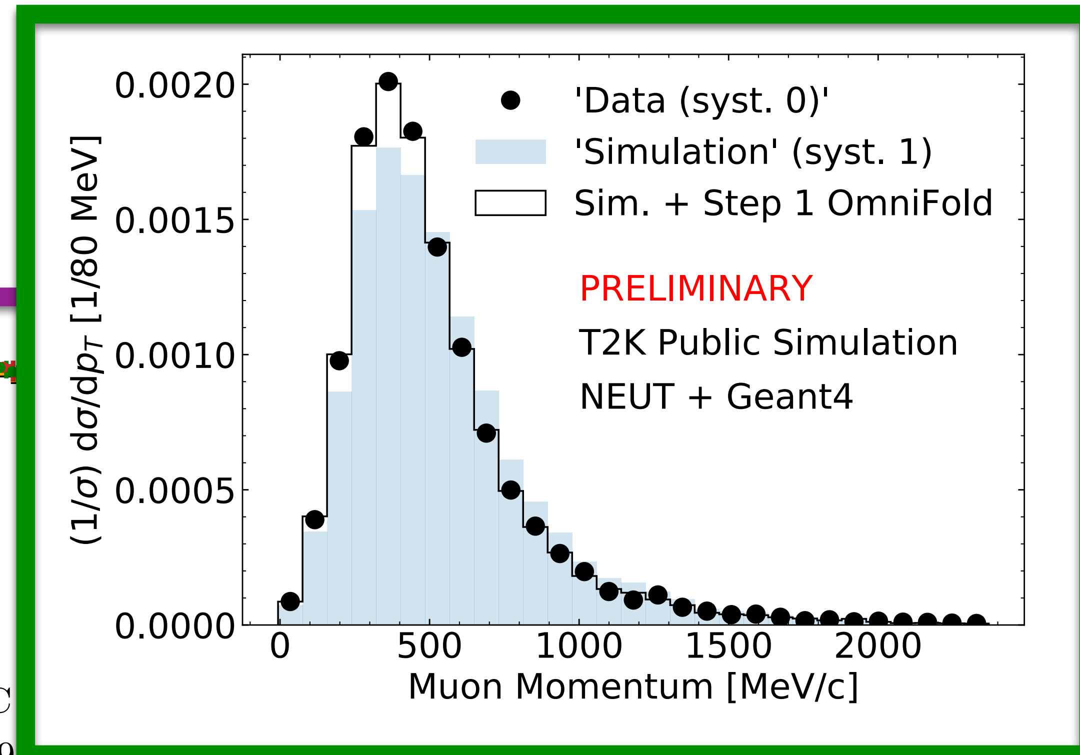
ML-based Unfolding: Science

We are already delivering science results with this methodology (more on the way!); R&D is required to extract the full benefits

ask Jing Pan

e+e- scattering

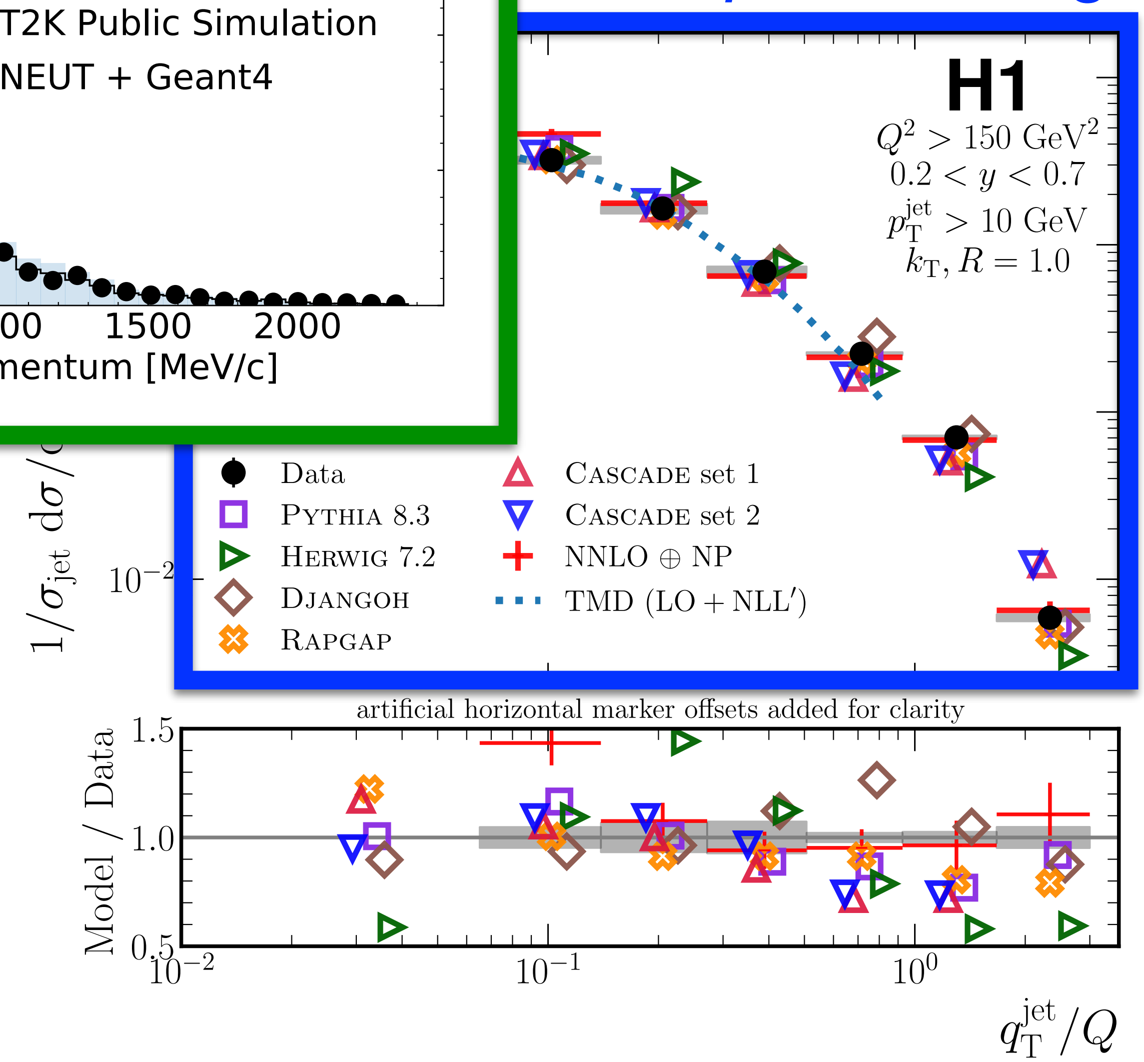




neutrino scattering

Data points = machine learning

ep scattering



ML-based Unfolding: Science

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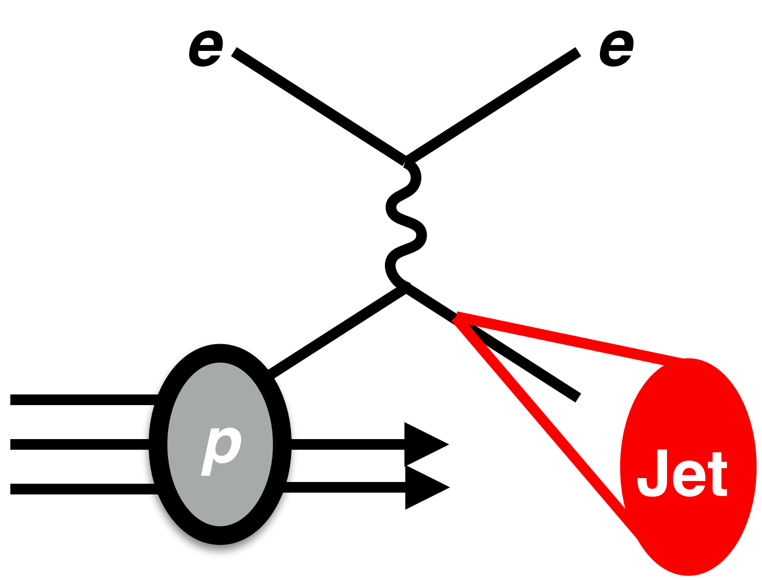
8-dimensional phase space for exploring proton structure & universality ("factorization")



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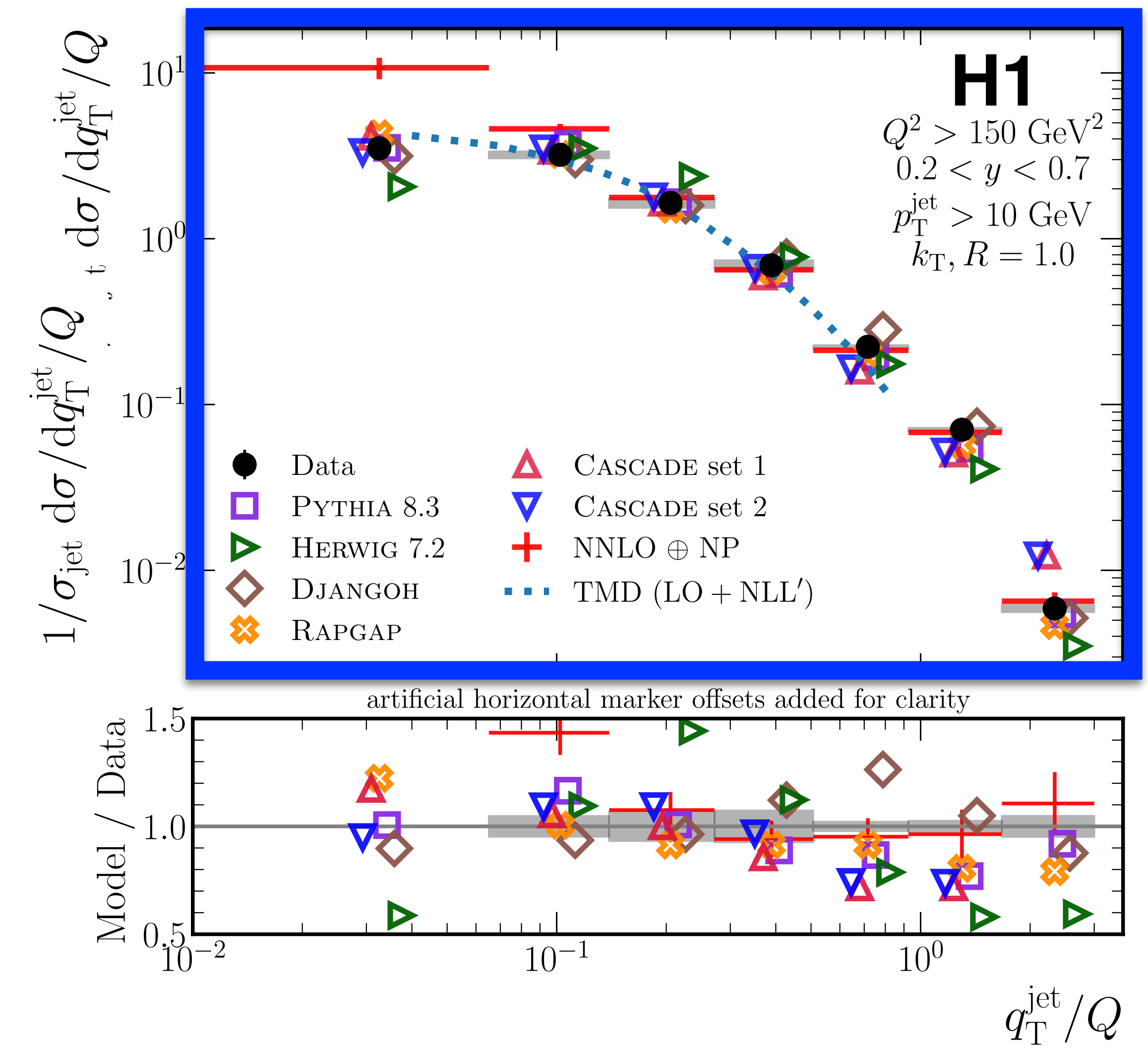


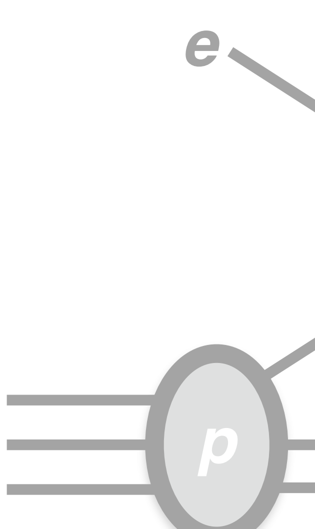
PRL 128 (2022) 132002, 2108.12376

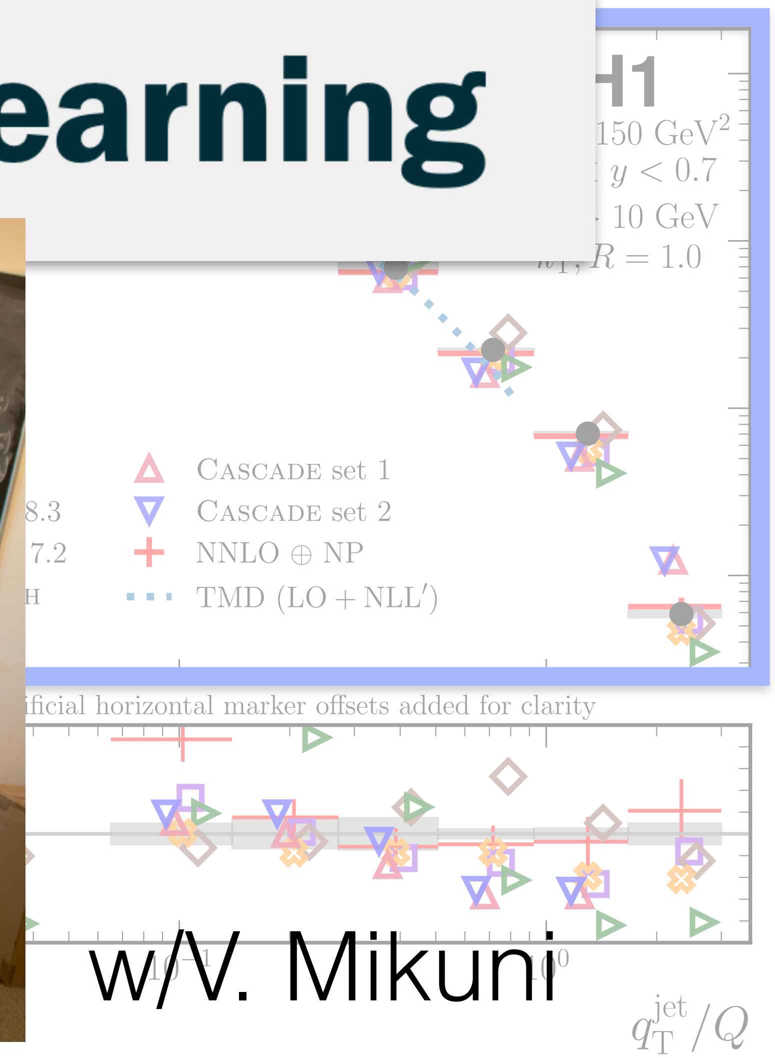
ML-based Unfolding: Science

ARTICLE • MYSTERIES OF MATTER

By Theresa Duque
October 25, 2022

How Do You Solve a Problem Like a Proton? You Smash It to Smithereens – Then Build It Back Together With Machine Learning





w/V. Mikuni

PRL 128 (2022) 13200

ML-based Unfolding: Science

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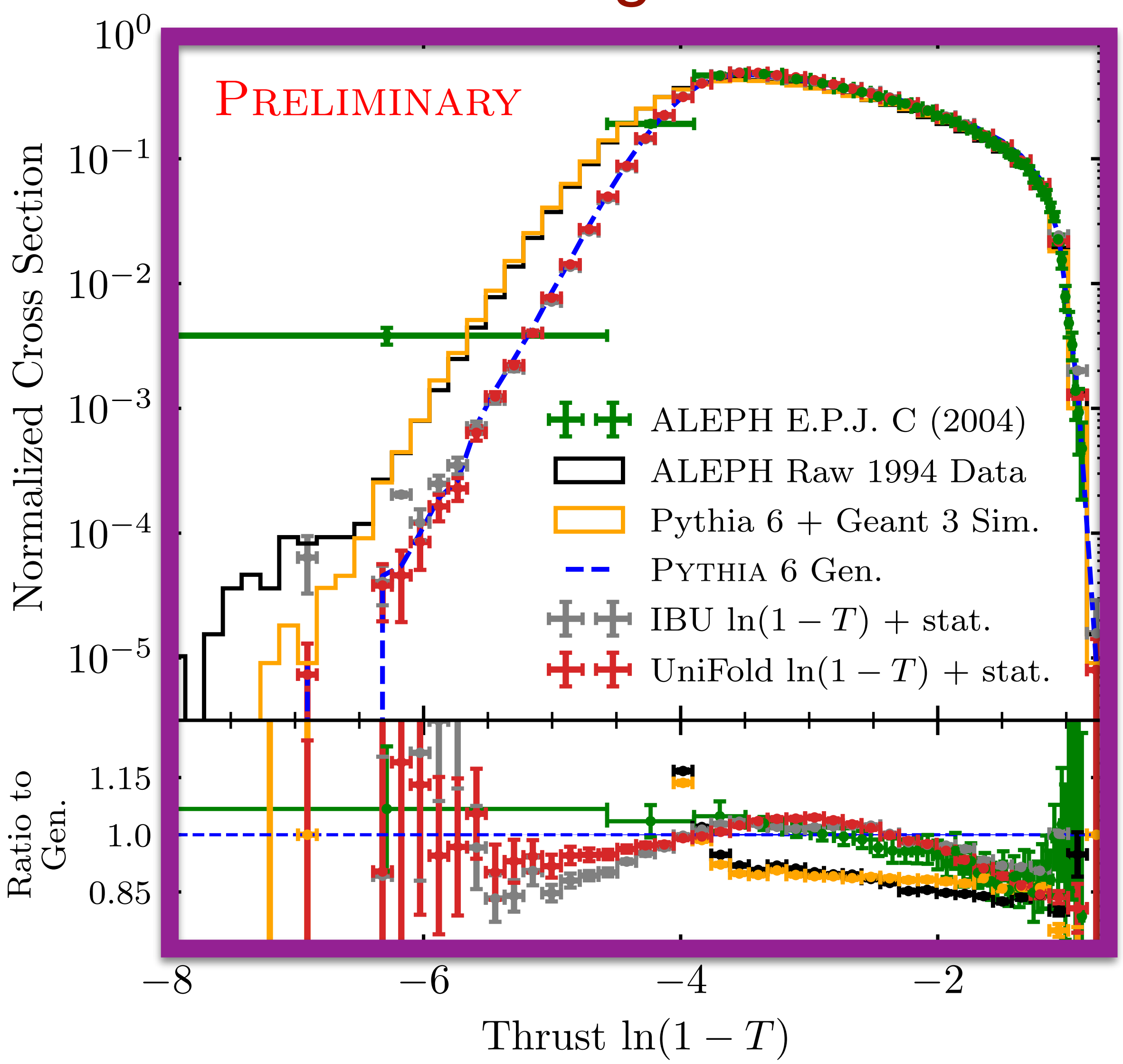
Data points = machine learning

e^+e^- scattering



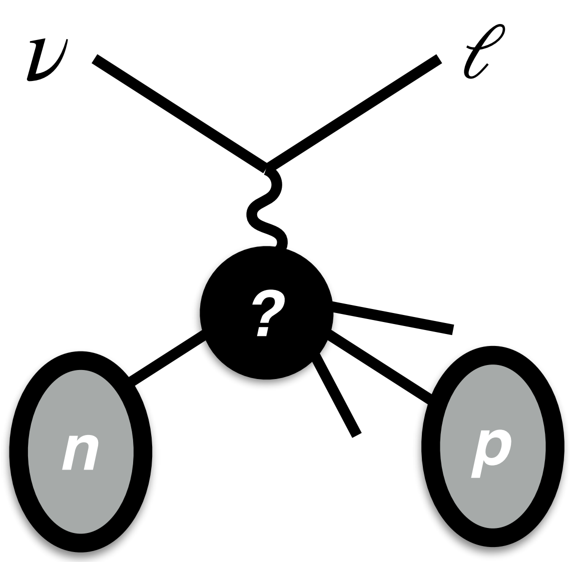
Long-standing tension (~3σ) between methods for measuring the strong coupling constant.

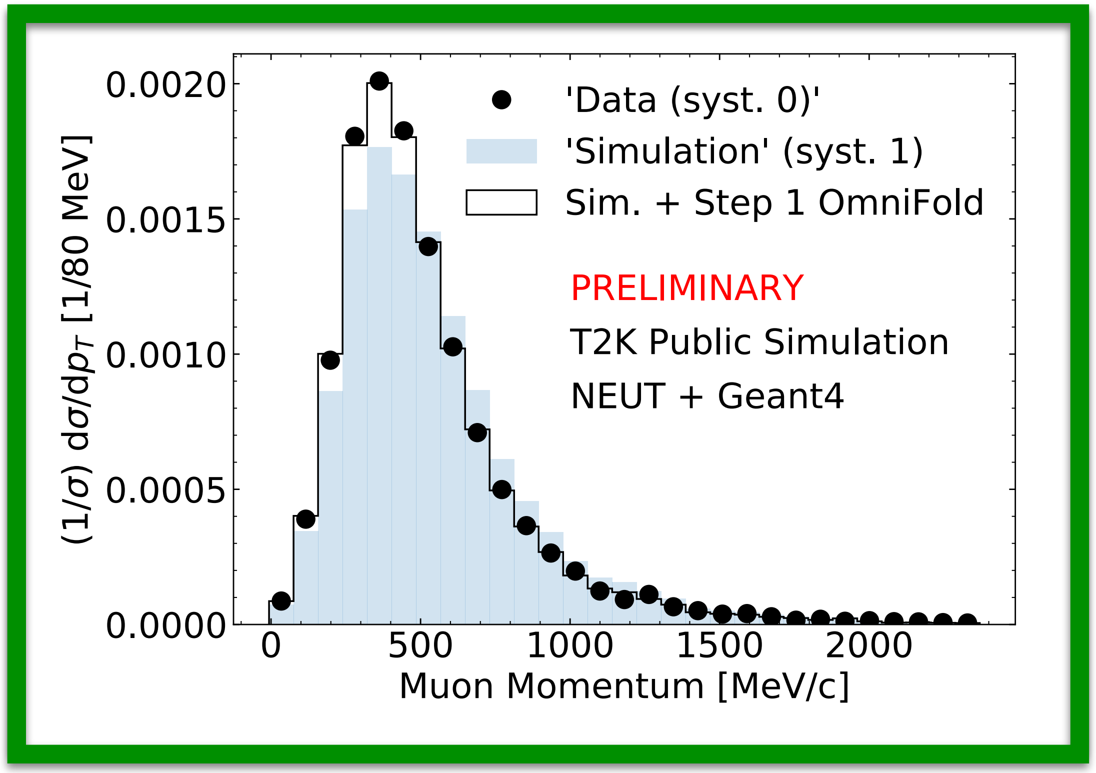
Goal: Use ML to shed light on this issue.

w/A. Badea, Y.-J. Lee, J. Thaler

ML-based Unfolding: Science

We are already delivering science results with this methodology (more on the way!); R&D is required to extract the full benefits





neutrino scattering

Data points = machine learning

Highly-variable detector response in T2K detector can be addressed with ML unfolding.

w/C. Wilkinson and T. Kikawa

The future of likelihood-free Inference

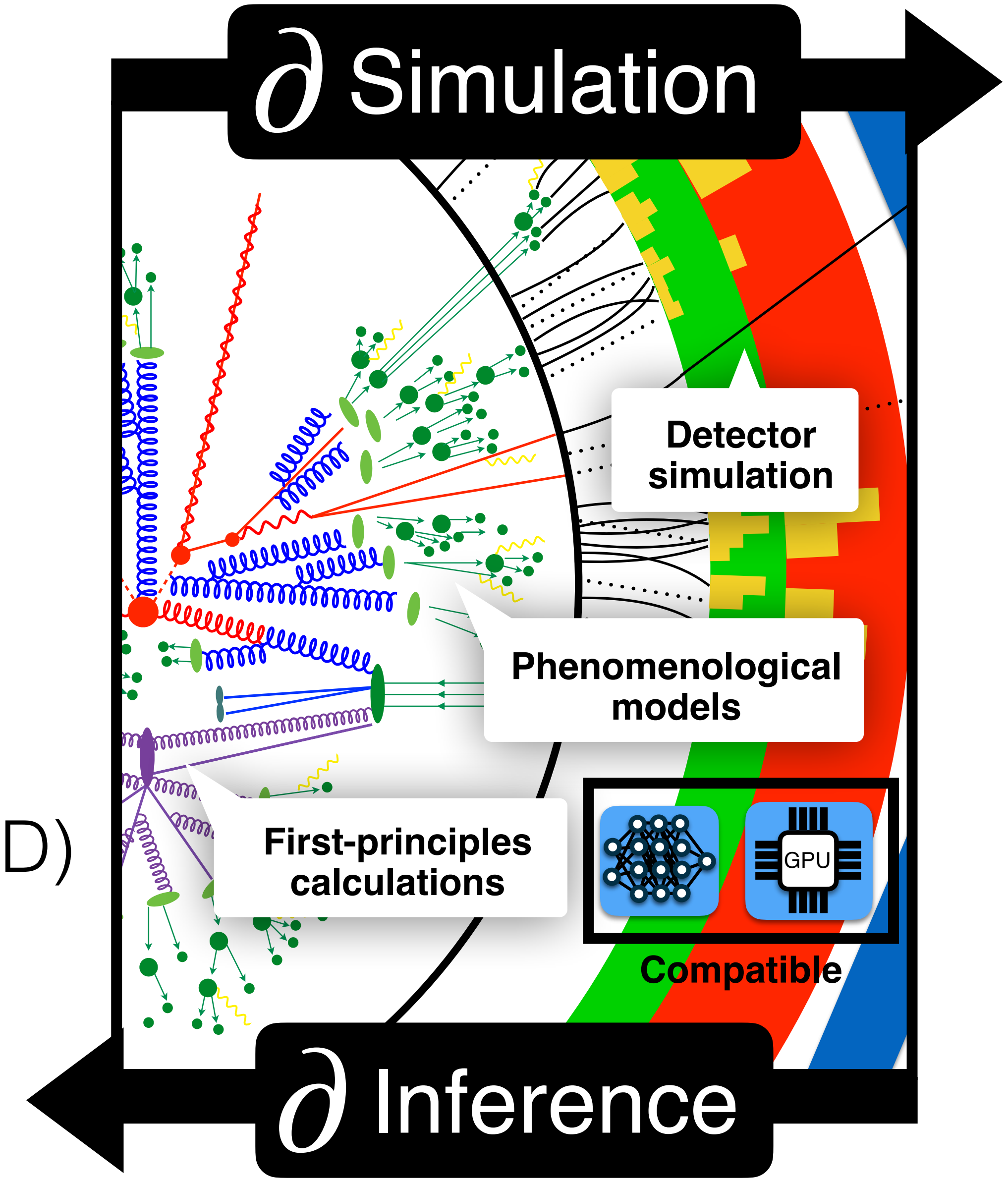
Goal: optimal combination of simulations & machine learning

Methods

Next frontier: **differentiable simulations**

Science

- Detector optimization
- Cross sections from ATLAS and T2K/LArTPC
- Cross sections from legacy data (HERA/LEP/SLD)



The future of likelihood-free Inference

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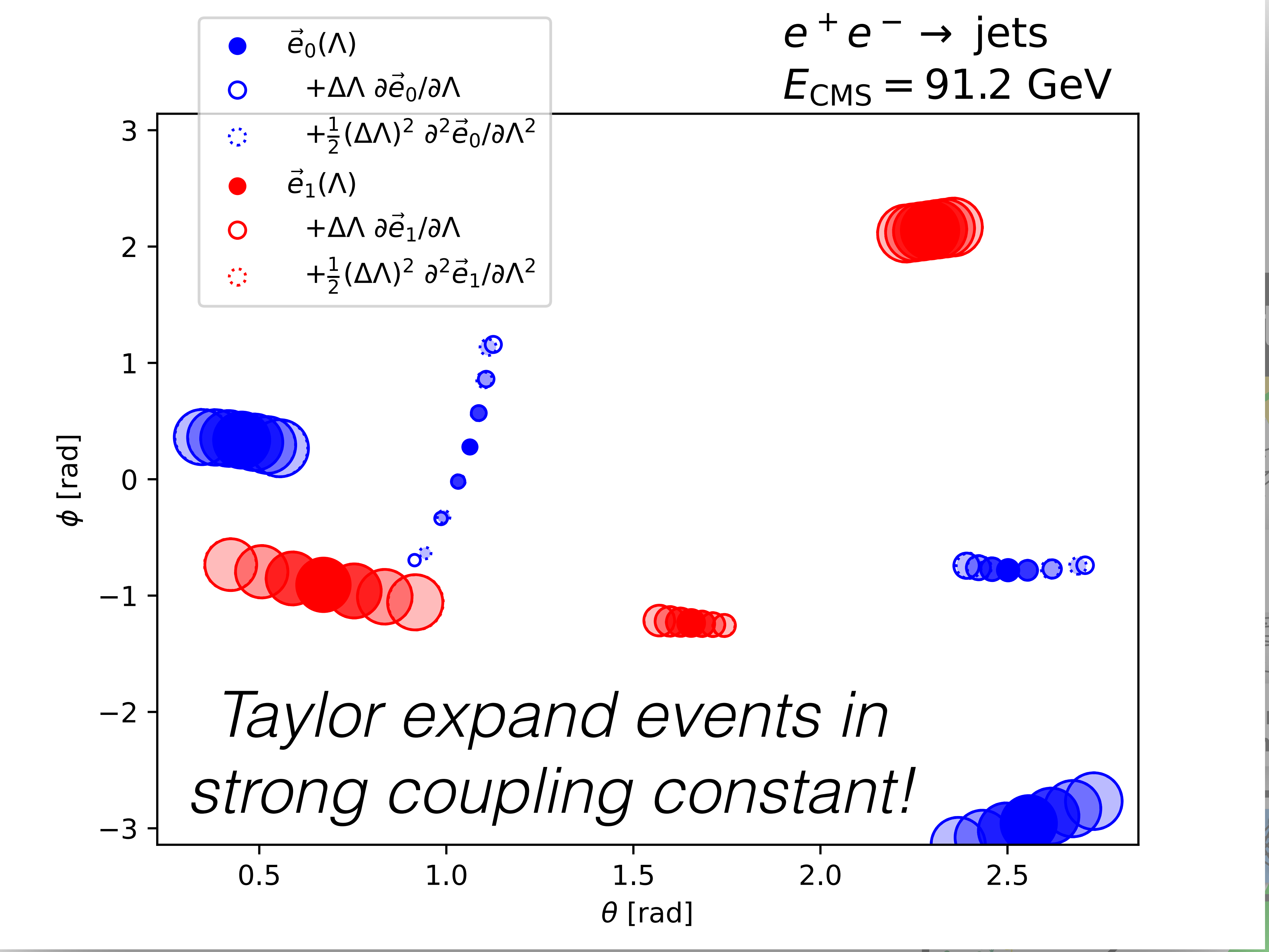
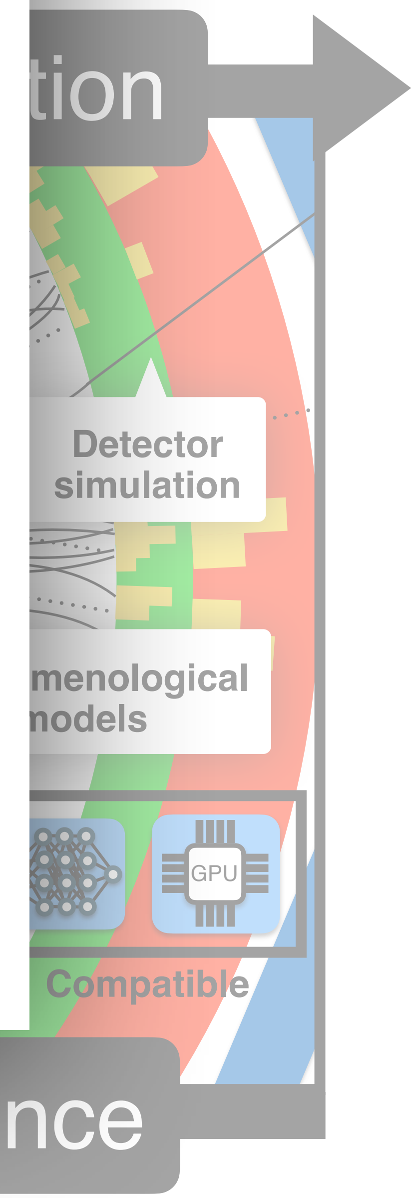
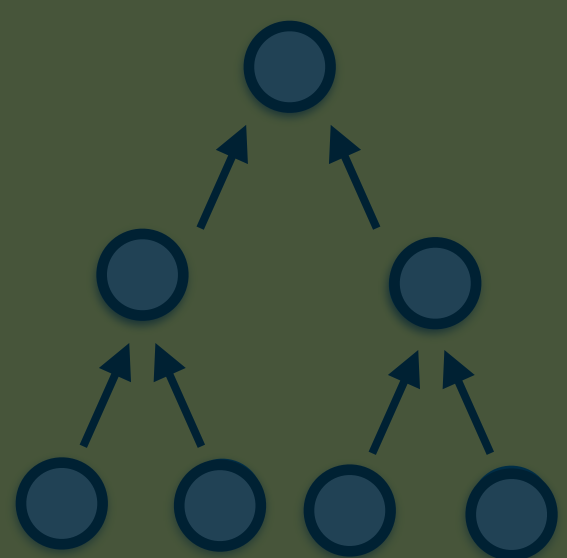




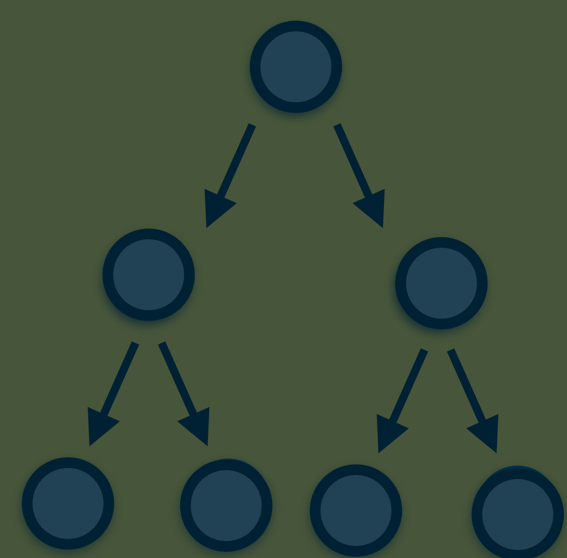
BN and S. Prestel, 2208.02274

Outline for today

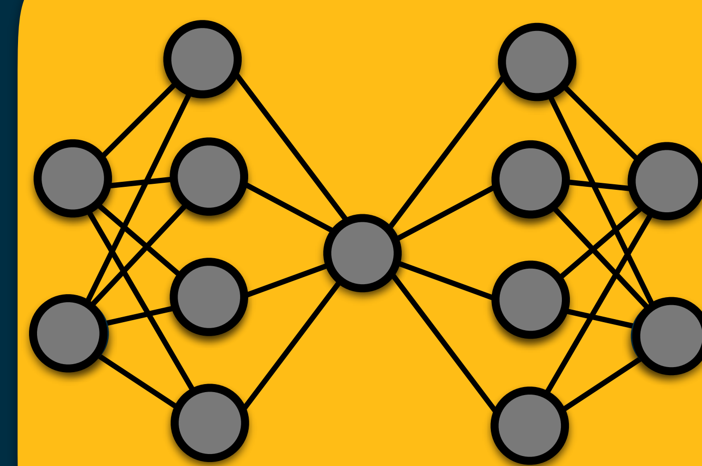
I'll focus on three core, cross-cutting areas of ML ∩ Physics



Forward Models
(fast simulation)



Inverse Models
(unfolding)



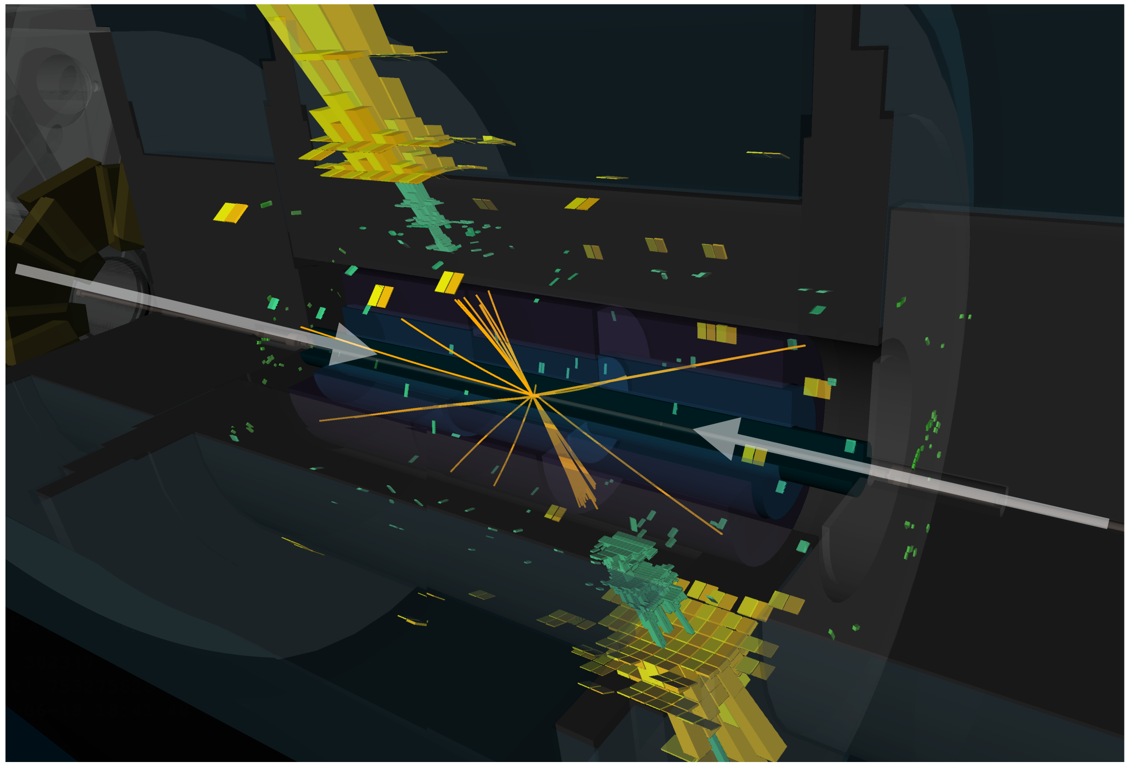
Simulation-free
(anomaly detection)

To illustrate these exciting topics, I'll give one vignette per area

Anomaly Detection

Nearly all searches for new particles are signal-model driven. We have introduced a new model agnostic program.

AD in fundamental physics is inherently different than other areas of science and industry - we need new approaches.



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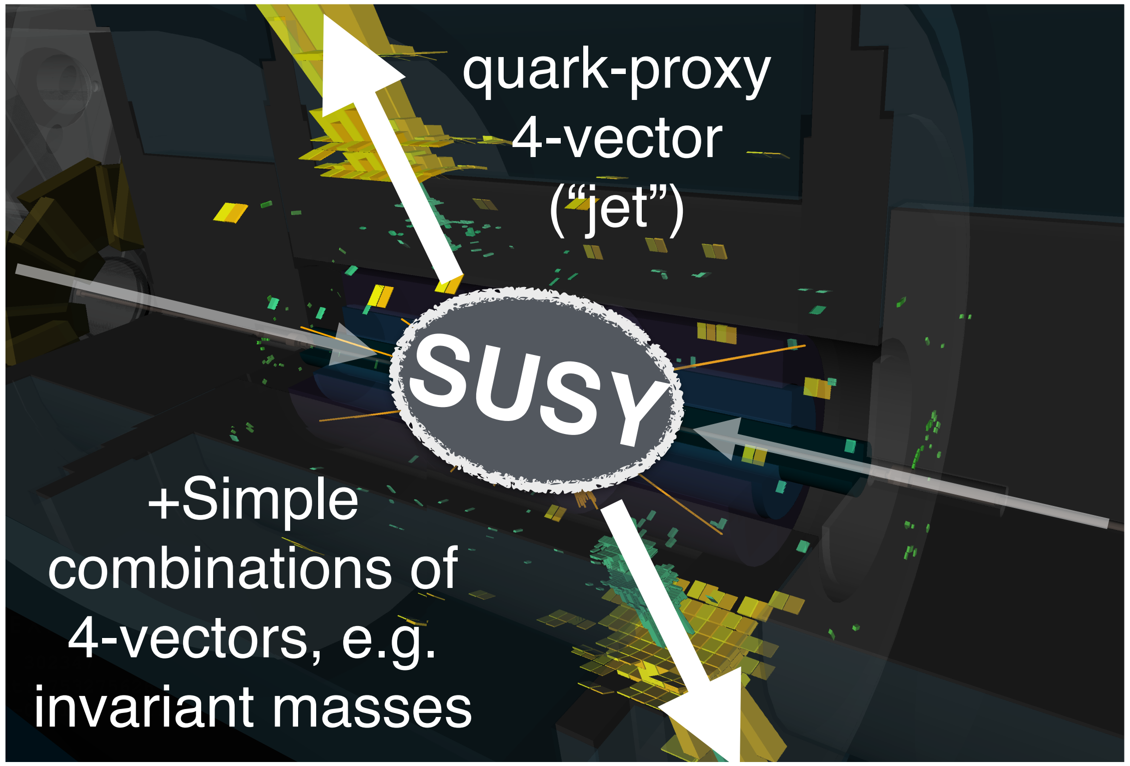

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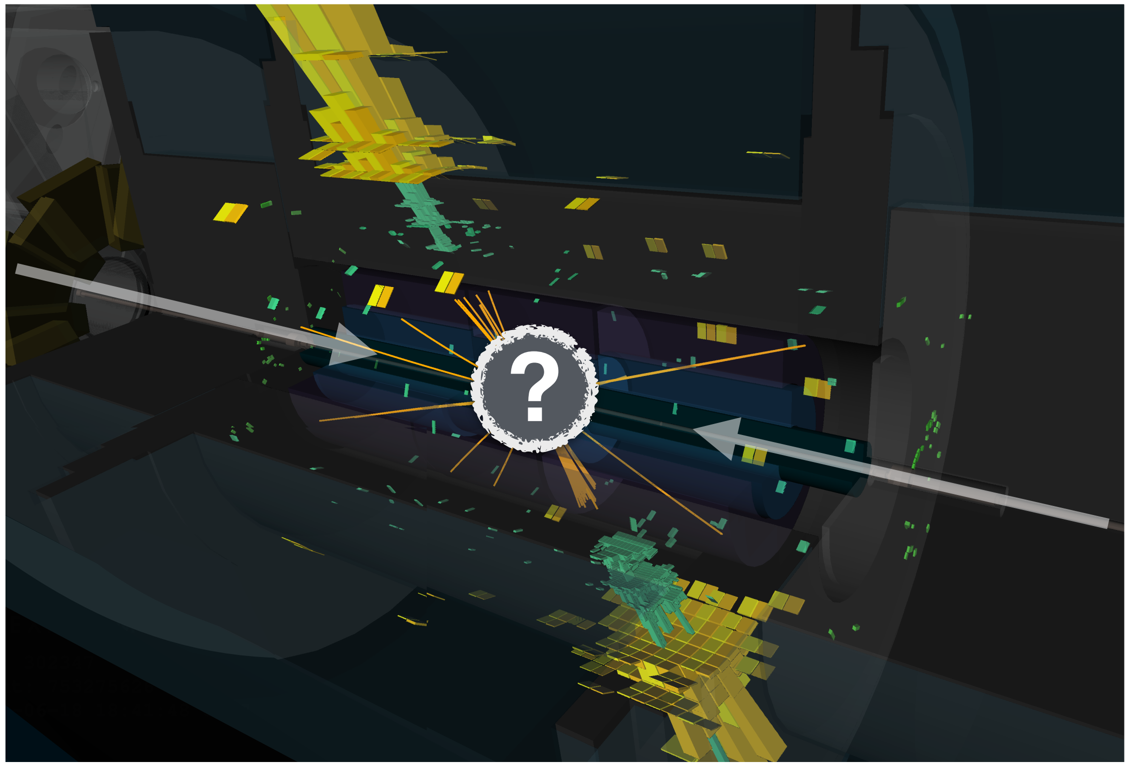


Overview of New Ideas

I like to categorize new ideas based on the core assumption about the new physics, which is intimately related to the technique ***supervision***

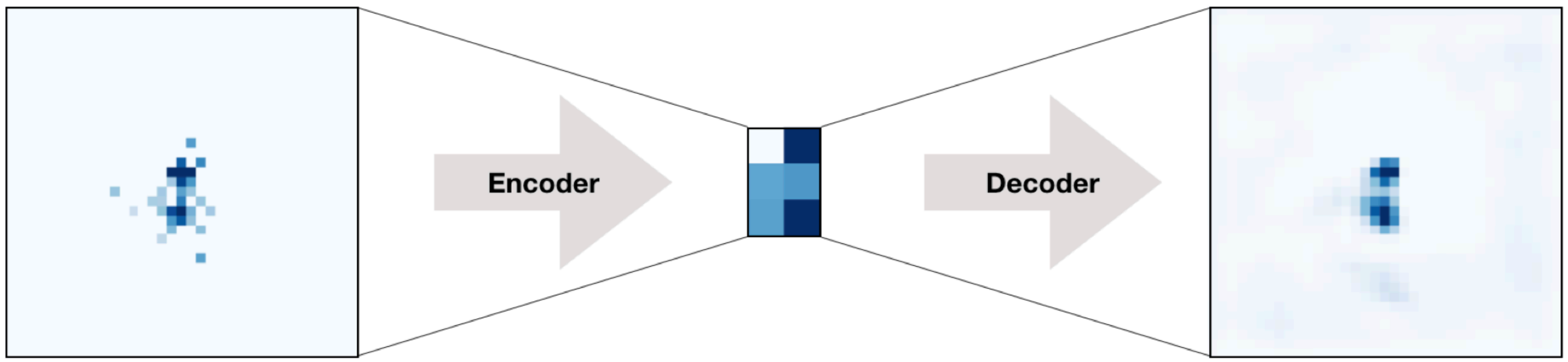
Unsupervised = no labels
Weakly-supervised = noisy labels
Semi-supervised = partial labels
Supervised = full label information

This is most searches. You simulate the signal (label = 1), simulate the background (label = 0) and "train" a classifier to distinguish the 1's from the 0's.

Unsupervised

Unsupervised = no labels

Typically, the goal of these methods is to look for events with **low *p(background)***



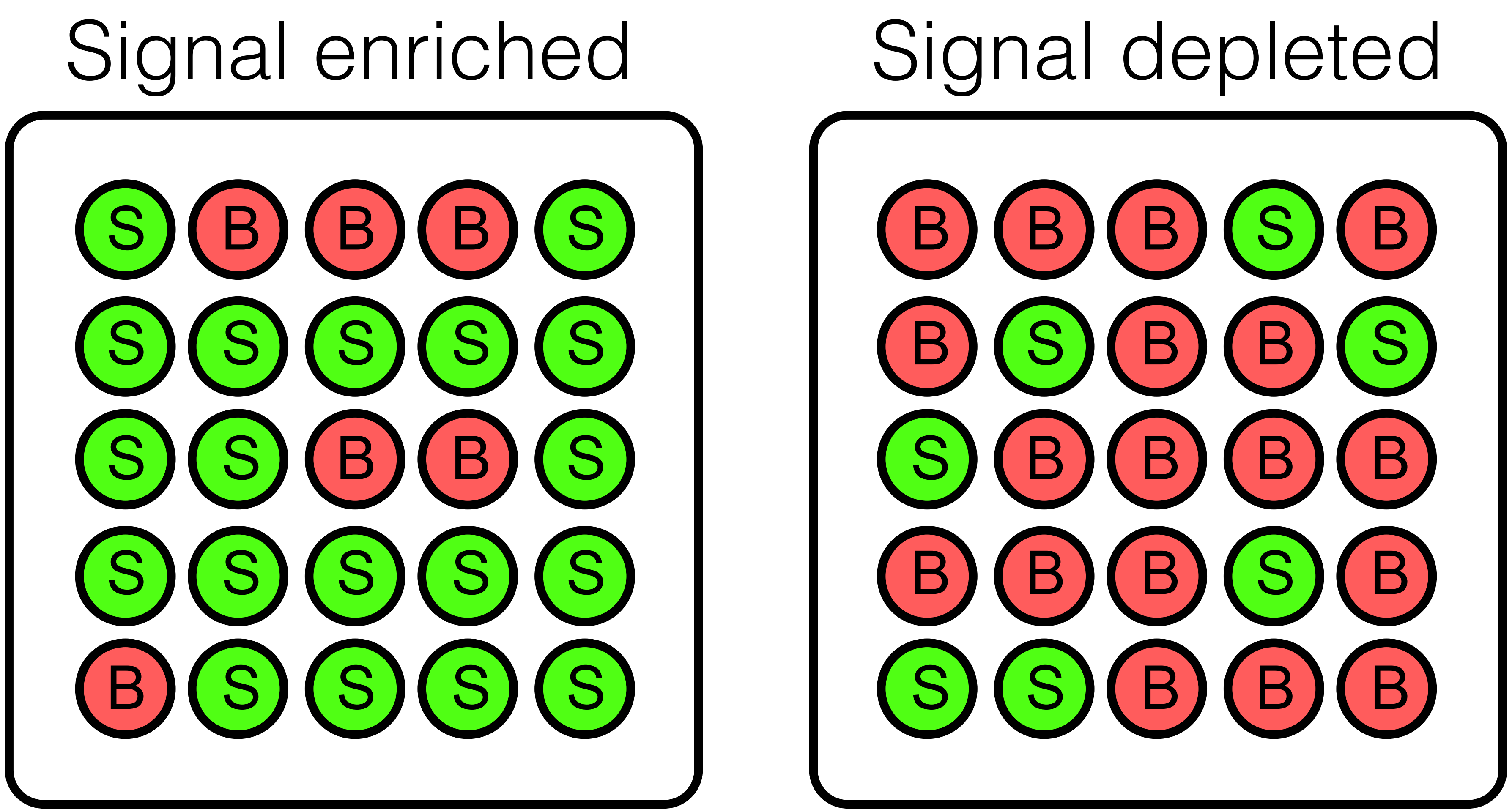
One strategy (autoencoders) is to try to compress events and then uncompress them. When x = uncompress(compress(x)), then x probably has low p(x).

M. Farina, Y. Nakai, D. Shih, 1808.08992; T. Heimel, G. Kasieczka, T. Plehn, J. Thompson, 1808.08979; … V. Mikuni, **BN**, D. Shih, 2111.06417+ many more

Weakly-supervised

Weakly-supervised = noisy labels

Typically, the goal of these methods is to look for events with high *p(possibly signal-enriched)/p(possibly signal-depleted)*



*E. Metodiev, **BN**, J. Thaler, 1708.02949; J. Collins, K. Howe, **BN**, 1805.02664; + many more*

Semi-supervised

Semi-supervised = partial labels

Typically, these methods use some signal simulations to build signal sensitivity

Image credit: https://www.particlezoo.net

vs

e.g. SM background versus many signals

Overview of New Ideas

Approach:	**Unsupervised**	**Weakly supervised**
BSM assumption	Signal is rare (low p)	Signal is an over density (high p ratio)
Main drawback	rare is not invariant* under coordinate transformations!	need two samples

*for a detailed discussion about this, see G. Kasieczka et al., 2209.06225

Overview of New Ideas

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BSM assumption	Signal is rare (low *p*)	Signal is an over density (high *p* ratio)
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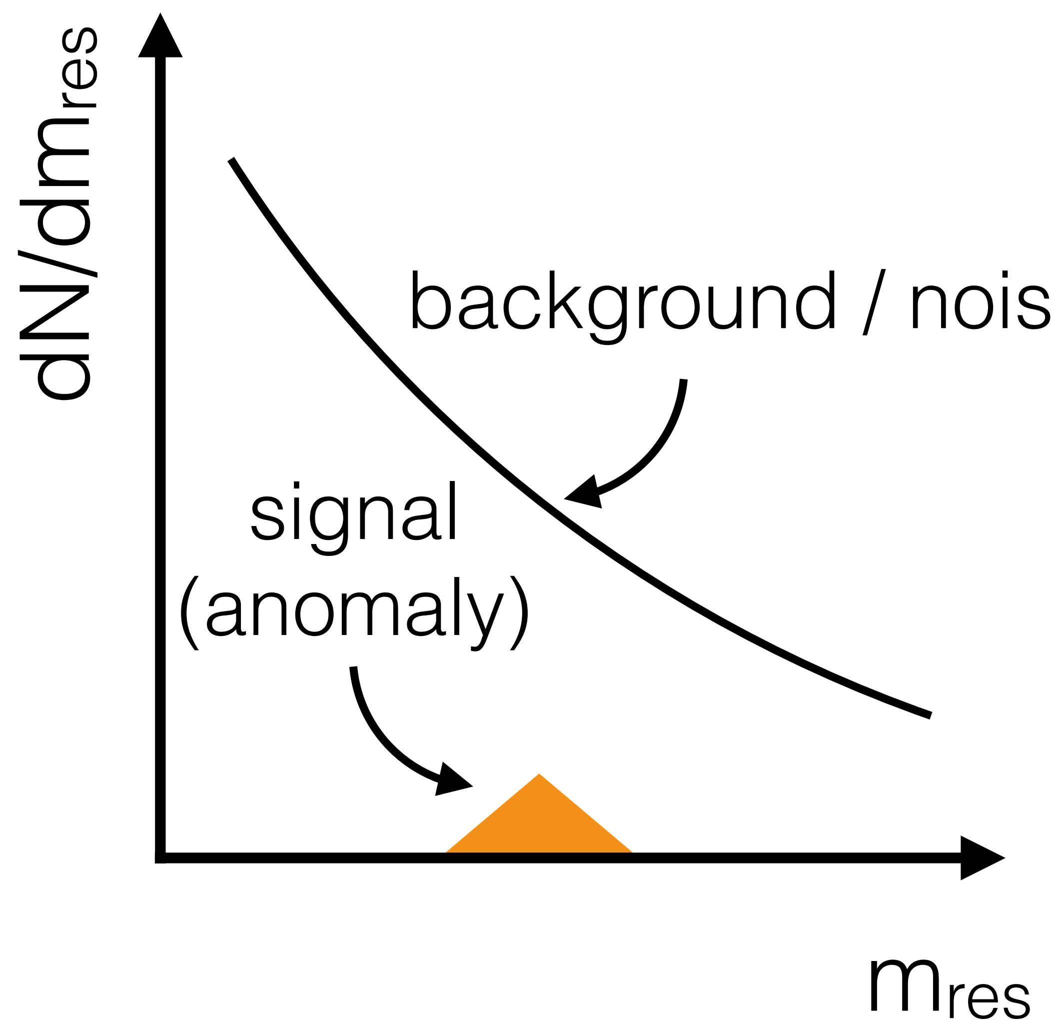
Cannonical example: resonances!

*for a detailed discussion about this, see G. Kasieczka et al., 2209.06225

Resonant Anomalies

A relatively general, but powerful assumption is that the anomaly is localized somewhere in phase space.



Generically true when there are on-shell new particles or transient phenomena in time series data

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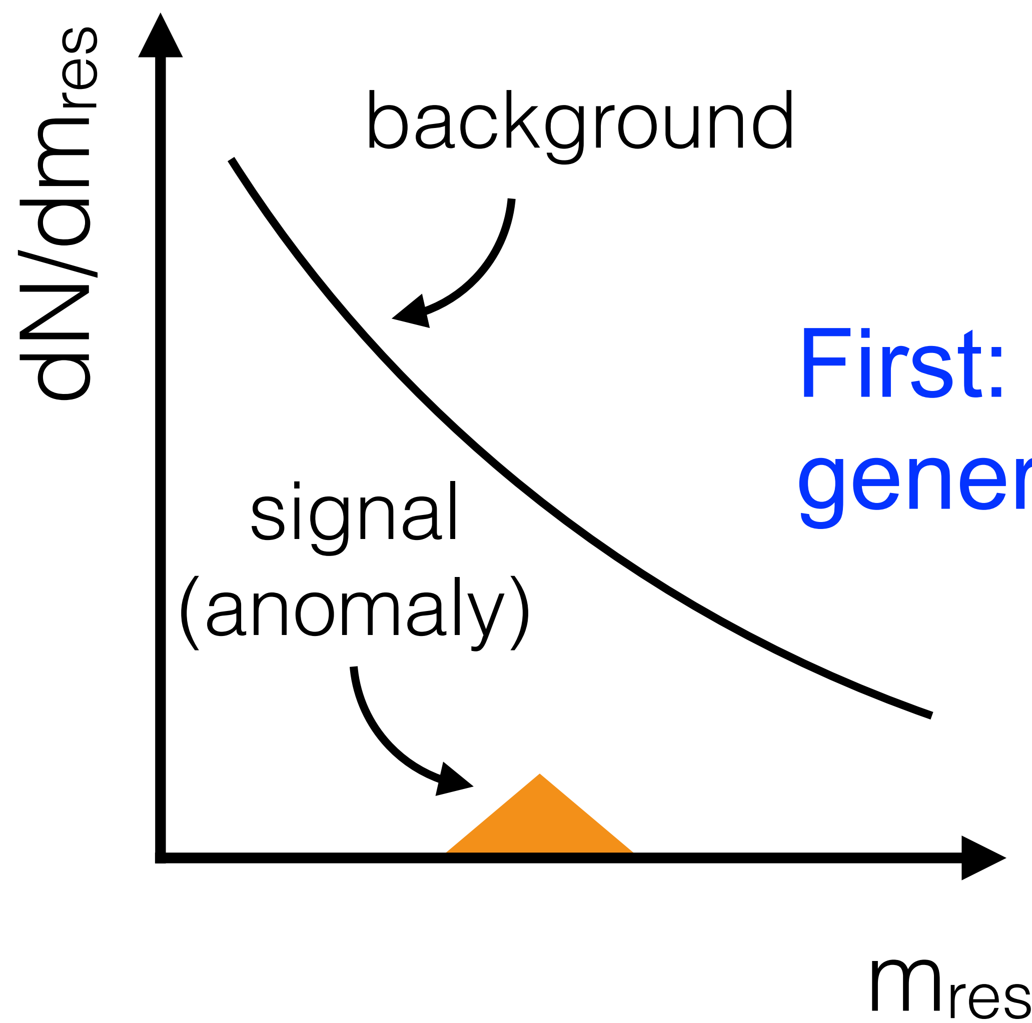
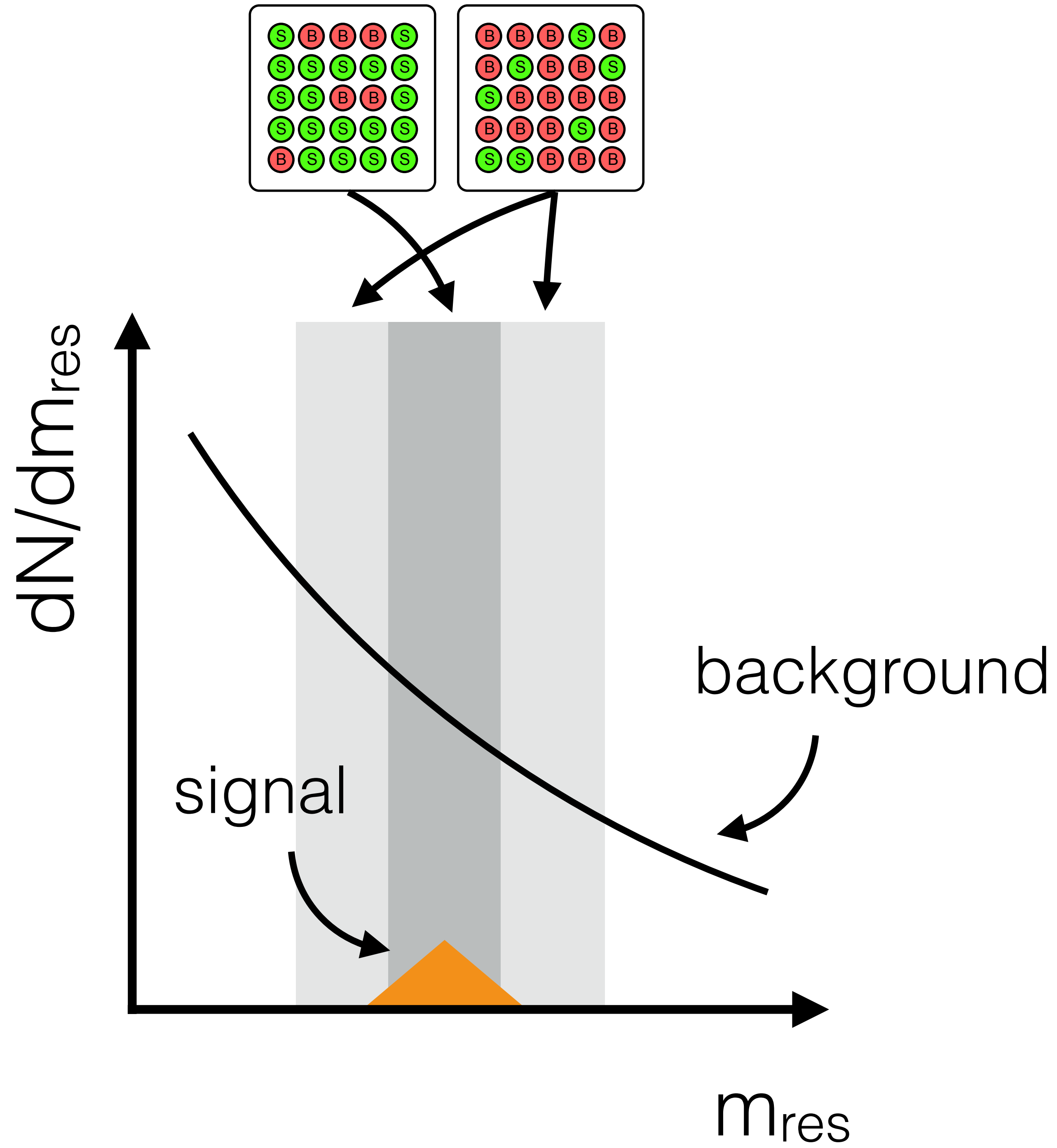


First: we will need to generate noisy labels.

Genericaly true when there are on-shell new particles or transient phenomena in time series data

Resonant Anomalies

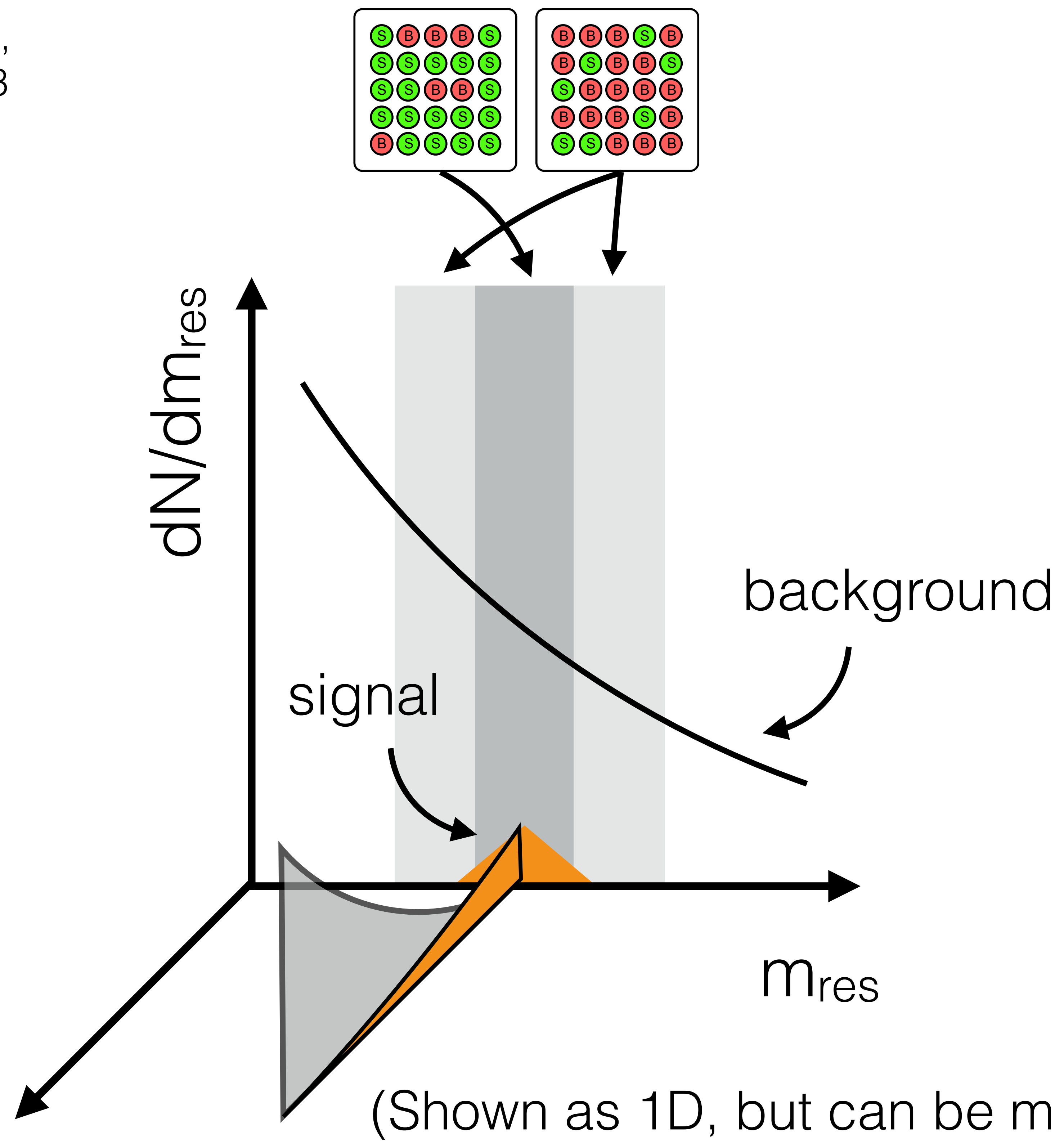


First: we will need to generate noisy labels.

Resonant Anomalies

J. Collins, K. Howe, **BN**,
PRL 121 (2018) 241803

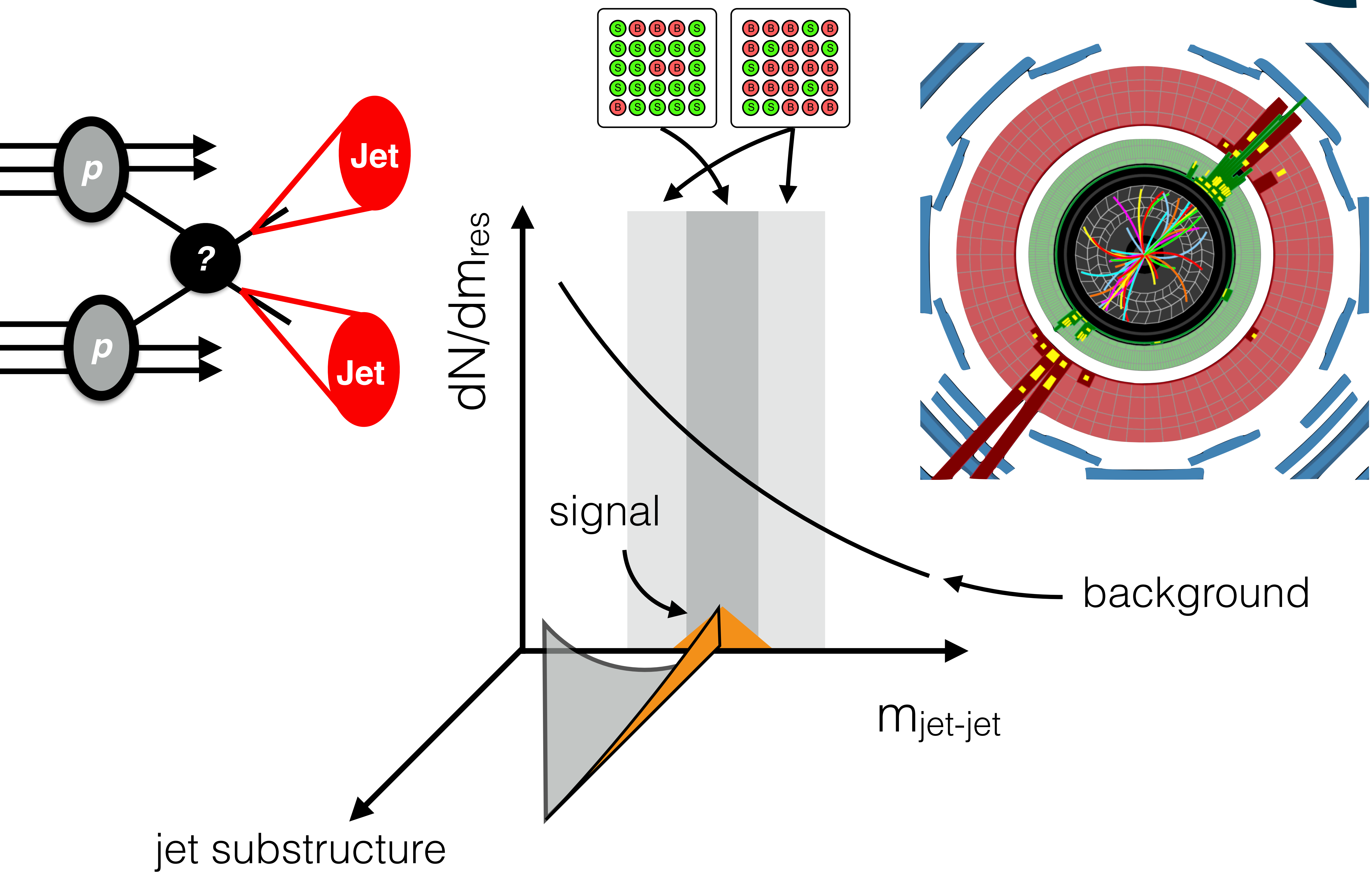
+many more



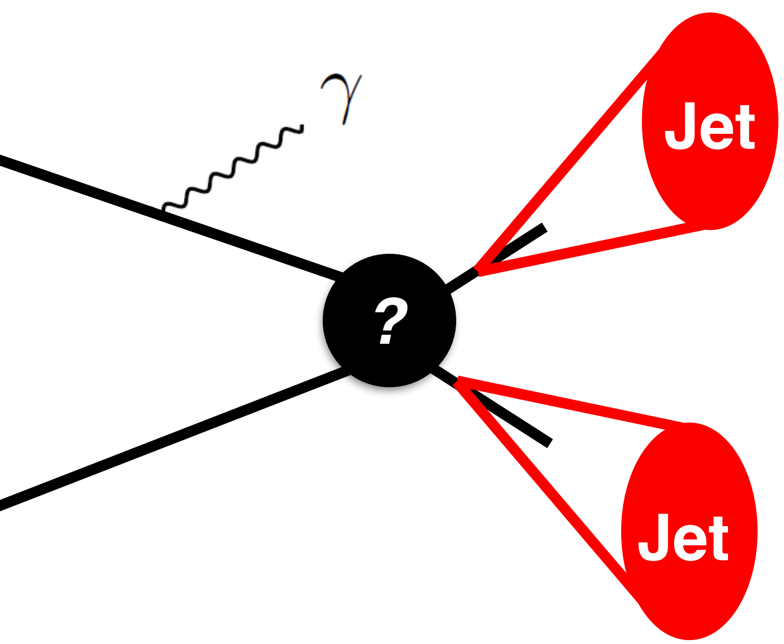
Extended feature space for machine learning

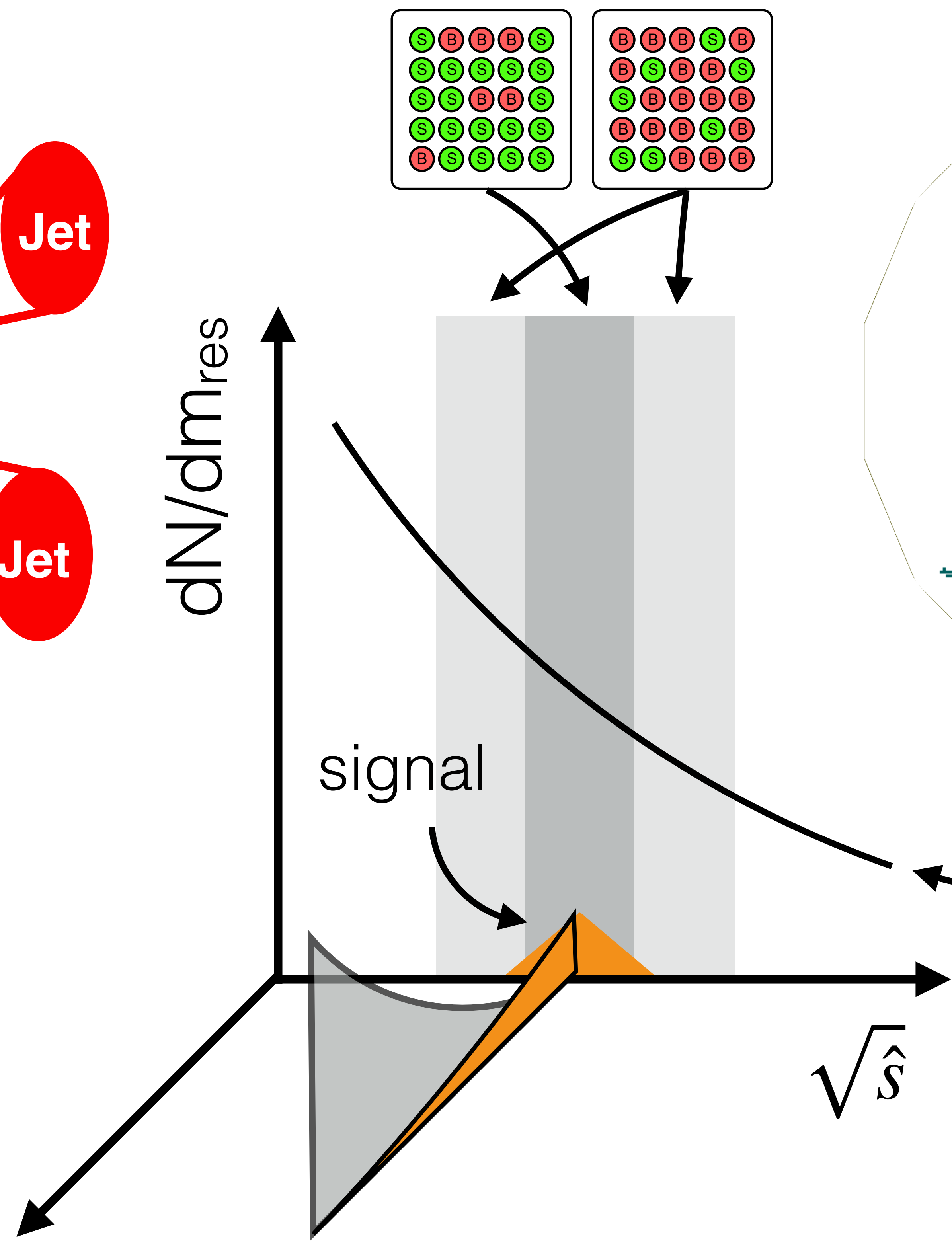
(Shown as 1D, but can be many-dimensional)

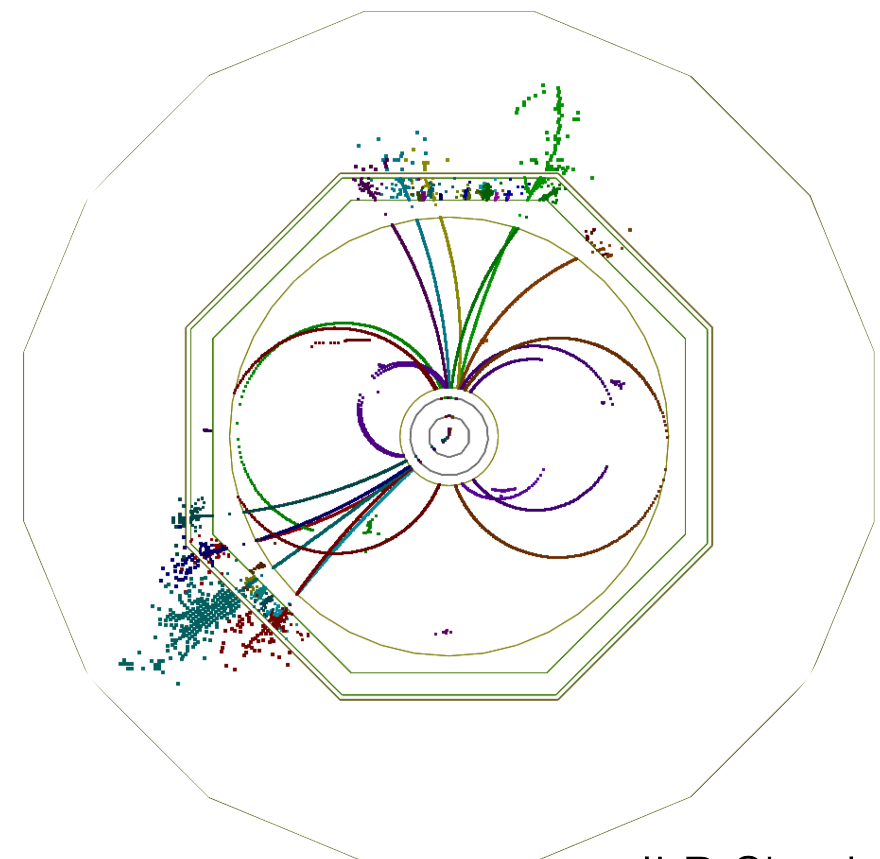
Resonant Anomalies



Resonant Anomalies







ILD Simulation

Resonant Anomalies

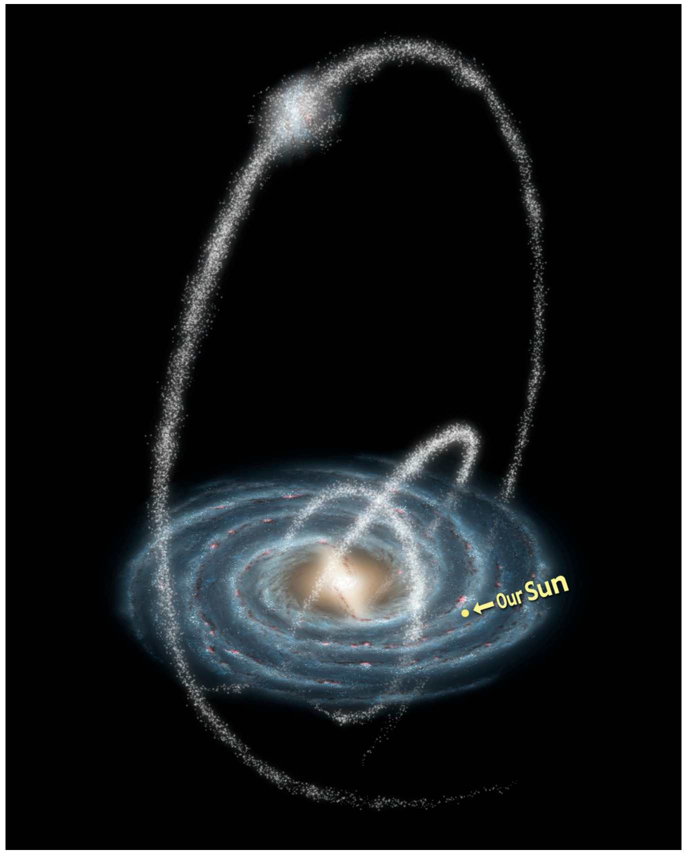
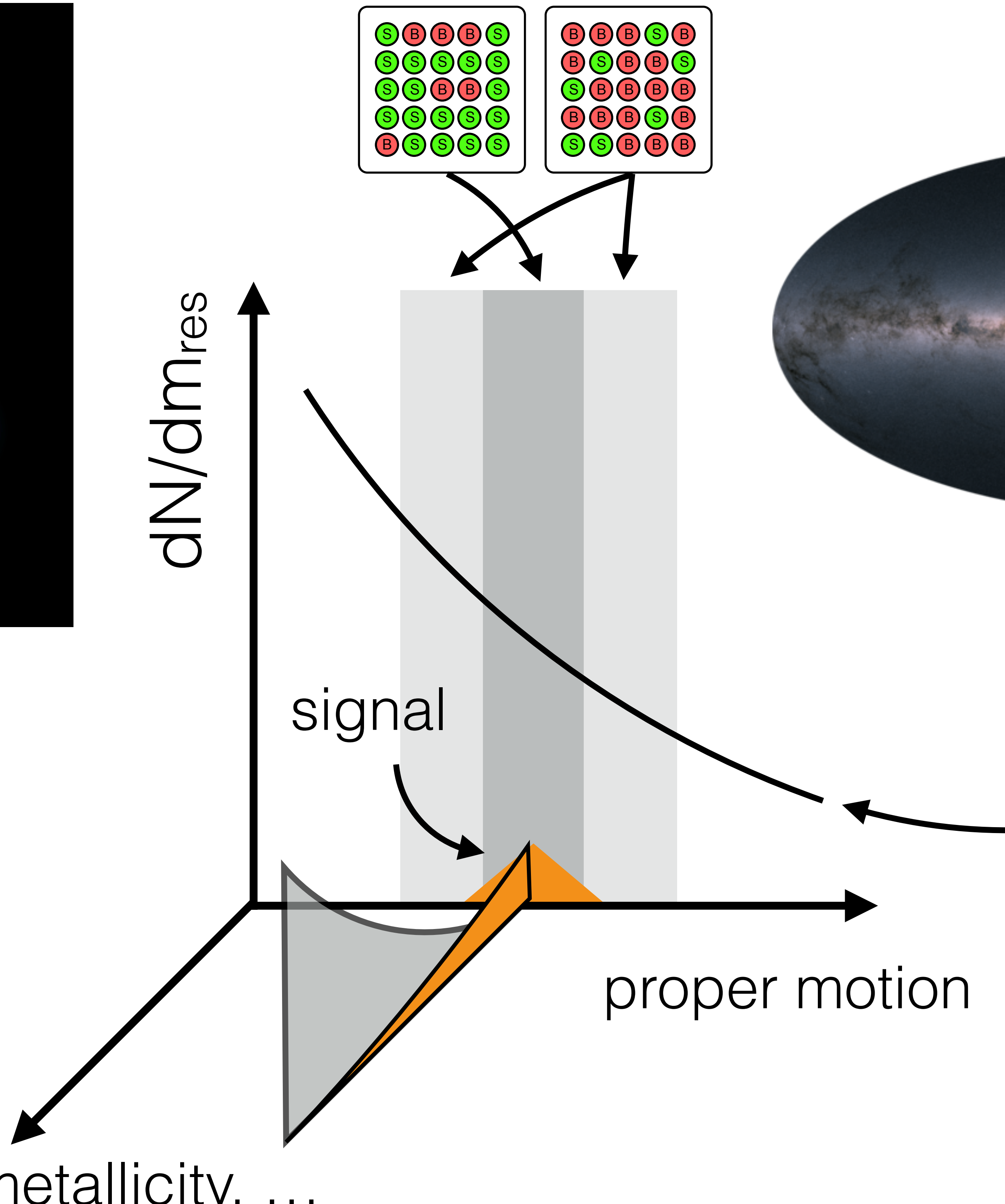
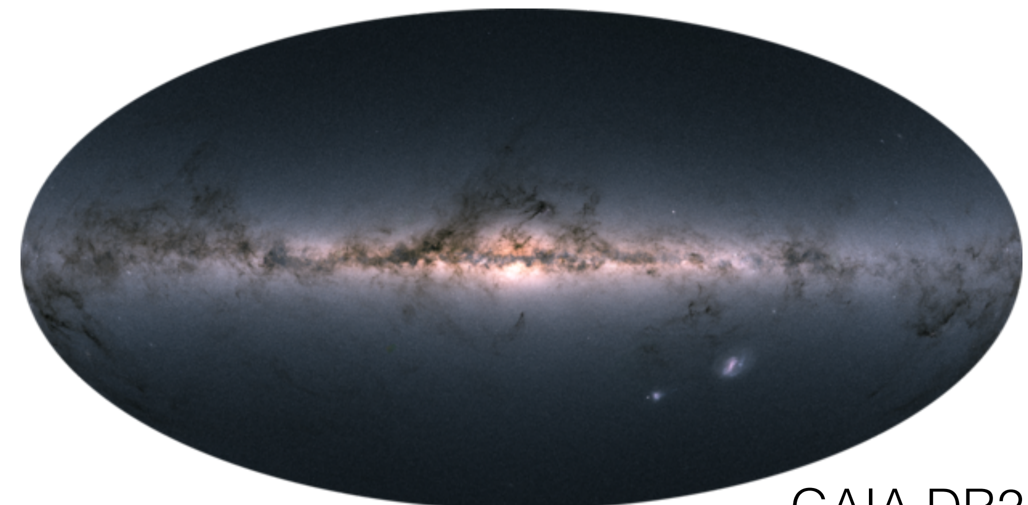


Image: NASA

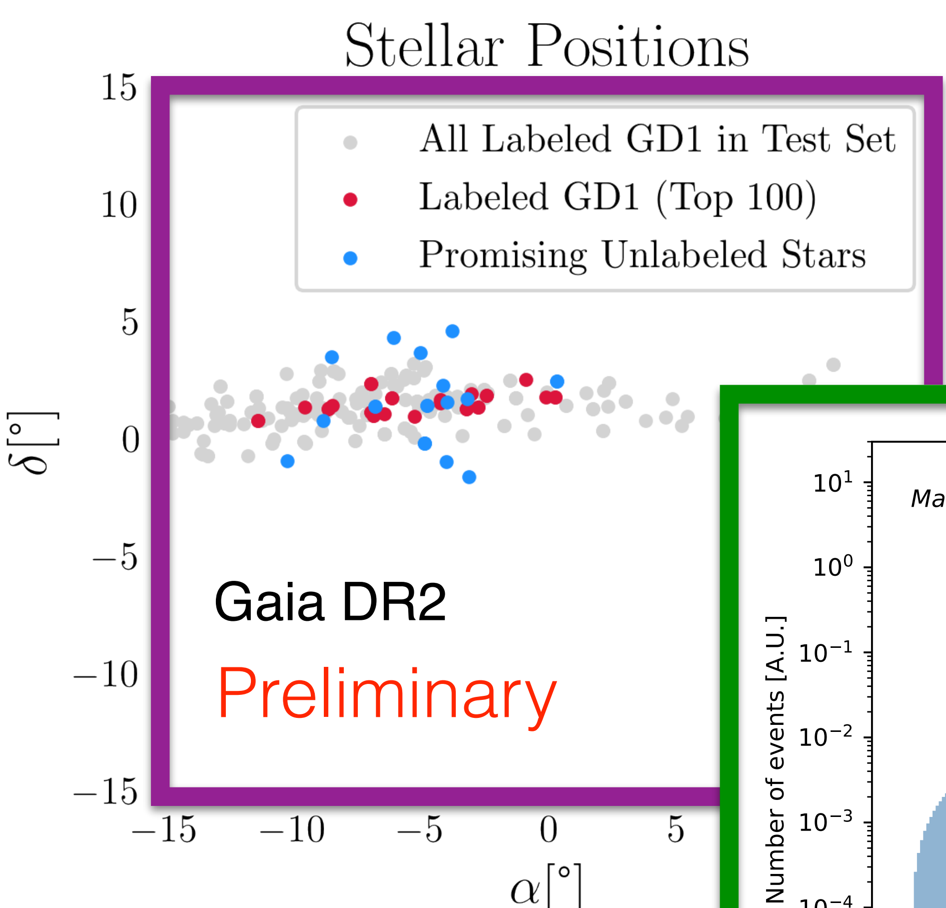




GAIA DR2

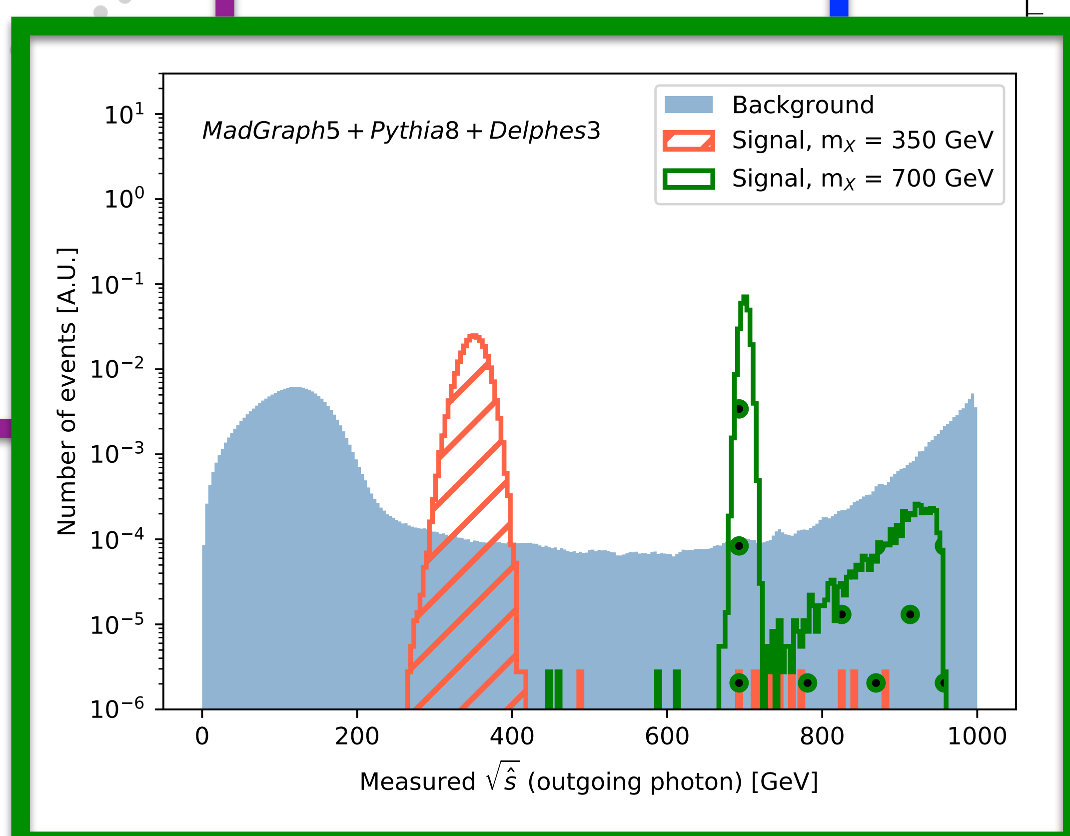
Anomaly Detection: Science

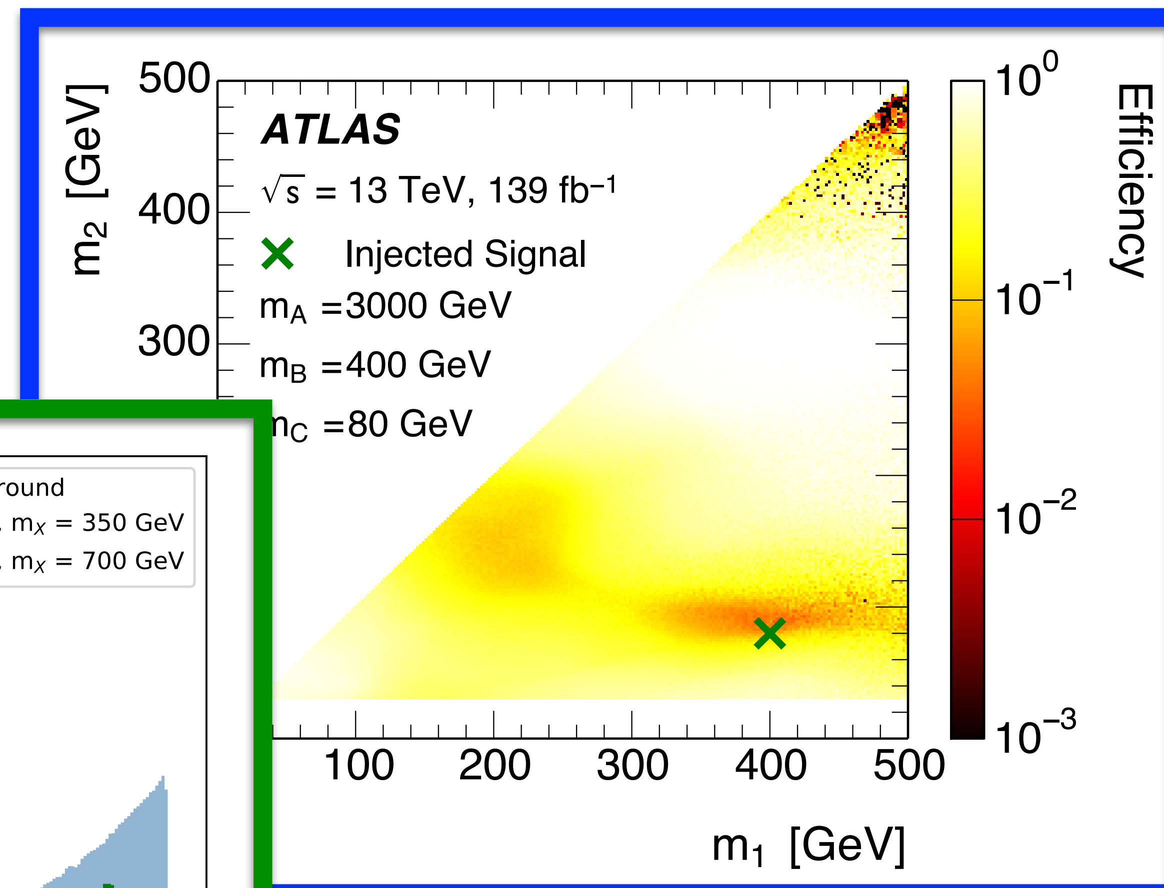
This program is really just getting started - there are many challenges to scale up (methods and computing*), but the early studies are exciting and cross-cutting



Cold, stellar streams

Future e^+e^-





LHC

*LHC result shown above required training 20k NNs!

Anomaly Detection: Science

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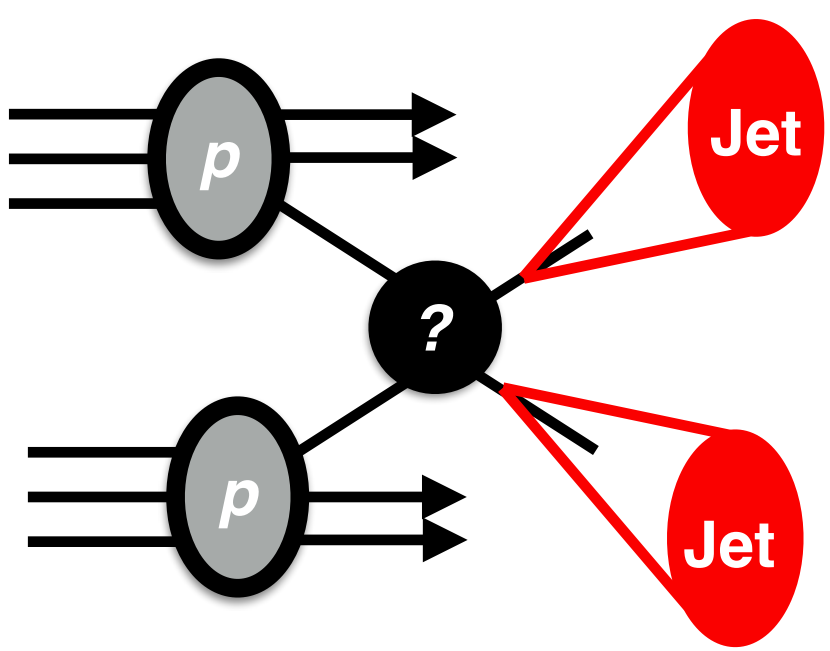
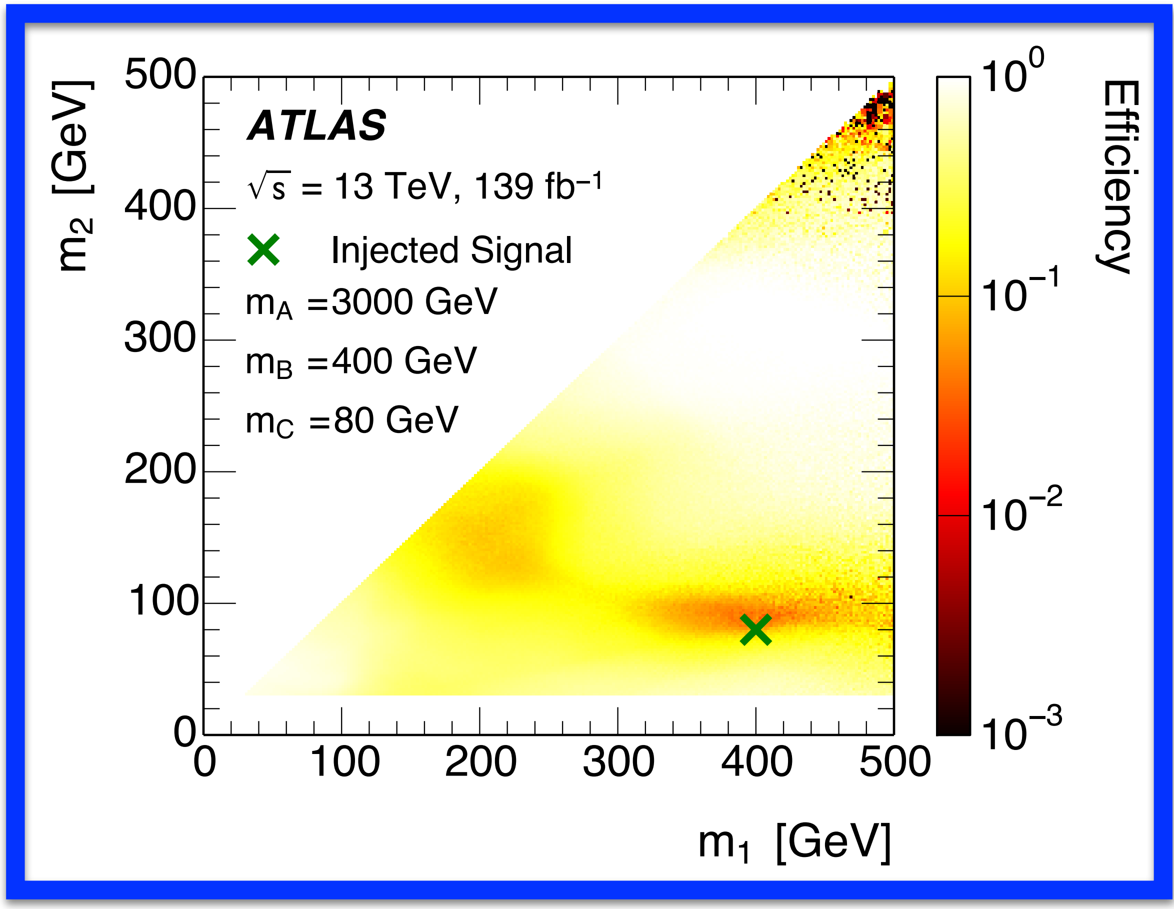
No new physics (yet), but significantly extended sensitivity





LHC

PRL 125 (2020) 131801

Anomaly Detection: Science

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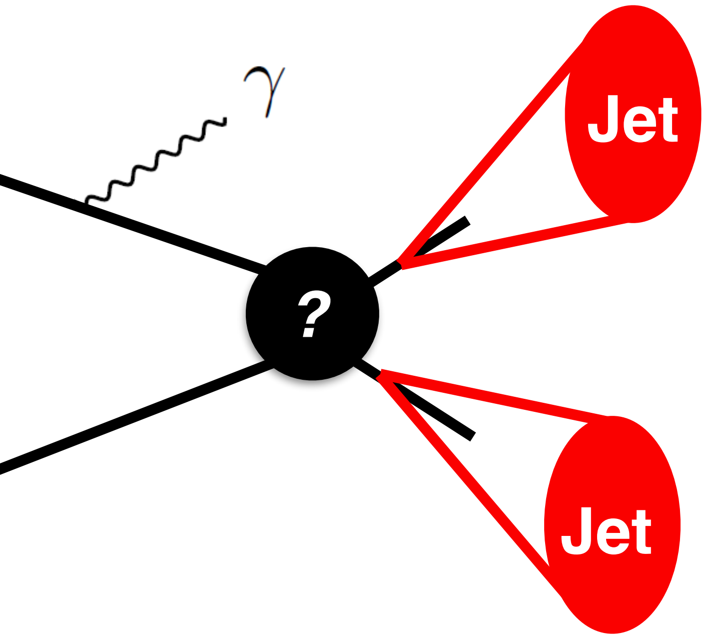
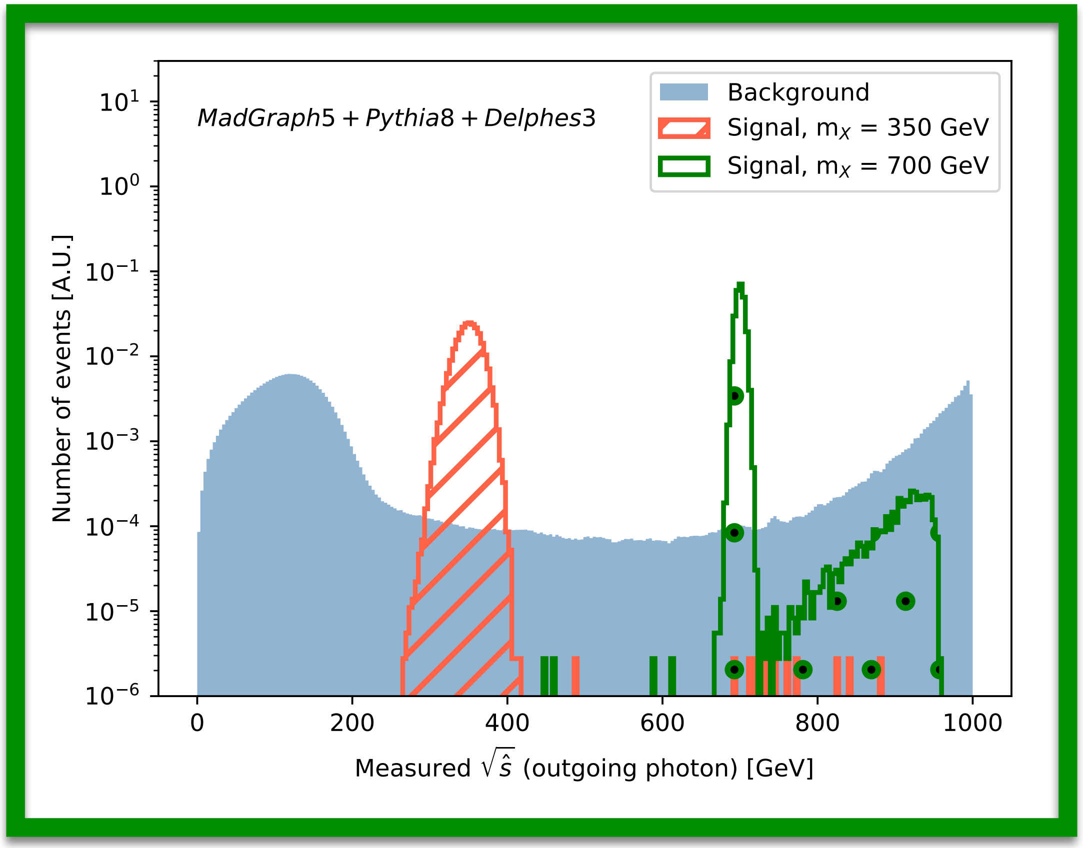
J. Gonski, J. Lai, **BN**, I Ochoa, JHEP (2022)

Future e^+e^-

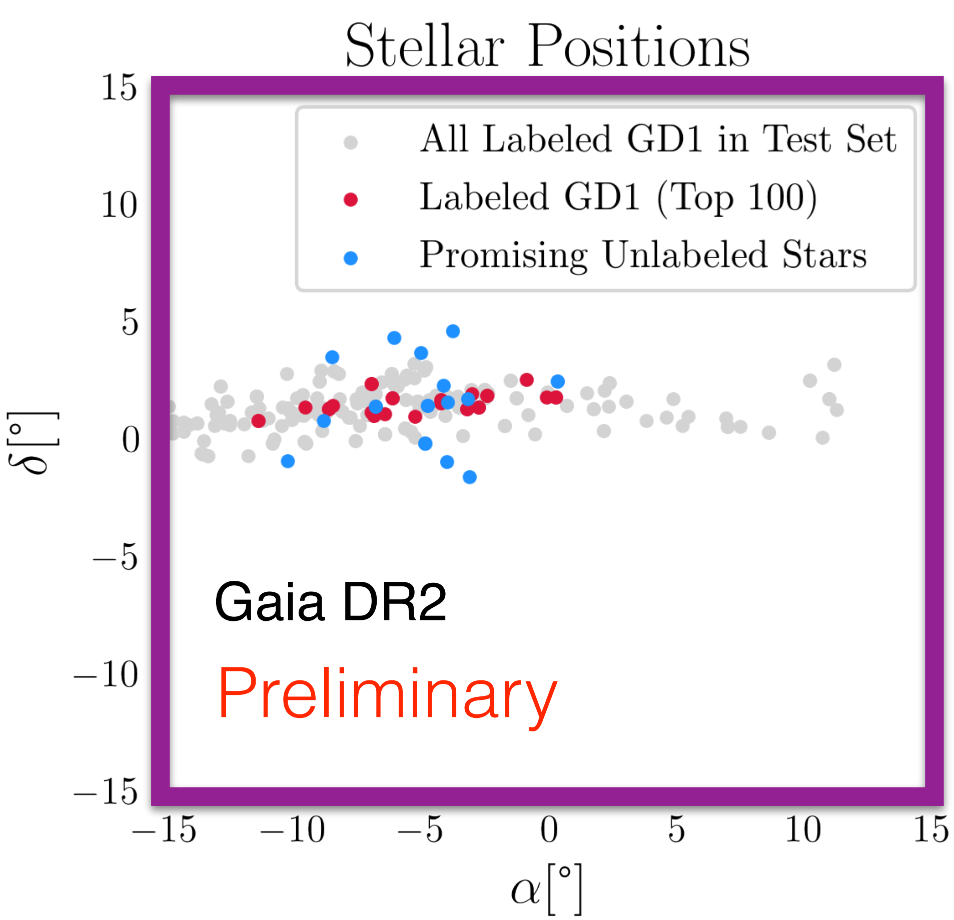




May have important implications for the design of future colliders

Anomaly Detection: Science

This program is really just getting started - there are many challenges to scale up (methods and computing*), but the early studies are exciting and cross-cutting



Cold, stellar streams

We have shown that we can find known streams

Will we be able to find new streams? Can weakly supervised learning help us categorize known streams?

w/M. Buckley, J. Collins, M. Pettee, D. Shih, S. Thanvantri

Future of Label-Free Learning

Goal: develop, deploy, and interpret anomaly detection

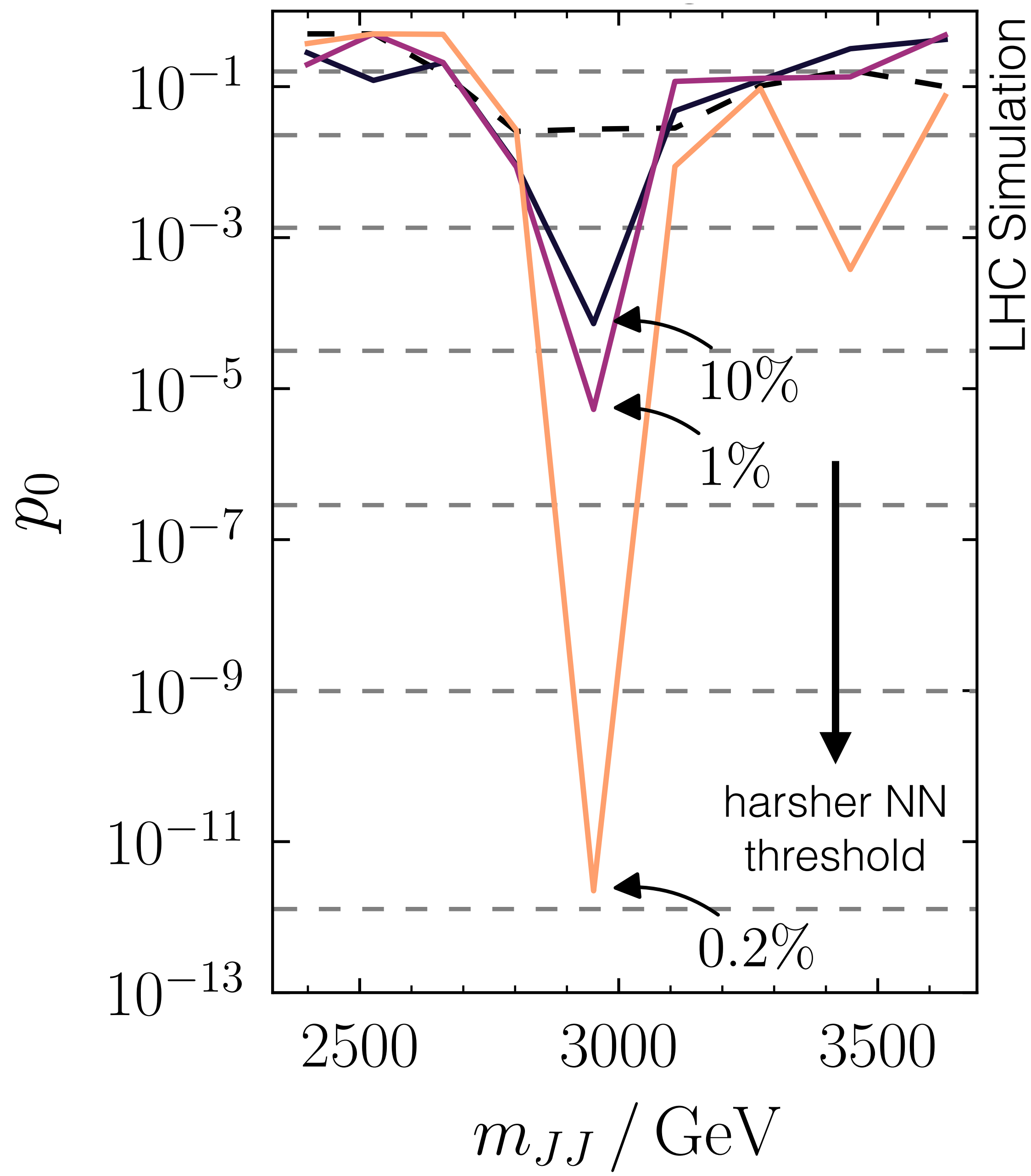
J. Collins, K. Howe, **BN**, PRL 121 (2018) 241803

Methods

Push the dimensionality, relax the assumptions (non-resonant, …)

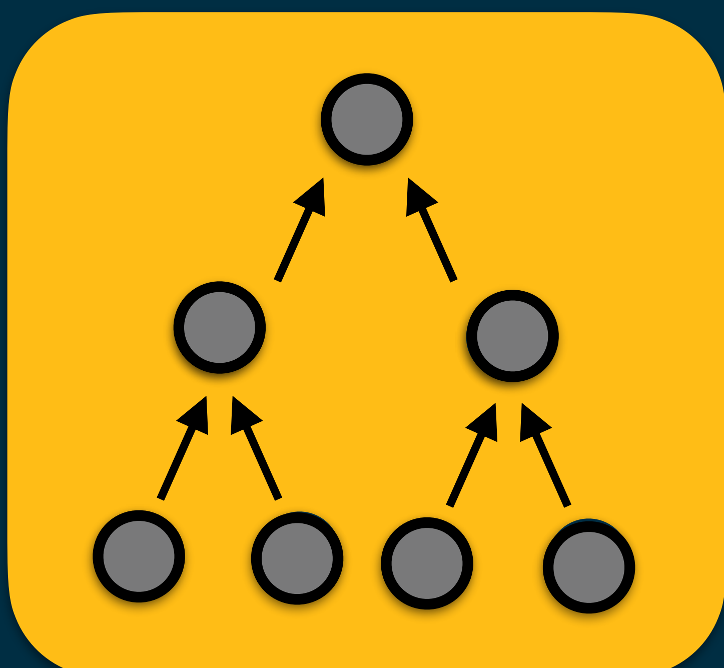
Science

- Anomalies @ colliders
- Anomalies @ astroparticle/cosmology
- Anomalies @ dark matter direct det.

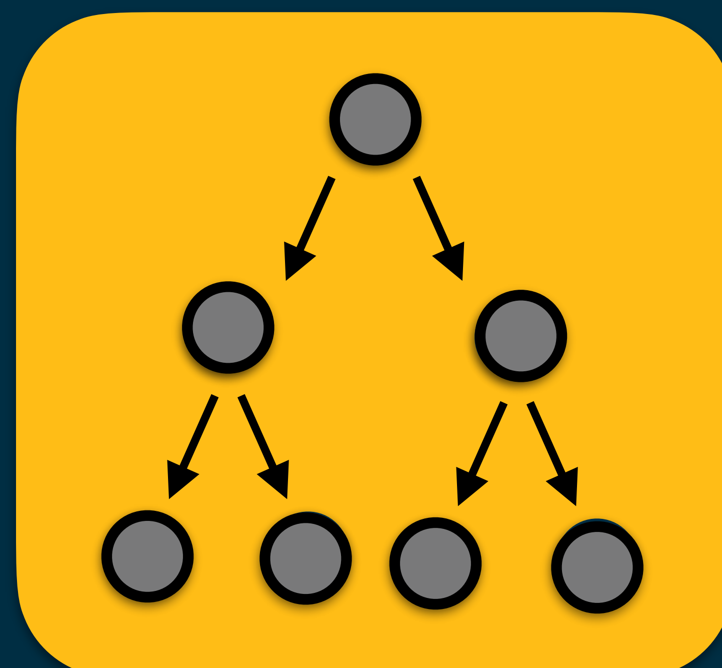


Outline for today

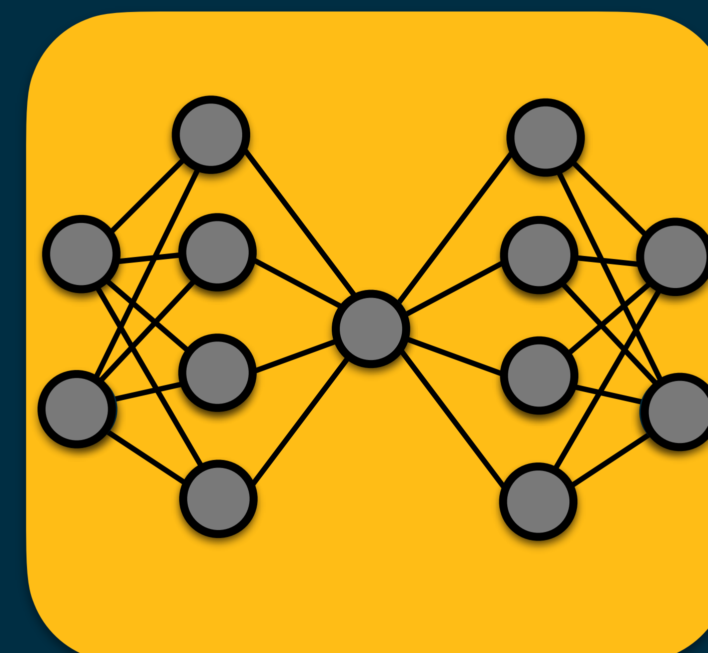
I'll focus on three core, cross-cutting areas of ML ∩ Physics



Forward Models
(fast simulation)



Inverse Models
(unfolding)



Simulation-free
(anomaly detection)

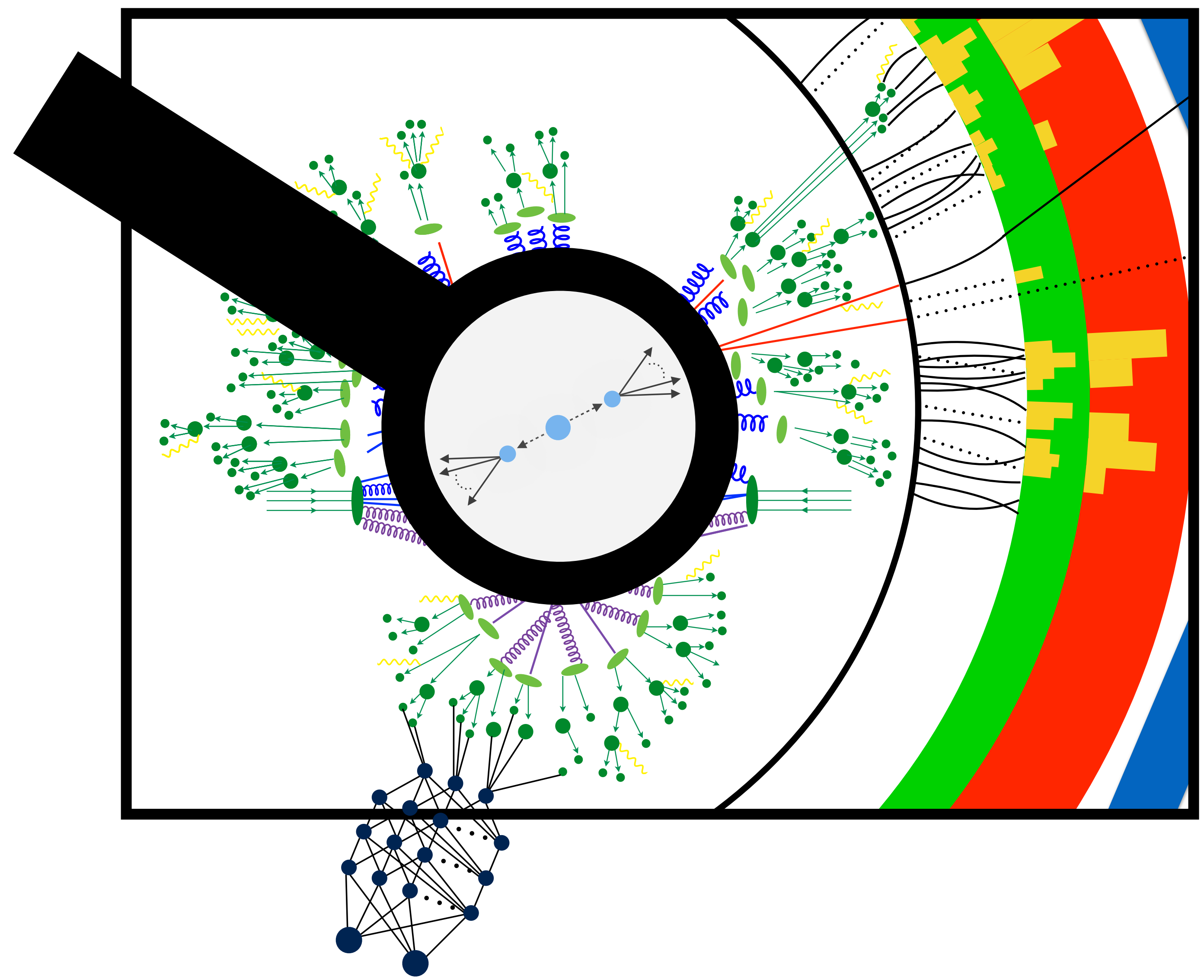
To illustrate these exciting topics, I'll give one vignette per area

Conclusions and Outlook

We need innovative computational techniques to make the **data-driven discoveries of the future**.

This is not just about improving precision, it is about enabling new science!

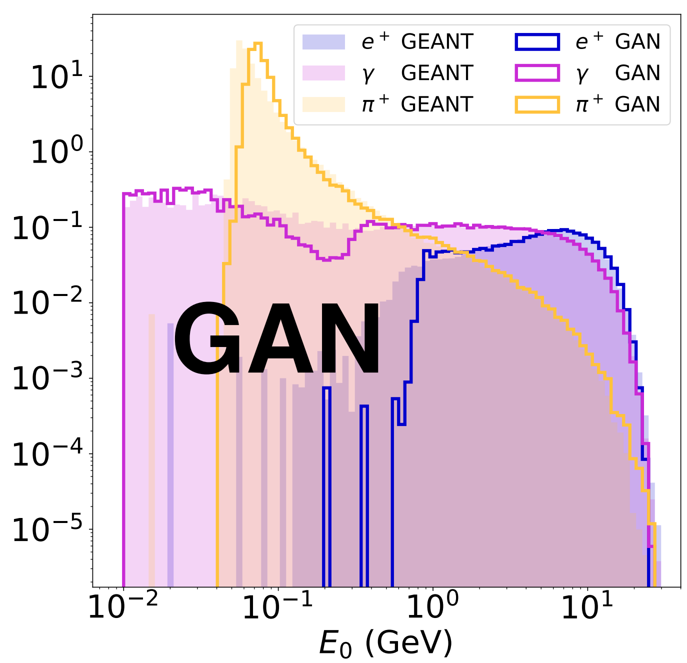
We need physicists
(theory + experiment) to address unique challenges

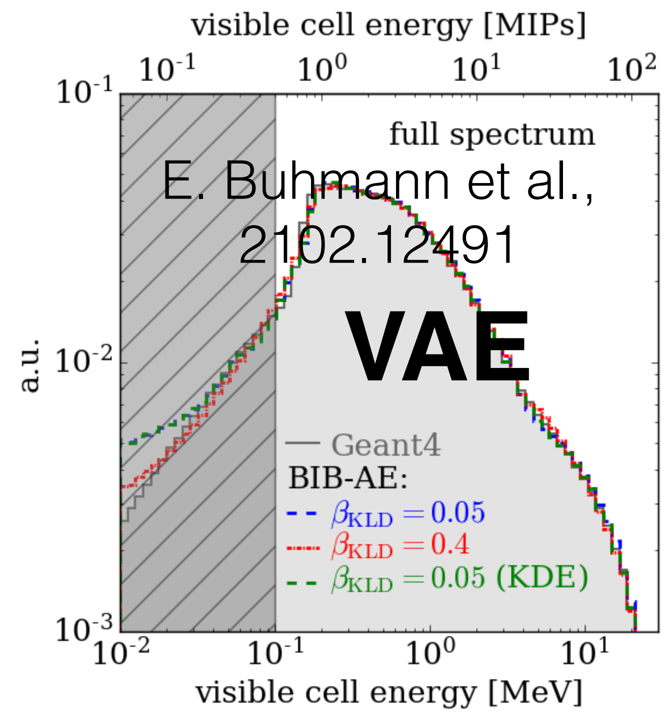


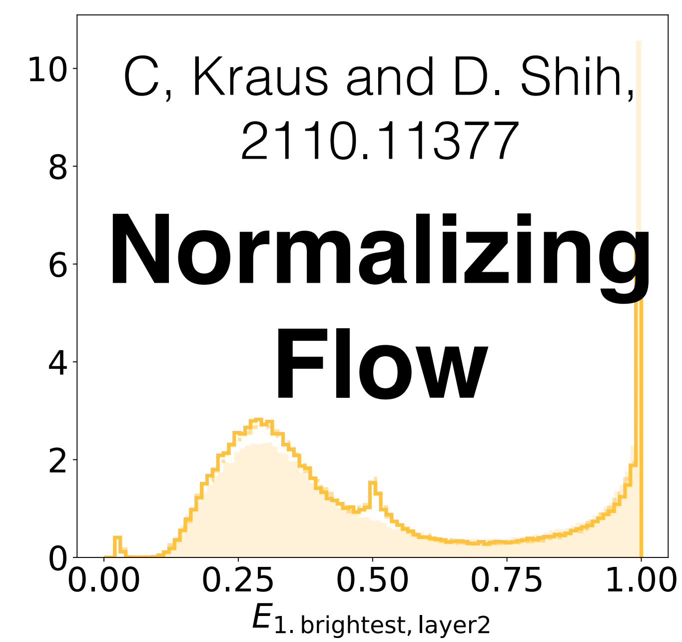

Questions?
Krish Desai
Yale BS/MS 2020
Mariel Pettee
Yale PhD 2021

Backup

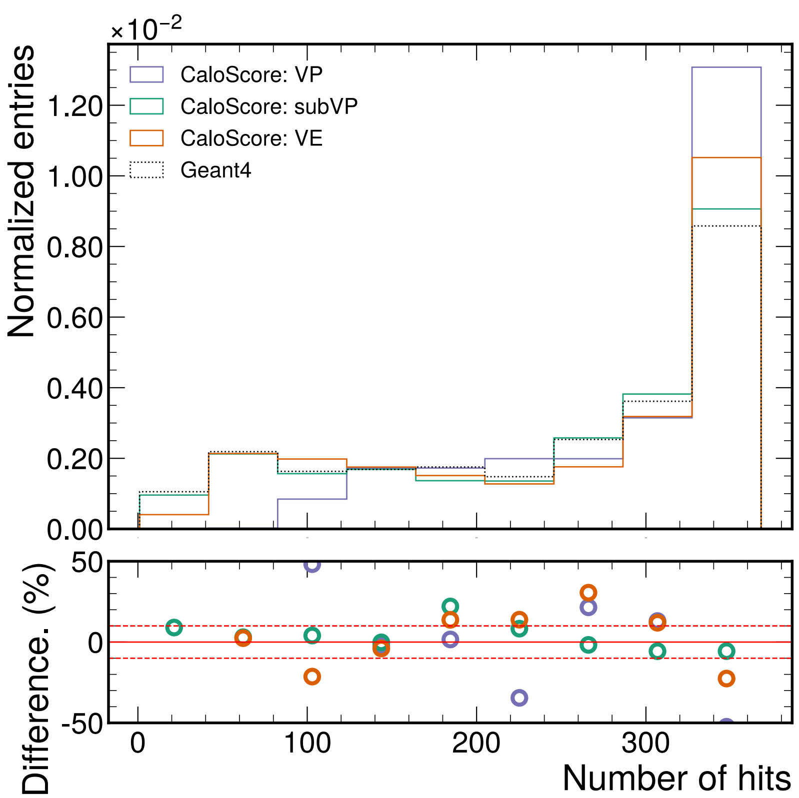
Calo(GAN,VAE,Flow,Score)

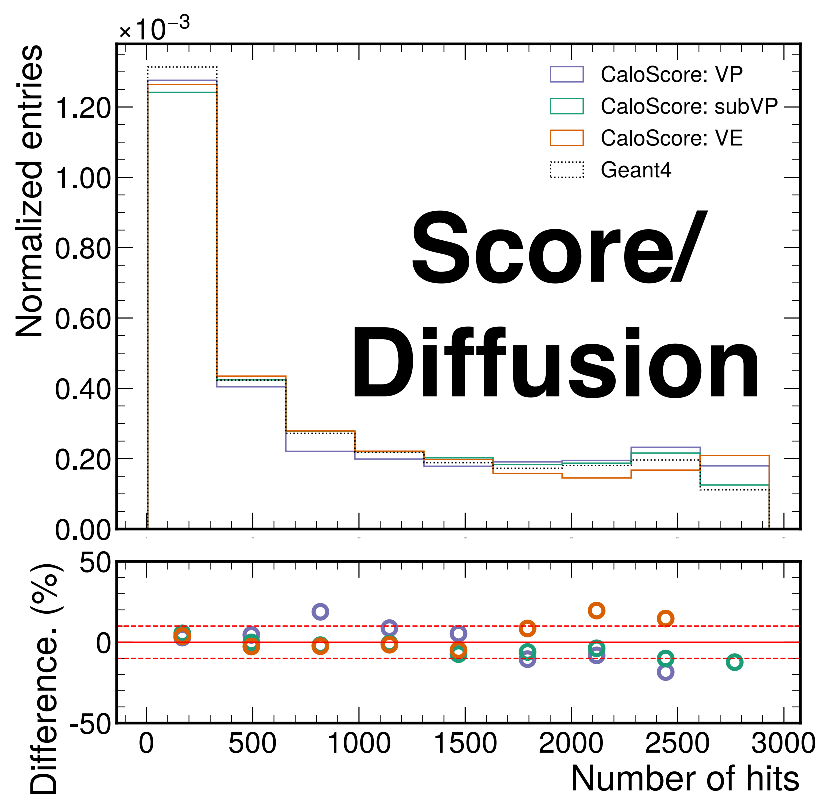


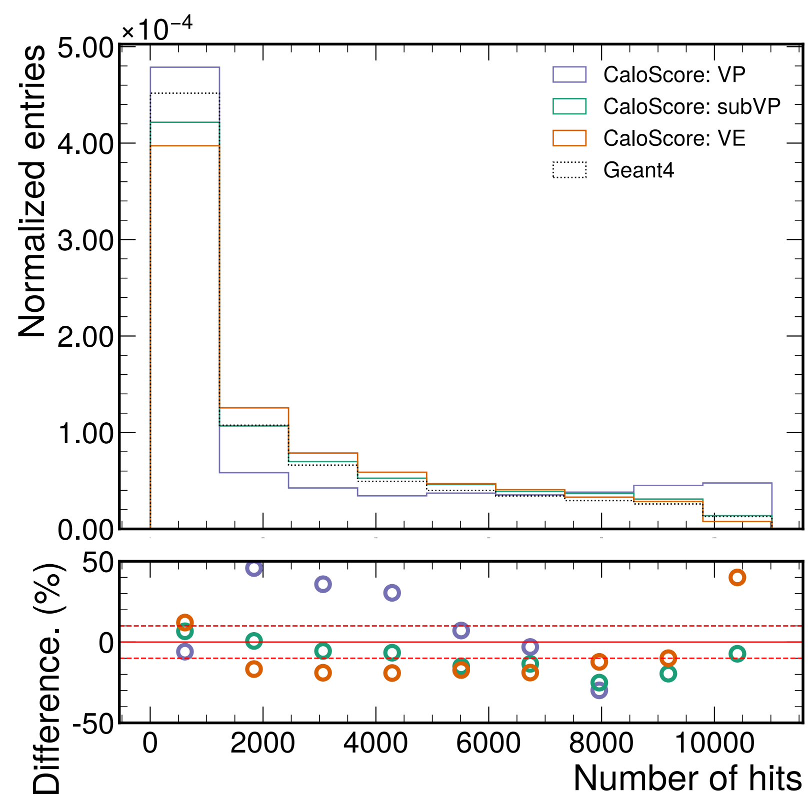




Multiple innovations beyond GANs



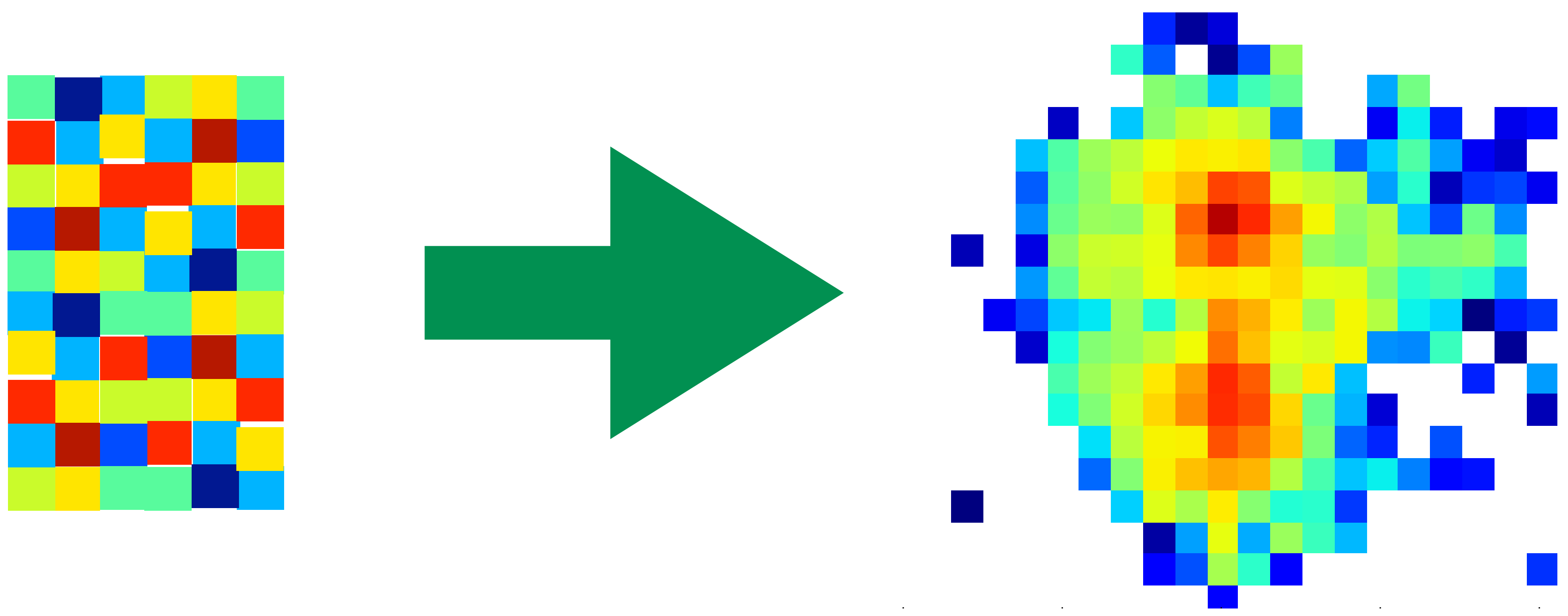




V. Mikuni and **BN**, 2206.11898

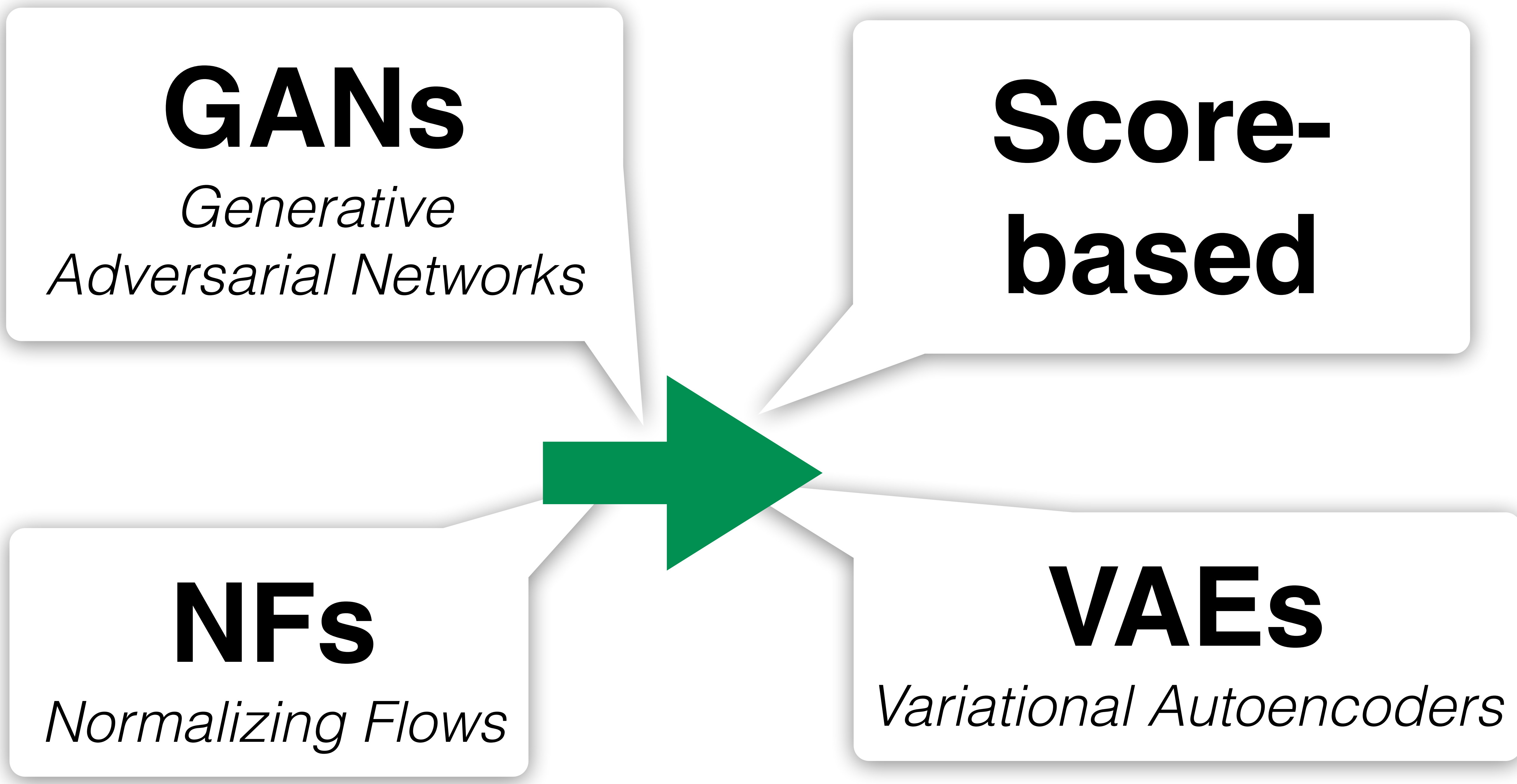
Introduction: generative models

A **generator** is nothing other than a function that maps random numbers to structure.



Deep generative models: the map is a deep neural network.

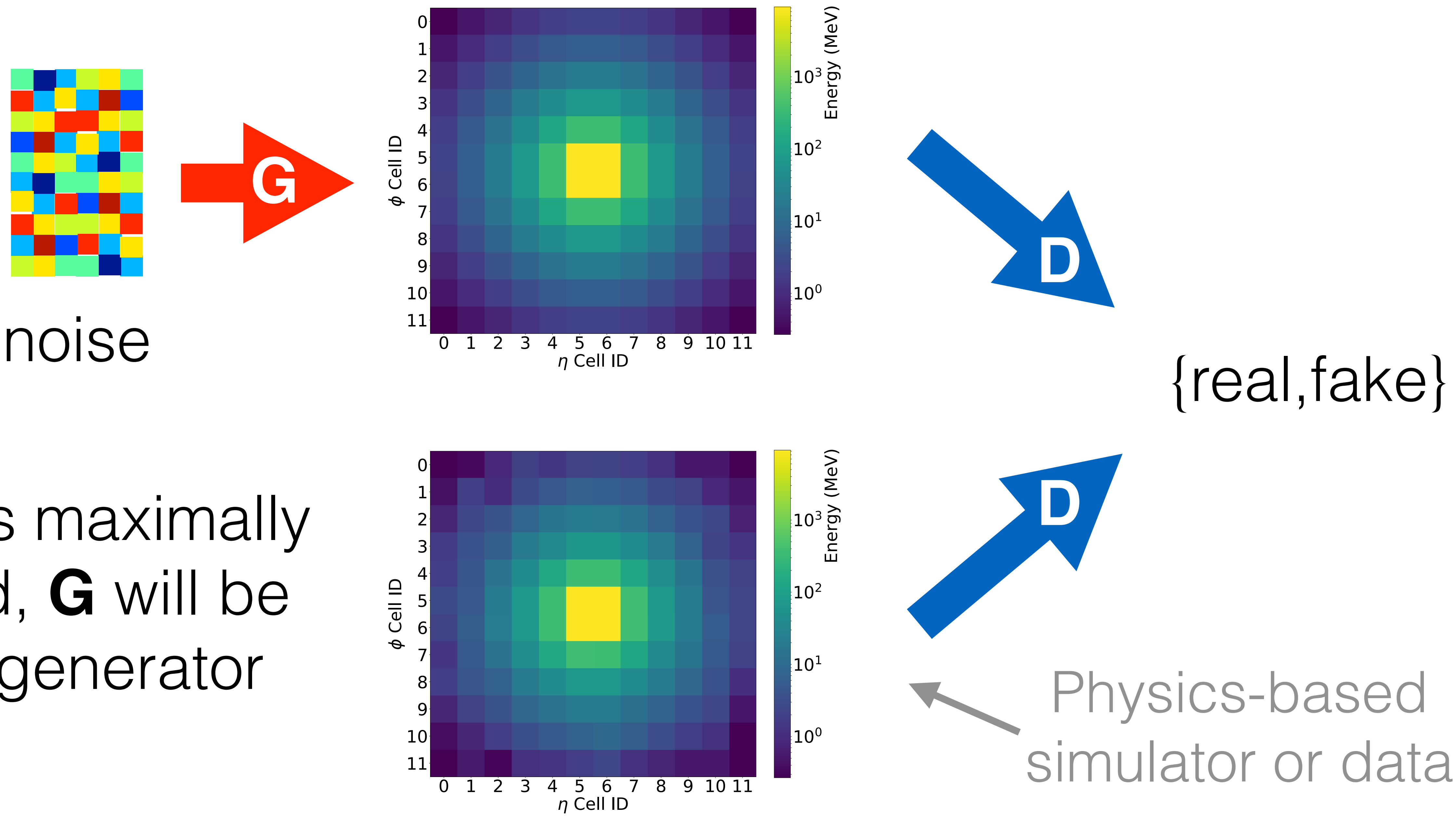
Tools



Deep generative models: the map is a deep neural network.

Introduction: GANs

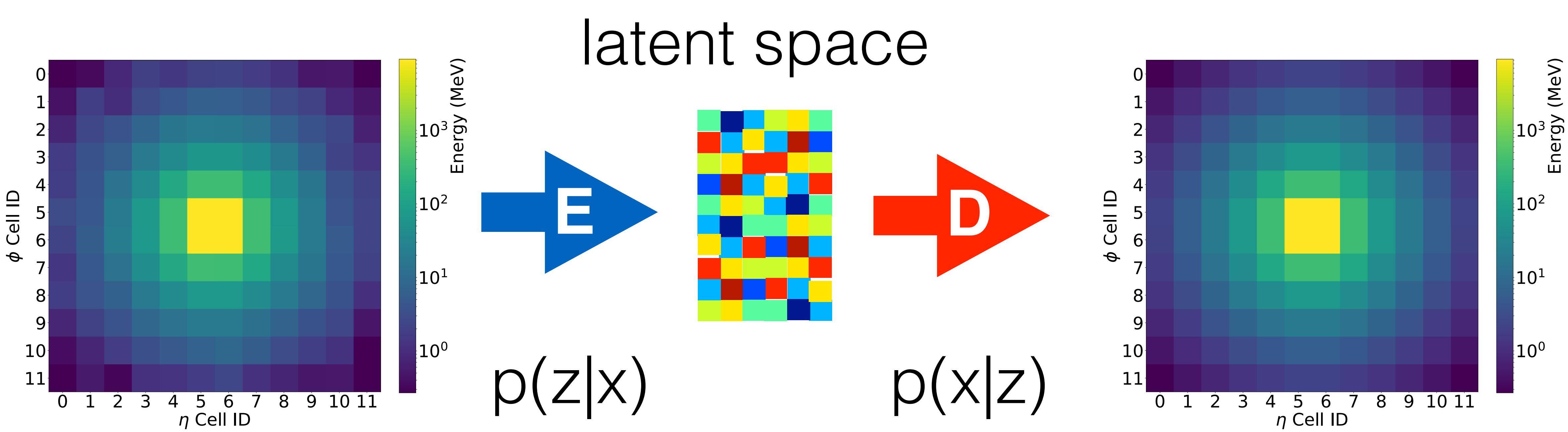
Generative Adversarial Networks (GANs):
A two-network game where one ***maps noise to structure*** *and one* ***classifies images as fake or real****.*



When **D** is maximally confused, **G** will be a good generator

Introduction: VAEs

Variational Autoencoders (VAEs):
A pair of networks that embed the data into a latent space with a given prior and decode back to the data space.



Physics-based simulator or data

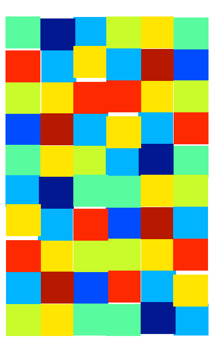
Probabilistic ***encoder***

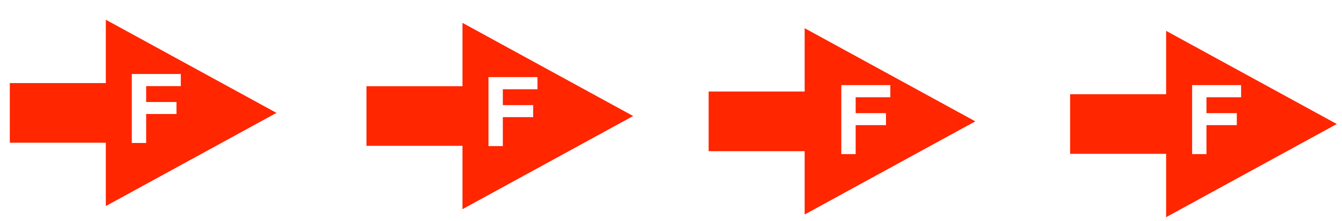
Probabilistic ***decoder***

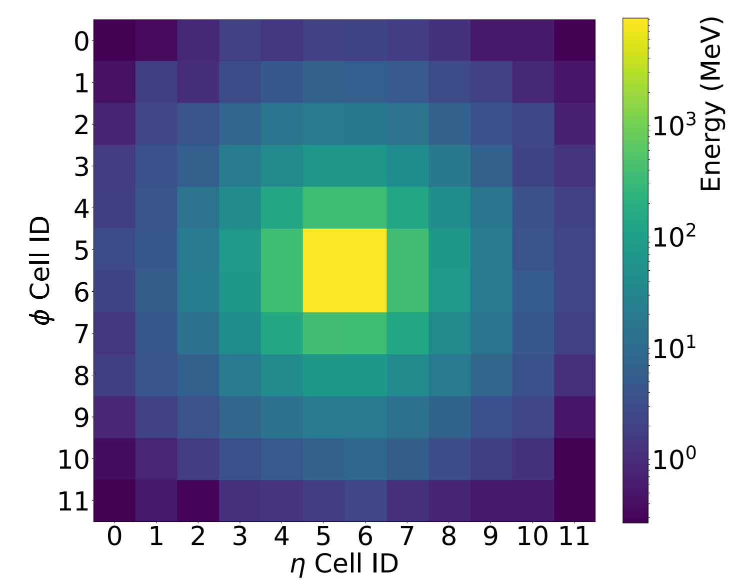
Introduction: NFs

Normalizing Flows (NFs):
A series of invertible transformations mapping a known density into the data density.

Optimize via maximum likelihood







latent space

Invertible transformations with tractable Jacobians

$p(z)$

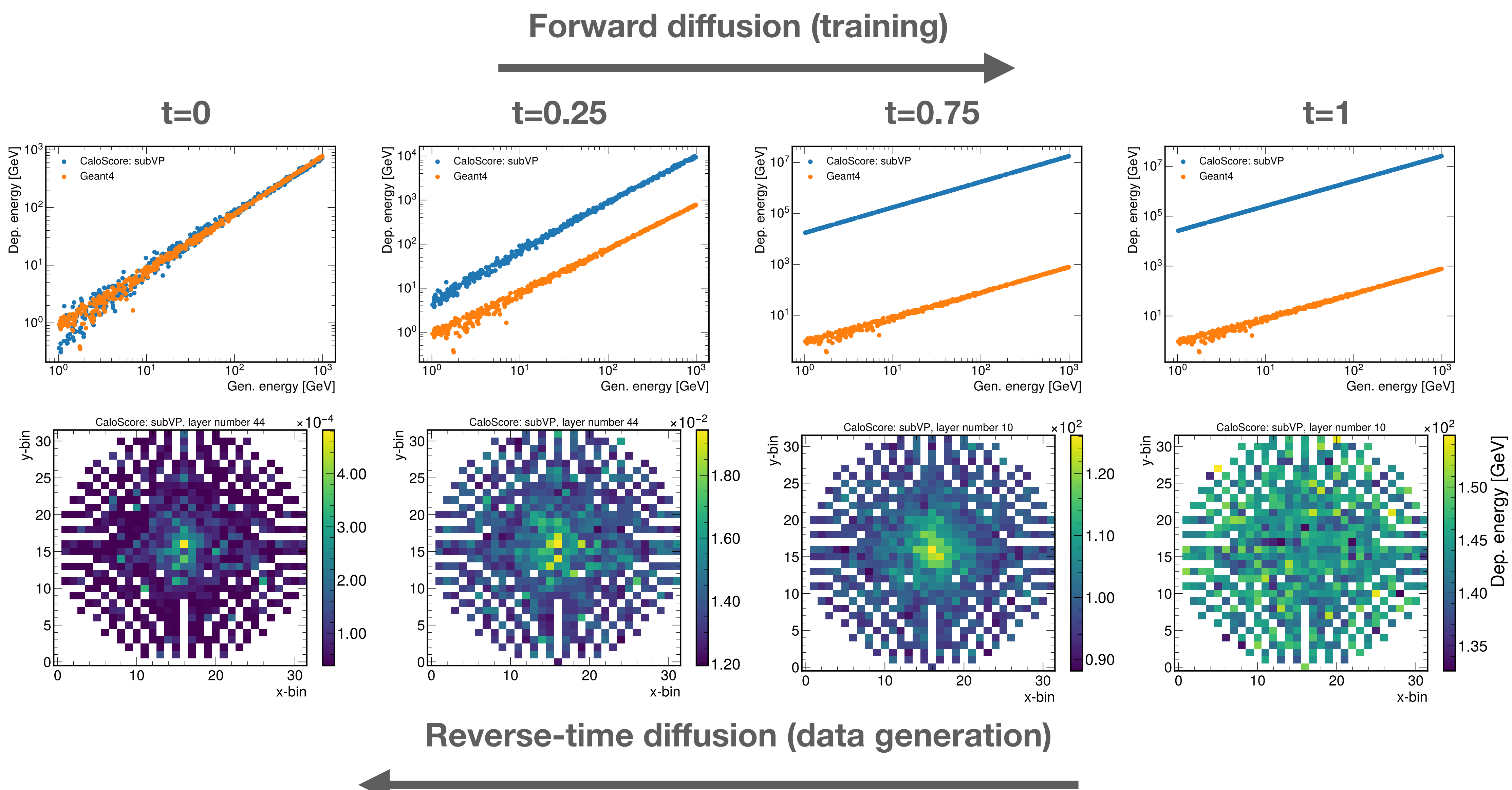
$p(x) = p(z)\ |dF^{-1}/dx|$

$p(x)$

Introduction: Score-based

Score-based

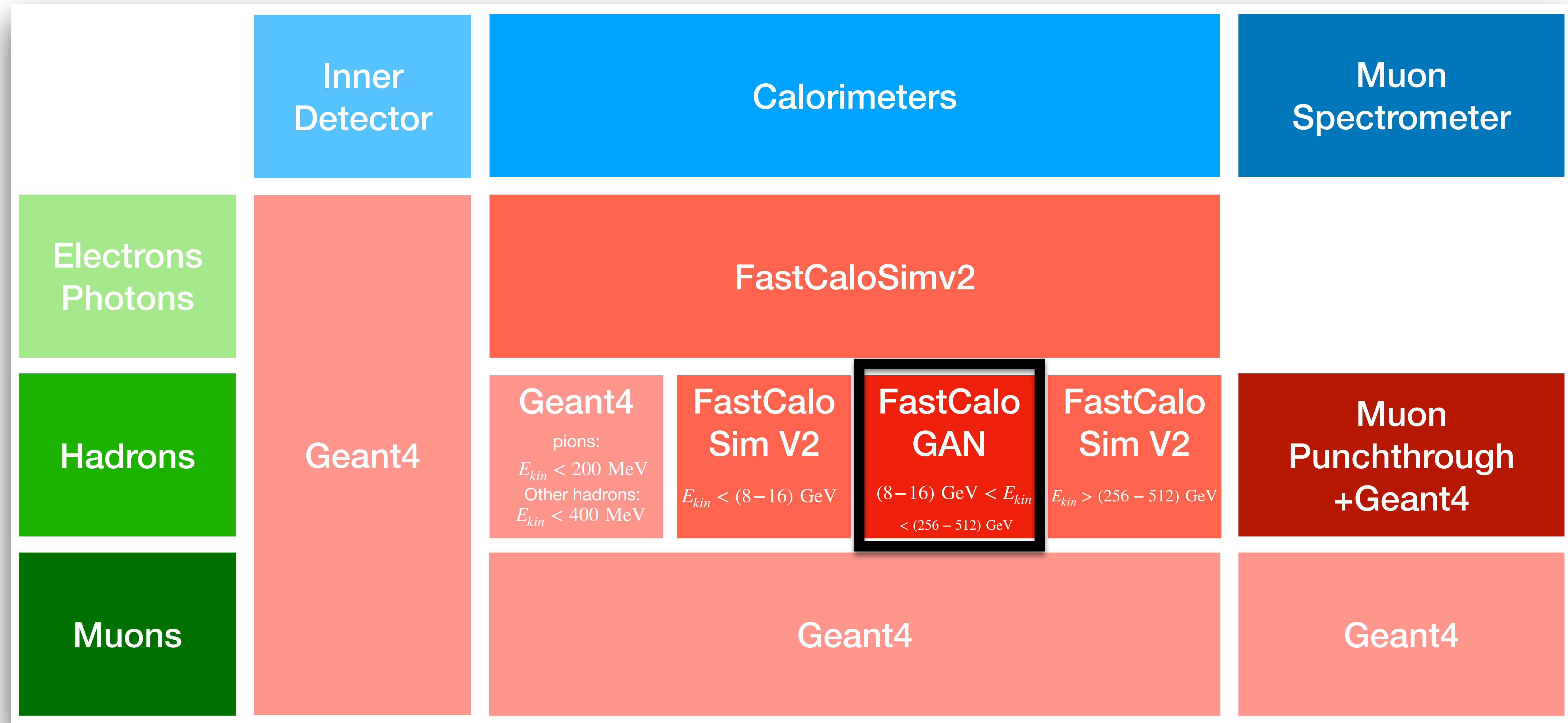
Learn the gradient of the density instead of the probability density itself.



From 2206.11898

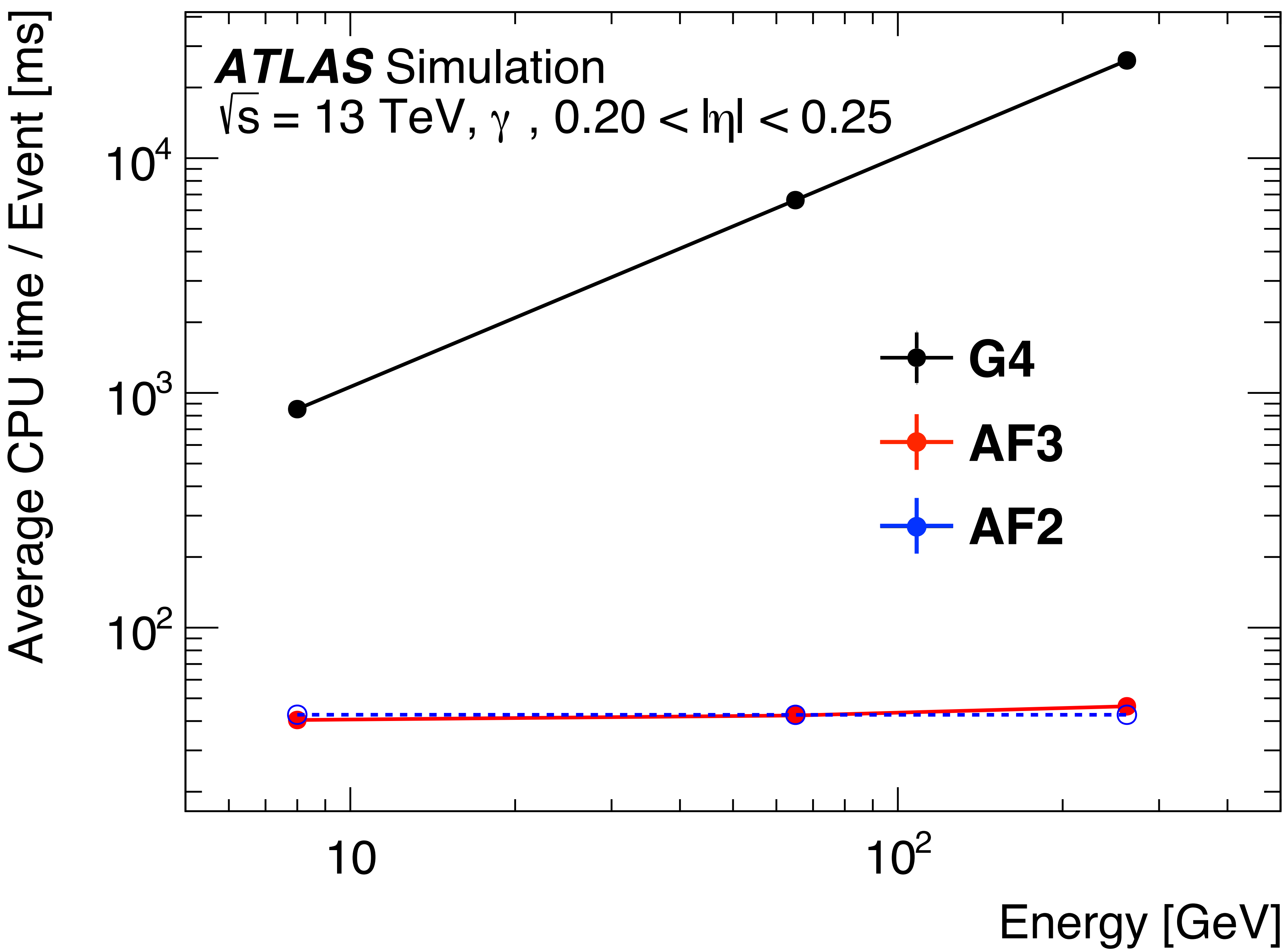
ATLAS Collaboration, 2109.02551

Integration into real detector sim.



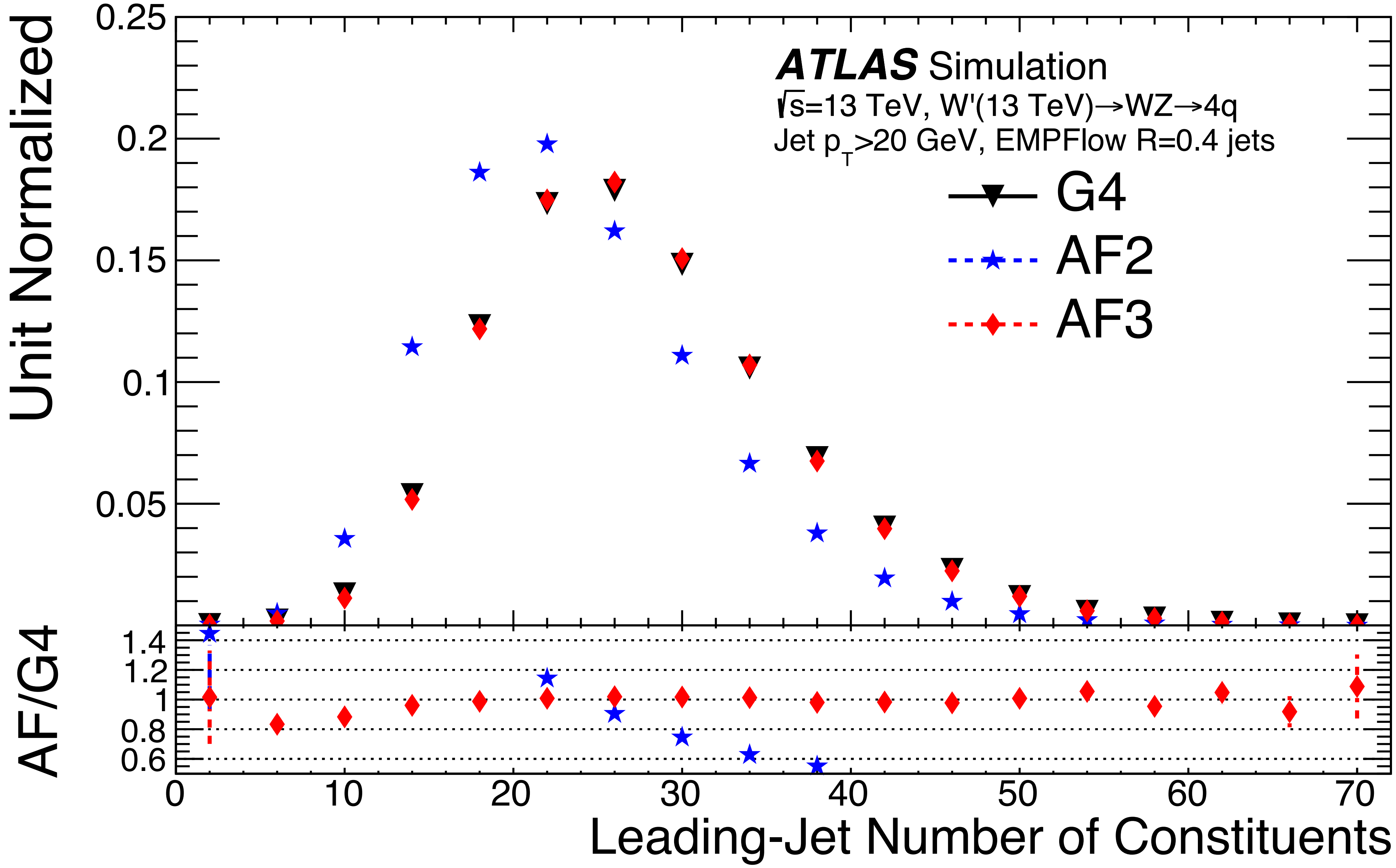
The ATLAS Collaboration fast simulation (AF3) now includes a GAN at intermediate energies for pions

Integration into real detector sim.



As expected, the fast sim. timing is independent of energy, while Geant4 requires more time for higher energy.

Integration into real detector sim.



The new fast simulation (**AF3**) significantly improves jet substructure with respect to the older one (**AF2**).

Differentiable Simulation

$$X \sim \mathcal{N}(\mu, \sigma)$$

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$$\downarrow$$

```
x = np.random.normal(mu,sigma)
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$\downarrow$

```
Z = np.random.uniform(0,1)
x = sigma*Phiinv(z)+mu
```

(**`Phiinv`** = inverse Gaussian CDF)

Removed randomness from simulator

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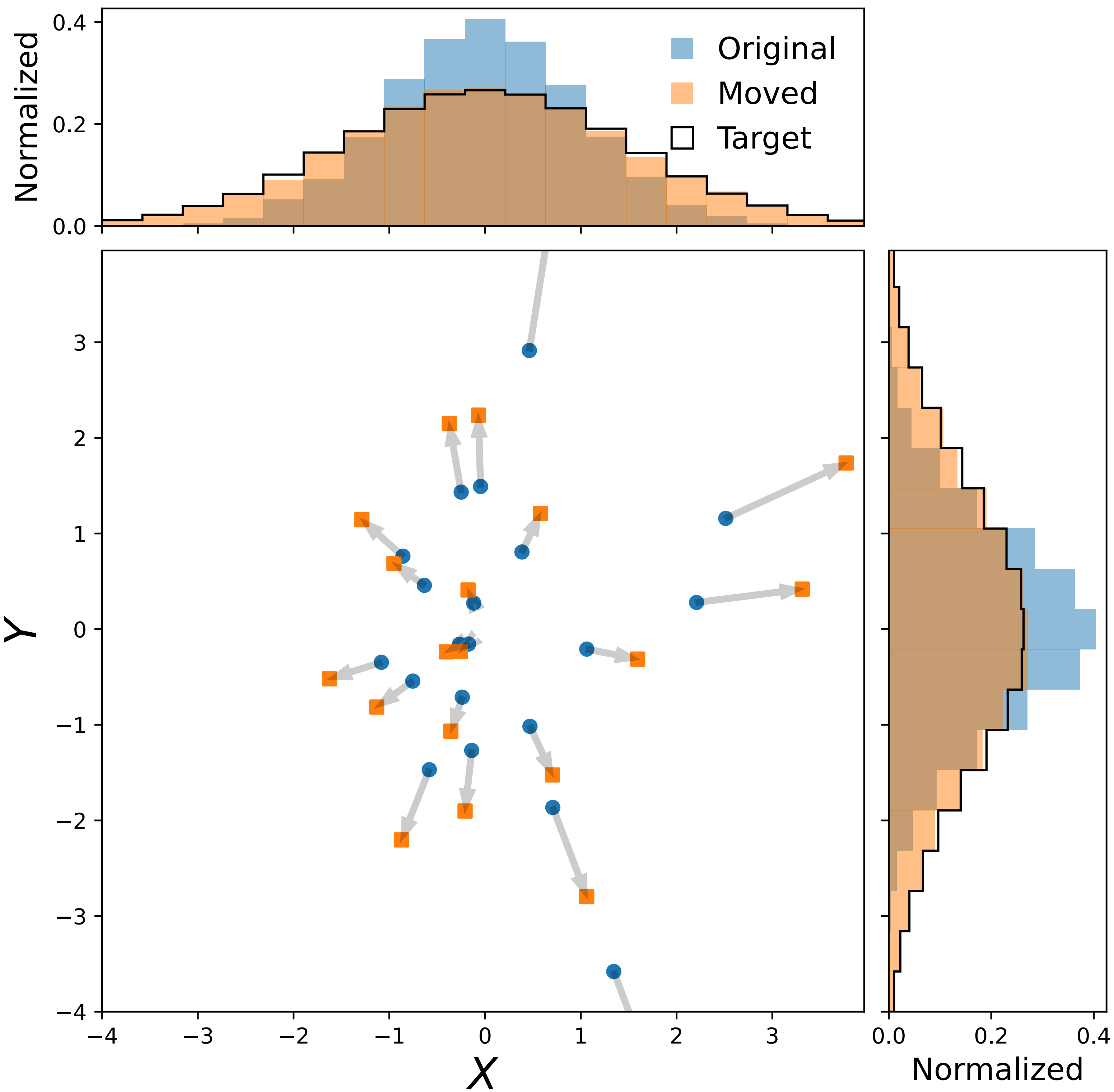
We can then do:

$$\text{sim}(\mu_0 + \epsilon) \approx \text{sim}(\mu_0) + \frac{\partial \text{sim}}{\partial \mu}\epsilon$$

Differentiable Simulation



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$$\text{sim}(\mu_0 + \epsilon) \approx \text{sim}(\mu_0) + \frac{\partial \text{sim}}{\partial \mu}\epsilon$$

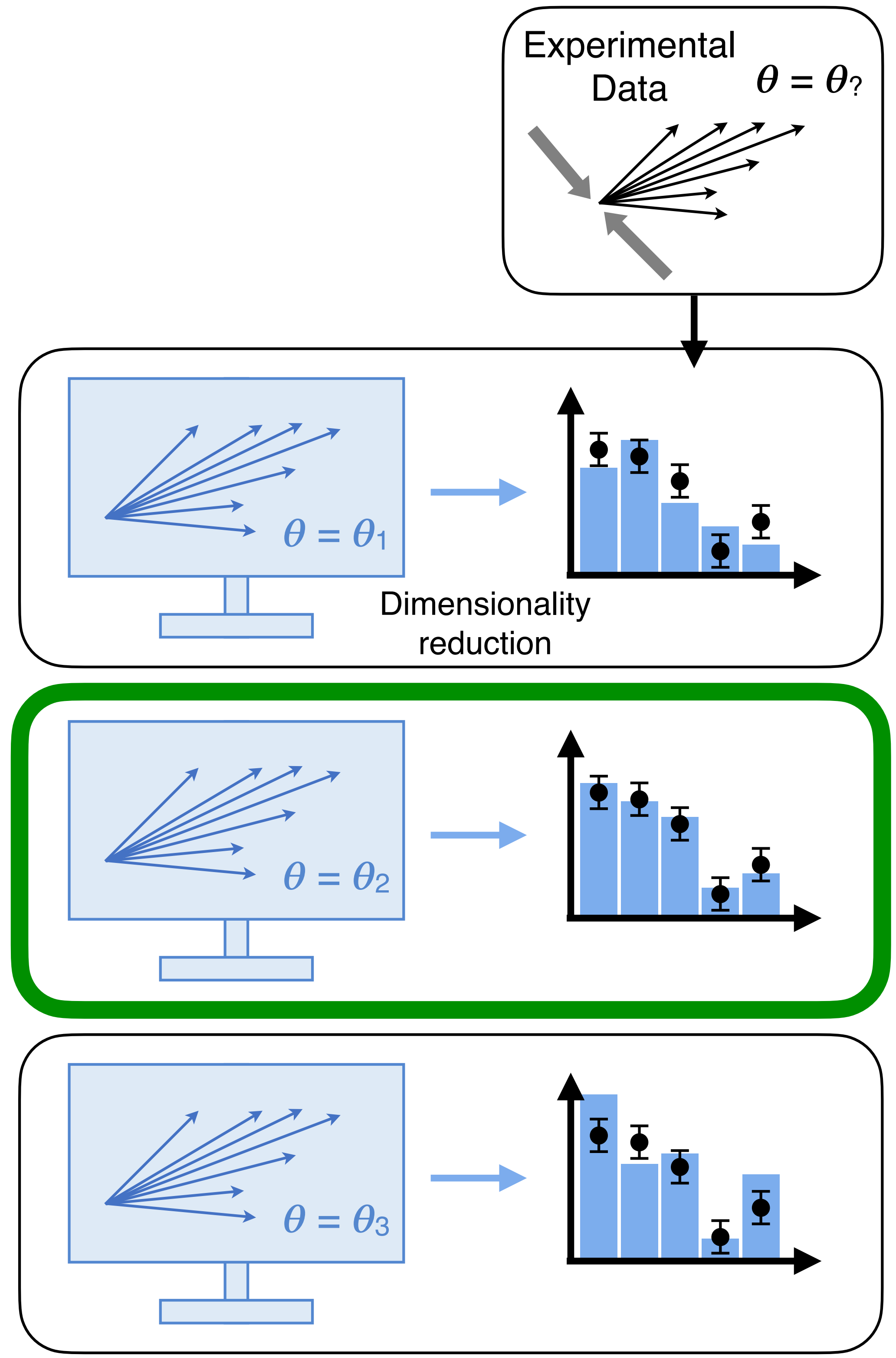
2208.02274

Why event moving?

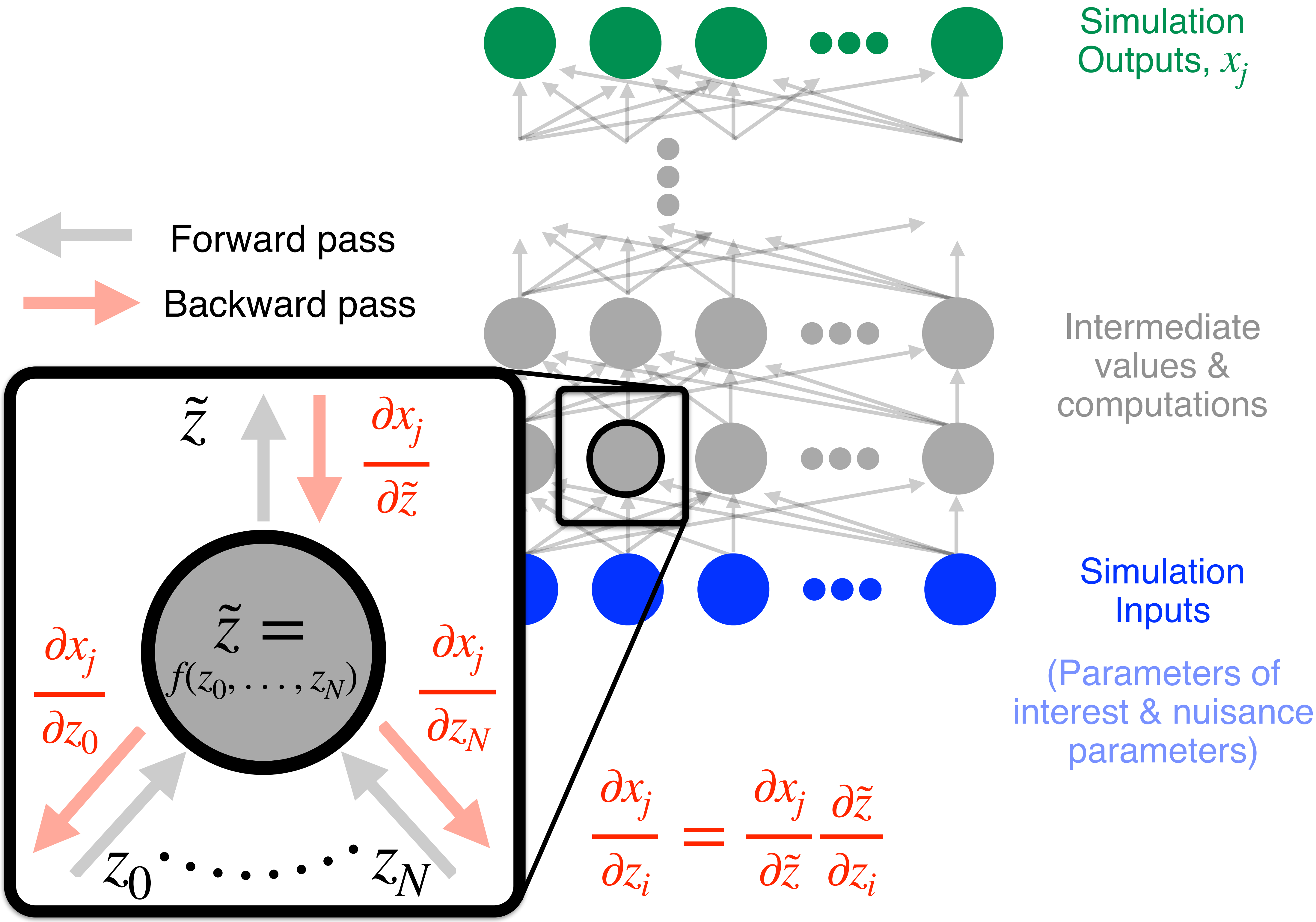
Often, we generate many simulations with different parameters (templates) and fit them to data.

We also often have to use histograms in order to interpolate.

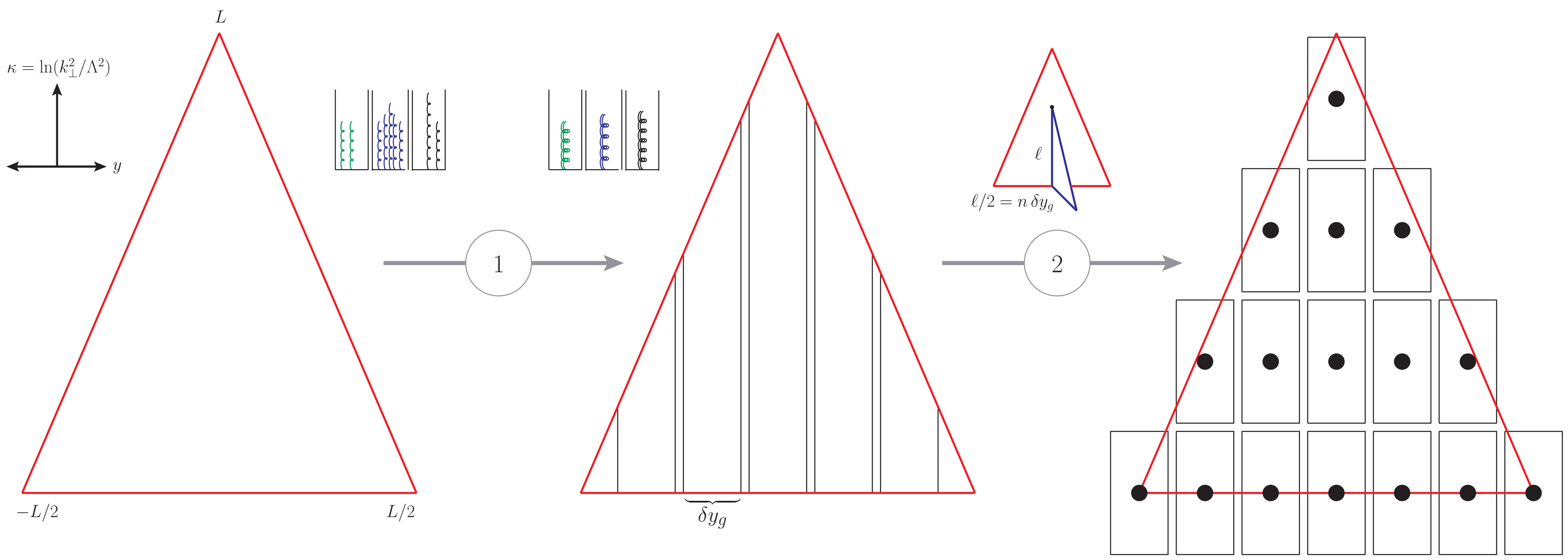
With event moving, we can interpolate in many dimensions and eliminate MC stat. uncertainties!

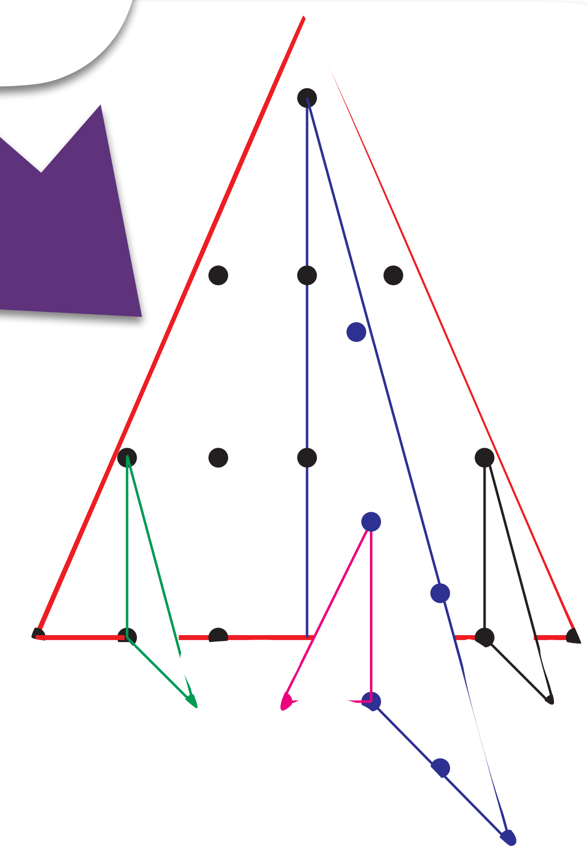


A brief word on Autodiff



Towards a differential parton shower

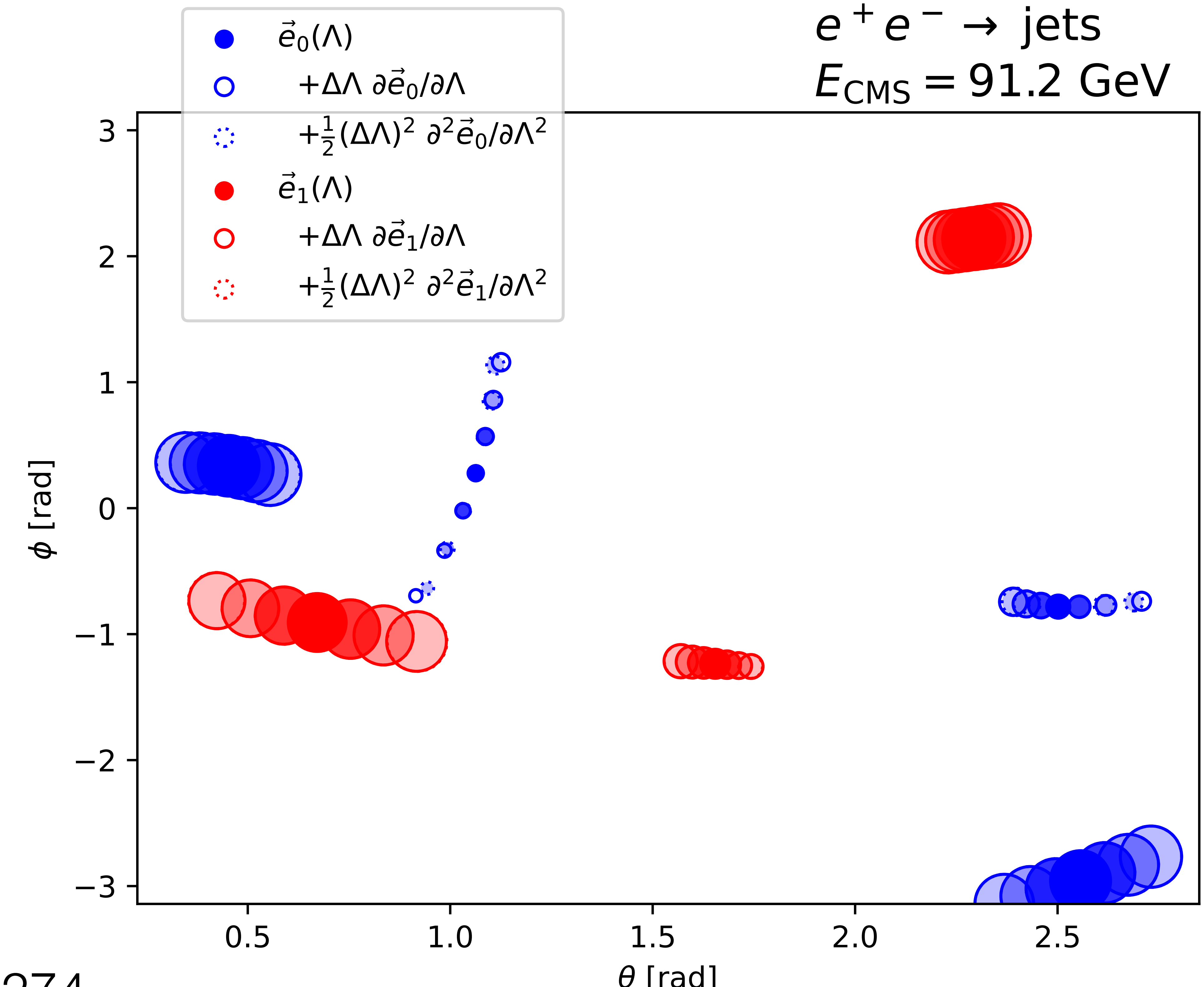




Full parton shower is a bit tricky since variable (unbounded) number of random numbers. Let's start with "Discrete QCD" where the number is fixed.

Images from 2207.10694; algorithm from Nuclear Physics B 463 (1996) 217

Towards a differential parton shower



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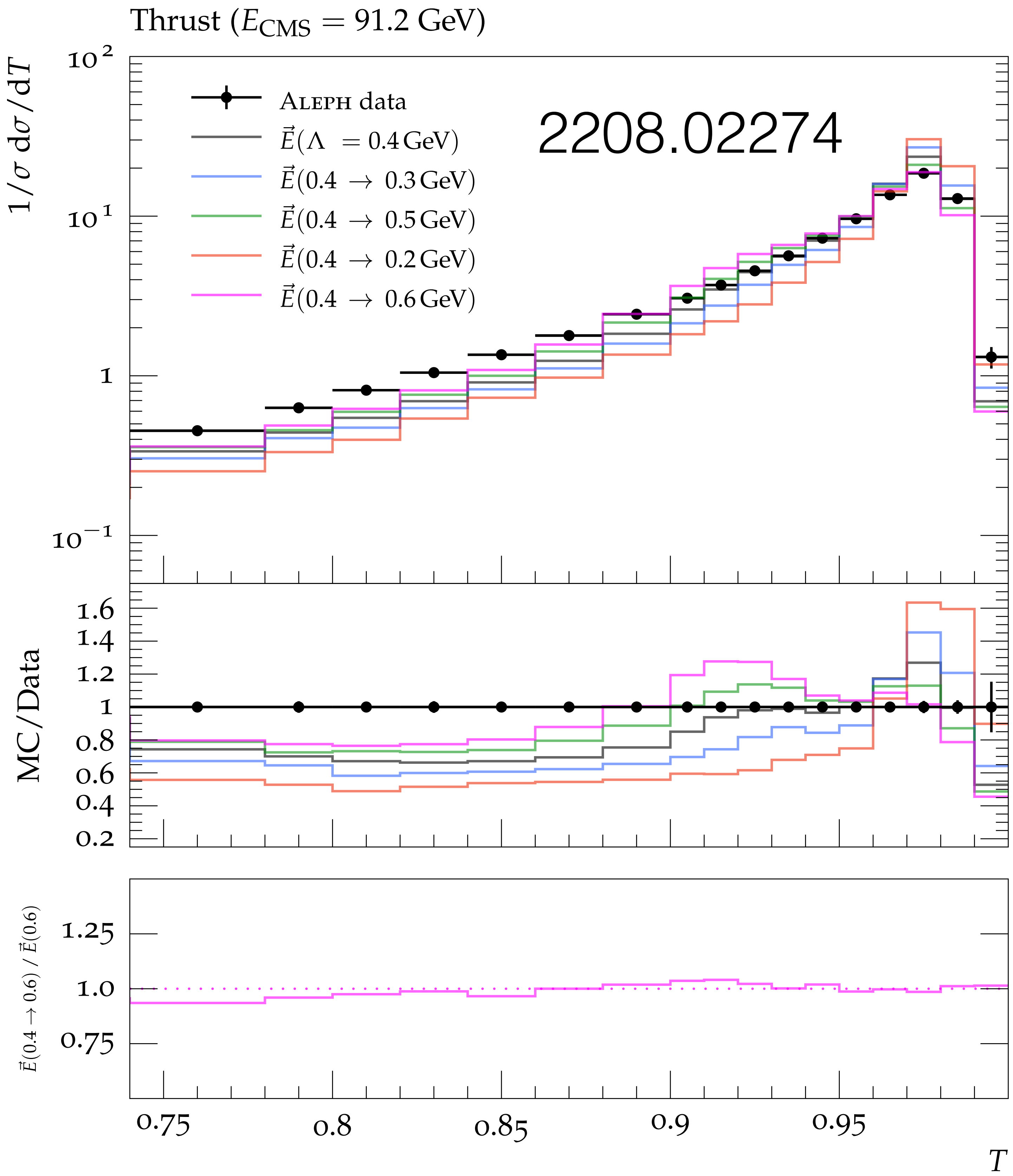
Towards a differential parton shower



As a first test, we show how this can be used to extract the strong coupling constant.

All of these samples have the same random numbers!