QCD ex-Machina: Development of a Deep Generative Hadronization Model

Andrzej Siódmok

HÆDML

Towards a Deep Learning Model for Hadronization

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2203.12660

Fitting a Deep Generative Hadronization Model

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2305.17169

Integrating Particle Flavor into Deep Learning Models for Hadronization

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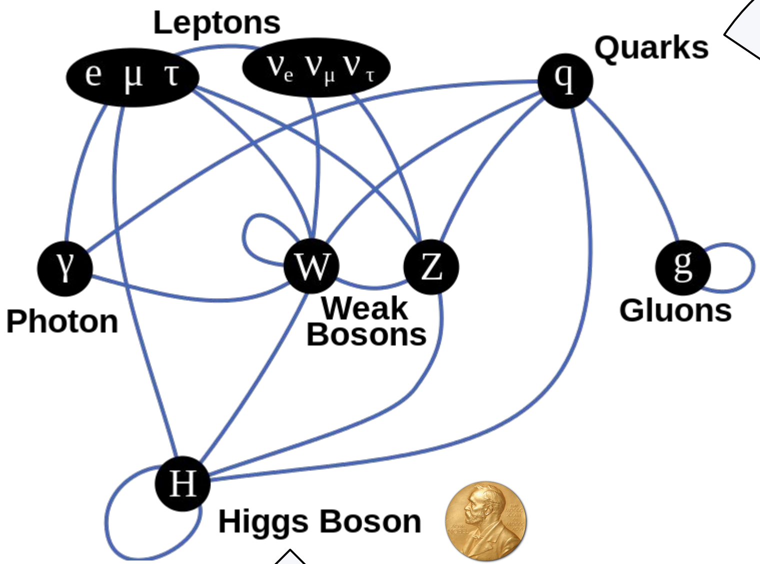
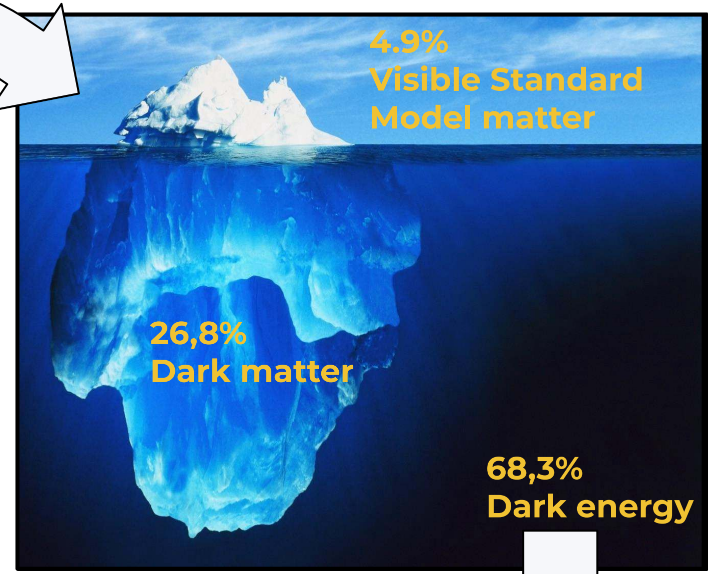
Motivation

Standard Model

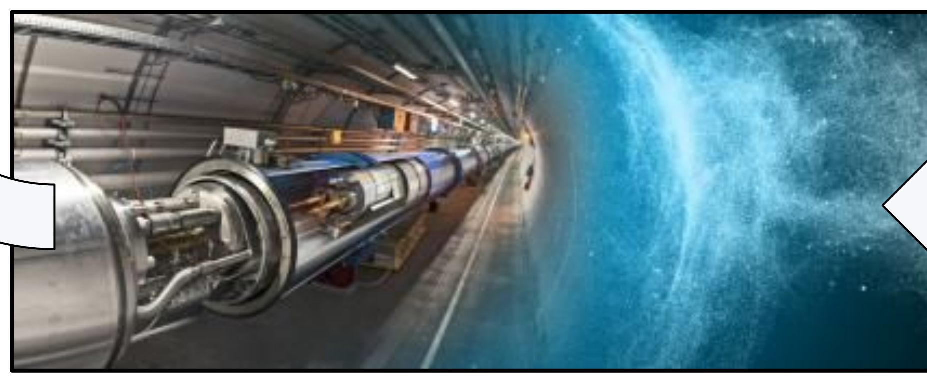
very successful theory



Physics beyond SM must exist



LHC



European Strategy for Particle Physics

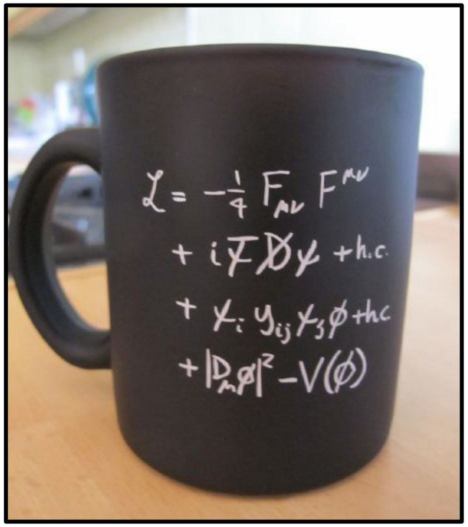
“Europe's top priority should be the exploitation of the full potential of the LHC”

Standard Model

There is a **huge gap** between a one-line formula of a fundamental theory, like the Lagrangian of the SM, and the experimental reality that it implies

Theory

Standard Model Lagrangian



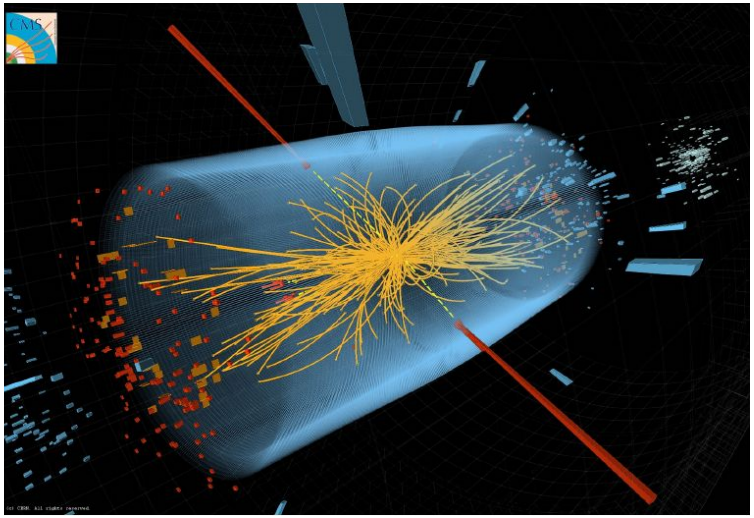
Data makes you smarter

It doesn't matter how beautiful your theory is, it doesn't matter how smart you are. If it doesn't agree with experiment, it's wrong.

Richard P. Feynman

Experiment

LHC event



Motivation - Monte Carlo Event Generators (MCEG)

Standard Model

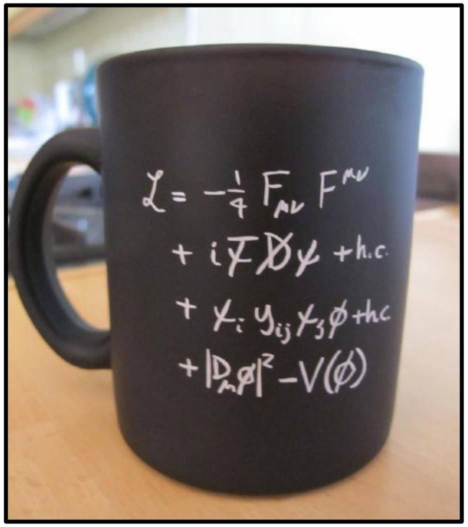
There is a **huge gap** between a one-line formula of a fundamental theory, like the Lagrangian of the SM, and the experimental reality that it implies

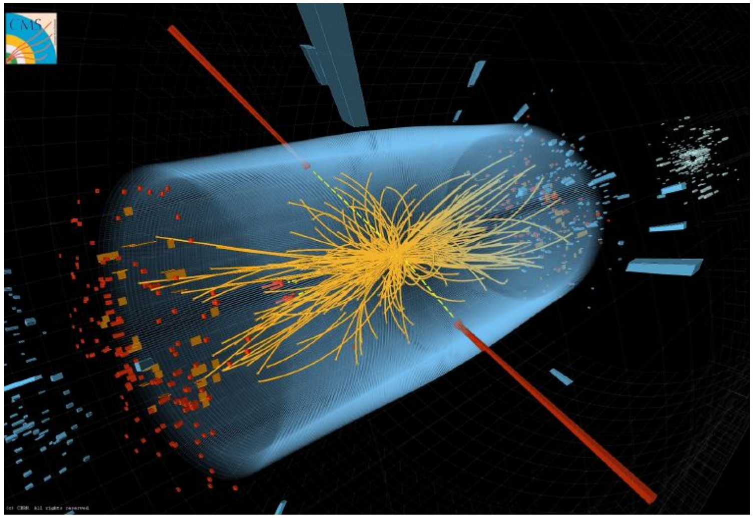
Theory

Standard Model Lagrangian

Experiment

LHC event





- MC event generators are designed to bridge the that **gap**
- “Virtual collider” ⇒ Direct comparison with data

Almost all **HEP measurements and discoveries** in the modern era have **relied on MCEG**, most notably the discovery of the Higgs boson.

(Herwig and Sherpa)@**UJ**, Pythia

Published papers by ATLAS, CMS, LHCb: **2252**
Citing at least 1 of 3 existing MCEG: **1888** (**84%**)

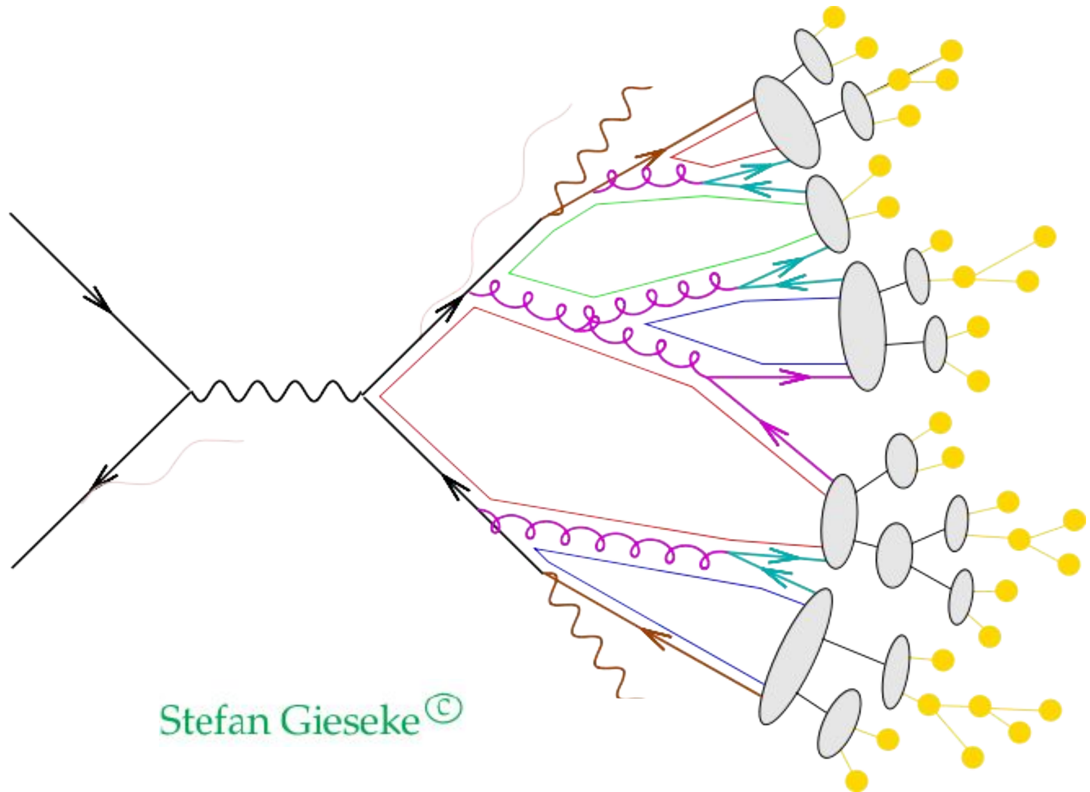
QCD correctly describes strong interactions in each energy range but it is very difficult to obtain precise predictions

High energy

- **perturbative QCD**
- **we have theoretical models**
- **but they are hard to use in practice**

Low energy

- **non-perturbative QCD**
- **we lack solid theoretical models**
- **so we use phenomenological models (with many free parameters)**



Quantum chromodynamics (QCD)

QCD correctly describes strong interactions in each energy range but it is very difficult to obtain precise predictions

High energy

- **perturbative QCD**
- **we have theoretical models**
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Low energy

- **non-perturbative QCD**
- **we lack solid theoretical models**
- **so we use phenomenological models (with many free parameters)**

Imagine that the BSM physics signal is at the LHC but due to lack of QCD understanding we missed it

We need:

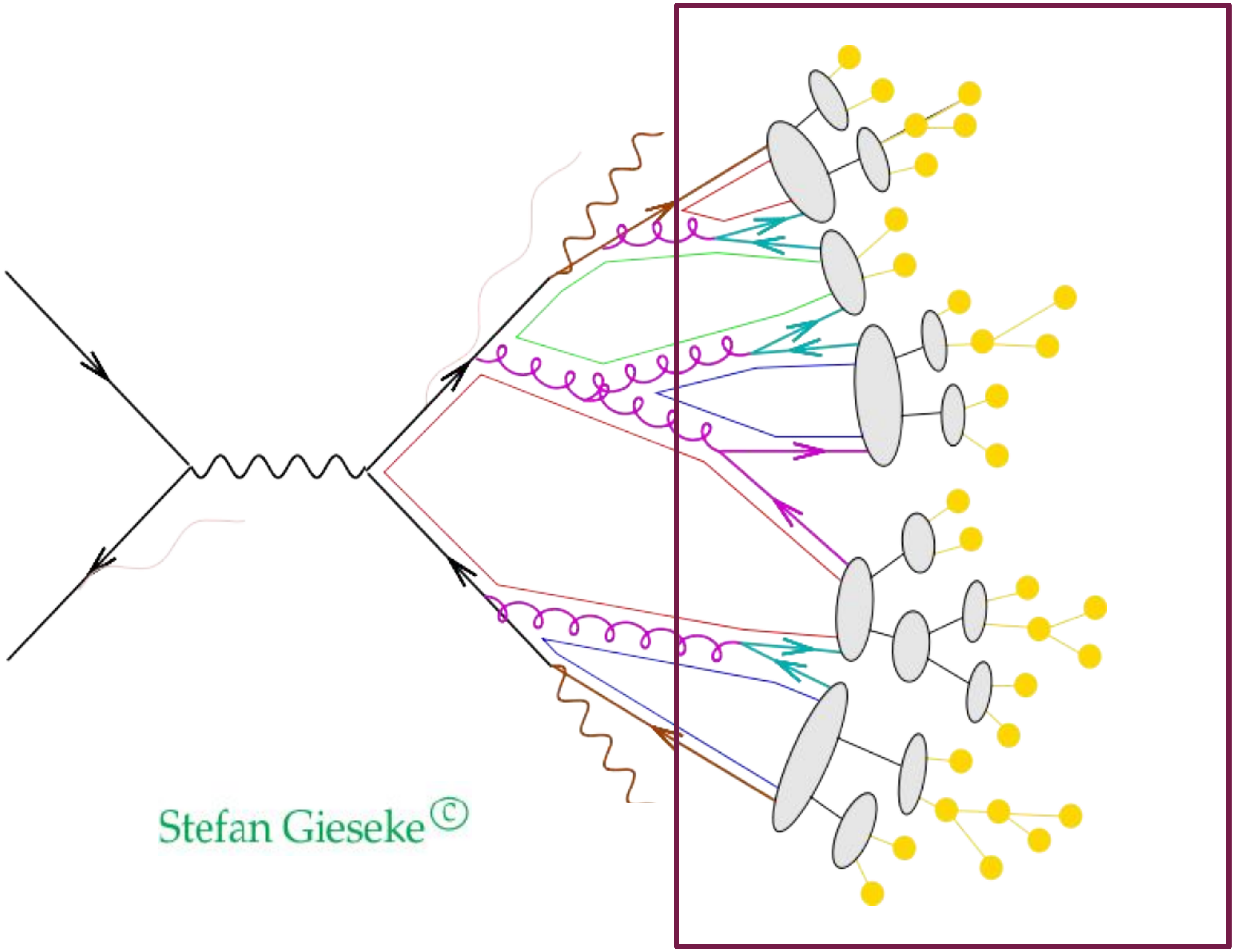
SIMPLIFICATIONS in perturbative QCD techniques [KrkNLO matching]

NEW IDEAS of treatment non-perturbative QCD

QCD ex-Machina

NARODOWE CENTRUM NAUKI
NCN: 2019/34/E/ST2/00457

Hadronization

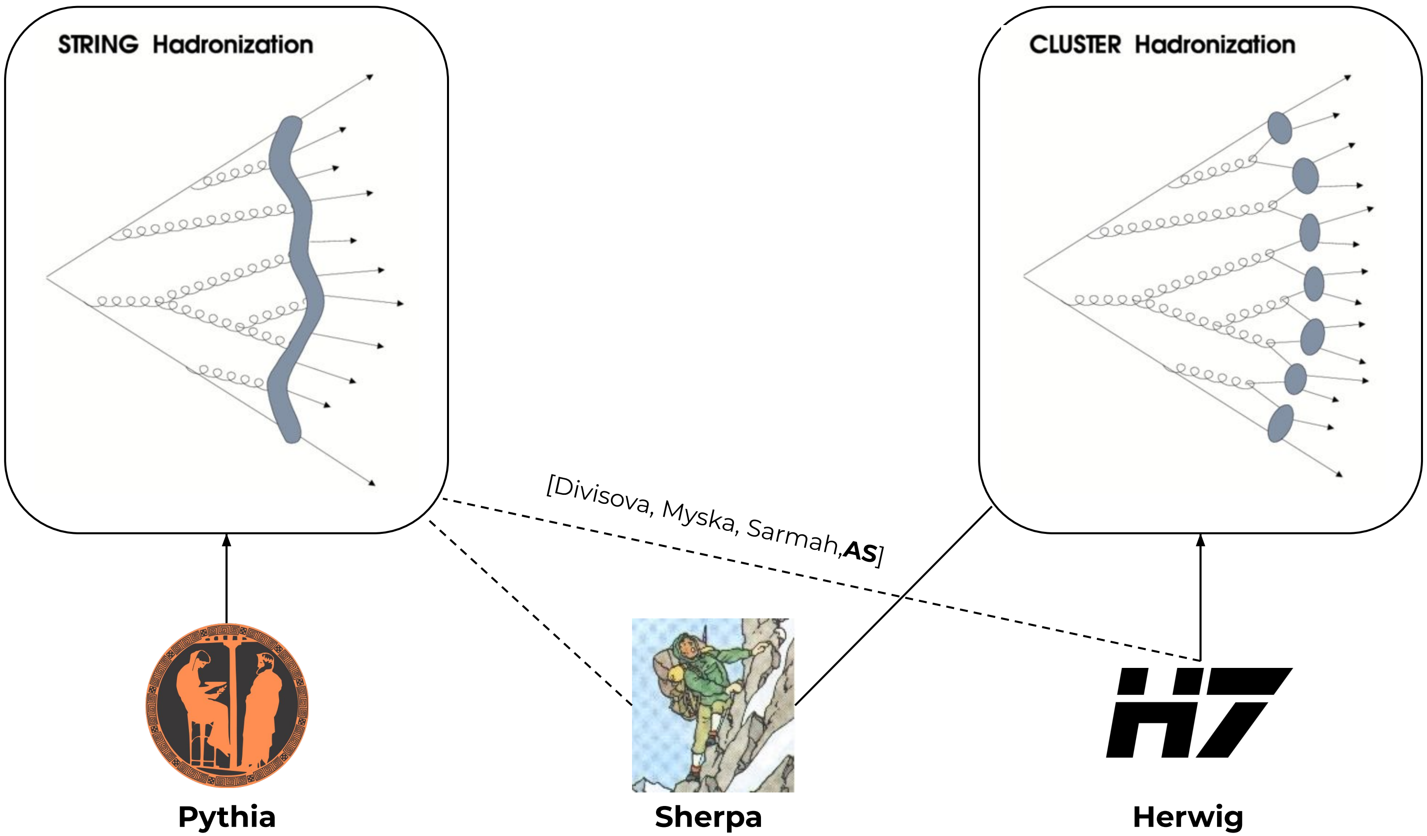


Hadronization:
one of the least understood elements of MCEG

Hadronization:

➔ Increased control of perturbative corrections ⇒ more often LHC measurements are limited by non-perturbative components, such as hadronization.

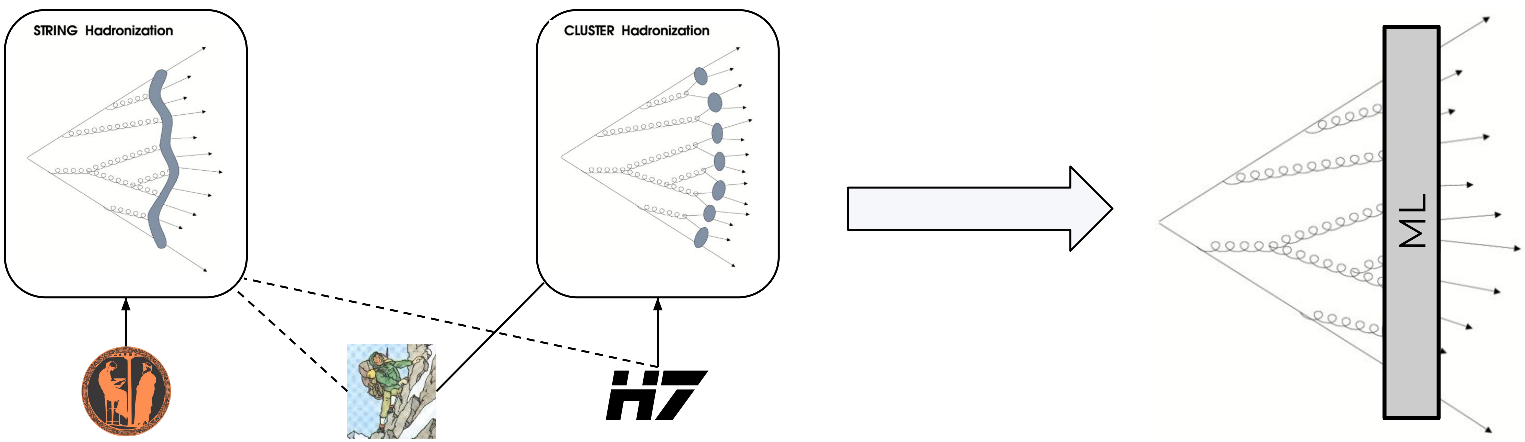
- W mass measurement using a new method [Freytsis at al. JHEP 1902 (2019) 003]
- Extraction of the strong coupling in [M. Johnson, D. Maître, Phys.Rev. D97 (2018) no.5]
- Top mass [S. Argyropoulos, T. Sjöstrand, JHEP 1411 (2014) 043]
- ...



Hadronization:

Early 1980's
(limited progress)

Early 2020's
(lot of progress in ML)



Pythia **Sherpa** **Herwig**

Idea of using Machine Learning (ML) for hadronization.

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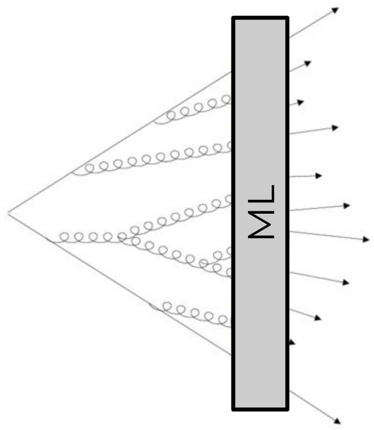
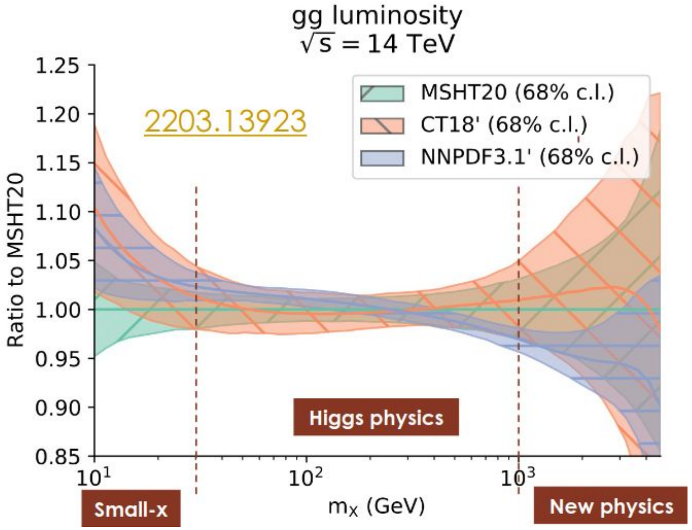


- Existing hadronization models are highly parameterized functions.
- Hadronization is a fitting problem
  - Can ML hadronization be more flexible to fit the data?
  - Can ML hadronization extract more information from the data? [can accommodate unbinned and high-dimensional inputs]

NNPDF

NNPDF used successfully ML to nonperturbative Parton Density Functions (PDF).
Hadronization is closely related to fragmentation functions (FF) which were considered the counterpart of PDFs.



Recent progress: Machine learning hadronization

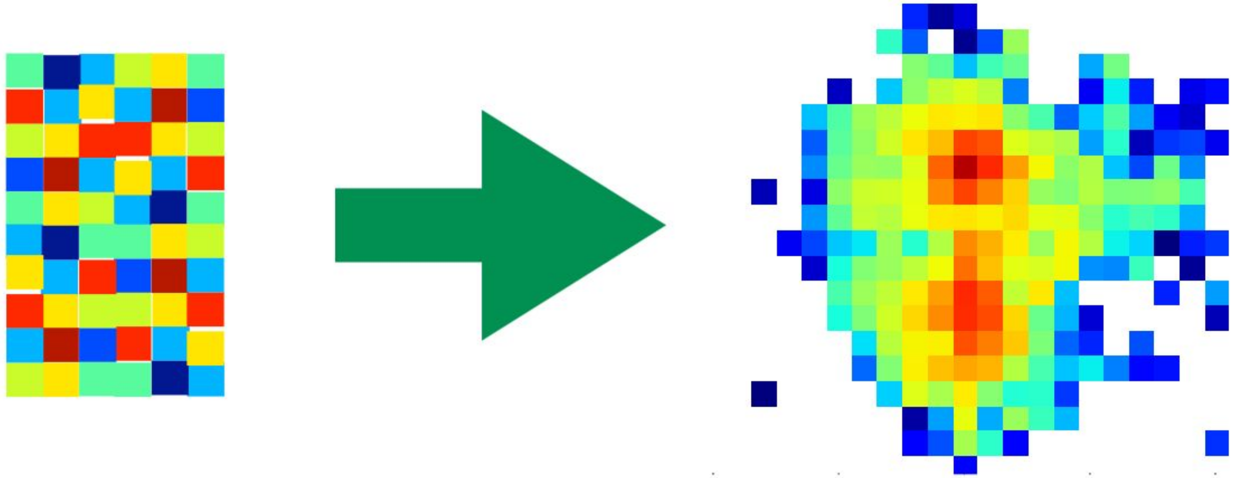
First steps for ML hadronization:

- HADML - [A. Ghosh, Xi. Ju, B. Nachman **AS**, *Phys.Rev.D* 106 (2022) 9]
- MLhad - [P. Ilten, T. Menzo, A. Youssef and J. Zupan, SciPost Phys. 14, 027 (2023)]

	MLhad	HADML
Deep generative model:	Variational Autoencoder	Generative Adversarial Networks
Trained on:	String model	Cluster model
Recent progress:	*“Reweighting Monte Carlo Predictions and Automated Fragmentation Variations in Pythia 8”* [Bierlich, Ilten, Menzo, Mrenna, Szewc, Wilkinson, Youssef, Zupan, 2308.13459] ...	*“Fitting a Deep Generative Hadronization Model”* [J. Chan, X. Ju, A. Kania, B. Nachman, V. Sangli and **AS**, JHEP 09 (2023) 084] ...

MLhadML

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

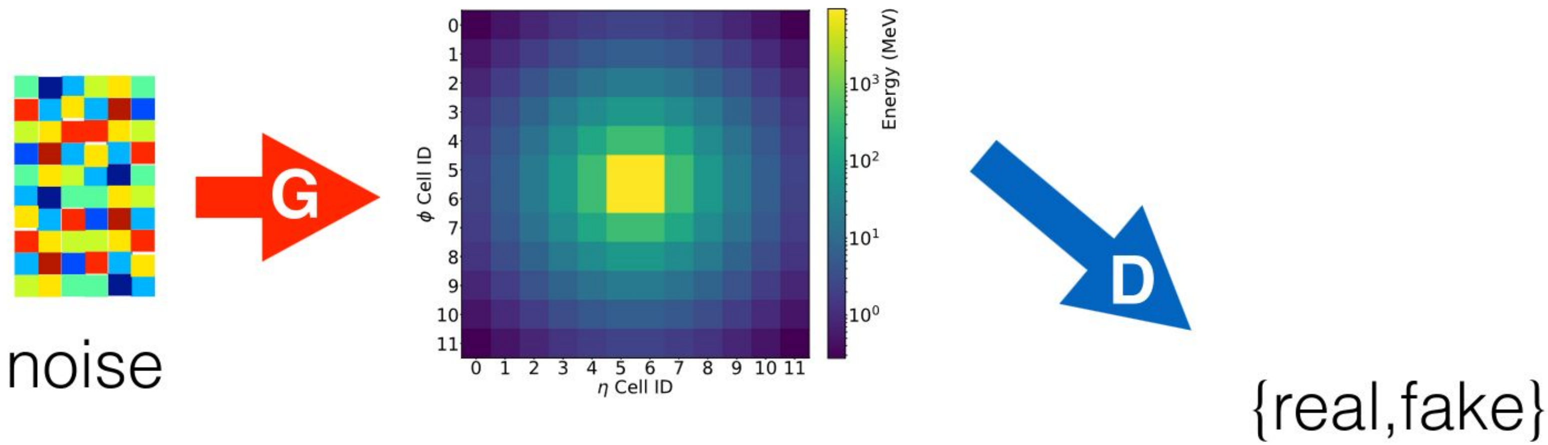


Deep generative models: the map is a deep neural network.

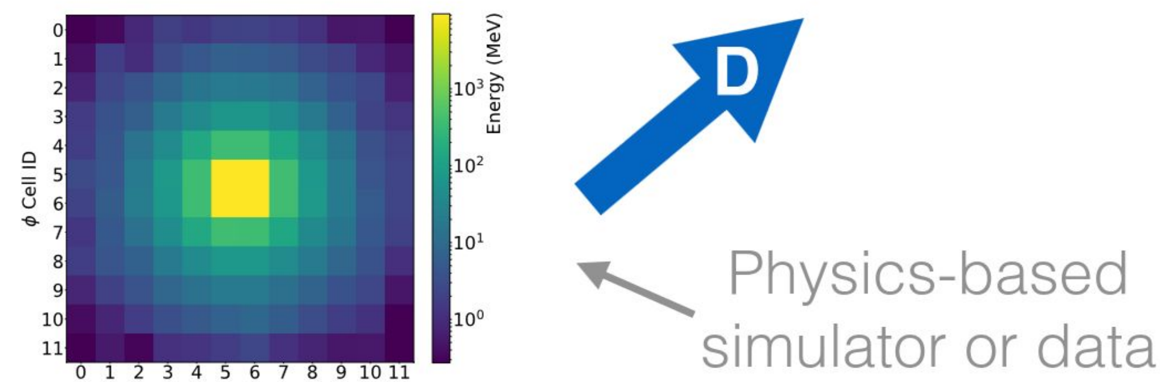
Our tool of choice: GANs

[Goodfellow et al. “Generative adversarial nets”. arxiv:1406.2661]

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

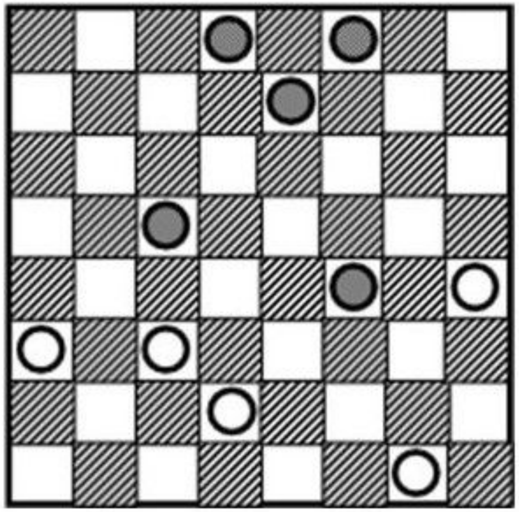


When **D** is maximally confused, **G** will be a good generator



Adversarial Networks

Arthur Lee Samuel (1959) wrote a program that learnt to play checkers well enough to beat him.

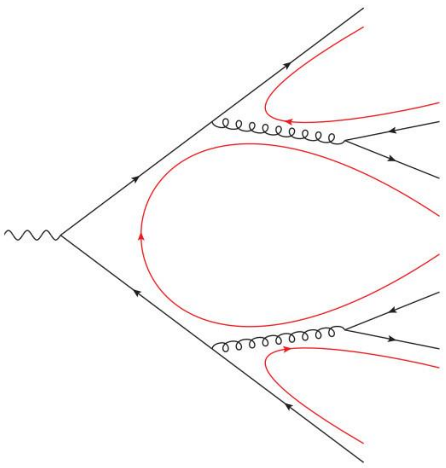


- He popularized the term **"machine learning"** in 1959.
- The program chose its move based on a **minimax** strategy, meaning it made the move assuming that the opponent was trying to optimize the value of the same function from its point of view.
- He also had it play thousands of **games against itself** as another way of learning.

Cluster hadronization model

The philosophy of the model: use information from perturbative QCD as an input for hadronization.

QCD **pre-confinement** discovered by Amati & Veneziano:



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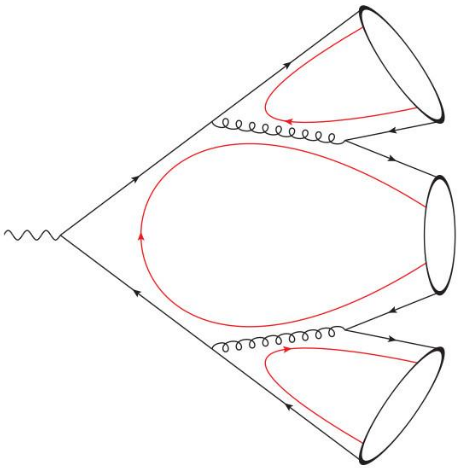

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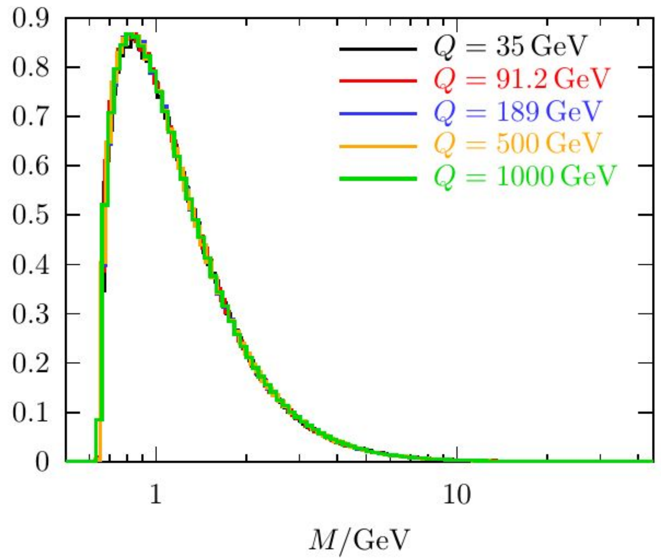

[S. Gieseke, A. Ribon, MH Seymour, P Stephens, B Webber JHEP 0402 (2004) 005]

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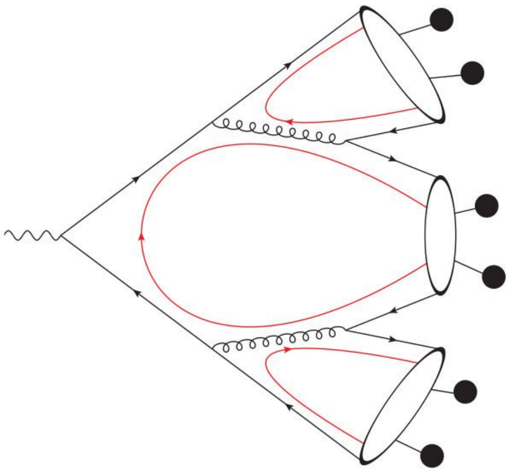

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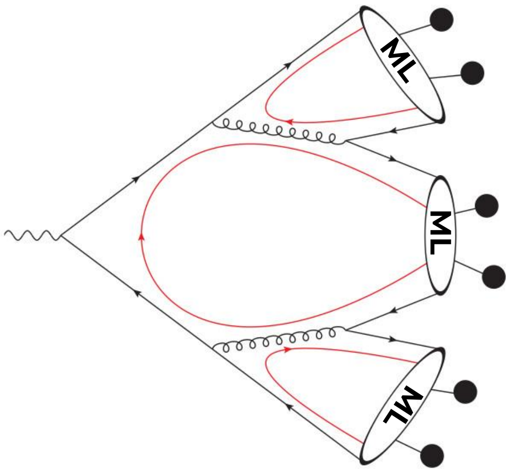

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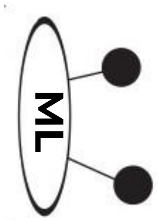
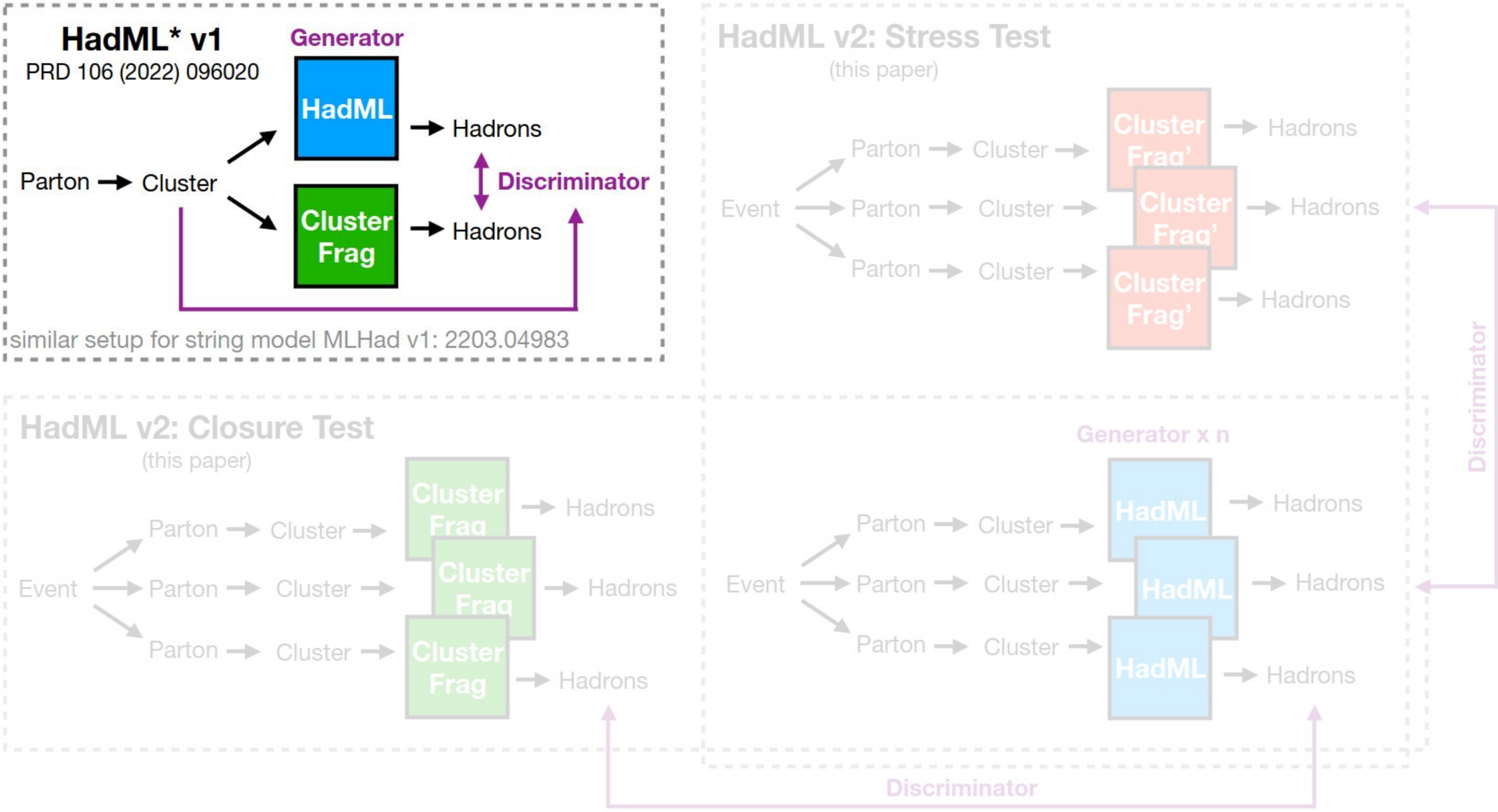
- **ML hadronization**
  1st step: generate kinematics of a cluster decay:



Road map for today



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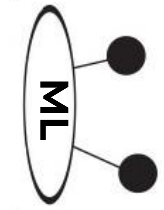

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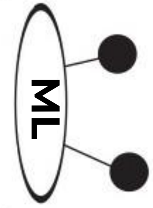
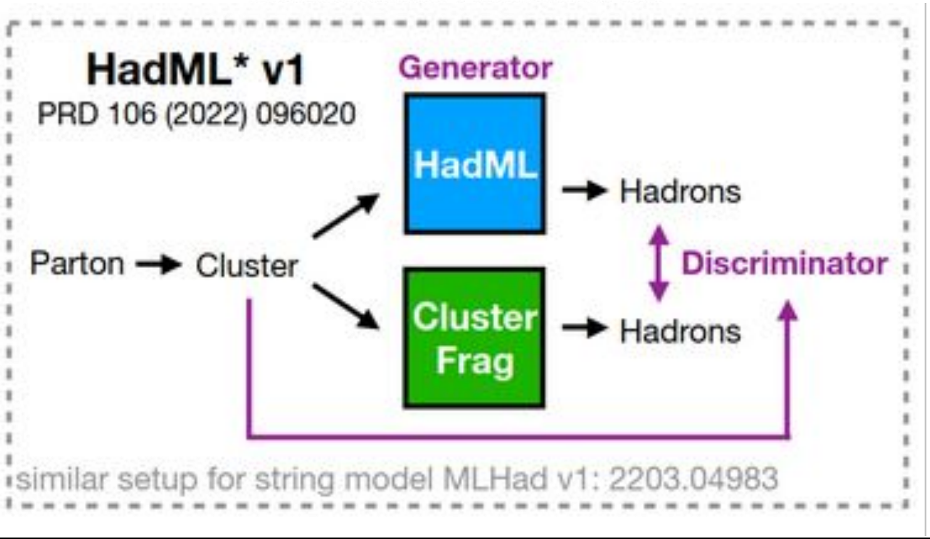


How?

We have a conditional GAN, with cluster 4-vector input and two hadron 4-vector outputs.

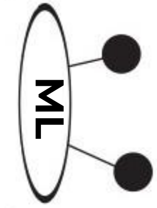
Generative Adversarial Net



Towards a Deep Learning Model for Hadronization

ML hadronization

1st step: generate kinematics of a cluster decay to 2 hadrons



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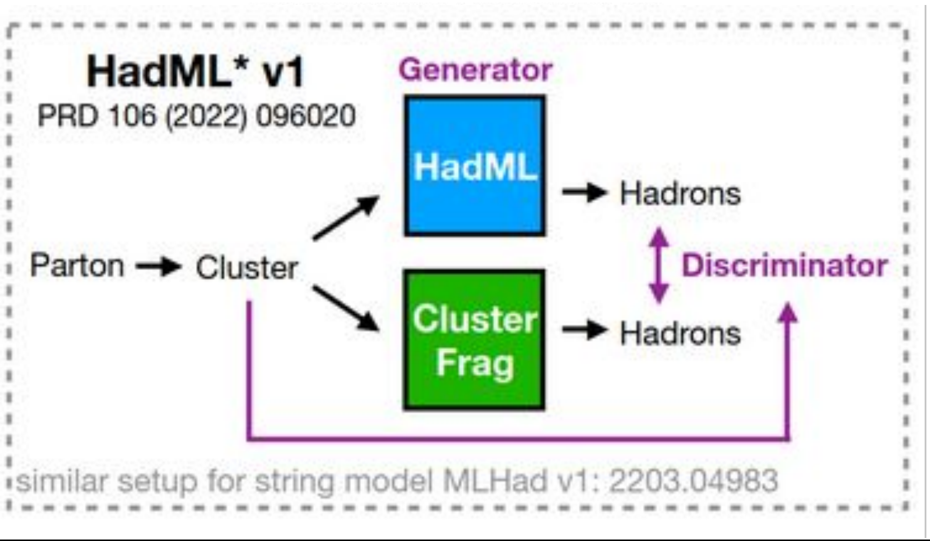
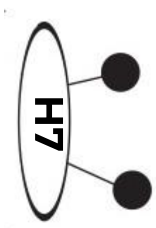


Training data:

e^+e^- collisions at $\sqrt{s} = 91.2$ GeV

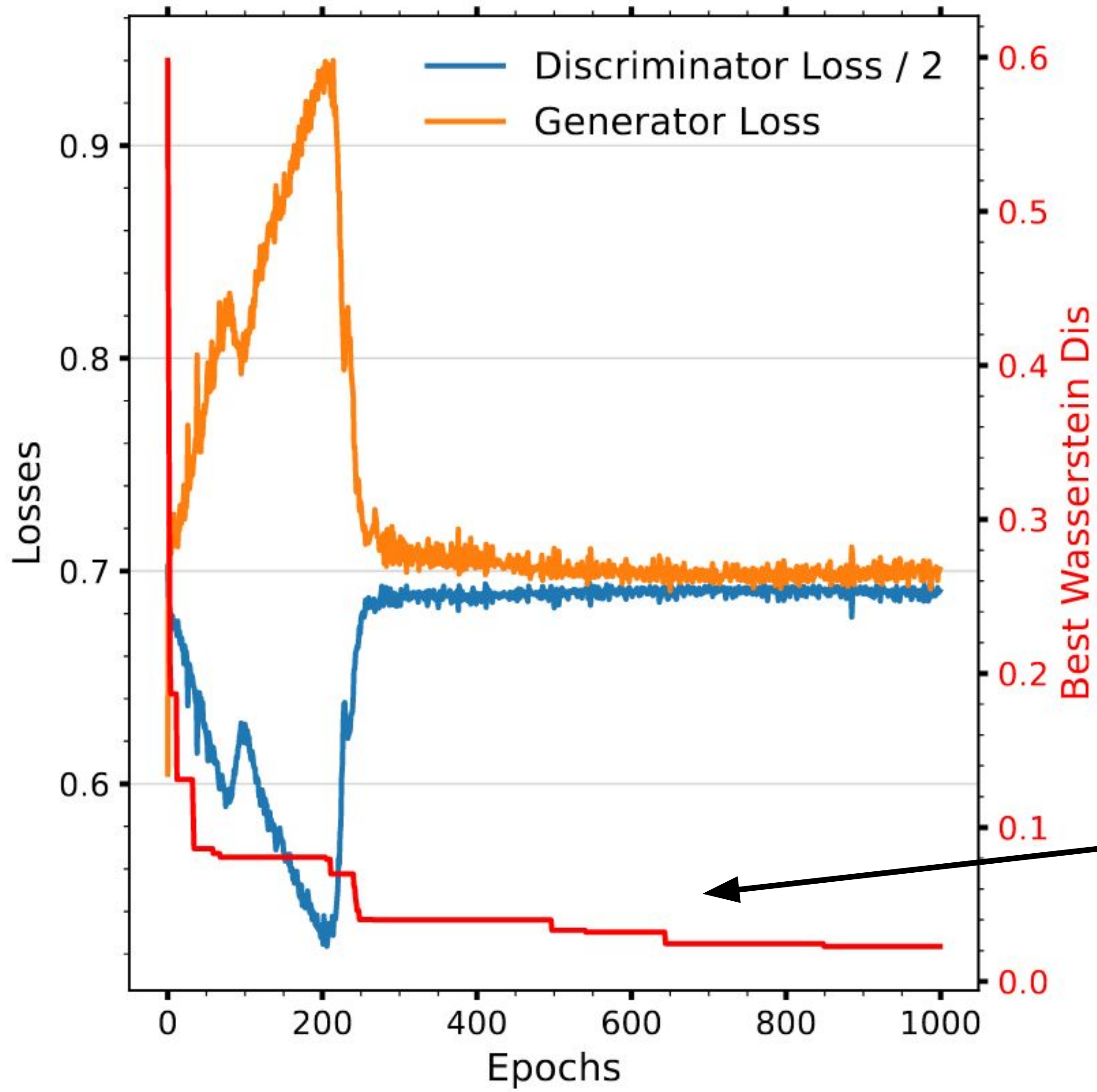
Cluster $(E,\ p_x,\ p_y,\ p_z)$



$\pi^0(E,\ p_x,\ p_y,\ p_z)$

$\pi^0(E,\ p_x,\ p_y,\ p_z)$

Simplification: considering only pions and generating two angles in the cluster rest frame.



We have a conditional GAN, with cluster 4-vector input and two hadron 4-vector outputs.

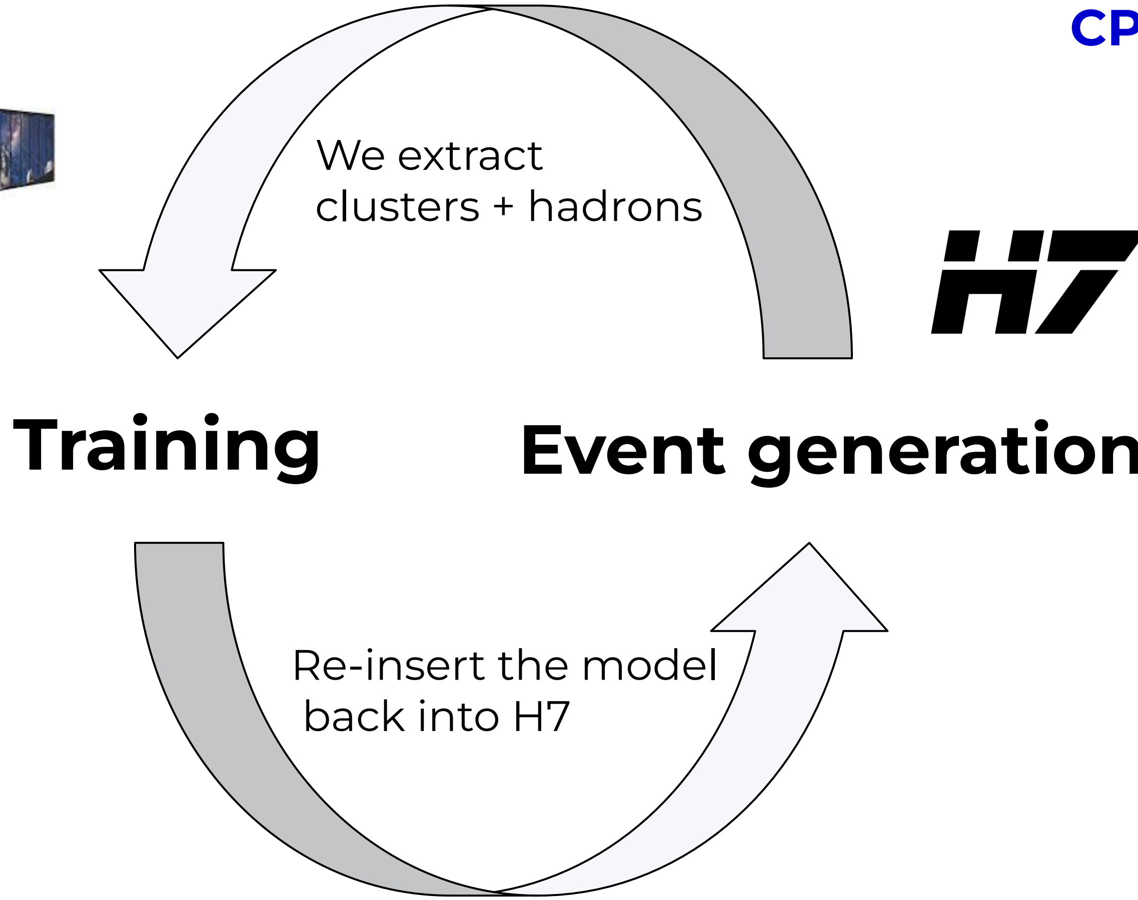
Simplification: considering only pions and generating two angles in the cluster rest frame.

This is a typical learning curve for GAN training

Integration into Herwig

GPU

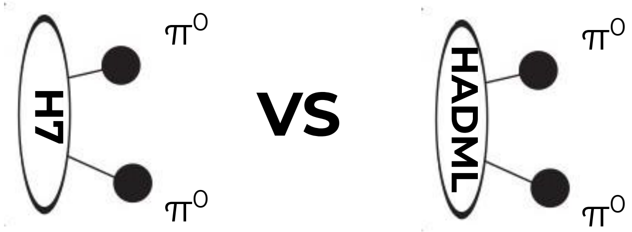
CPU



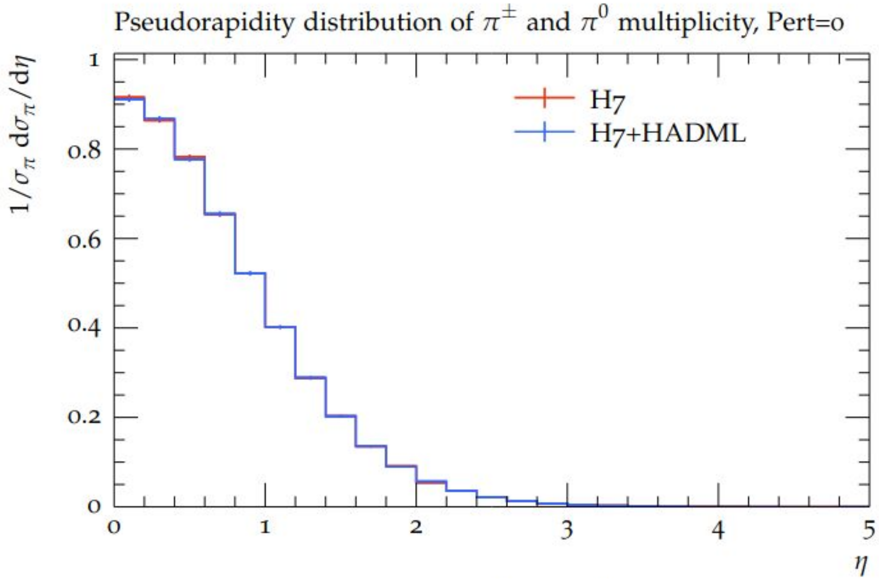
This then allows us to run a full event generator and produce plots

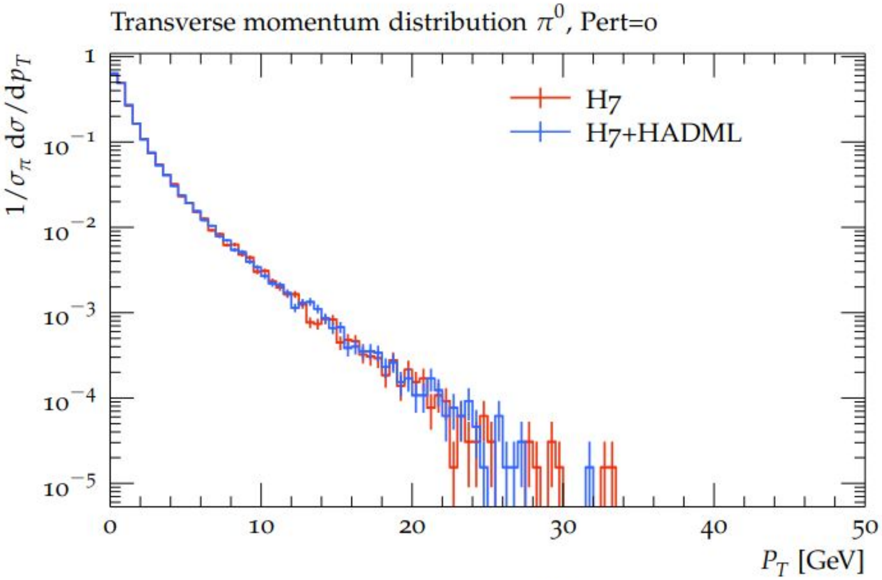
Low-level Validation
(similar to training data)

e^+e^- collisions at
$\sqrt{s} = 91.2$ GeV



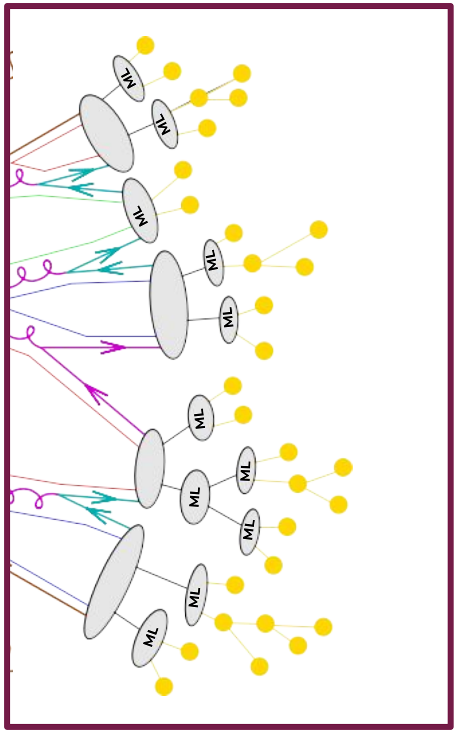
π^0 kinematic variables

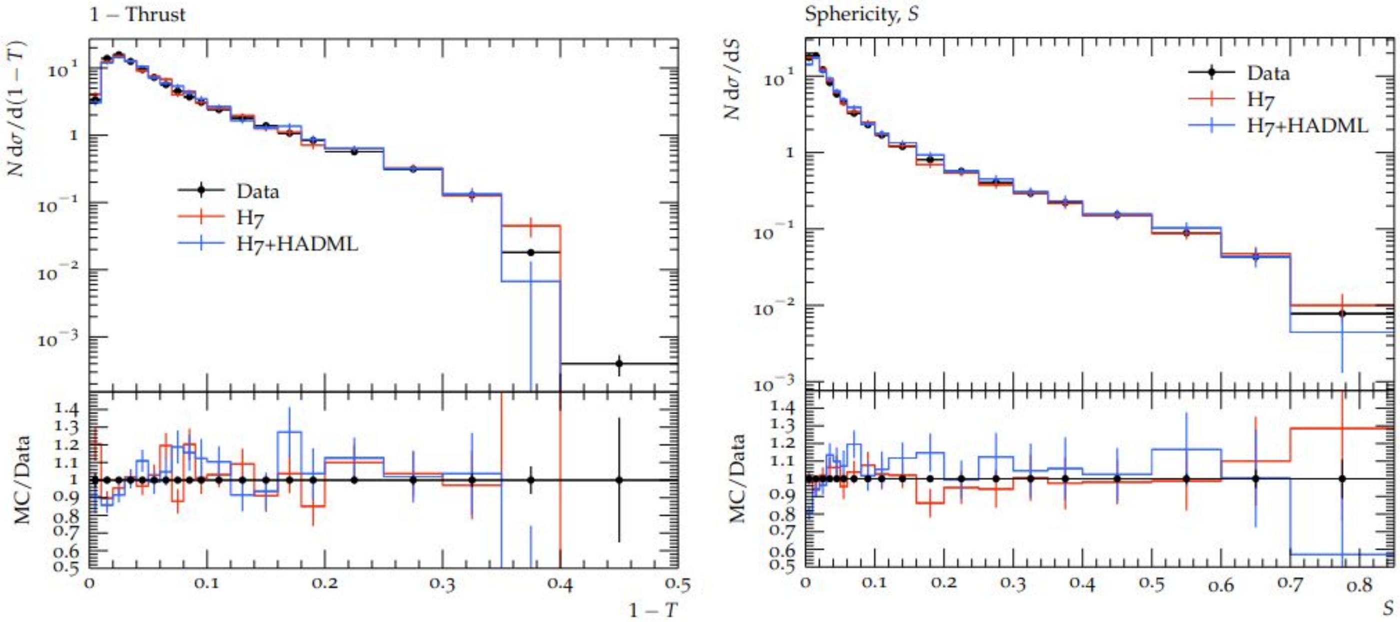




With a “full” model, we can compare directly to data!

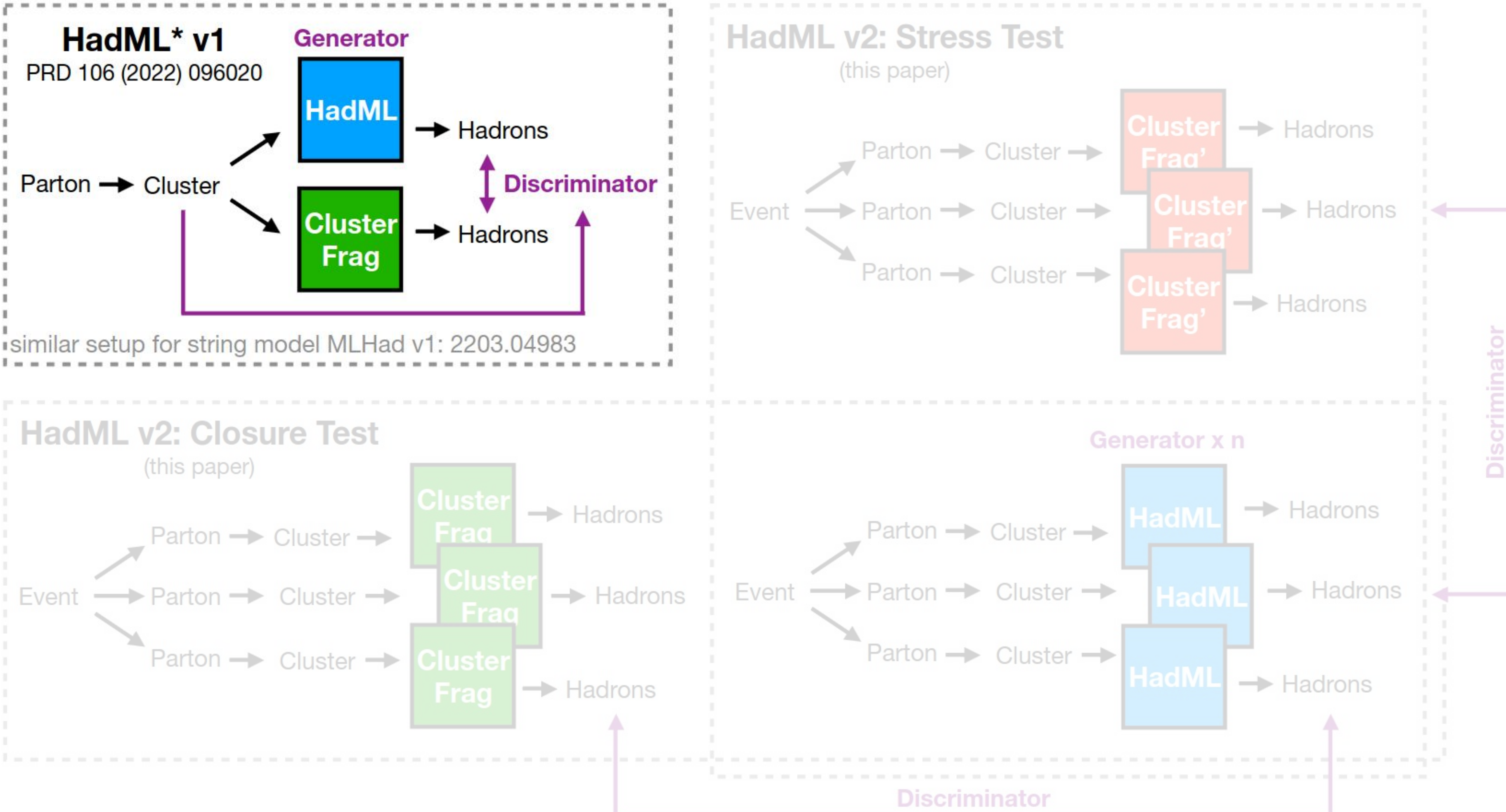
LEP DELPHI **Data**

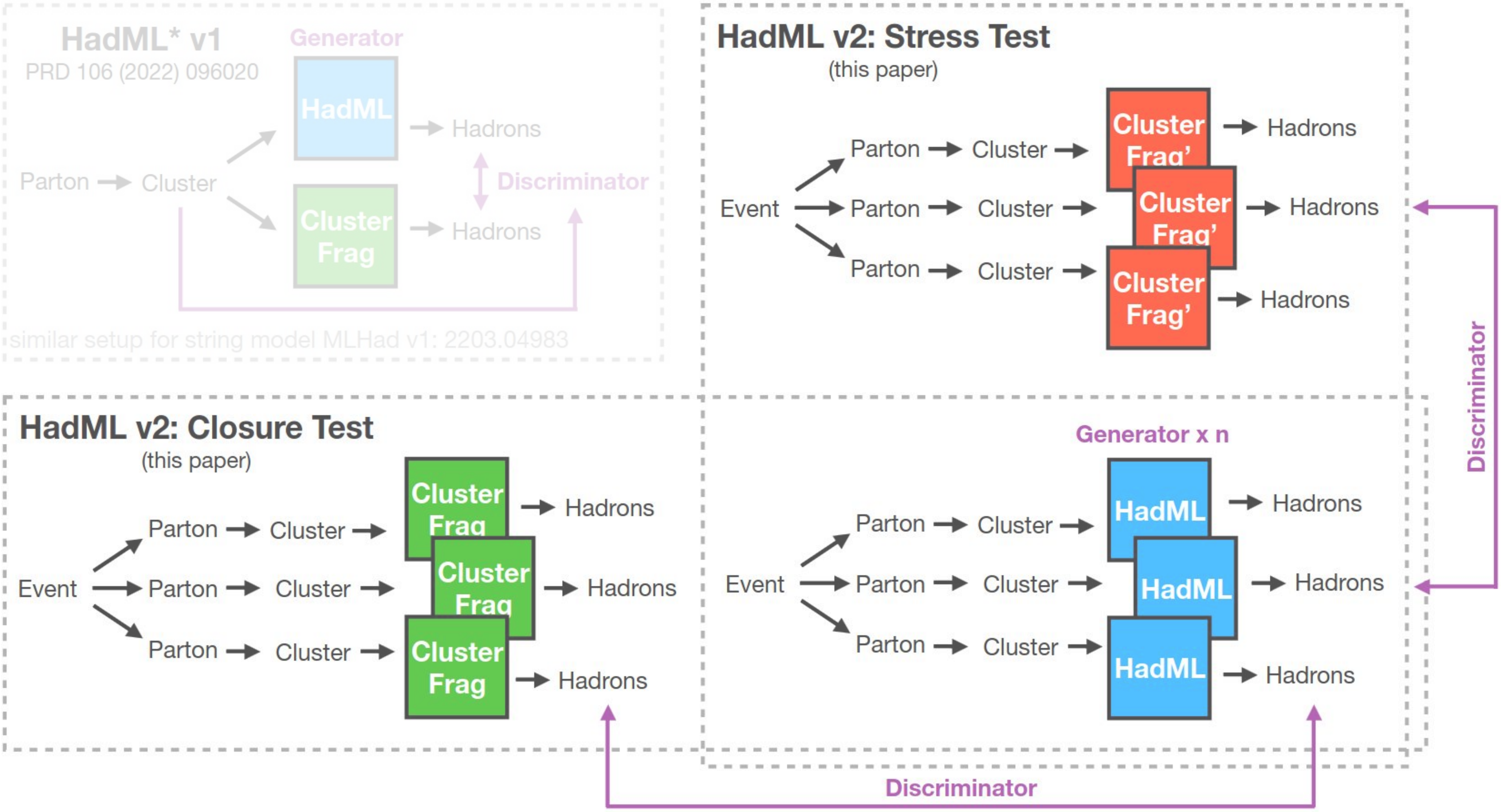




N.B. we have trained on H7, so we don’t expect to be any better than it at modeling the data.

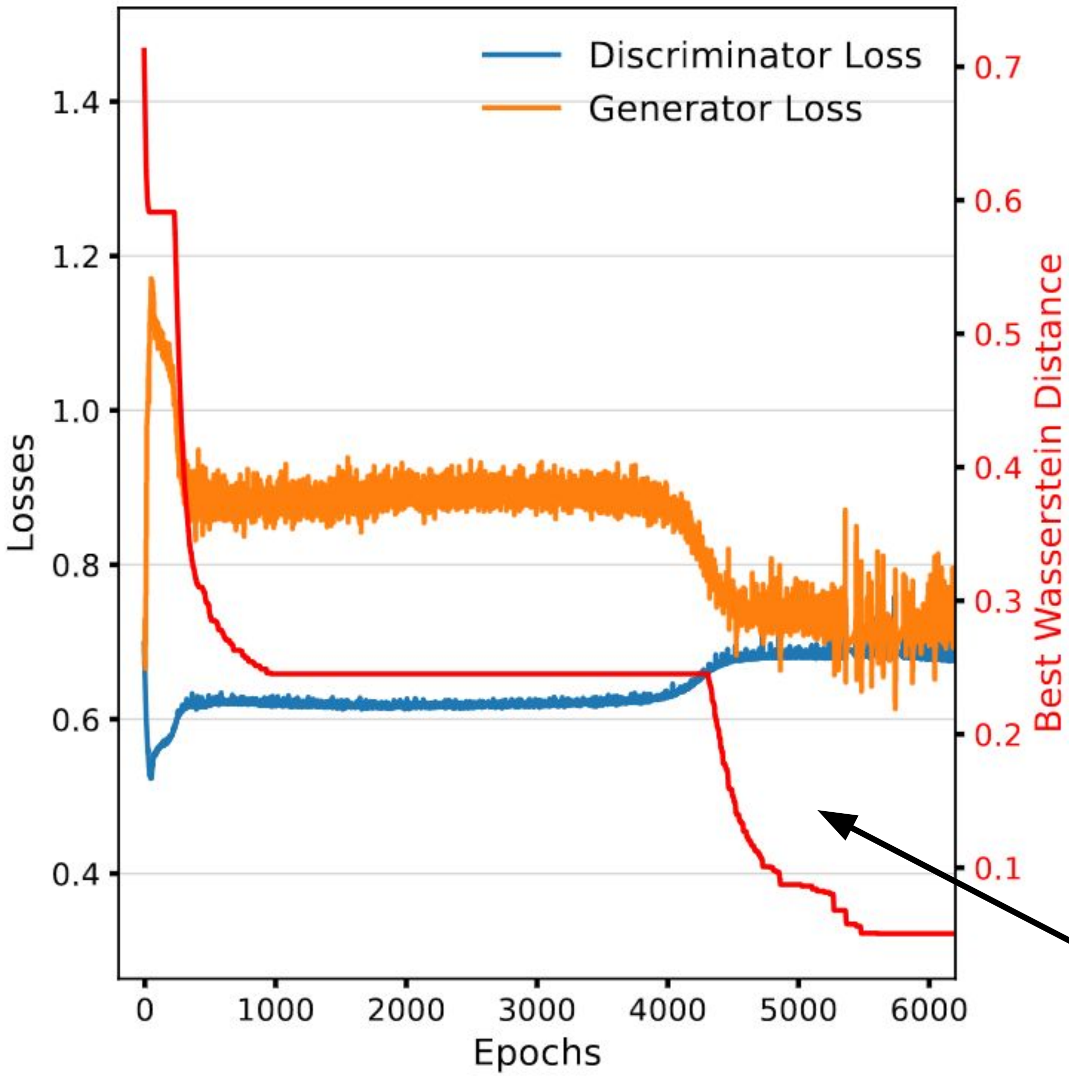
Road map for today





Protocol for fitting a deep generative hadronization model in a realistic data setting, where we only have access to a set of hadrons in data.

Training HADML v2

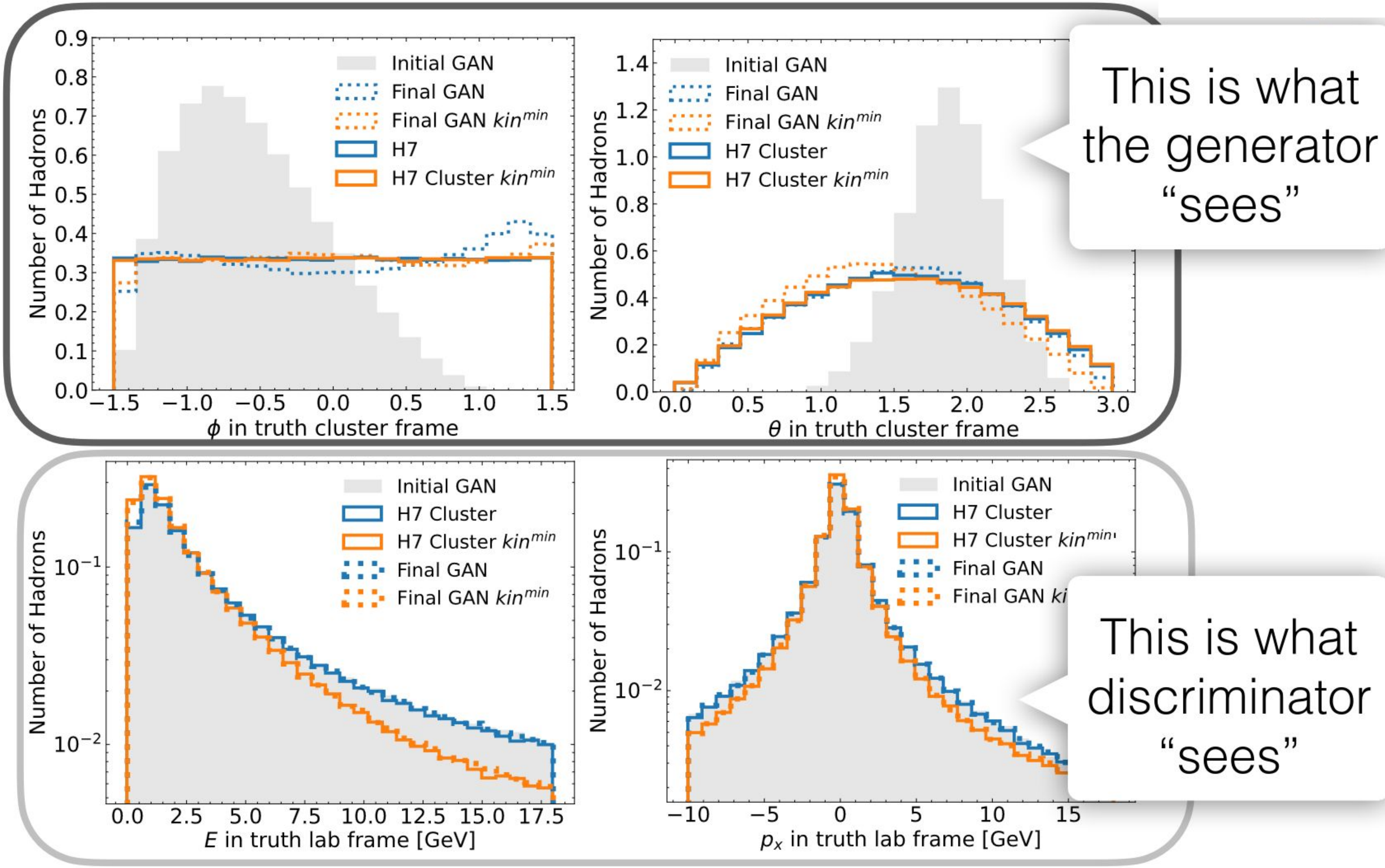


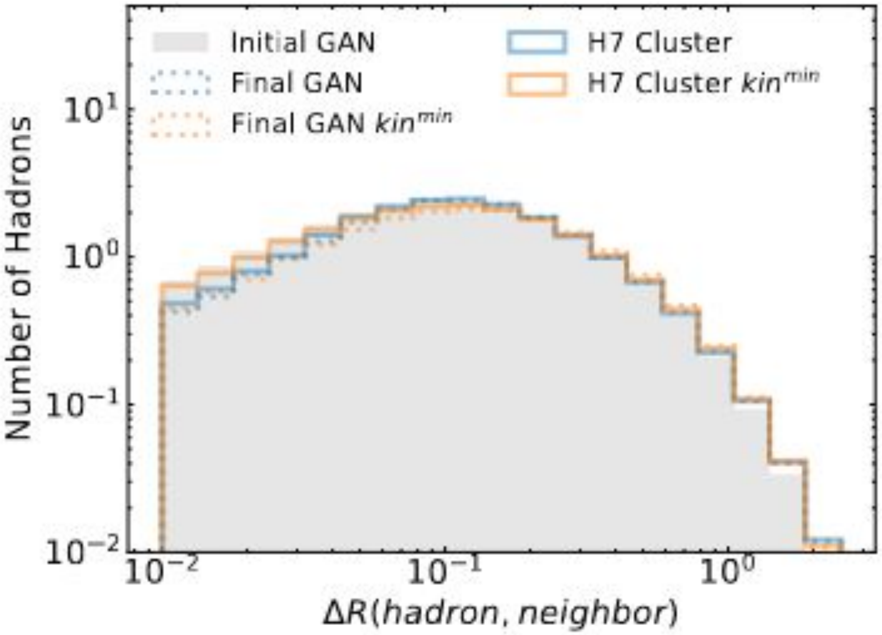
Now, the generator is local (per cluster), but the discriminator is global (whole event).

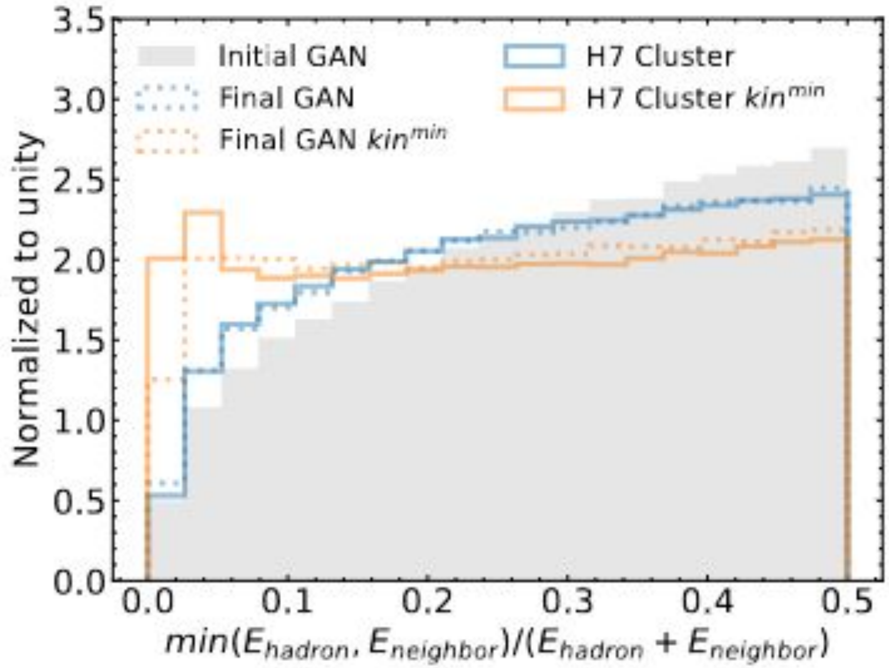
Discriminator is a permutation-invariant architecture called Deep Sets.

Simplification only Pions

Still works !

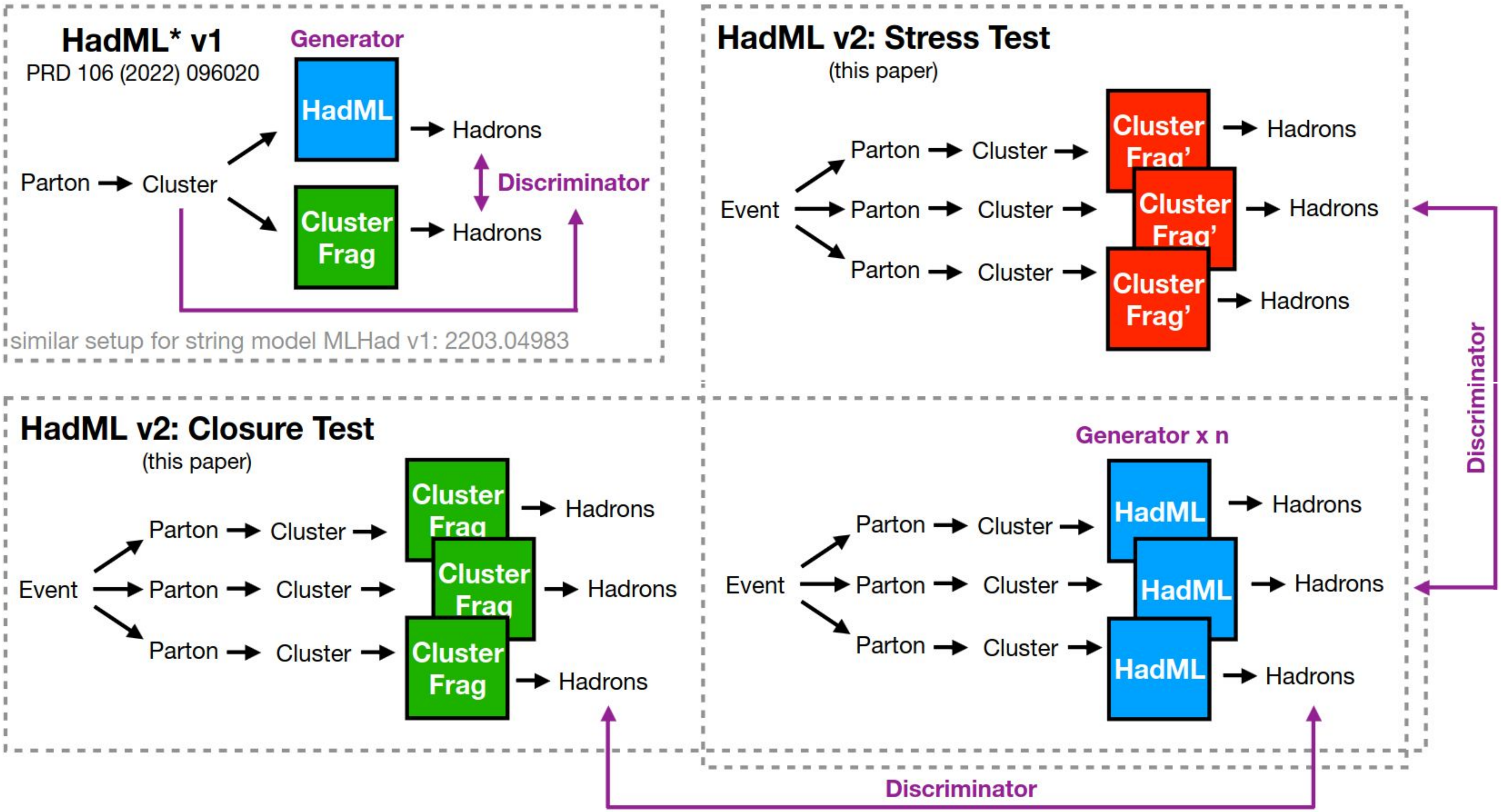

Initial GAN
Final GAN
Final GAN kin^{min}
H7
H7 Cluster kin^{min}
Number of Hadrons
ϕ in truth cluster frame
H7 Cluster
θ in truth cluster frame
This is what the generator "sees"
E in truth lab frame [GeV]
p_x in truth lab frame [GeV]
This is what discriminator "sees"





MINIMAL $\Delta R^2 = \Delta\phi^2 + \Delta\eta^2$

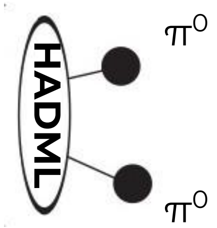
Summary



A key advantage of this fitting protocol over other methods is that it can accommodate unbinned and high-dimensional inputs.

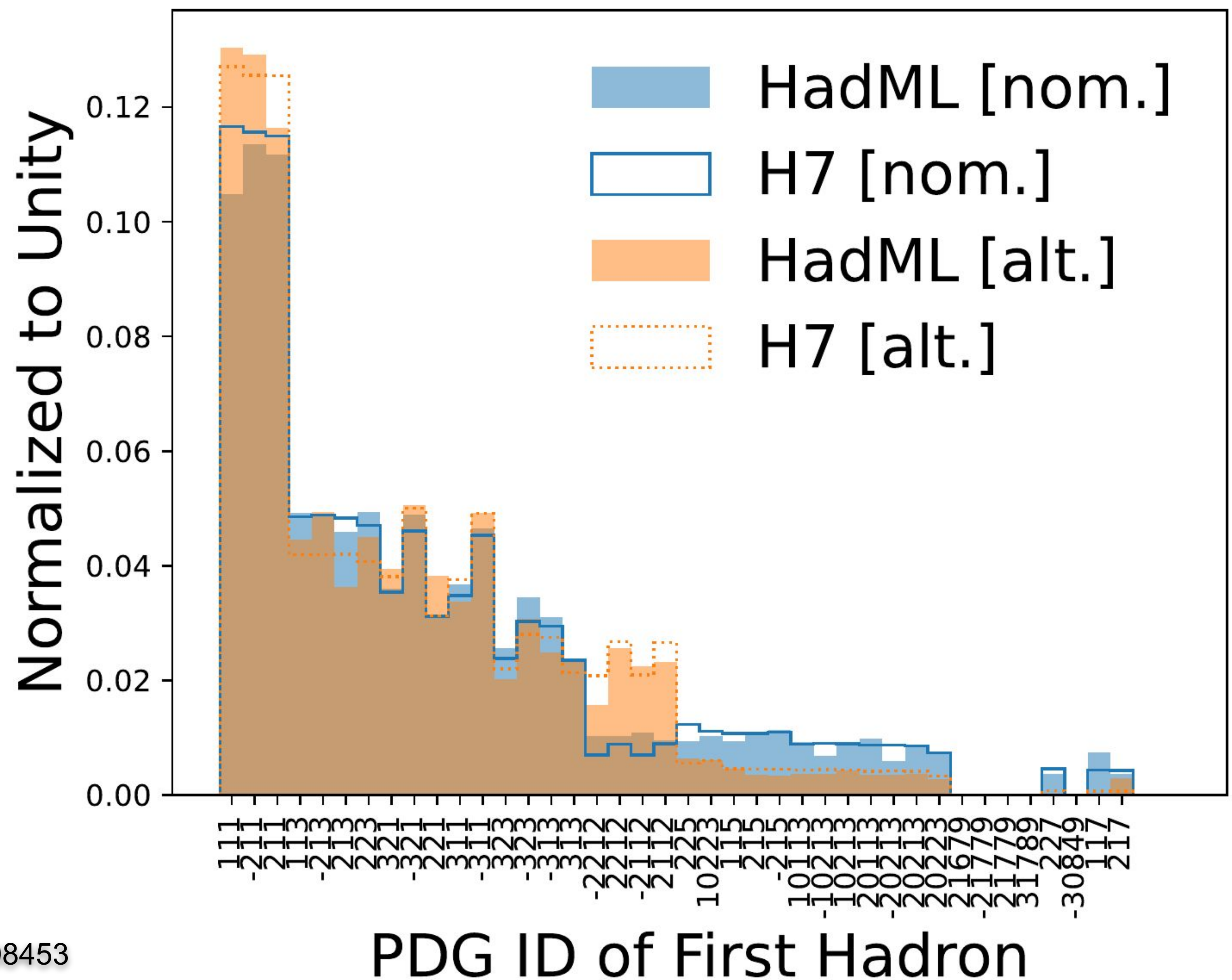
The approach could also be used to tune (without binning) data to a parametric physics model (for example cluster) as well. However, this would require making the cluster model differentiable.

- For HADML, we have made significant progress, but there are still multiple steps to build and tune a full-fledged hadronization model.



What is next?

- Number of technical and methodological step needed:
  - ➔ Directly accommodate multiple hadron species with their relative probabilities


HadML [nom.]
H7 [nom.]
HadML [alt.]
H7 [alt.]
Normalized to Unity
0.00
0.02
0.04
0.06
0.08
0.10
0.12
PDG ID of First Hadron

2312.08453

Outlook

- For HADML, we have made significant progress, but there are still multiple steps to build and tune a full-fledged hadronization model.

- HADML is naturally suited for GPUs

What is next?

- Number of technical and methodological step needed:

    ➔ Include heavy clusters (so far done by Herwig)

    ➔ Hyperparameter optimization, including the investigation of alternative generative models

    ➔ More flexible model with a capacity to mimic the cluster or string models and beyond.

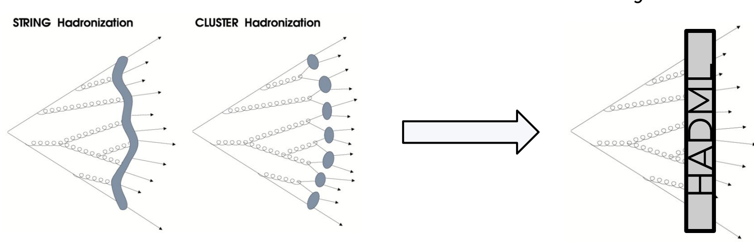
    ➔ MLhadML joining idea of MLhad reweighting and HadML fitting deep generative models

    ➔ Tune to the LEP data

There is still a multi-year program ahead of us, but it will be worth it!

Early 1980's

Early 2020's



So Stay tuned!

HadML v1

The loss function:

$$L = - \sum_{\lambda \sim \textsc{Herwig},\, z \sim p(z)} \left(\log \left(D \left(\tau \left(\lambda \right) \right) \right) + \log \left(1 - D \left(G \left(z, \lambda \right) \right) \right) \right)$$

HadML v2

The discriminator function is modified, we parameterize is as a Deep Sets model

$$D_E \left(x \right) = F \left(\frac{1}{n} \sum_{i=1}^{n} \Phi \left(h_i, \omega_{D_\Phi} \right), \omega_F \right)$$

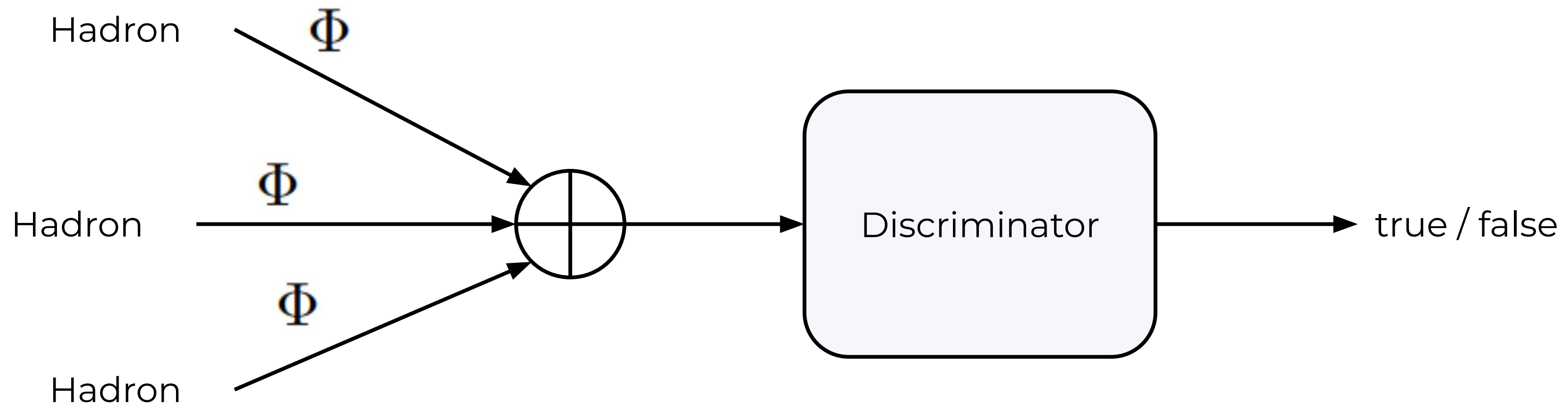
invariant under permutations of hadrons

Φ embeds a set of hadrons into a fixed-length latent space and F acts on the average

$$L = - \sum_{x \sim \text{data}} \log \left(D_E \left(x \right) \right) - \sum_{\{G\} \sim \textsc{Herwig},\, z \sim p(z)} \log \left(1 - D_E \left(\{ G \left(z, \lambda \right) \} \right) \right)$$

The approach could also be used to fit (without binning) data to a parametric physics model (for example cluster) as well. However, this would require making the cluster model differentiable.

Discriminator HadML v2



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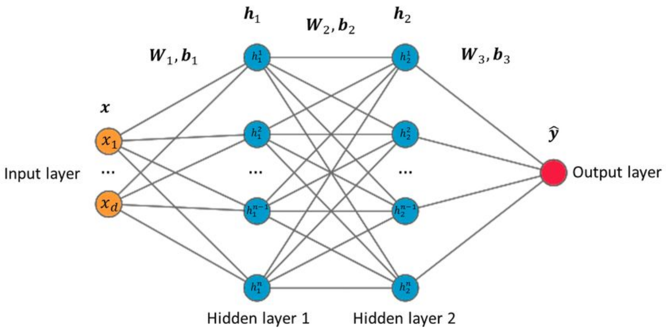
invariant under permutations of hadrons

Architecture: conditional GAN

Generator and the Discriminator are composed of two-layer perceptron
(each a fully connected, hidden size 256, a batch normalization layer, LeakyReLU activation function)



Generator

Input

Cluster $(E,\ p_x,\ p_y,\ p_z)$ and 10 noise features sampled from a Gaussian distribution

Output (in the cluster frame)

ϕ - polar angle
θ - azimuthal angle

we reconstruct the four vectors of the two outgoing hadrons

Discriminator

Input

ϕ and θ labeled as signal (generated by Herwig) or background (generated by Generator)

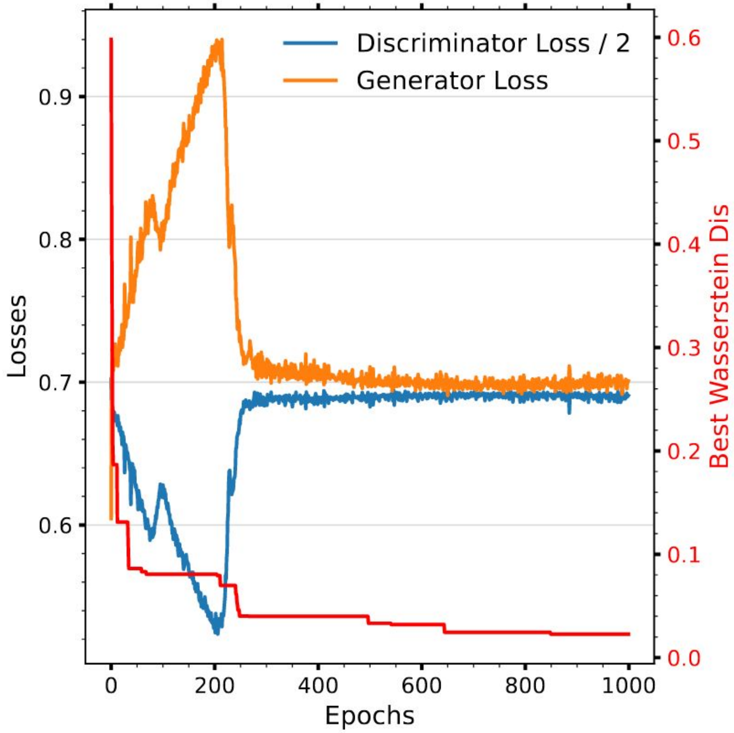
Output

Score that is higher for events from Herwig and lower for events from the Generator

Training

- **Data normalization:**
  cluster's four vector and angular variables are scaled to be between -1 and 1 (tanh activation function as the last layer of the Generator)

- **Discriminator** and the **Generator** are trained separately and alternately by two independent Adam optimizers with a learning rate of 10^{-4}, for 1000 epochs



- **The best model** for events with partons of Pert = 0, is found at the epoch 849 with a total Wasserstein distance of 0.0228.

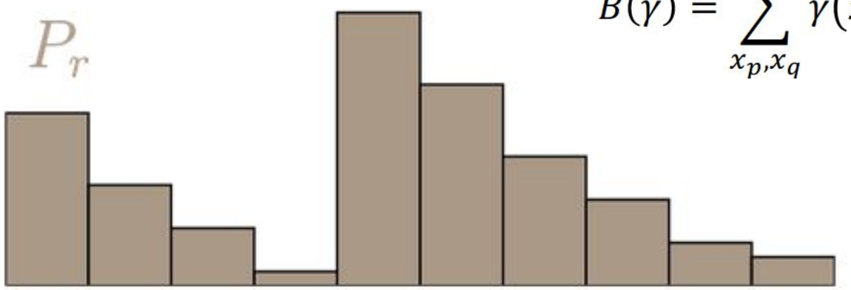
The Wasserstein distance

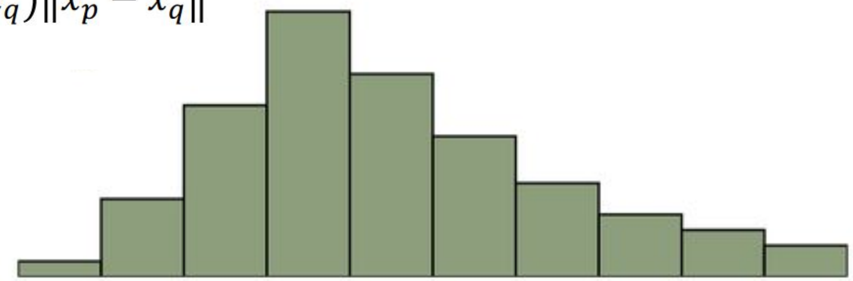
- For discrete probability distributions, the Wasserstein distance is called the earth mover's distance (EMD):
- EMD is the minimal total amount of work it takes to transform one heap into the other.

$$W(P,Q) = \min_{\gamma \in \Pi} B(\gamma)$$

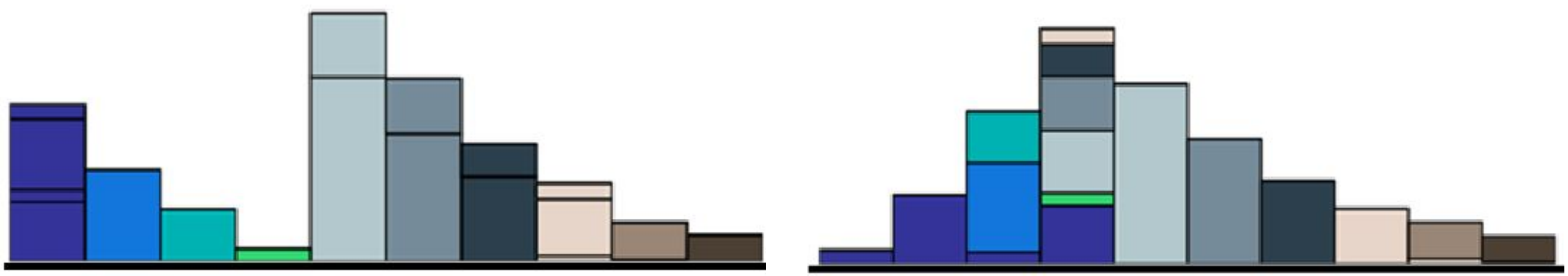
- Work is defined as the amount of earth in a chunk times the distance it was moved.

$$B(\gamma) = \sum_{x_p, x_q} \gamma(x_p, x_q) \|x_p - x_q\|$$

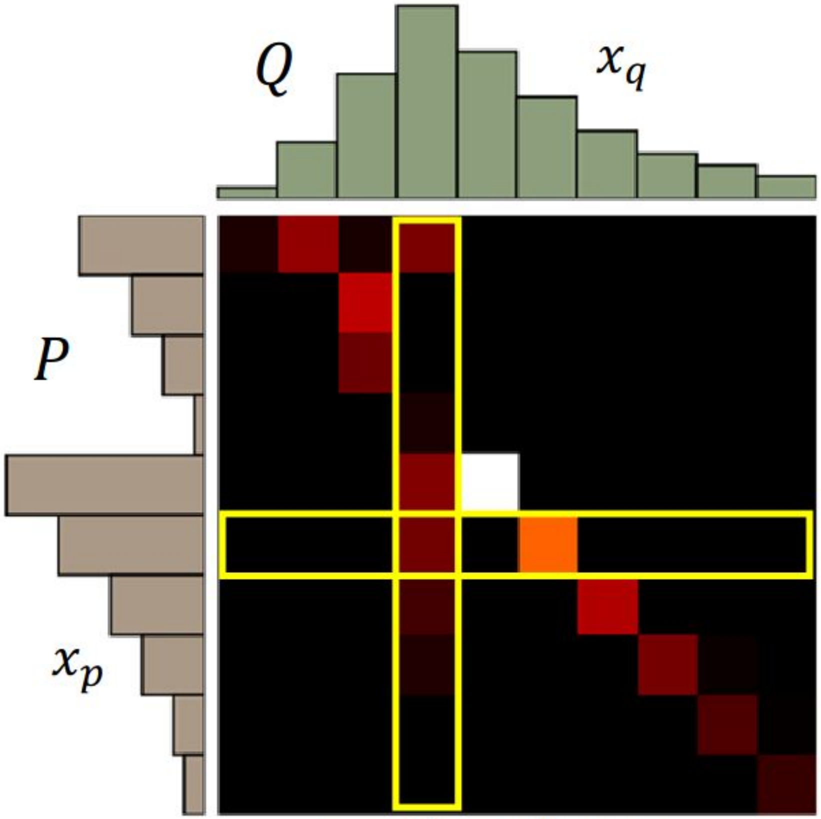




Best "moving plans" of this example



Wasserstein distance



moving plan γ

All possible plan Π

A “moving plan” is a matrix

The value of the element is the amount of earth from one position to another.

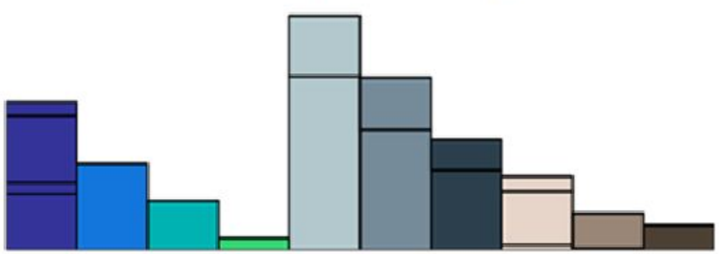
Average distance of a plan γ:

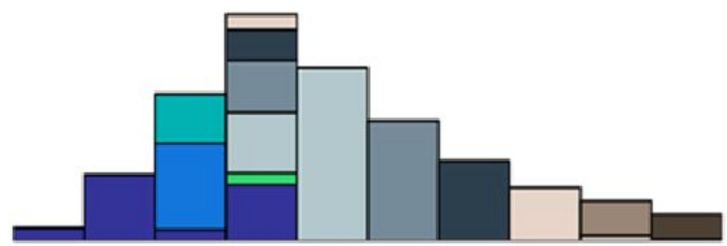
$$B(\gamma) = \sum_{x_p, x_q} \gamma(x_p, x_q) \|x_p - x_q\|$$

Earth Mover’s Distance:

$$W(P, Q) = \min_{\gamma \in \Pi} B(\gamma)$$

The best plan





Minimax Loss

In the paper that introduced GANs, the generator tries to minimize the following function while the discriminator tries to maximize it:

$$E_x[log(D(x))] + E_z[log(1 - D(G(z)))]$$

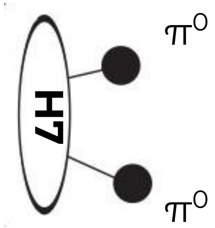
In this function:

- `D(x)` is the discriminator's estimate of the probability that real data instance x is real.
- E_x is the expected value over all real data instances.
- `G(z)` is the generator's output when given noise z.
- `D(G(z))` is the discriminator's estimate of the probability that a fake instance is real.
- E_z is the expected value over all random inputs to the generator (in effect, the expected value over all generated fake instances G(z)).
- The formula derives from the cross-entropy between the real and generated distributions.

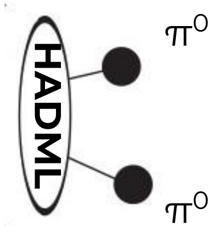
The generator can't directly affect the `log(D(x))` term in the function, so, for the generator, minimizing the loss is equivalent to minimizing `log(1 - D(G(z)))`.

Low-level Validation
(**beyond** training data **different energy**)

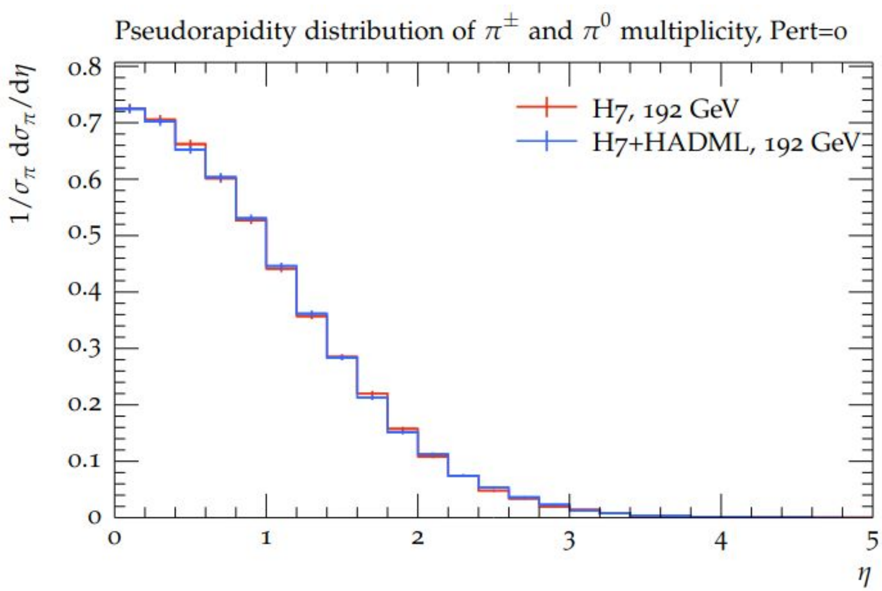
e^+e^- collisions at $\boxed{\sqrt{s} = 192\ \text{GeV}}$

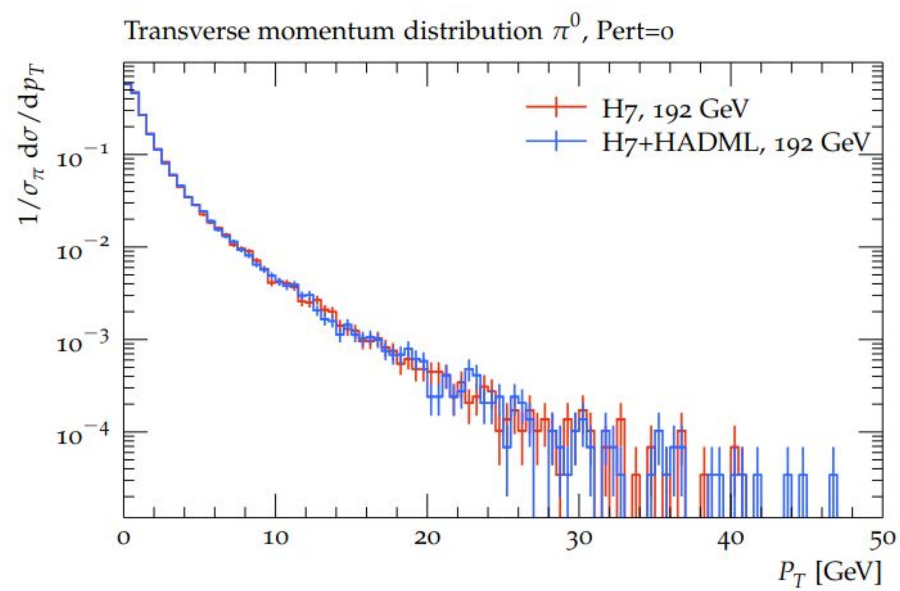


VS



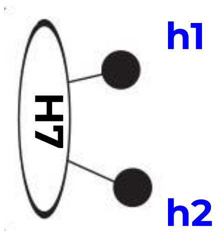
π^0 kinematic variables



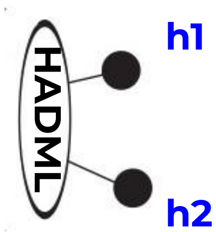


Low-level Validation
(**beyond** training data **different hadrons**)

e^+e^- collisions at
$\sqrt{s} = 91.2$ GeV



VS



h kinematic variables

As a crude "full" model, we simply take the PIDs from Herwig and the kinematics from the GAN.

Kaons

Lambda