

Studying hadronization with Machine Learning techniques

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Techniques in Physics Research

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GÁBOR BÍRÓ

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arXiv:2111.15655

arXiv:2210.10548



UNIVERSITY OF
OXFORD

Data, data, and more data

LHC numbers in **2013** vs. **now**:

Data: **15 PB/y** vs **200+ PB/y**

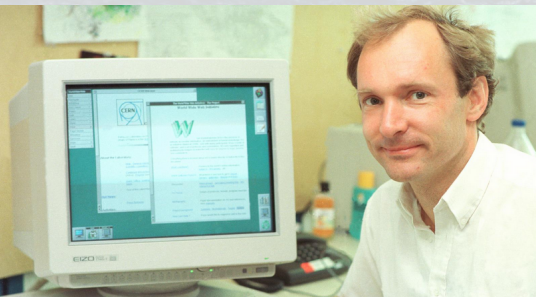
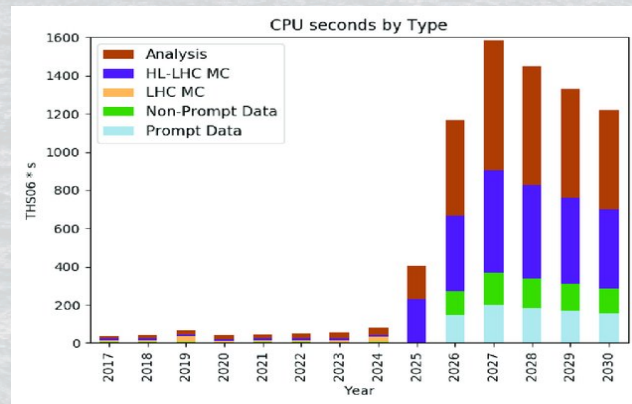
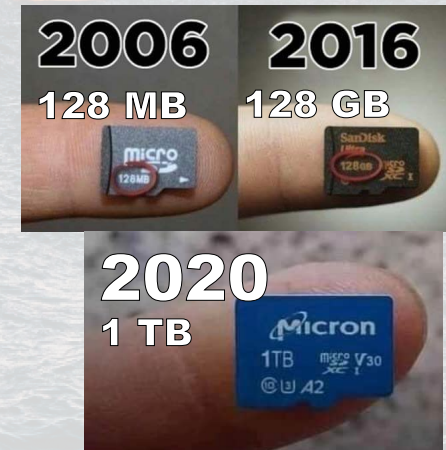
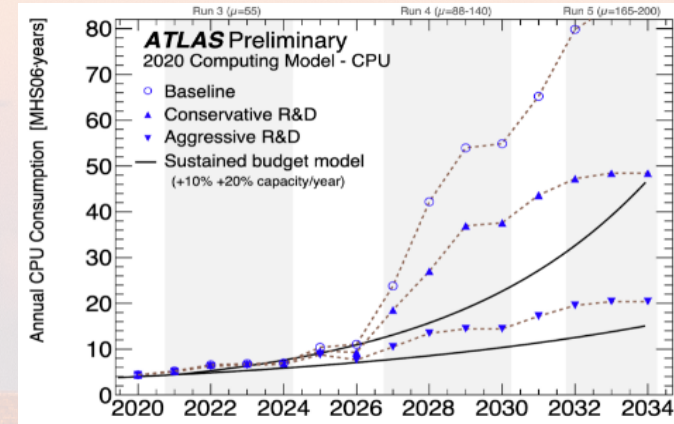
Tape: **180 PB** vs **740+ PB**

Disk: **200 PB** vs **570+ PB**

HS06 hours: **2M** vs **100+ B**

Storing the data is not the only challenge

→ analysis, simulation



Machine Learning in HEP

A Living Review of Machine Learning for Particle Physics

<https://iml-wg.github.io/HEPML-LivingReview/>

Matthew Feickert, Benjamin Nachman, arXiv:2102.02770

2021 May: **417** references

2021 November: **568** references

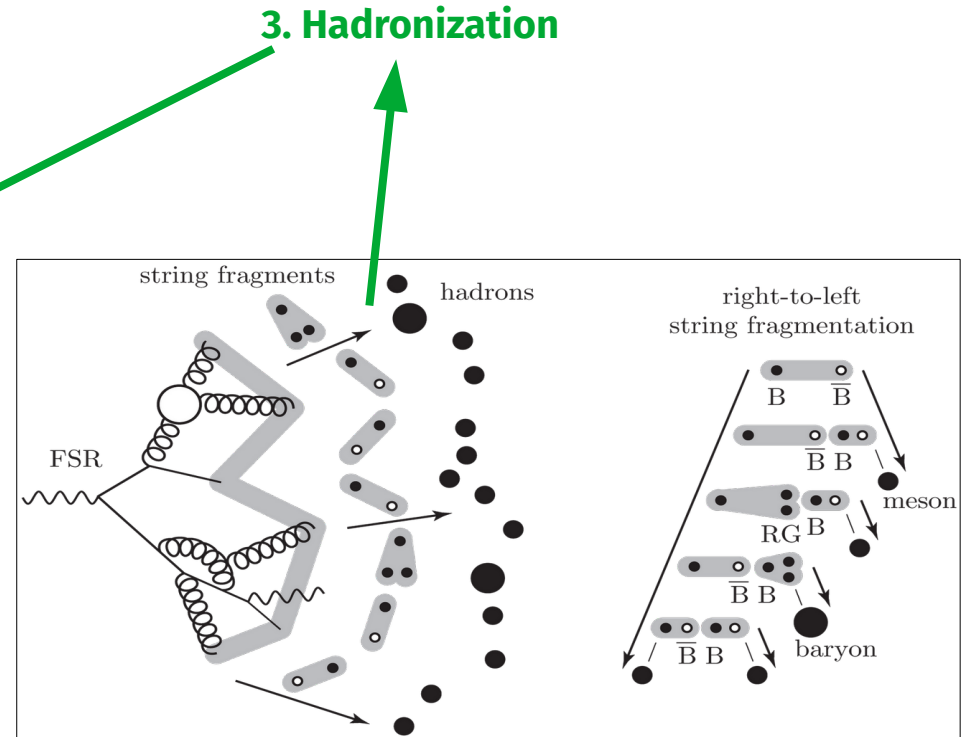
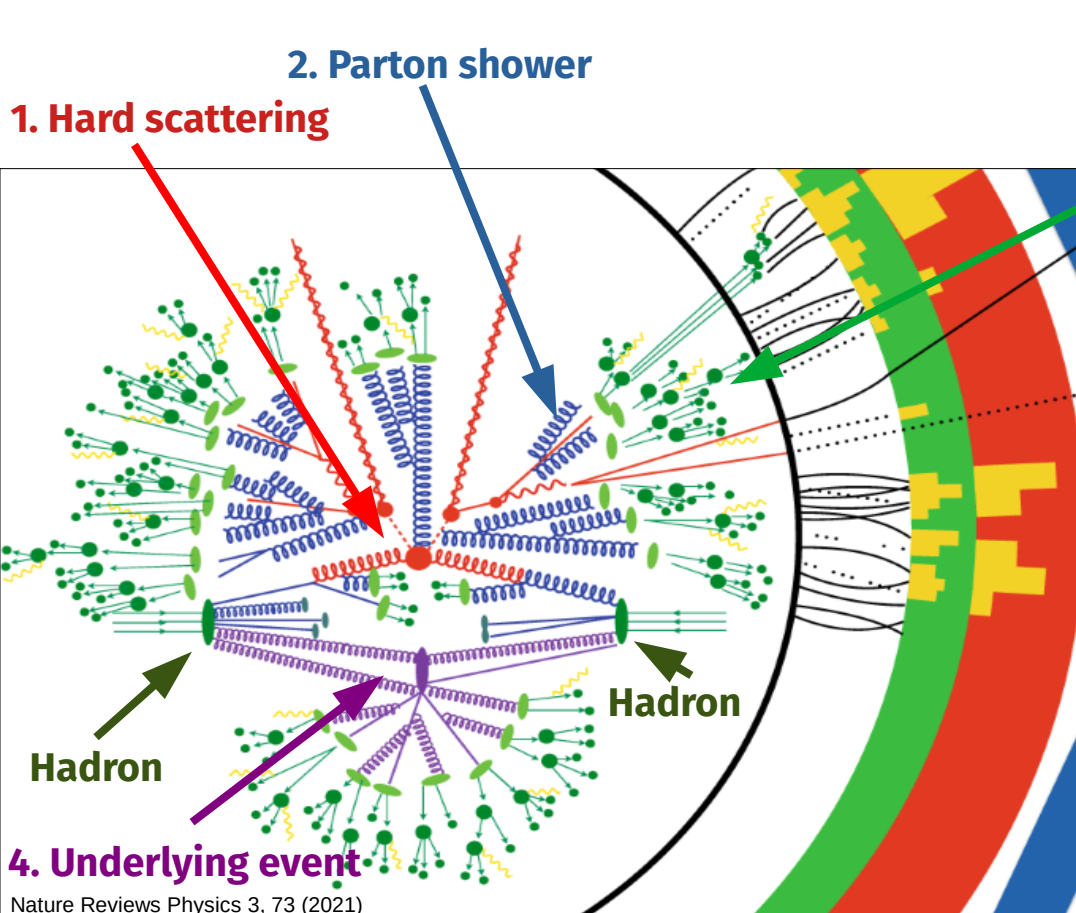
Today: **724** references

- Track reconstruction
- Quark/gluon jet separation
- Jet reconstruction
- Tuning Monte Carlo event generators
- GAN of detectors
- ...

- Accelerated Charged Particle Tracking with Graph Neural Networks on FPGAs
- Particle Track Reconstruction using Generative Deep Learning
- Jet tagging in the Lund plane with graph networks [DOI]
- Vertex and Energy Reconstruction in JUNO with Machine Learning Methods
- MLPN: Efficient machine-learned particle-flow reconstruction using graph neural networks
- 25th International Conference on Computing in High-Energy and Nuclear Physics
- 25th International Conference on Computing in High-Energy and Nuclear Physics
- Graph Neural Network for Object Reconstruction in Liquid Argon Time Projection Chambers
- Instance Segmentation GNNs for One-Shot Conformal Tracking at the LHC
- Charged particle tracking via edge-classifying interaction networks
- Jet characterization in Heavy Ion Collisions by GCD-Aware Graph Neural Networks
- Graph Generative Models for Fast Detector Simulations in High Energy Physics
- Segmentation of EM showers for neutrino experiments with deep graph neural networks
- Sets (point clouds)
 - Energy Flow Networks: Deep Sets for Particle Jets [DOI]
 - ParticleNet: Jet Tagging via Particle Clouds [DOI]
 - ABCNet: An attention-based method for particle tagging [DOI]
 - Secondary Vertex Finding in Jets with Neural Networks
 - Equivalent Energy Flow Networks for Jet Tagging
 - Permutation-Invariant Many-Jet Event Reconstruction with Symmetry Preserving Attention Networks
 - Zero-Permutation Jet-Pariton Assignment using a Self-Attention Network
 - Learning to Isolate Muons
 - Point Cloud Transformers applied to Collider Physics
- Physics-inspired bas
 - Automating the Construction of Jet Observables with Machine Learning [DOI]
 - How Much Information is in a Jet? [DOI]
 - Novel Jet Observables from Machine Learning [DOI]
 - Energy flow polynomials: A complete linear basis for jet substructure [DOI]
 - Deep-learned Top Tagging with a Lorentz Layer [DOI]
 - Resurrecting S/\bar{S} with kinematic shapes
- S/\bar{S} tagging
 - Jet-Images — deep learning edition [DOI]
 - Parlon Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks [DOI]
 - GCD-Aware Recursive Neural Networks for Jet Physics [DOI]
 - Identification of heavy, energetic, hadronically decaying particles using machine-learning techniques [DOI]
 - Boosted S/\bar{S} and SZ tagging with jet charge and deep learning [DOI]
 - Suppressed Jet Clustering with Graph Neural Networks for Lorentz Boosted Bosons [DOI]
 - Jet tagging in the Lund plane with graph networks [DOI]
 - A S/\bar{S} μ ns polarization analyzer from Deep Neural Networks
- S/\bar{S} μ ns \bar{S} μ ns
 - Automating the Construction of Jet Observables with Machine Learning [DOI]
 - Boosting S/\bar{S} μ ns \bar{S} μ ns with Machine Learning [DOI]
 - Interaction networks for the identification of boosted S/\bar{S} μ ns \bar{S} μ ns decays [DOI]
 - Interpretable deep learning for two-prong jet classification with jet spectra [DOI]
 - Identification of heavy, energetic, hadronically decaying particles using machine-learning techniques [DOI]
 - Distinguishing Boosted Higgs Boson Production Modes with Machine Learning
 - Benchmarking Machine Learning Techniques with Di-Higgs Production at the LHC
 - The Boosted Higgs Jet Reconstruction via Graph Neural Network
 - Extracting Signals of Higgs Boson From Background Noise Using Deep Neural Networks
 - Learning to increase matching efficiency in identifying additional b-jets in the S/\bar{S} μ ns \bar{S} μ ns process
- quarks and gluons
 - Quark versus Gluon Jet Tagging Using Jet Images with the ATLAS Detector
 - Deep learning in color: towards automated quark/gluon [DOI]
 - Recursive Neural Networks in Quark/Gluon Tagging [DOI]
 - DeepJet: Generic physics object based jet multiclass classification for LHC experiments
 - Probing heavy ion collisions using quark and gluon jet substructure
 - JEDI-net: a jet identification algorithm based on interaction networks [DOI]
 - Quark-Gluon Jettagging: Machine Learning vs Detector [DOI]
 - Towards Machine Learning Analysis for Jet Substructure [DOI]
 - Quark-Gluon Jet Discrimination with Weakly Supervised Learning [DOI]

- Classification
 - Parameterized classifiers
 - Parameterized neural networks for high-energy physics [DOI]
 - Approximating Likelihood Ratios with Calibrated Discriminative Classifiers
 - E-Fluoribus Uram Ex Machina: Learning from Many Collider Events at Once
 - Jet images
 - How to tell quark jets from gluon jets
 - Jet-Images: Computer Vision Inspired Techniques for Jet Tagging [DOI]
 - Playing Top with ANN: Boosted Top Identification with Pattern Recognition [DOI]
 - Jet-Images — deep learning edition [DOI]
 - Quark versus Gluon Jet Tagging Using Jet Images with the ATLAS Detector
 - Boosting S/\bar{S} μ ns \bar{S} μ ns with Machine Learning [DOI]
 - Learning to classify from imprecise samples with high-dimensional data [DOI]
 - Parlon Shower Uncertainties in Jet Substructure Analyses with Deep Neural Networks [DOI]
 - Deep learning in color: towards automated quark/gluon [DOI]
 - Deep-learning Top Taggers or the End of GCD? [DOI]
 - Pulling Out All the Tops with Computer Vision and Deep Learning [DOI]
 - Reconstructing boosted Higgs jets from event image segmentation
 - An Attention Based Neural Network for Jet Tagging
 - Quark-Gluon Jet Discrimination Using Convolutional Neural Networks [DOI]
 - Learning to Isolate Muons
 - Deep learning jet modifications in heavy-ion collisions
 - Event images
 - Topology classification with deep learning to improve real-time event selection at the LHC [DOI]
 - Convolutional Neural Networks with Event Images for Pileup Mitigation with the ATLAS Detector
 - Boosting S/\bar{S} μ ns \bar{S} μ ns with Machine Learning [DOI]
 - End-to-End Physics Event Classification with the CMS Open Data: Applying Image-based Deep Learning on Detector Data to Directly Classify Collision Events at the LHC [DOI]
 - Distinguishing Boosted Higgs Boson Production Modes with Machine Learning
 - Identifying the nature of the GCD transition in relativistic collision of heavy nuclei with deep learning [DOI]
 - Sequences
 - Jet Flavor Classification in High-Energy Physics with Deep Neural Networks [DOI]
 - Topology classification with deep learning to improve real-time event selection at the LHC [DOI]
 - Jet Flavor Classification Using DeepJet [DOI]
 - Development of a Vertex Finding Algorithm using Recurrent Neural Network
 - Sequence-based Machine Learning Models in Jet Physics
 - Trees
 - GCD-Aware Recursive Neural Networks for Jet Physics [DOI]
 - Recursive Neural Networks in Quark/Gluon Tagging [DOI]
 - Graphs
 - Neural Message Passing for Jet Physics
 - Graph Neural Networks for Particle Reconstruction in High Energy Physics detectors
 - Probing stop pair production at the LHC with graph neural networks [DOI]
 - Pileup mitigation at the Large Hadron Collider with graph neural networks [DOI]
 - Unveiling CP property of top-Higgs coupling with graph neural networks at the LHC [DOI]
 - JEDI-net: a jet identification algorithm based on interaction networks [DOI]
 - Learning representations of irregular particle-detector geometry with distance-weighted graph networks [DOI]
 - Interpretable deep learning for two-prong jet classification with jet spectra [DOI]
 - Neural Network-based Top Tagger with Two-Point Energy Correlations and Geometry of Soft Emissions [DOI]
 - Probing triple Higgs coupling with machine learning at the LHC
 - Casting a graph net to catch dark showers [DOI]
 - Graph neural networks in particle physics [DOI]
 - Distance-Weighted Graph Neural Networks on FPGAs for Real-Time Particle Reconstruction in High Energy Physics [DOI]
 - Supervised Jet Clustering with Graph Neural Networks for Lorentz Boosted Bosons [DOI]
 - Track Seeding and Labeling with Embedded-space Graph Neural Networks
 - Graph neural network for 3D classification of ambiguities and optical crosstalk in scintillator-based neutrino detectors [DOI]

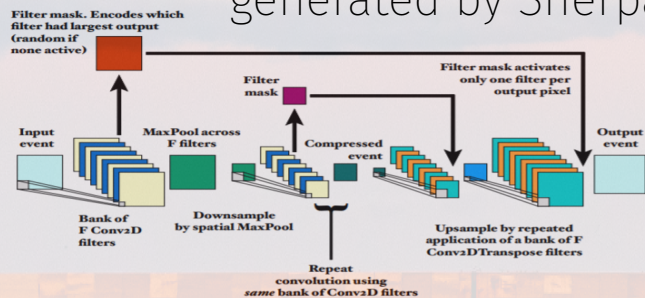
Parton shower and hadronization



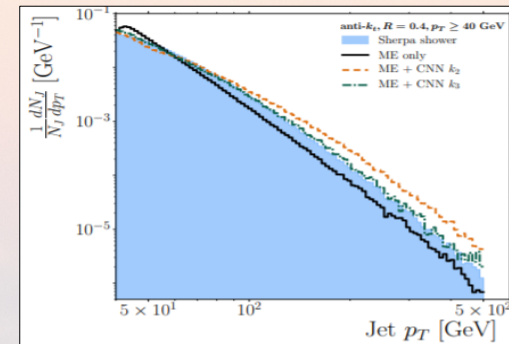
The goal of this study

J.W. Monk: Deep Learning as a Parton Shower (arXiv:1807.03685)

Dataset: 500 000 QCD pp event @ 7 TeV,
generated by Sherpa



parameter	model k_2	model k_3
Kernel size, k	2	3
Input image size, N	64	81
Size of filter bank, F	9	7
Levels of decomposition	5	3
Regularisation, λ	500	300
Learning rate	5×10^{-5}	1×10^{-5}
Loss weight w_1	5	4
Loss weight w_2	2	2
Loss weight w_3	1	1
Total number of trained weights	72	126

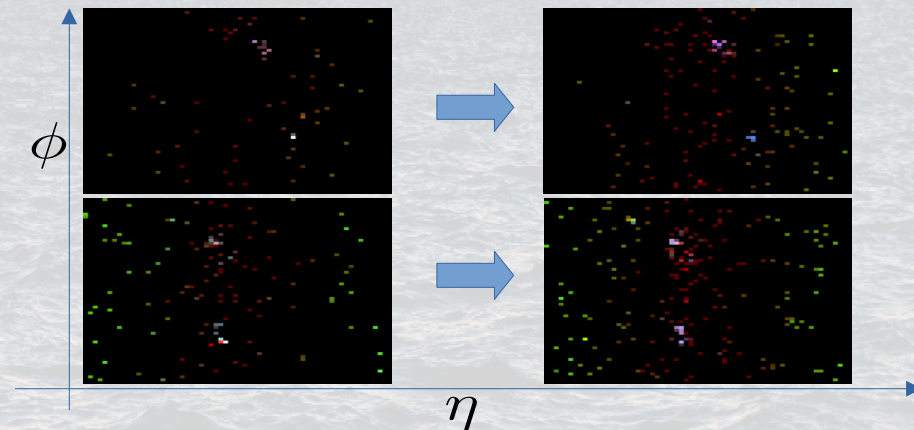
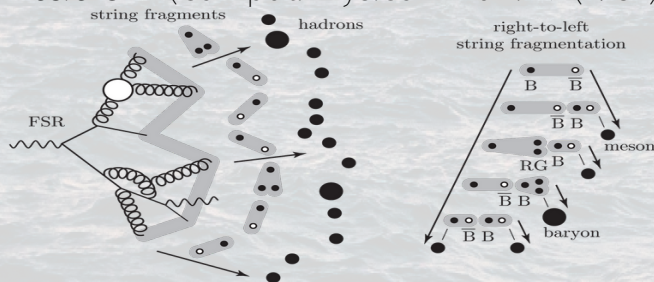


Hadronization

Partons \rightarrow hadrons

Non-perturbative process

Lund-fragmentation (Comput.Phys.Commun. 27 (1982) 243)

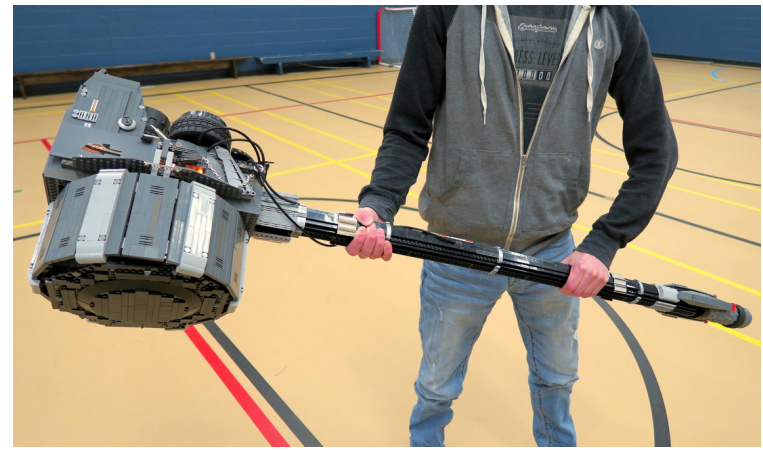
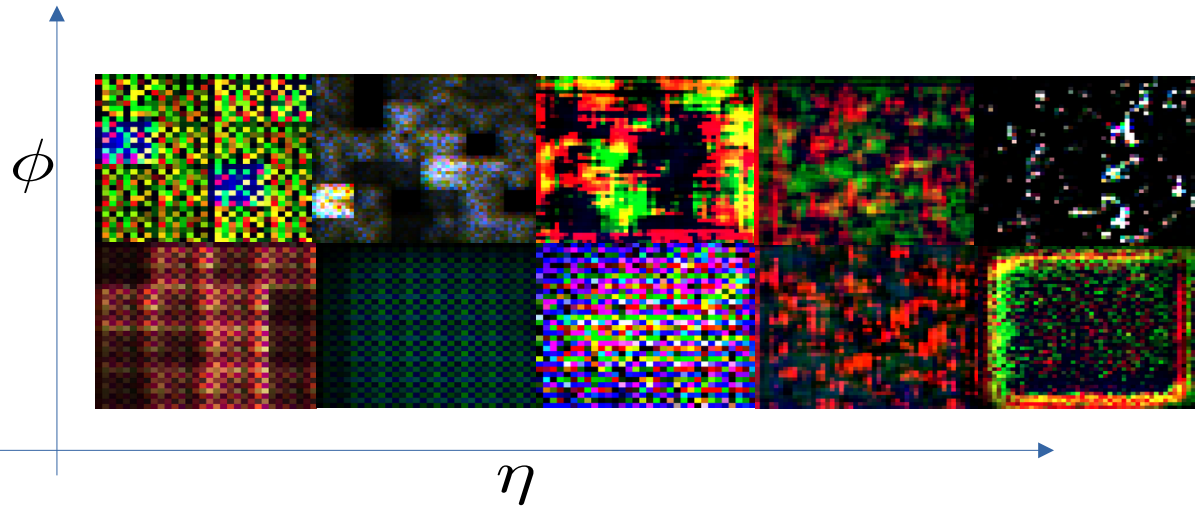


ML: a great tool..

ML: a great tool..



ML: a great tool..



“The nice thing about artificial intelligence is that at least it’s better than artificial stupidity.”

Terry Pratchett, Stephen Baxter: The Long War

Train and validation sets

Monte Carlo data: Pythia 8.303

Monash tune

Rescattering and decays turned off
ISR, FSR, MPI: turned on (*)

Selection:

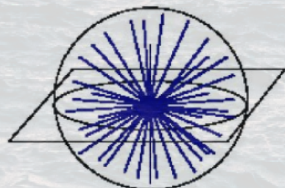
- All final particles with $|y| < \pi$
- At least 2 jets
 - Anti- k_T
 - $R=0.4$
 - $p_T > 40$ GeV

Event number:

- Train: 750 000, $\sqrt{s} = 7$ TeV
- Validation and test: 100 000
- ~20 GB raw data



S=3/4 A=0



S=1 A=1/2

Input:

Parton level

Discretized in the (y, ϕ) plane: p_T , m , multiplicity $\times \sqrt{s}/1\text{GeV}$

$y \in [\pi, \pi]$ 32 bins

$\phi \in [0, 2\pi]$, 32 bins

Hadron level output:

(Charged) event multiplicity, (tr-)sphericity, mean jet p_T , -mass, -width, -multiplicity

$$M_{xyz} = \sum_i \begin{pmatrix} p_{xi}^2 & p_{xi}p_{yi} & p_{xi}p_{zi} \\ p_{yi}p_{xi} & p_{yi}^2 & p_{yi}p_{zi} \\ p_{zi}p_{xi} & p_{zi}p_{yi} & p_{zi}^2 \end{pmatrix}$$

Eigenvalues:

$$\lambda_1 > \lambda_2 > \lambda_3 \quad \sum_i \lambda_i = 1$$

Sphericity:

$$S = \frac{3}{2}(\lambda_2 + \lambda_3)$$

Transverse sphericity:

$$S_{\perp} = \frac{2\lambda_2}{\lambda_1 + \lambda_2}$$

Models

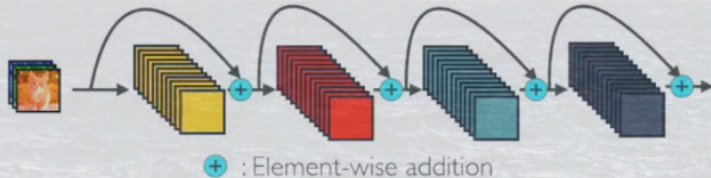
Stacking more layers: solve complex problems more efficiently, get highly accurate results

BUT:

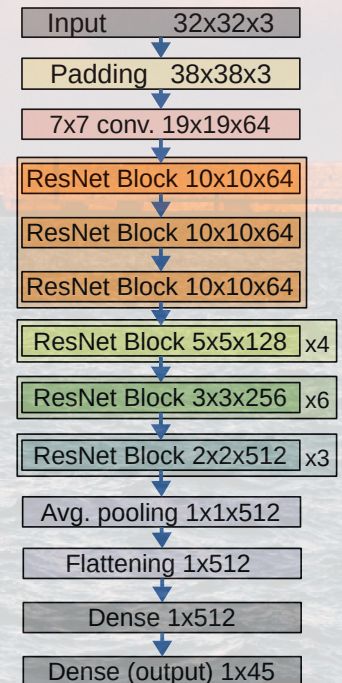
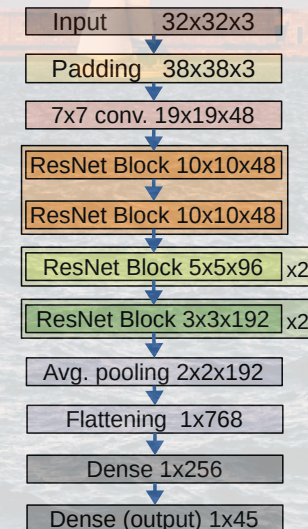
Vanishing/exploding gradients

ResNet:

Residual blocks with “skip connections”



	Model S	Model K
Trainable parameters	1.7 M	20 M

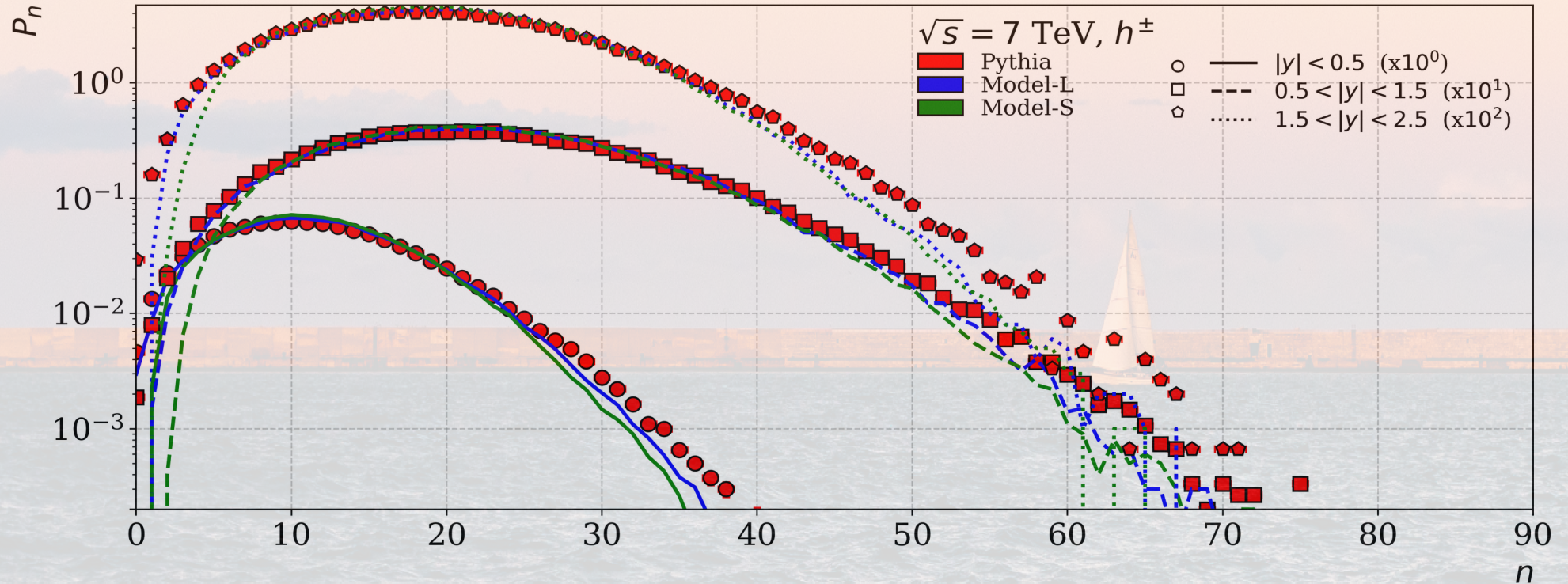


Used hardwares: Nvidia Tesla T4, GeForce GTX 1080
@ Wigner Scientific Computing Laboratory

Framework: Tensorflow 2.4.1, Keras 2.4.0

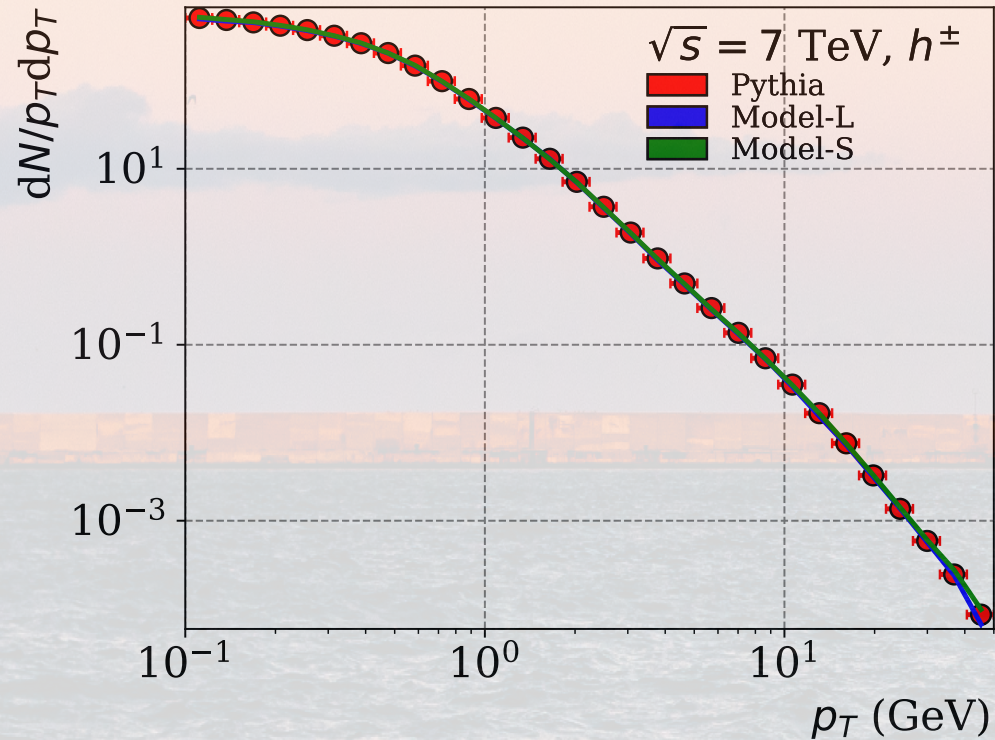
Results

Proton-proton @ 7 TeV, Training + Validation

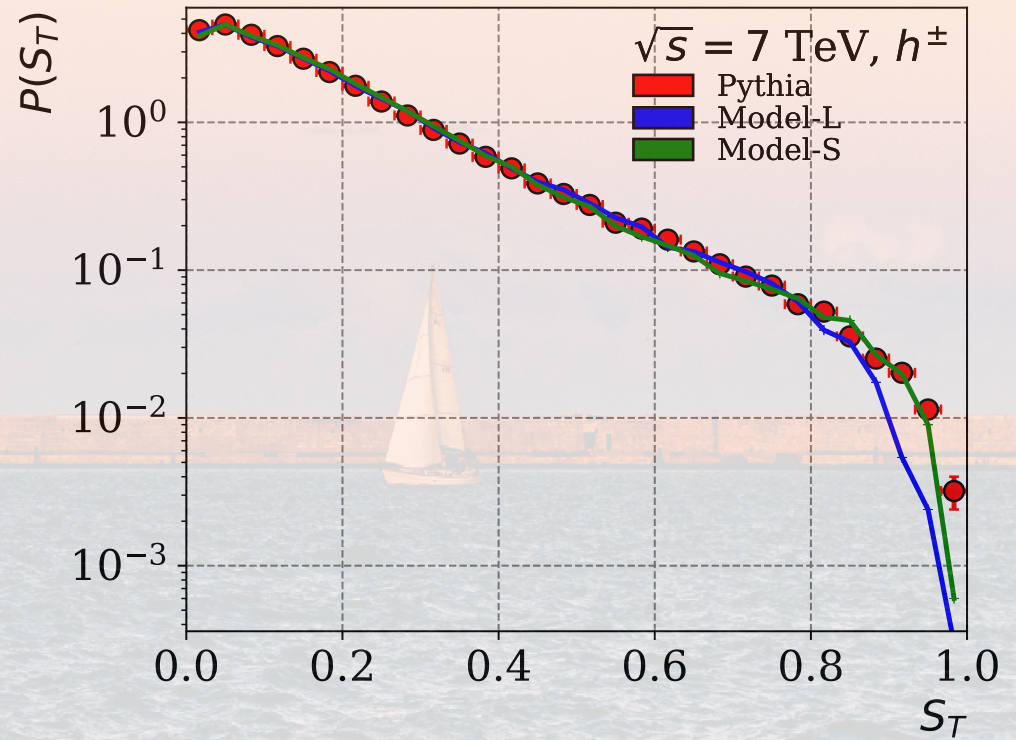


Charged hadron multiplicity at various rapidity windows
Comparison to reference MC model
Good agreement for both models

Proton-proton @ 7 TeV, Training + Validation

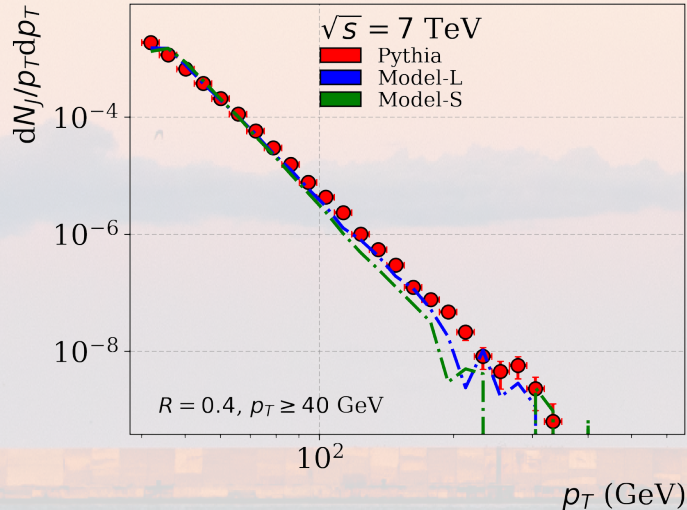


Charged hadron transverse momentum
 $0.1 \text{ GeV} \leq p_T \leq 50 \text{ GeV}$



Event transverse sphericity
The smaller model performs better

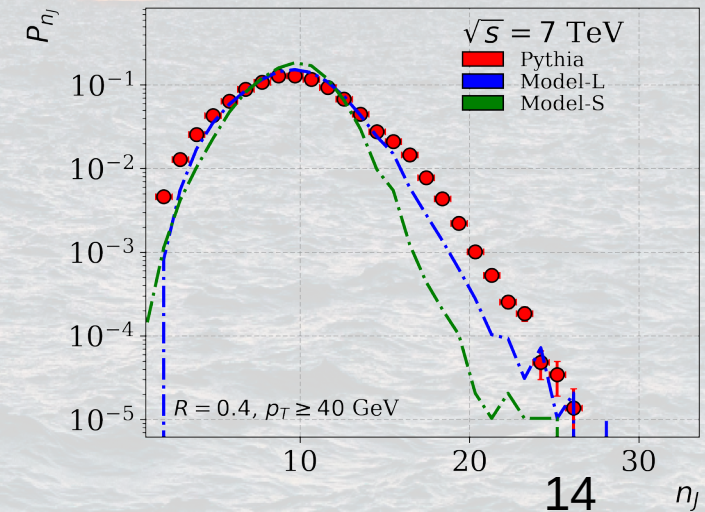
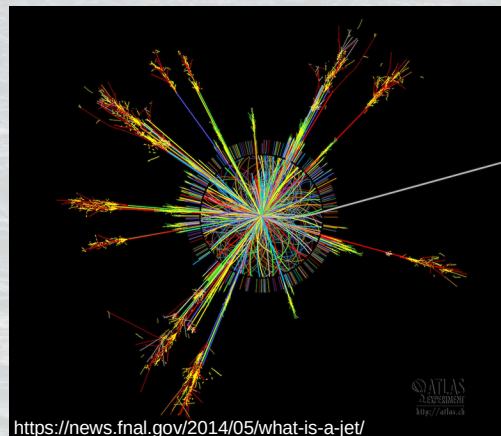
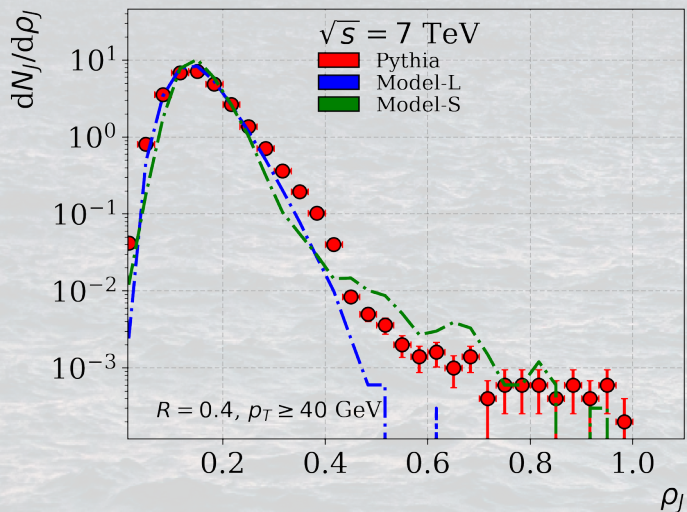
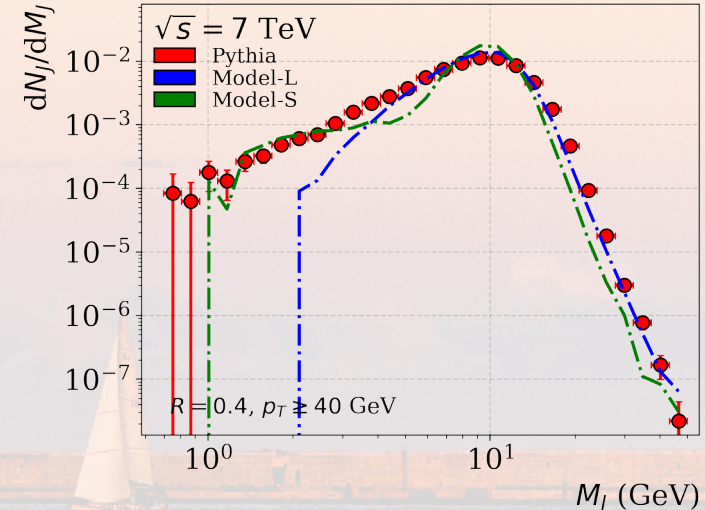
Proton-proton @ 7 TeV, Training + Validation



Jets:

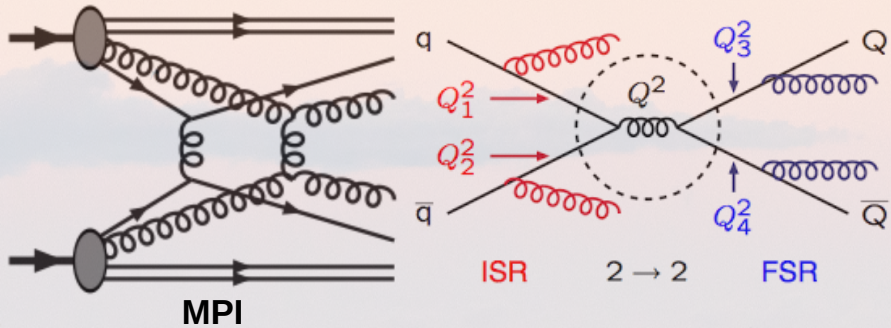
- Mean $p_T \leq 400 \text{ GeV}$
- Mean mass $p_T \leq 400 \text{ GeV}$
- Mean multiplicity
- Mean width

The smaller model performs better

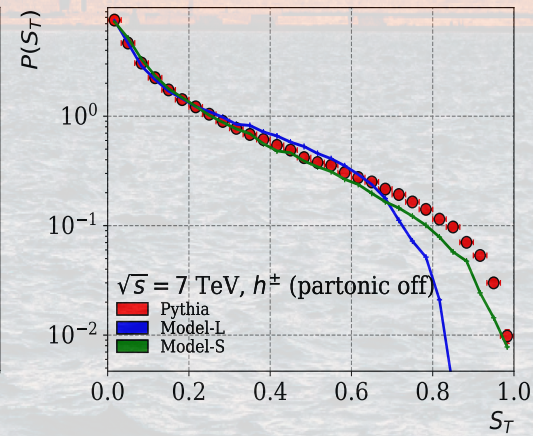
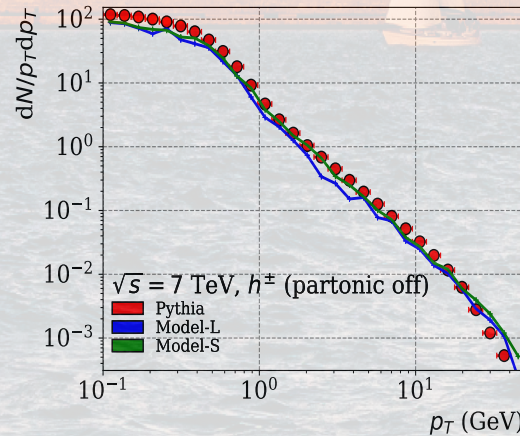
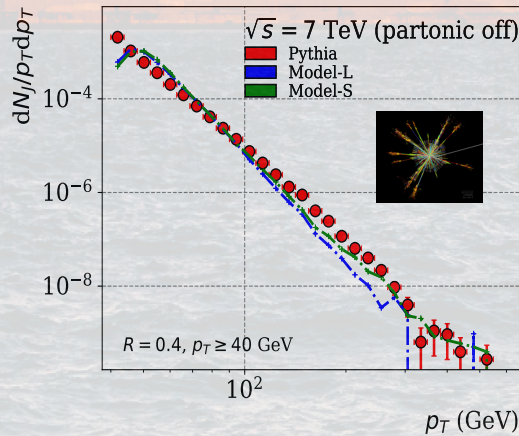
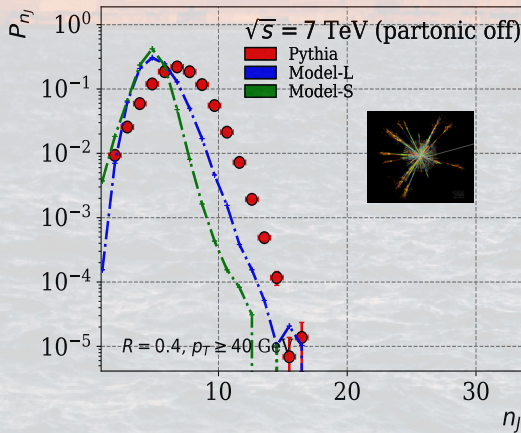
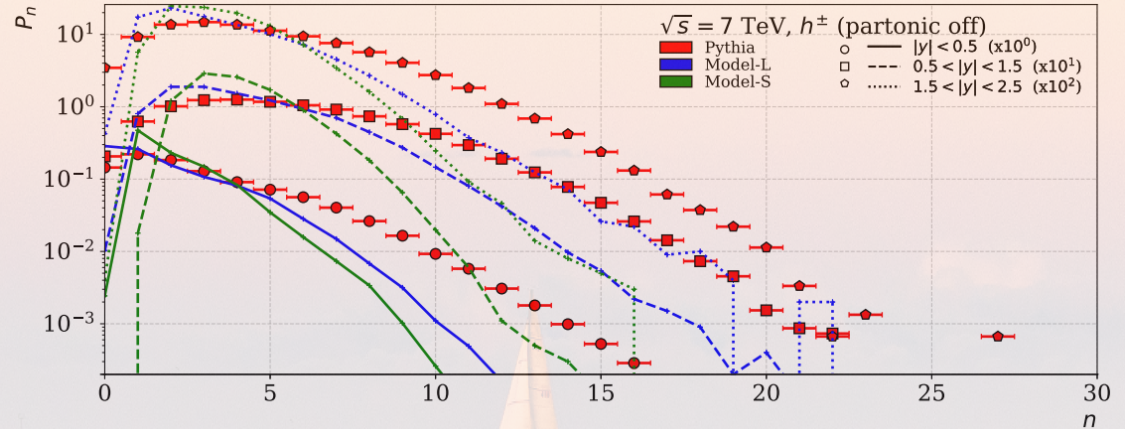


Proton-proton @ 7 TeV, Training + Validation

(* What about the partonic processes?)

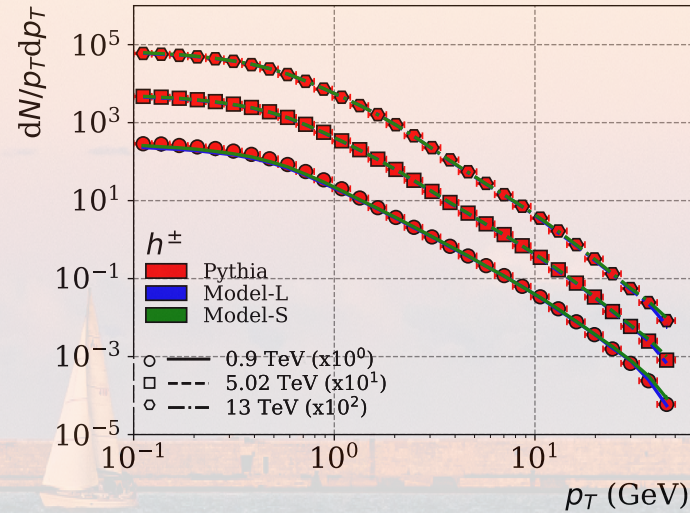
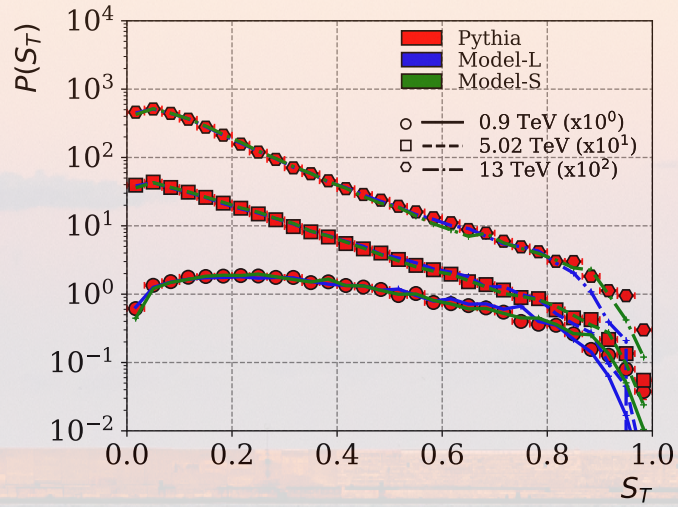
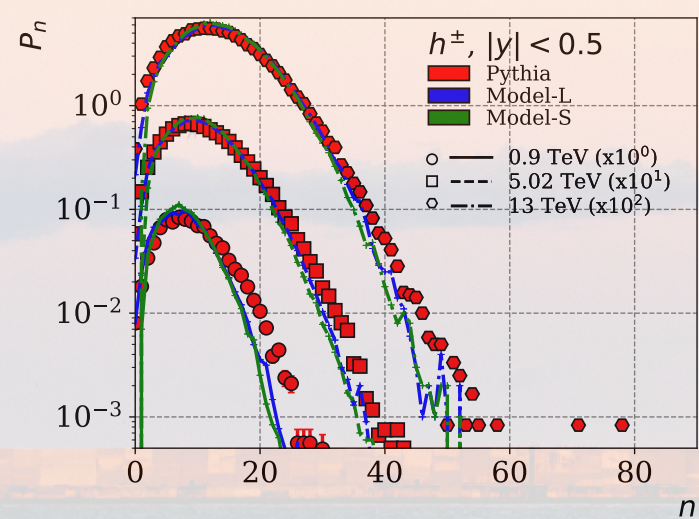


<http://home.thep.lu.se/~torbjorn/talks/cern18cosmic.pdf>

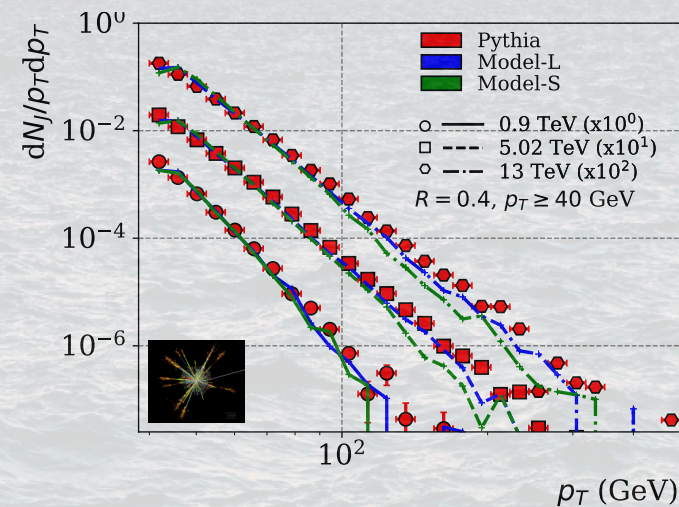


Qualitative agreement → the models adopted the hadronization properties

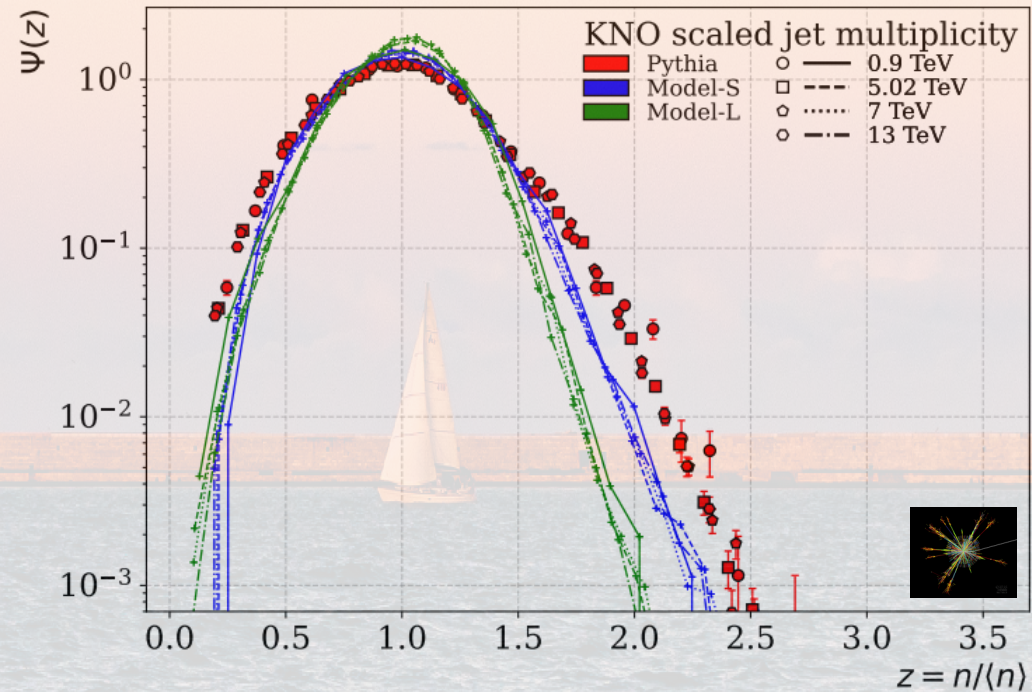
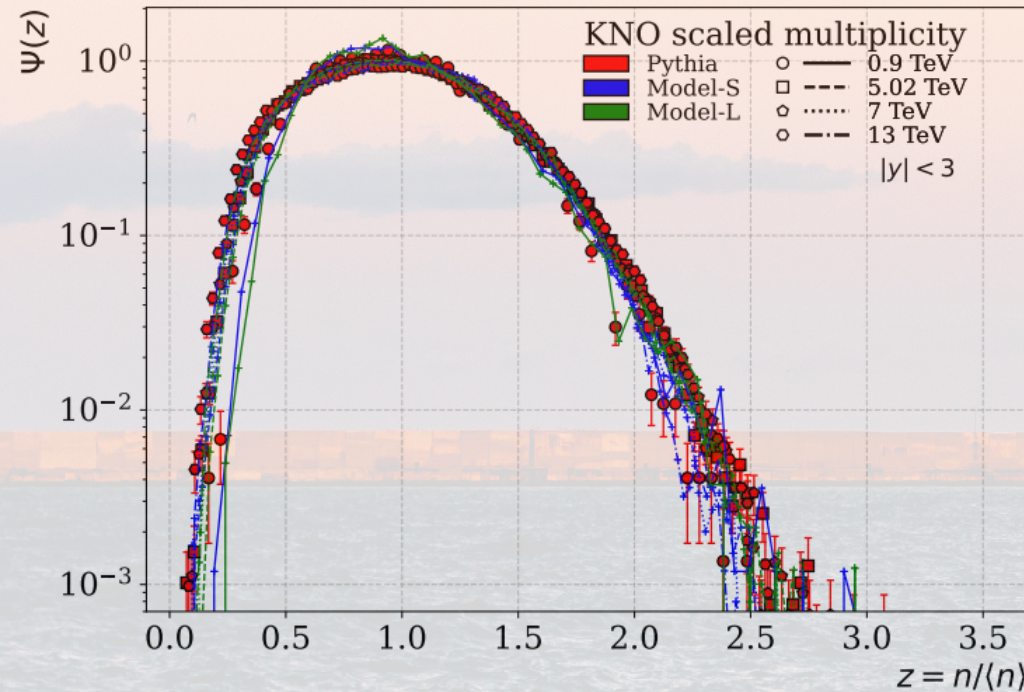
Proton-proton @ 0.9-13 TeV, Predictions



- So far: everything at $\sqrt{s} = 7$ TeV \rightarrow the **ONLY** energy, where the models were trained
- Good agreement for all observable quantities as **predictions** for other LHC energies
- **Multiplicity scaling?**



Test of KNO-scaling for the predictions



Scaling function for multiplicities at various energies: $P_n = \frac{1}{\langle n \rangle} \Psi \left(\frac{n}{\langle n \rangle} \right)$

Charged hadron multiplicities in **jetty** events: good overlap and agreement

Mean jet multiplicities: different scaling for the models



Summary

ACAT 2022

24-28 OCTOBER 2022

Developed hadronization models with different complexities

Traditional computer vision algorithms capture the main features of high-energy event variables successfully → training only at a **single** c.m. energy, predictions at other energies

Generalization to other CM energies: KNO scaling in jetty events

Prospects

Architecture variations (hyperparameter fine-tuning)

Heavy ion (centralities, collective effects)

Thank you for your attention!

The research was supported by OTKA grants K135515, NKFIH 2019-2.1.6-NEMZKI-2019-00011, 2020-2.1.1-ED-2021-00179, the **Wigner Scientific Computing Laboratory** (former Wigner GPU Laboratory) and RRF-2.3.1-21-2022-00004 within the framework of the Artificial Intelligence National Laboratory.



Dimensionality

Input:

Parton level

Discretized in the (y, ϕ) plane: $p_{T,m}$, multiplicity

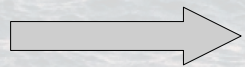
$$\left. \begin{array}{l} y \in [\pi, \pi], \quad 32 \text{ bins} \\ \phi \in [0, 2\pi], \quad 32 \text{ bins} \end{array} \right\} := M$$

Reduction with Singular Value Decomposition:

$$M_{n \times m} = U_{n \times n} \Sigma_{n \times m} V_{m \times m}^T$$

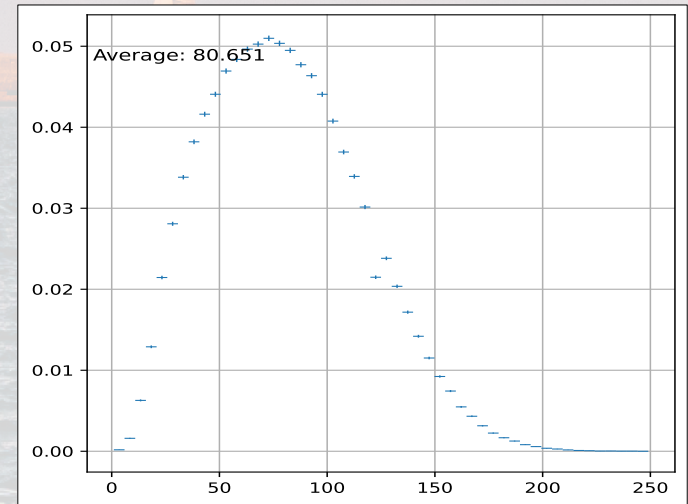
- Unitarity
- Ordered by importance
- Guaranteed to exist, unique

$$M \approx \sum_{i=1}^r \sigma_i u_i v_i^T + \mathcal{O}(\epsilon), \quad r \leq \min\{n, m\}$$



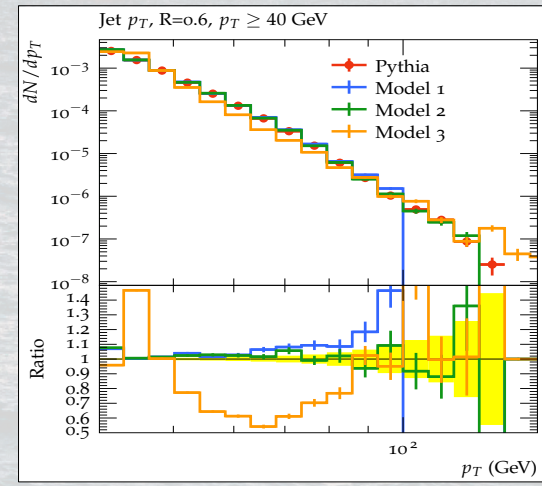
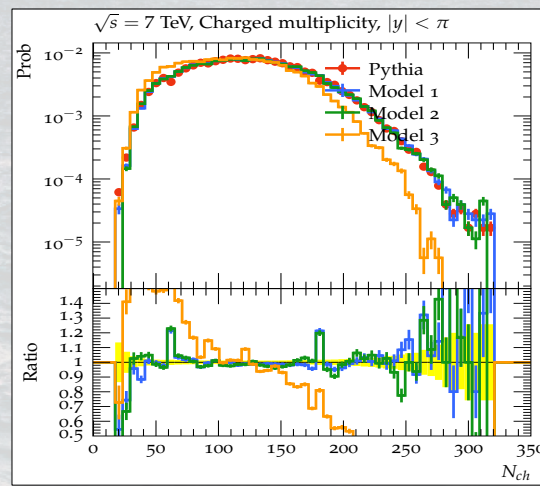
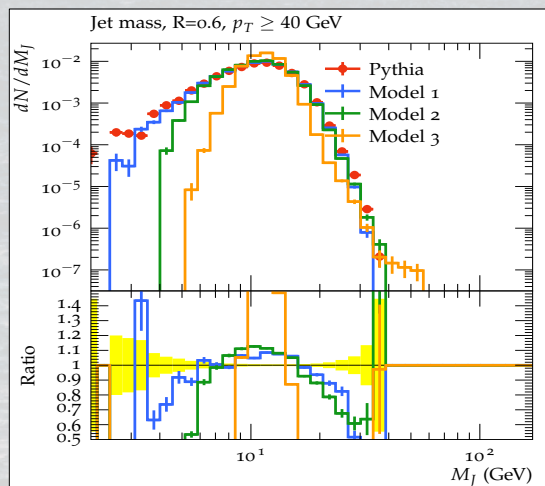
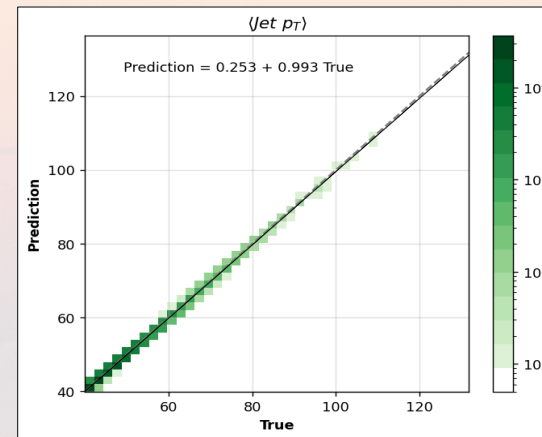
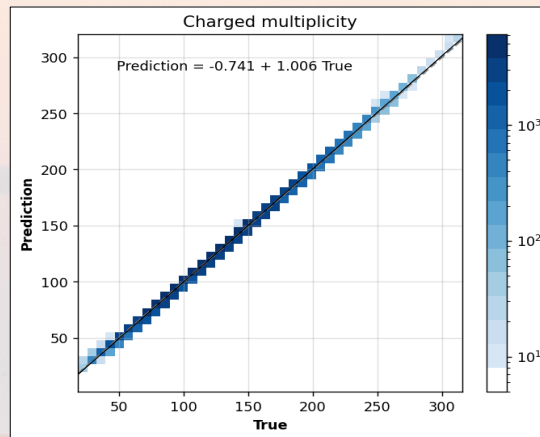
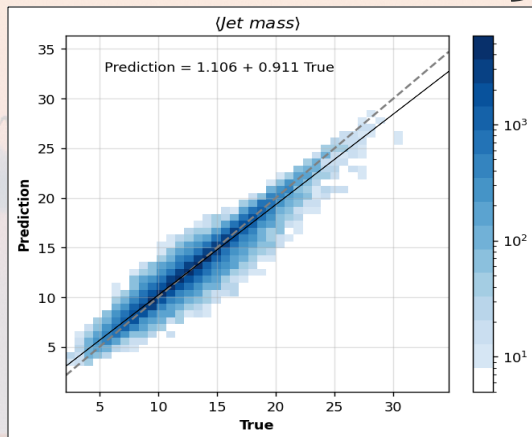
Reduce the input to $\mathcal{O}(10^2)$

$\left. \begin{array}{l} \mathcal{O}(10^3 - 10^4) \text{ Total pixels} \\ \text{vs } \mathcal{O}(10^2) \end{array} \right\}$
Pixels with information



doi:10.1007/BF02288367

Dimensionality (work in progress)



Machine Learning in HEP

Track reconstruction

Particle Track Reconstruction with Deep Learning

Steven Farrell, Paolo Calafiura, Mayur Mudigonda, Prabhat
Lawrence Berkeley National Laboratory
{SFarrell,PCalafiura,Mudigonda,Prabhat}@lbl.gov

**Dustin Anderson, Josh Bendavid, Maria Spiropoulou,
Jean-Roch Vlimant, Stephan Zheng**
California Institute of Technology
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**Giuseppe Cerati, Lindsey Gray, Keshav Kapoor, Jim Kowalkowski,
Panagiotis Spentzouris, Aristeidis Tsaris, Daniel Zurawski**
Fermi National Accelerator Laboratory
{cerati,lgray,kkapoor,jbk,spentz,
atsaris,zurawski}@fnal.gov

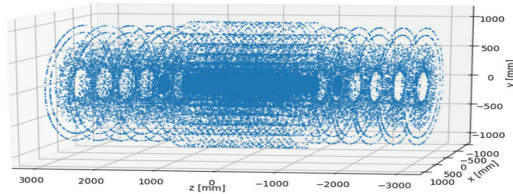
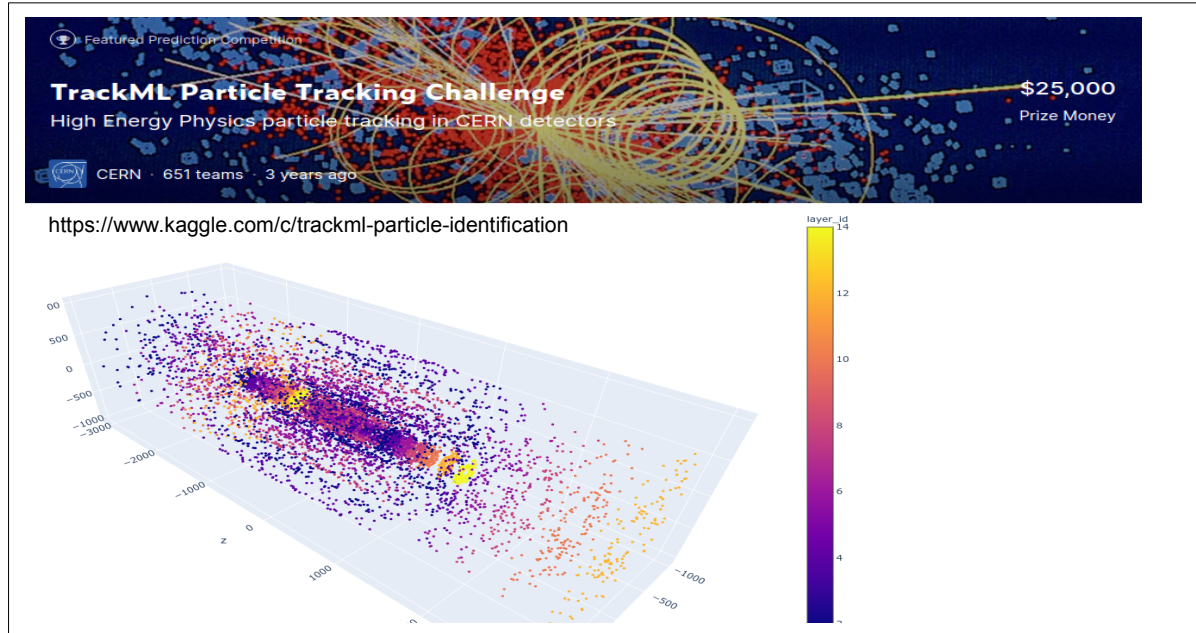
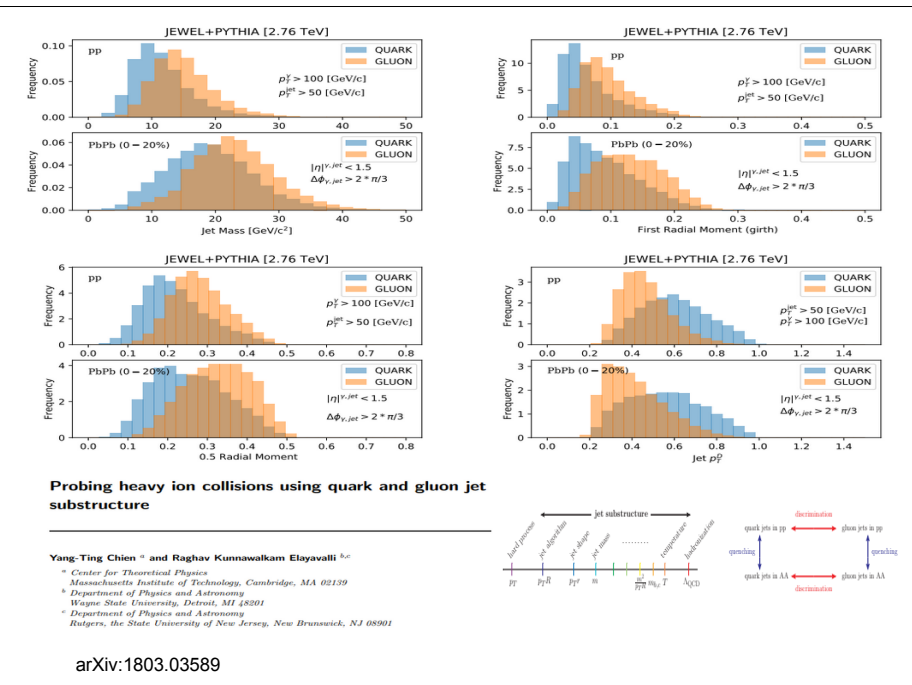


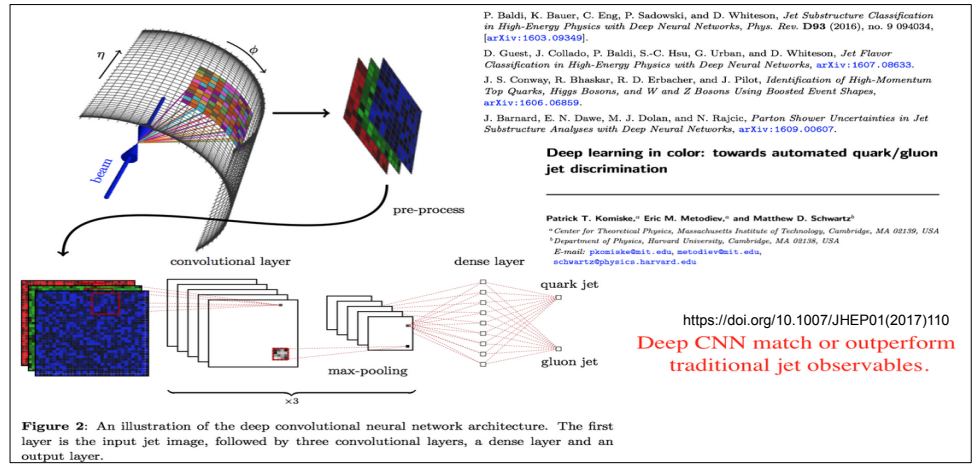
Figure 1: Distribution of particle spacepoints in a particle collision event in a generic simulated HL-LHC tracking detector.



Machine Learning in HEP



Quark/gluon jet separation



Machine Learning in HEP

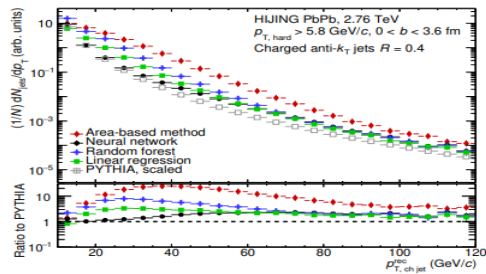
Machine Learning based jet momentum reconstruction in heavy-ion collisions

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(Dated: June 24, 2019)



Feature	Score	Feature	Score
Jet p_T (no corr.)	0.1355	$p_{T, \text{const}}^1$	0.0012
Jet mass	0.0007	$p_{T, \text{const}}^2$	0.0039
Jet area	0.0005	$p_{T, \text{const}}^3$	0.0015
Jet p_T (area-based corr.)	0.7876	$p_{T, \text{const}}^4$	0.0011
LeSub	0.0004	$p_{T, \text{const}}^5$	0.0009
Radial moment	0.0005	$p_{T, \text{const}}^6$	0.0009
Momentum dispersion	0.0007	$p_{T, \text{const}}^7$	0.0008
Number of constituents	0.0008	$p_{T, \text{const}}^8$	0.0007
Mean of const. p_T	0.0585	$p_{T, \text{const}}^9$	0.0006
Median of const. p_T	0.0023	$p_{T, \text{const}}^{10}$	0.0007

FIG. 9. Reconstructed charged jet spectra in HIJING events and the ratio to (N_{coll} -scaled) PYTHIA jet spectra.

<https://doi.org/10.1103/PhysRevC.99.064904>

Jet reconstruction

Machine Learning based jet momentum reconstruction in Pb–Pb collisions measured with the ALICE detector

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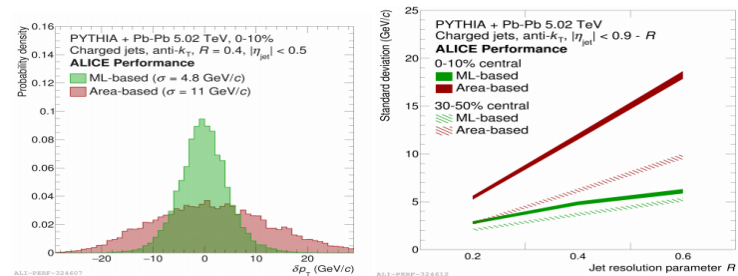


Figure 1: Residual p_T -distributions of embedded jet probes of known transverse momentum.

<https://doi.org/10.22323/1.364.0312>

Machine Learning in HEP

Tuning Monte Carlo event generators

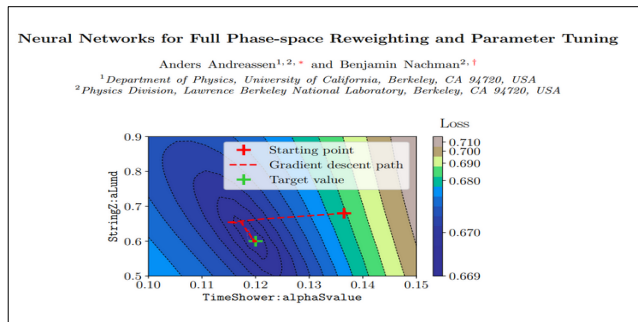
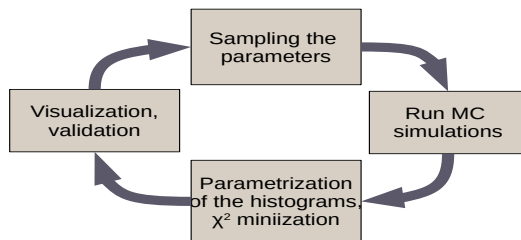


Figure 1: An illustration of the parametrization of the generator response as implemented in the Per Bin Model.

Figure 2: An illustration of the Inverse Model strategy.

MCNNTUNES: tuning Shower Monte Carlo generators with machine learning

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<https://doi.org/10.1016/j.cpc.2021.107908>

Accelerating Science with Generative Adversarial Networks: An Application to 3D Particle Showers in Multi-Layer Calorimeters

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<https://doi.org/10.1103/PhysRevLett.120.042003>