Modeling charged-particle spectra in pp collisions with deep neural networks

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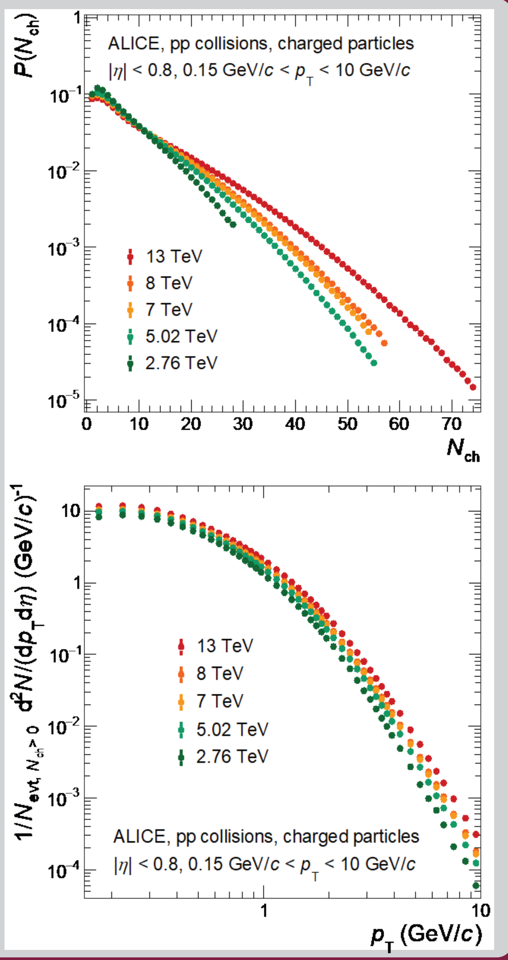
Motivation

Fundamental observables, like the inclusive charged-particle multiplicity (N_{ch}) distributions and transverse momentum (p_T) spectra, precisely characterize the final state of pp collisions

ALICE published a comprehensive dataset of N_{ch} distributions and p_T spectra within 0.15 GeV/c < p_T < 10 GeV/c and $|\eta| < 0.8$ for pp collisions ranging from $\sqrt{s}$ = 2.76-13 TeV [1]

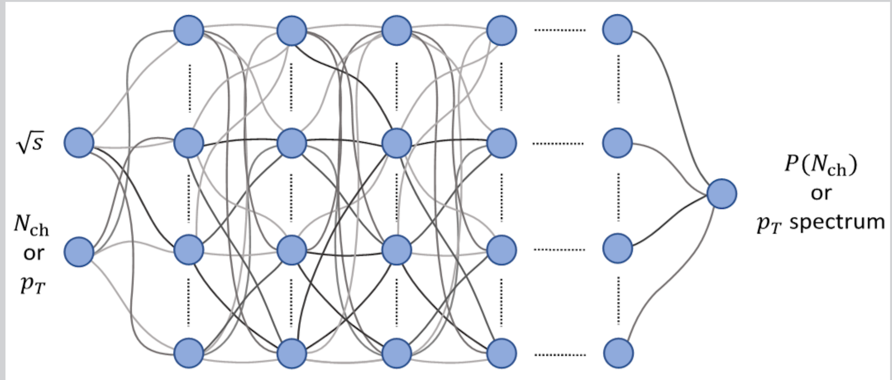
Those results demonstrate that predicting the collision-energy dependence of these observables remains a challenging task for PYTHIA simulations using the Monash13 tune [2]

Deep neural networks (DNNs) provide a purely data-driven alternative to predict these observables at unmeasured energies
→ Proof of principle with provided by MC-based study in [3]



Approach

Model sketch:



- Fully connected DNN implemented with Tensorflow & Keras
- Two separate models for the prediction of N_{ch} and p_T yields
- Two inputs each N_{ch} | p_T and $\sqrt{s}$
- Fixed number of nodes per layer
- Model configuration determined in hyperparameter scan

Data preparation:

- Logarithmic scaling of p_T, N_{ch} and $\sqrt{s}$
  → More linear tail for better extrapolation capabilities
- Data shuffeling and splitting into training and validation sets (80% / 20%)
- Data augementation by redinifing each initial data point N times within its range of uncertainties
  → Better training performance and stability

Model Tuning & Uncertainties

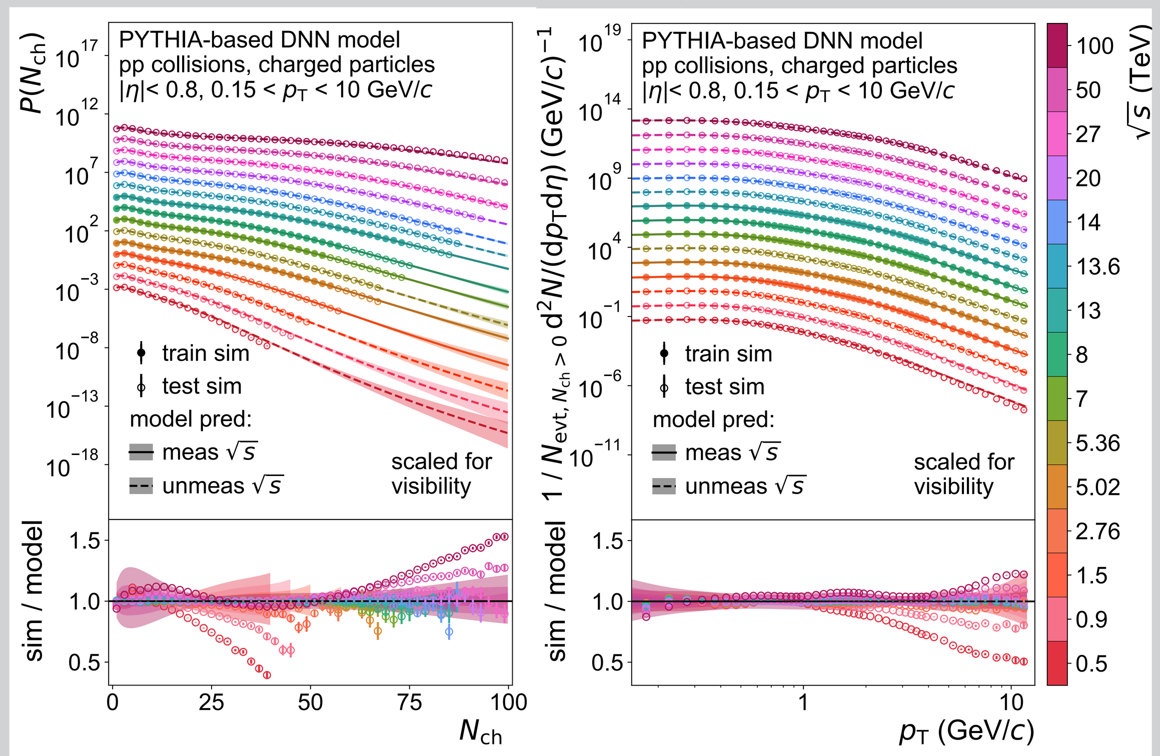
Hyperparameter scan:
Bayesian-optimization [4] search for best model architecture

sampling: discrete values			
layers	neurons per layer	activation function	initializer
2	32	TanH (TH)	RandomUniform (RU)
3	64	ReLU (RE)	RandomNormal (RN)
4	128	SeLU (SE)	TruncatedNormal (TN)
5	256	Swish (SW)	GlorotUniform (GN)
	512	Mish (MI)	GlorotNormal (GU)
		Softplus (SP)	
sampling: intervals (logarithmic)			
	λ_1	λ_2	learning rate (lr)
min	$5 \cdot 10^{-8}$	$5 \cdot 10^{-8}$	$1 \cdot 10^{-5}$
max	$5 \cdot 10^{-1}$	$5 \cdot 10^{-1}$	$1 \cdot 10^{-3}$

- Extrapolation capability evaluated with PYTHIA simulations
  → ALICE-equivalent energies (training/validation)
  → Selected energies within 0.5 – 100 TeV (test)
- Target score: Quadratic mean of validation MAE & test MAE
→ Best-performing architecture retrained on ALICE data

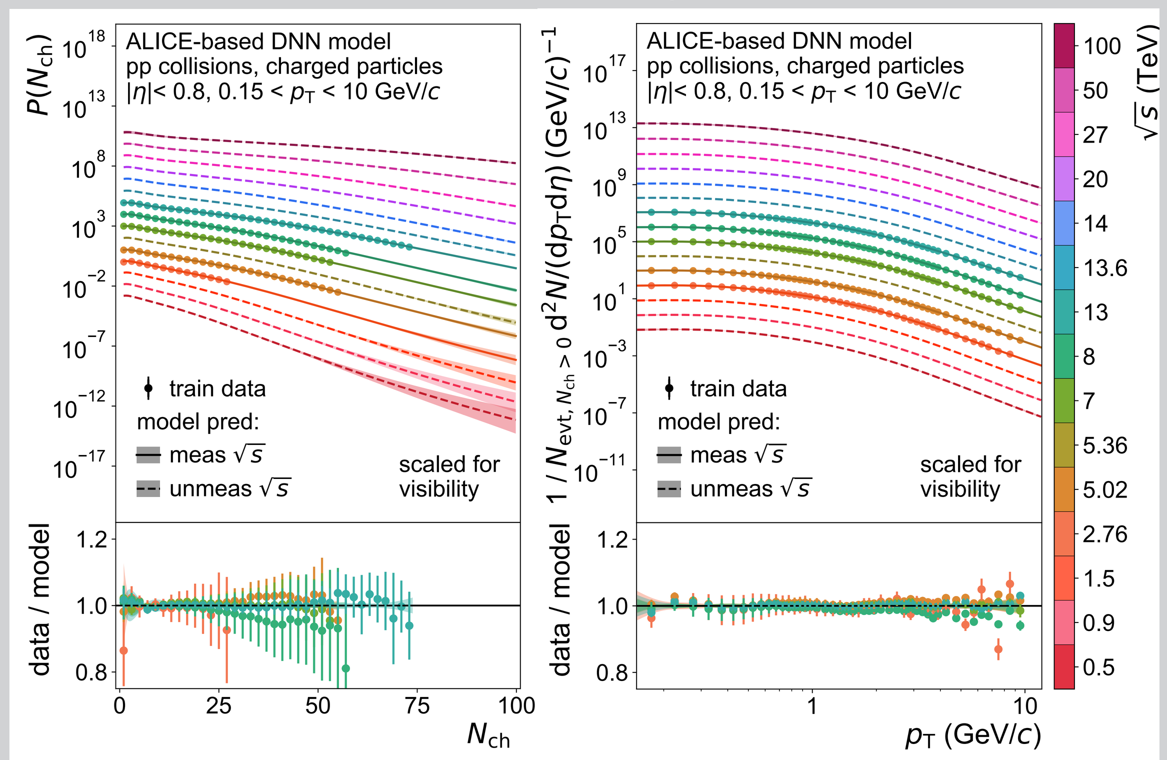
Uncertainty estimation:
Two different sources are added in quadrature
- Spread of Top5 perfroming hyperparameter configurations
- Ensemble of 20 random initializations of the top model

PYTHIA-based DNN predictions



Regression performance :
- Good description of training data with deviation < 2%
- Extrapolation for 2.76 ≤ $\sqrt{s}$ ≤ 20 TeV within 5%
- Inside 1.5 ≤ $\sqrt{s}$ ≤ 27 TeV accuracy drops to 10%
- For the highest and lowest energeis the model fails to describe the simulation within its uncertainties

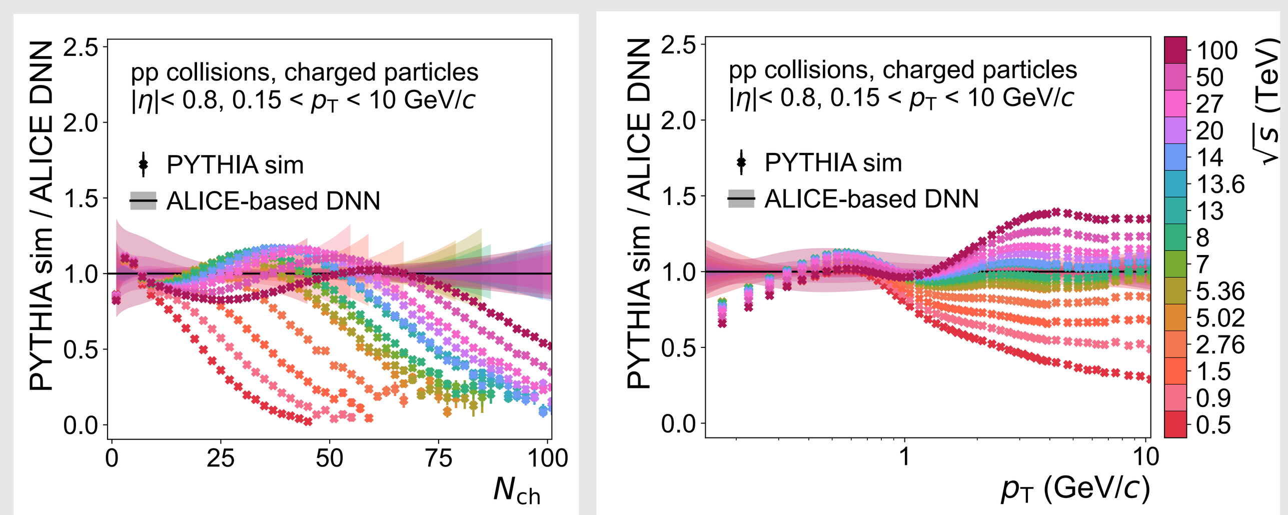
ALICE-based DNN predictions



Retrained on ALICE data:
- Similar performance compared to PYTHIA-based model
- All available data within their corresponding uncertainties
- Solid extrapolation in N_{ch} and p_T by about 20%

→ Reliable interpolation to unmeasured energies

PYTHIA Comparison



Ratio of PYTHIA to DNN predictions:

The simulations are compared to a wide range of energies:
- For lower N_{ch} (< 20) and p_T (< 1 GeV/c), PYTHIA deviates from the predictions by up to 20% for all studied energies
- At higher N_{ch} and p_T, the comparison indicates an energy dependence of PYTHIA's accuracy decreasing beyond the energy range used in the tuning process
- The trend observed for the training energies is further extended to unmeasured energies
- Especially at lower energies a larger tension is observed

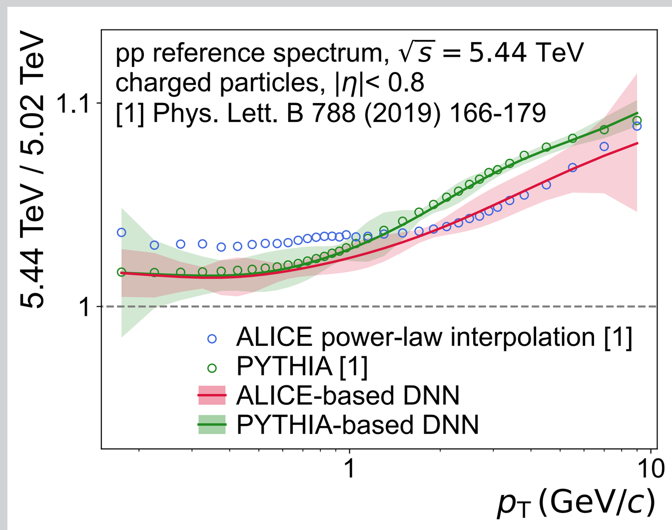
→ These deviations between the PYTHIA simulations and the data-driven predictions could provide feedback for future PYTHIA tunes

Model Application

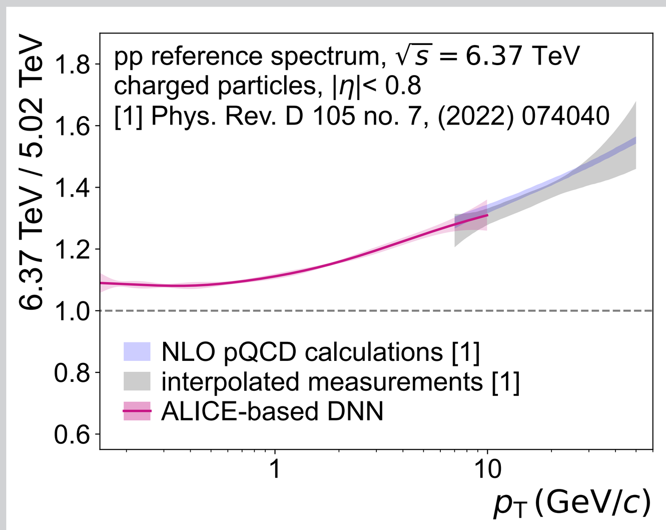
Construction of pp reference spectra for the nuclear modification factor:

- Extract relative change of the p_T spectra at different energies
- Apply to a chosen baseline pp measurement
  → Allows consistent event class definition between pp and AA

A suitable baseline provided by the ALICE measurement at $\sqrt{s}$ = 5.02 TeV
→ High precision & close in energy to the interpolation targets



Xe–Xe at $\sqrt{s}$ = 5.44 TeV [5]:
- Consistent with established power-law interpolation at high p_T
- Reduced fluctuations and matching with PYTHIA at low p_T



O–O at $\sqrt{s}$ = 6.37 TeV [6]:
- Extending the pp reference to much lower p_T
- At high p_T, good agreement with functional interpolation & theory

Conclusion & Outlook

This approach could provide a more accurate reference than established methods or PYTHIA estimations.
It could be helpful for future heavy-ion runs where no explicit pp reference measurements are foreseen.
In the future, the procedure could be extended to the measured correlation of N_{ch} and p_T to further constrain the particle production or to identified particle spectra in other analyses.

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[2] P. Skands, S. Carrazza, and J. Rojo, "Tuning PYTHIA 8.1: the Monash 2013 Tune", Eur. Phys. J. C 74 no. 8, (2014) 3024,
[3] E. Shokr, A. De Roeck, and M. A. Mahmoud, "Modeling of N_{ch} and p_T distributions in pp collisions using a DNN", Sci. Rep. 12 no. 1, (2022) 8449.
[4] R. Garnett, Bayesian Optimization. Cambridge University Press, 2023
[5] ALICE, "Transverse momentum spectra and nuclear modification factors of charged particles in Xe-Xe collisions at $\sqrt{s}$ =5.44 TeV", Phys. Lett. B 788 (2019) 166–179
[6] J. Brewer, A. Huss, A. Mazeliauskas, and W. van der Schee, "Ratios of jet and hadron spectra at LHC energies: Measuring high-p_T suppression without a pp reference", Phys. Rev. D 105 no. 7, (2022) 074040

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