Effective denoising diffusion probabilistic models for fast and high fidelity whole-event simulation in high-energy heavy-ion experiment

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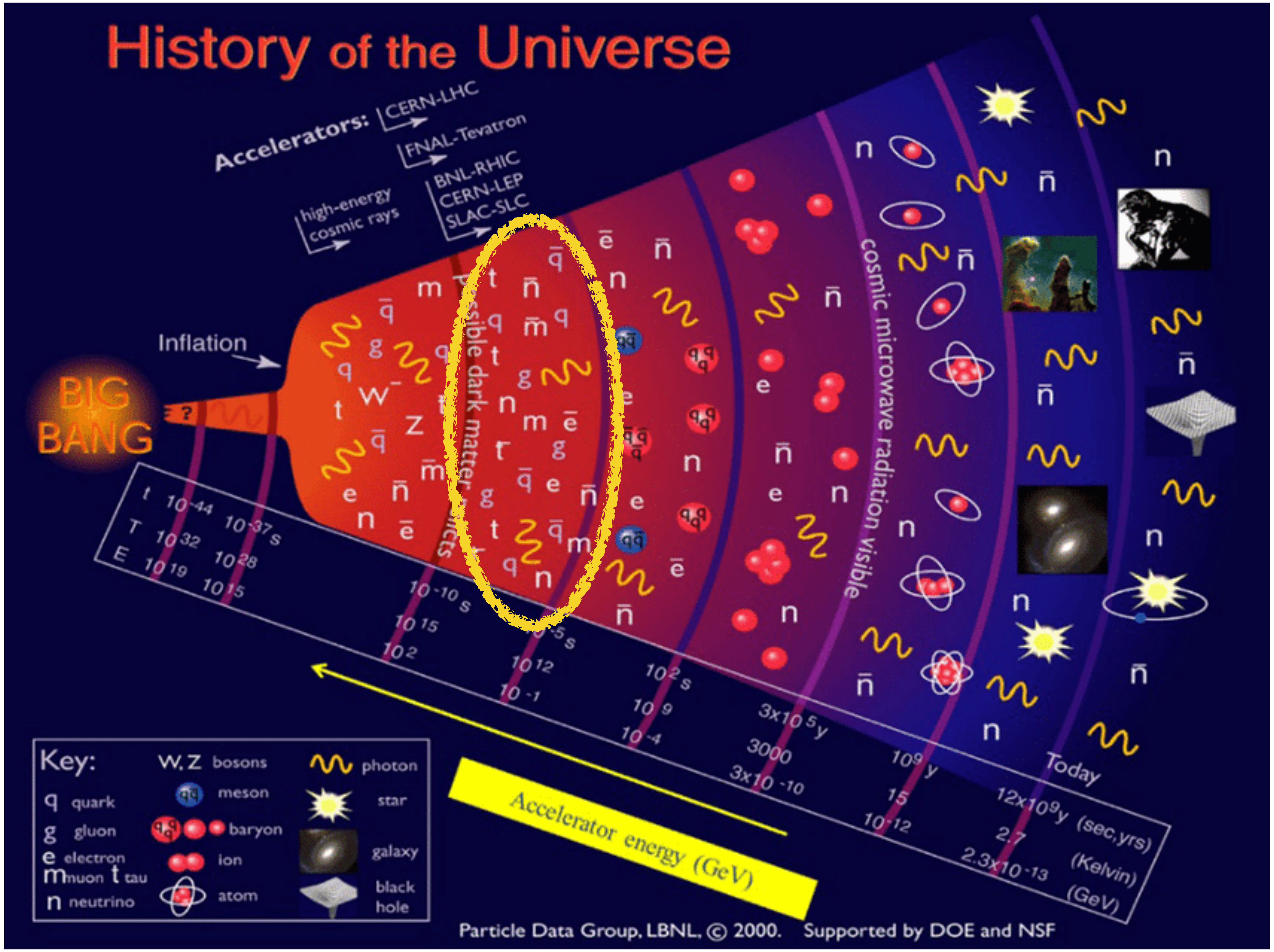
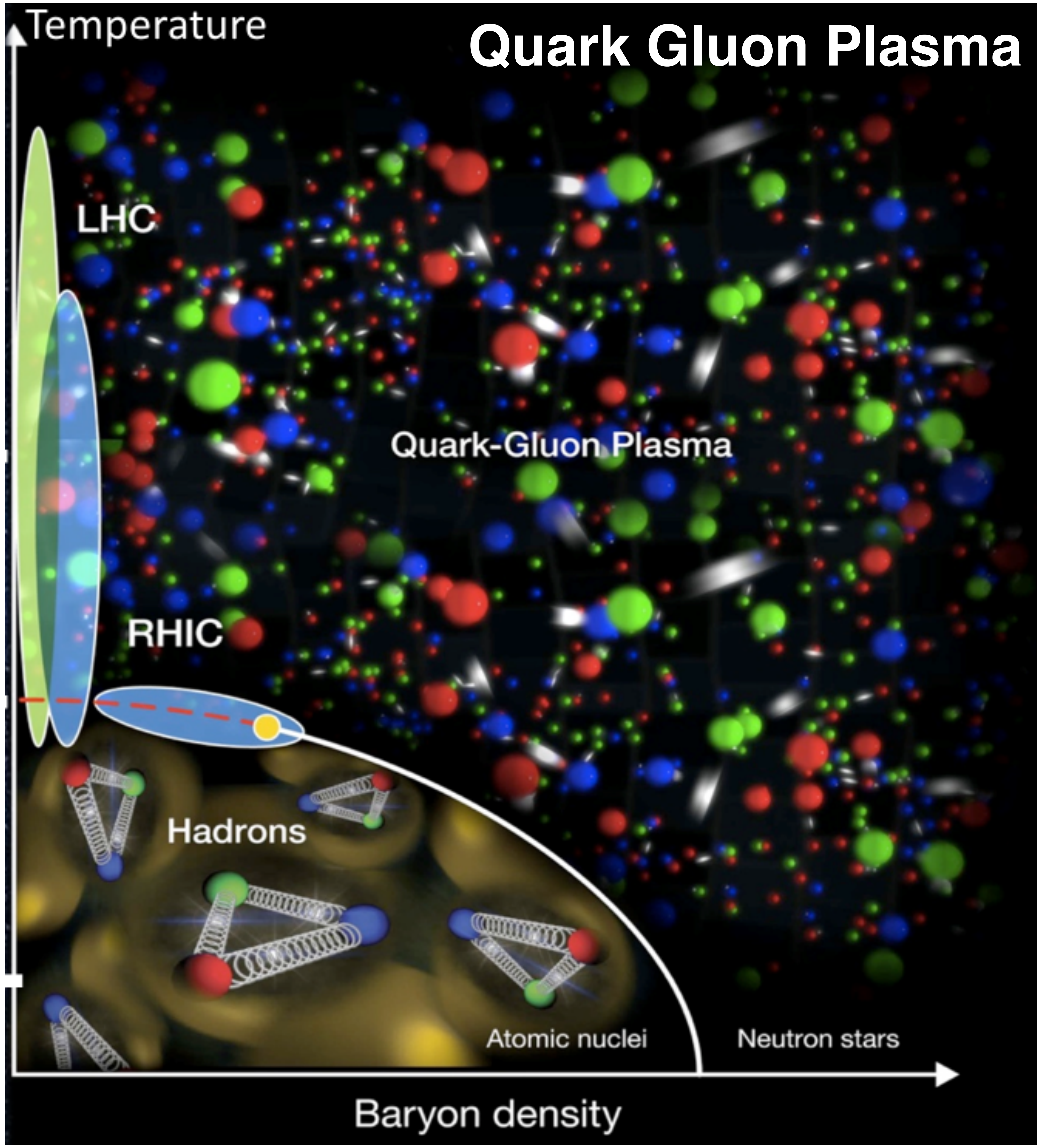
BNL Physics 8th Joint Meeting on AI/ML
Apr. 3, 2024

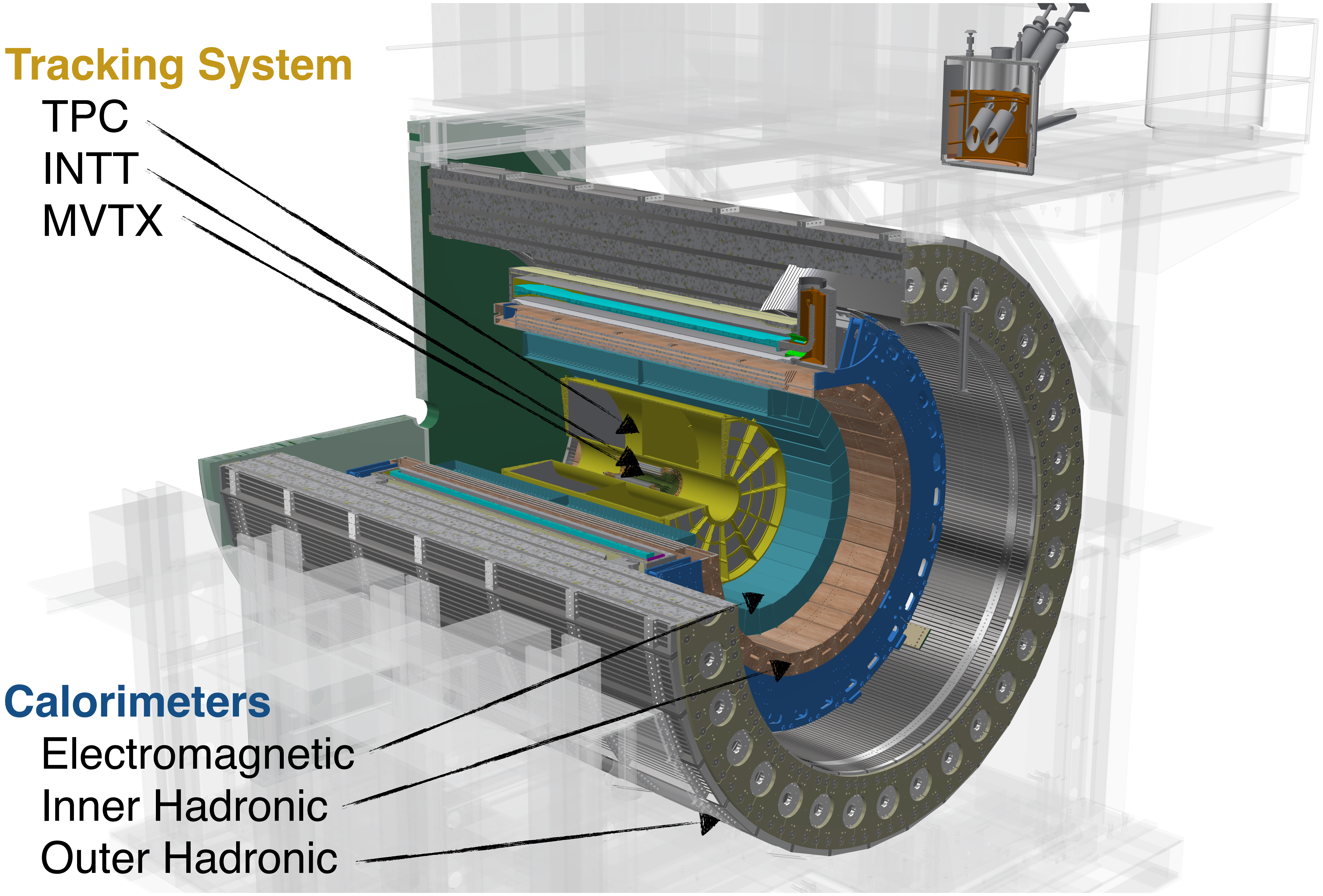
Brookhaven National Laboratory

Early Universe and Quark Gluon Plasma





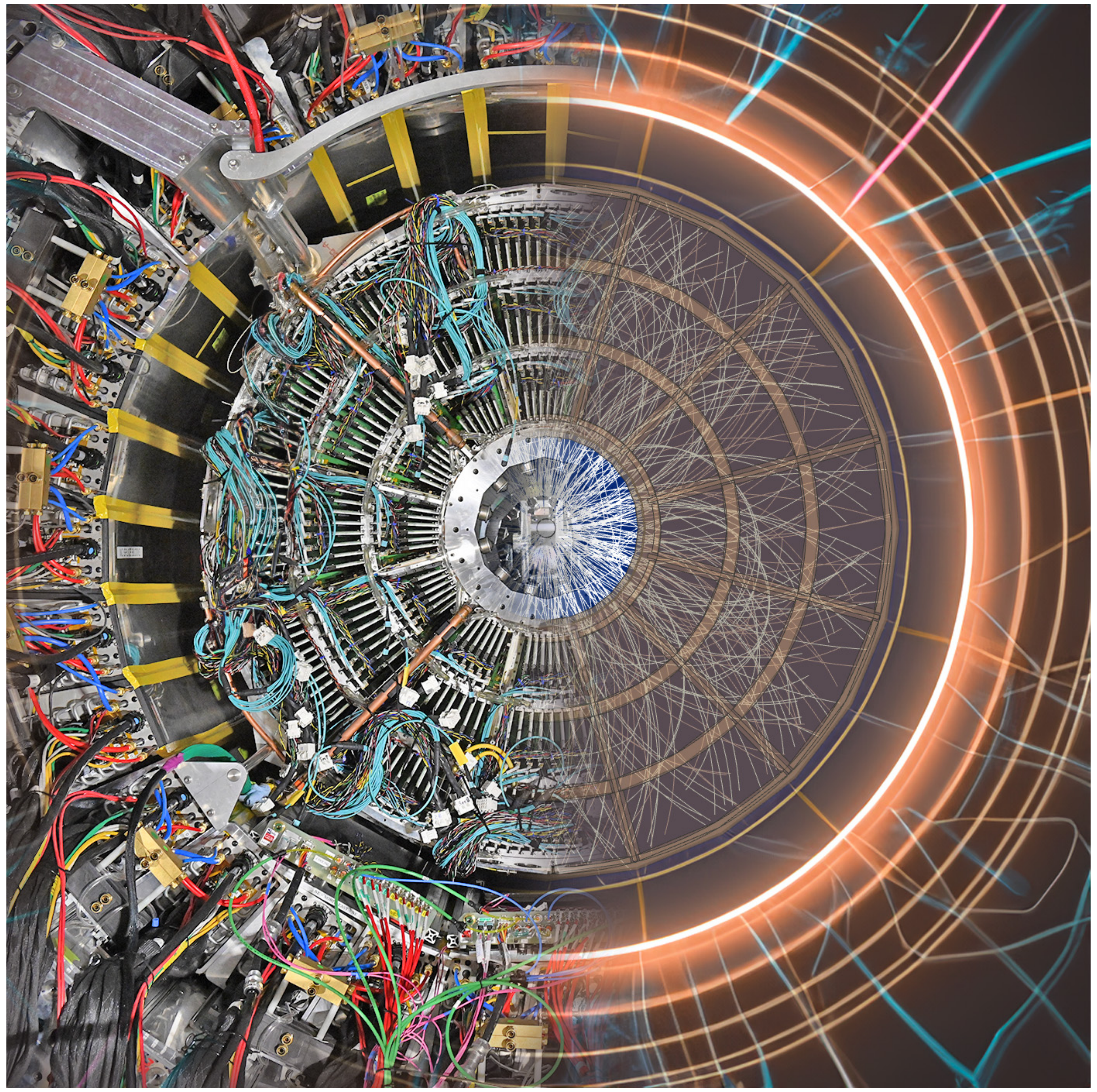
sPHENIX Detector at RHIC



- Data taking began last year!
- High-precision tracking system + Hermetic Electromagnetic & Hadronic calorimeters

Simulations of Relativistic Heavy Ion Collisions

- ***O(1000) particles*** in one nuclear collision event
  + ***thousands shower steps*** per particle
  ➡ Simulation of the interaction of particles with detectors is **high complexity and computationally intensive work**



sPHENIX TPC

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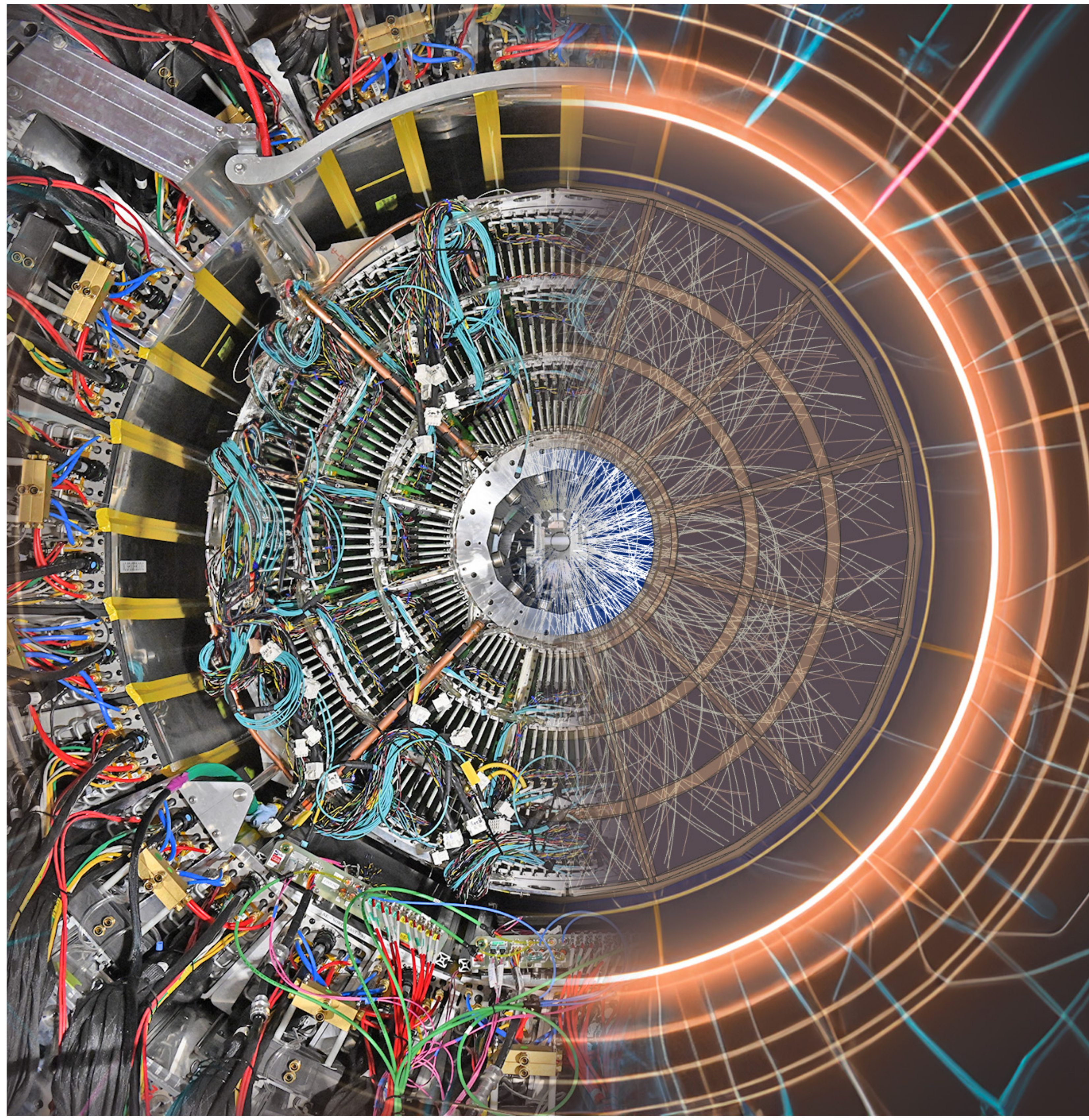

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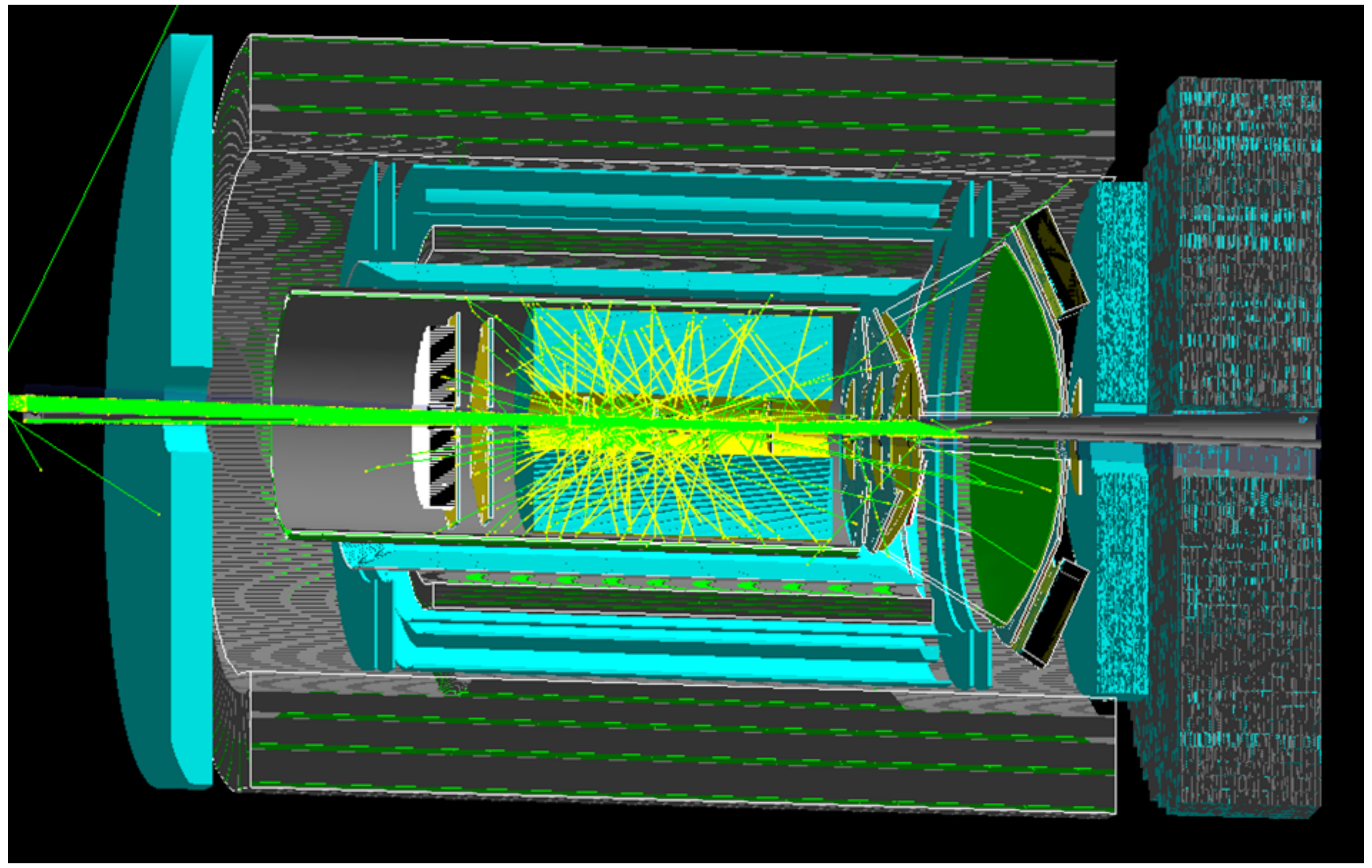

EIC CDR

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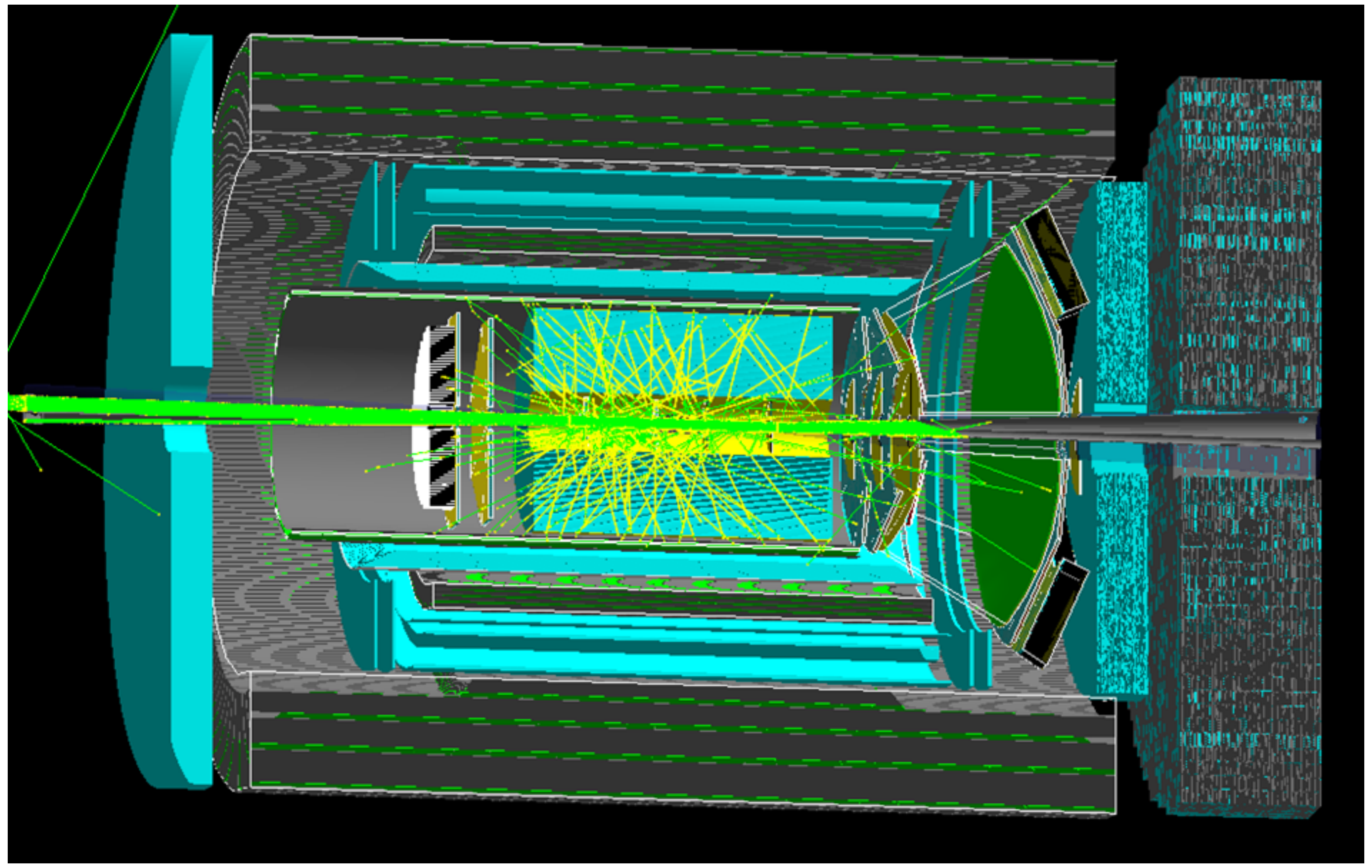
  ➡ Simulation of the interaction of particles with detectors is **high complexity and computationally intensive work**
- *Electron-Ion Collider* will need a large amount of simulations of full detector with both physics and machine background
- ML can speed up and produce large amount of the heavy ion event simulations!



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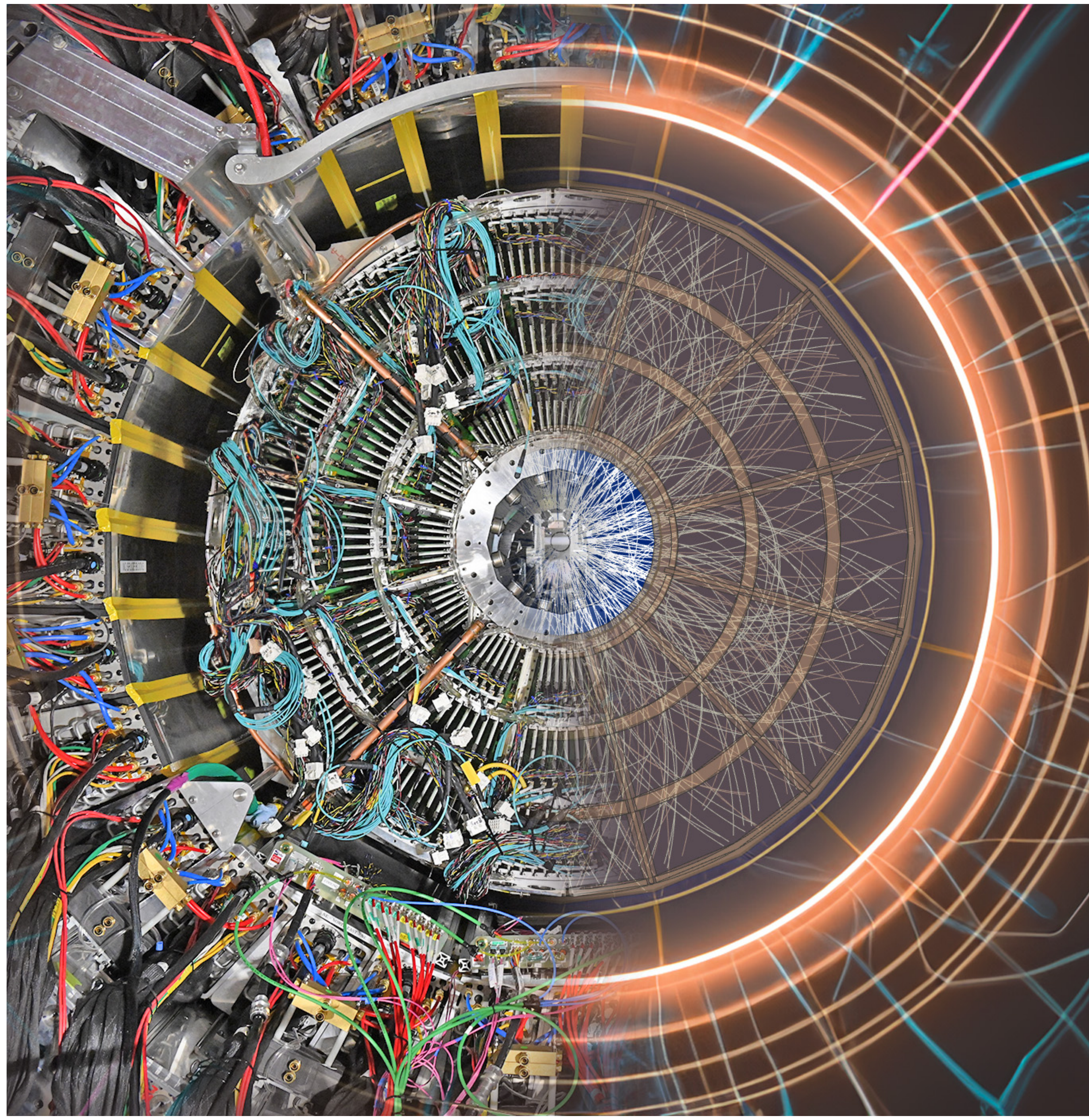


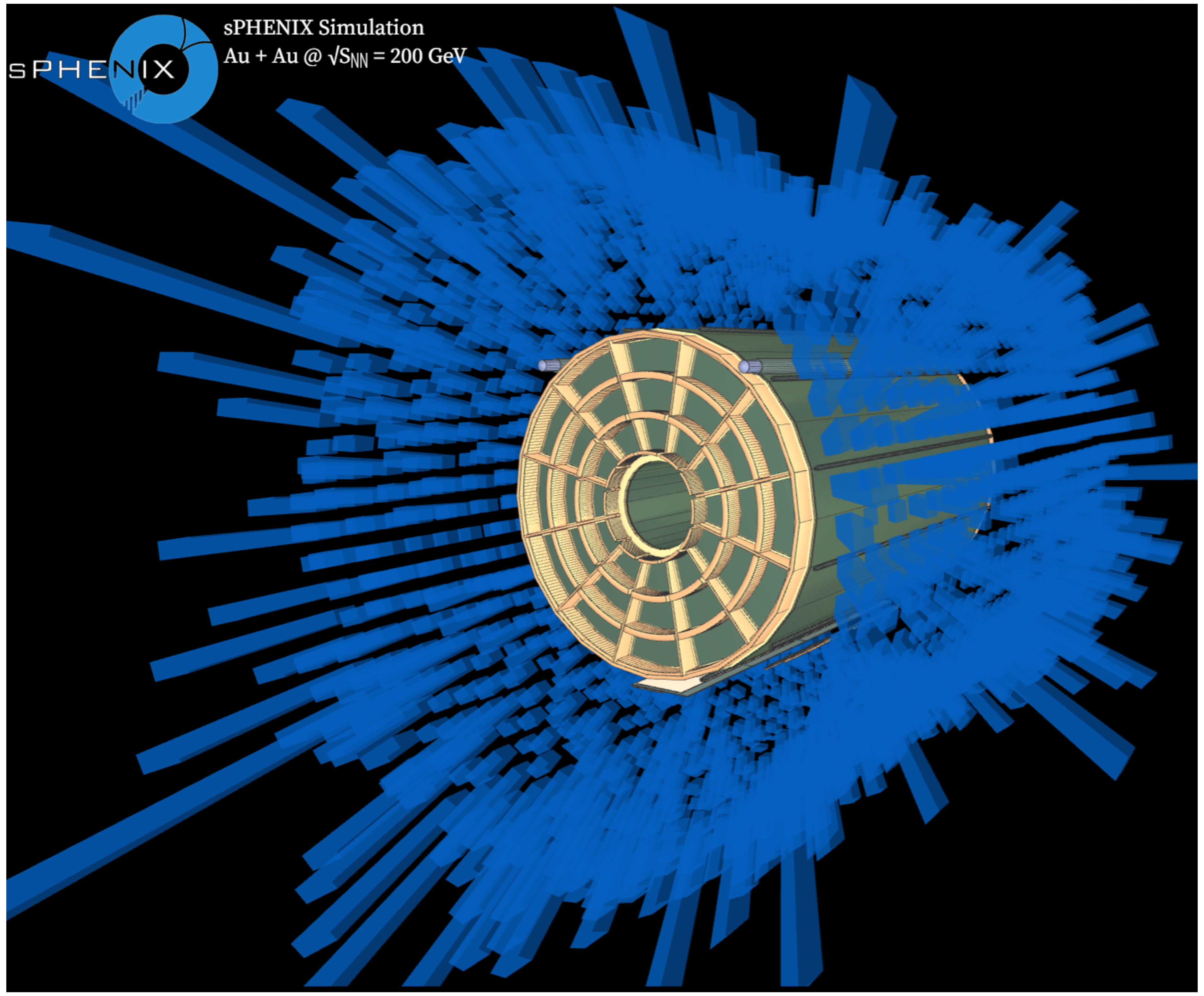
sPHENIX TPC

We introduce ***full detector whole-event ML simulations*** for heavy ion collisions

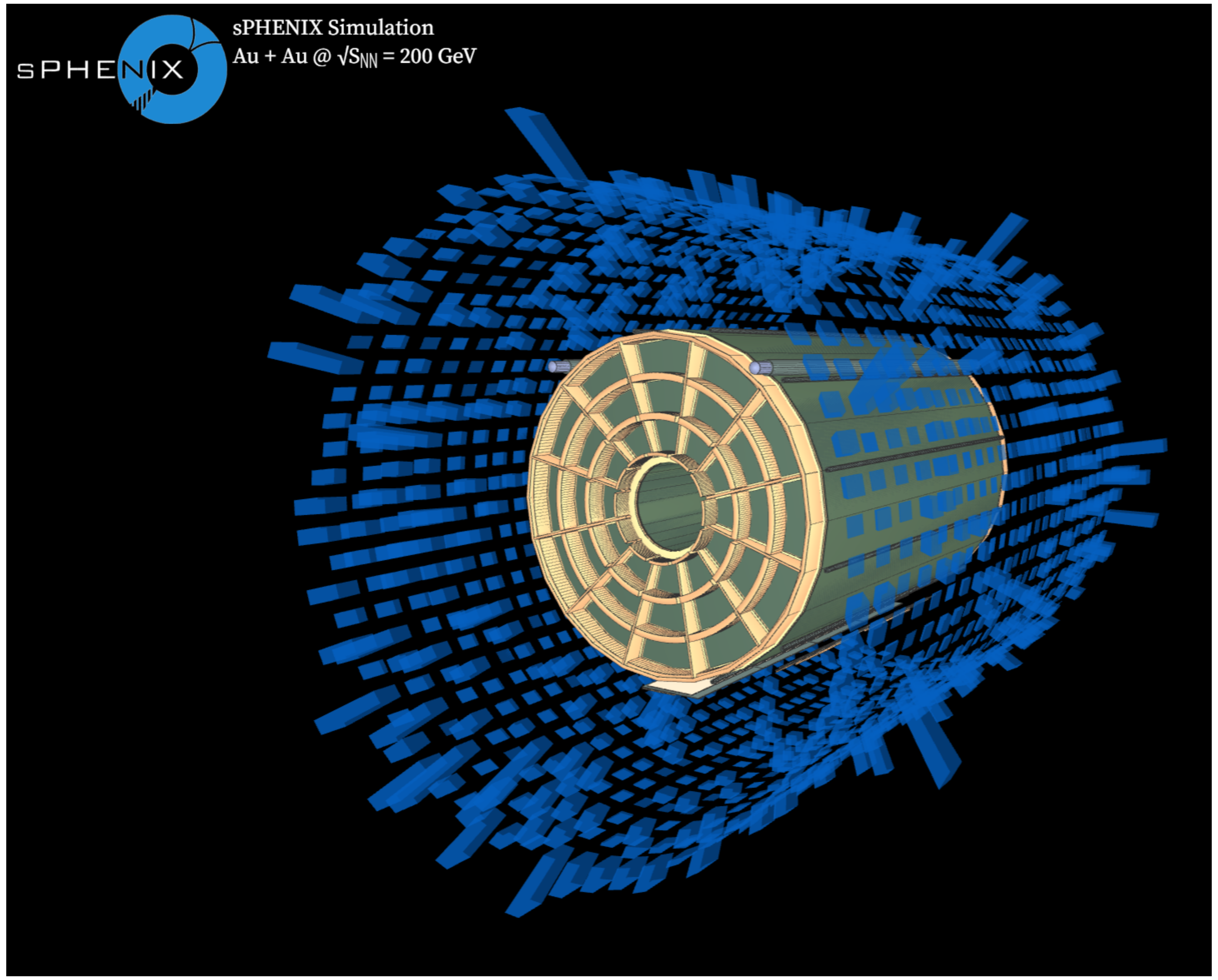
Heavy Ion Collision Event

- **HIJING** Monte Carlo event generator for Au+Au collisions at $\sqrt{s_{NN}}$=200 GeV
- **Geant4** full detector simulation with the sPHENIX geometry

Head-on collision (0-10% Centrality)

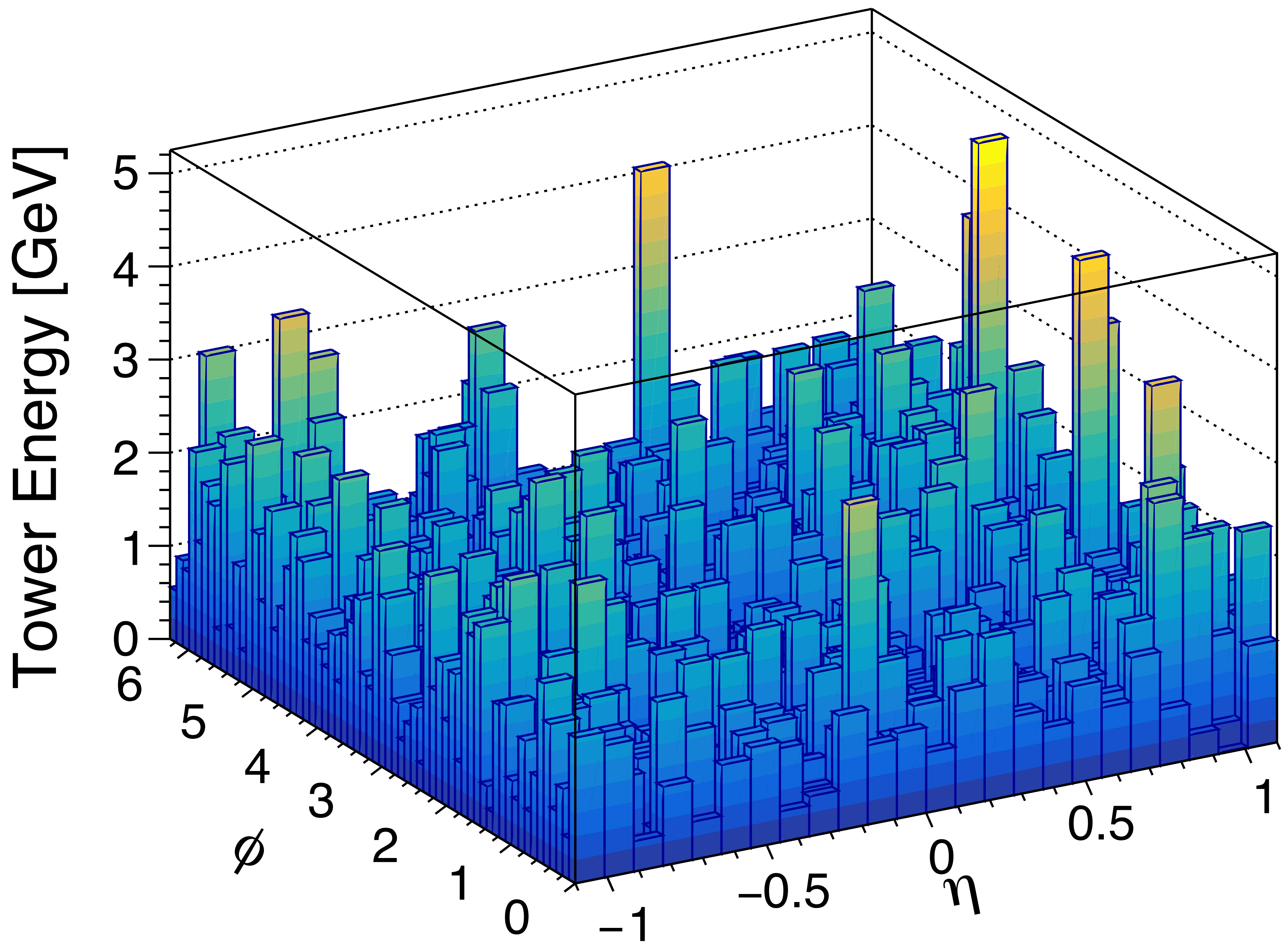


Side collision (40-50% Centrality)



Tower Distributions

0-10% Centrality



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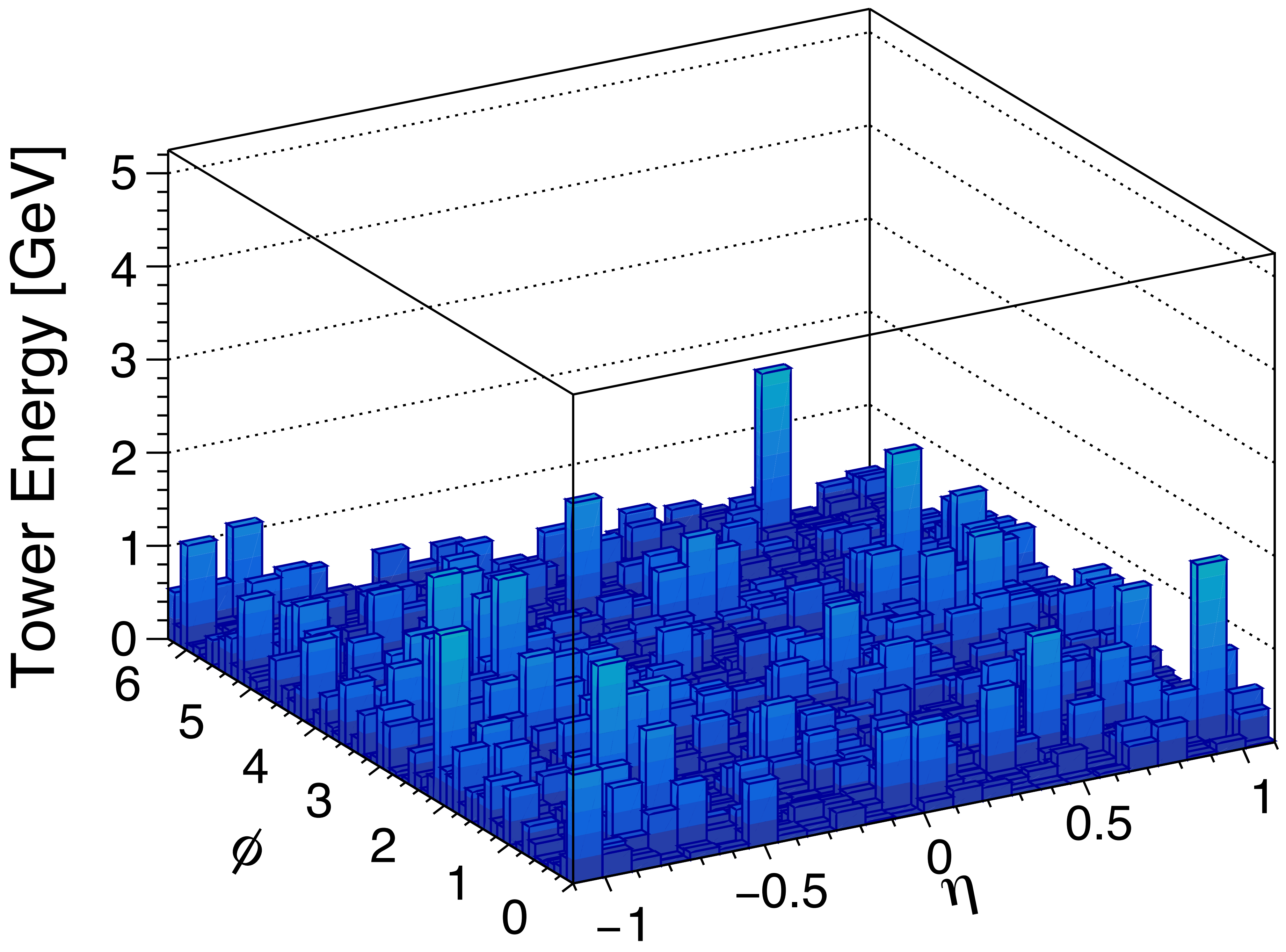
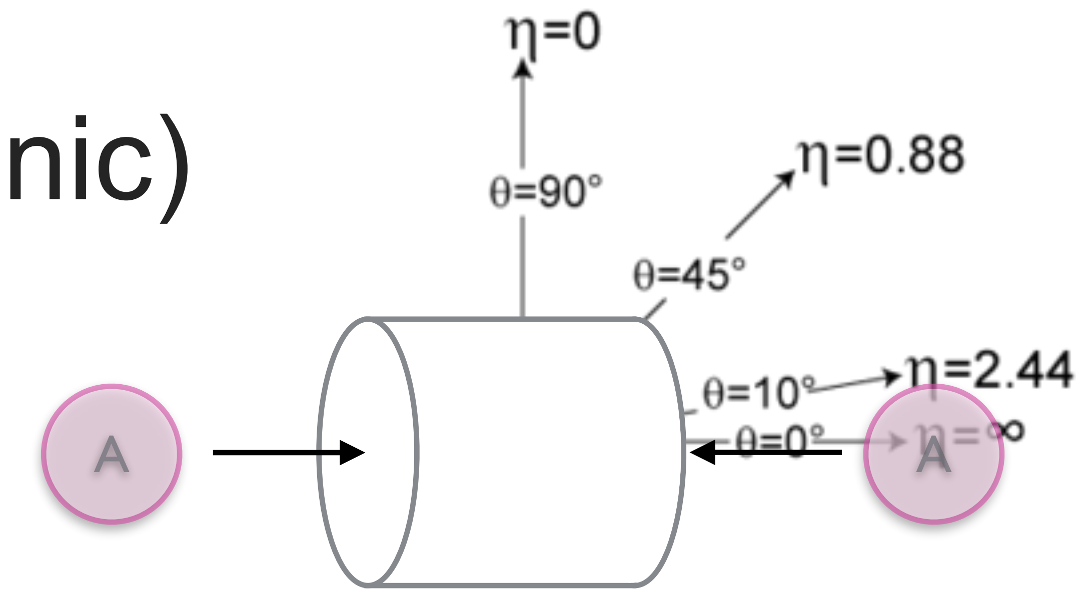


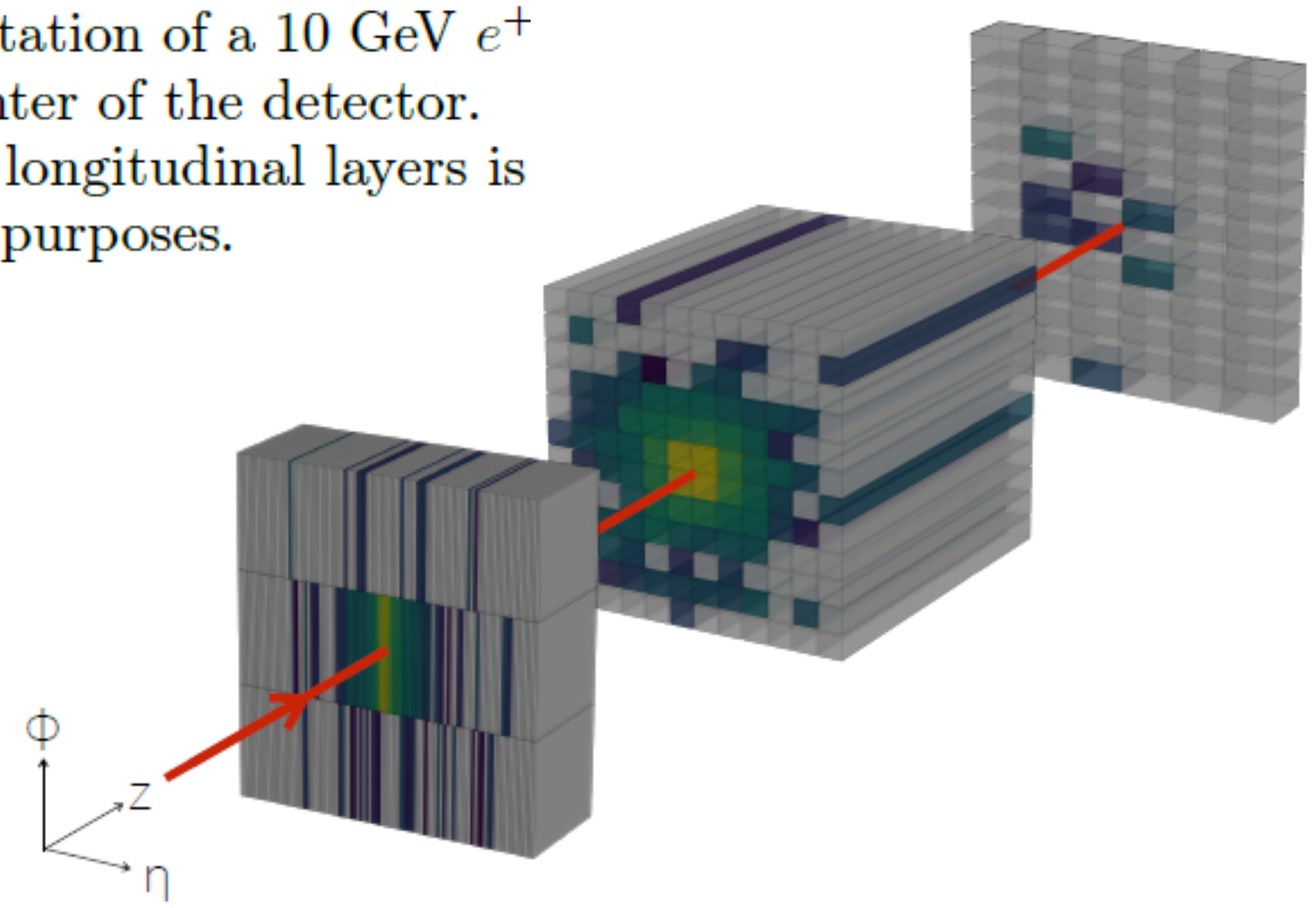
- Full calorimeter **towers** (Electromagnetic + Inner hadronic + Outer hadronic)
  - ➡ $-1.1 < \eta < 1.1, \quad 0 < \phi < 2\pi$
  - ➡ (24 x 64) bins in (η, ϕ)



Generative AI

- **Generative Adversarial Networks (GAN)**
  - ➡ actively used in high energy physics *(e.g. arXiv:1712.1032, arXiv:2209.07559, EPJC 80 (2020) 688, arXiv:2210.14245)*

FIG. 2: Three-dimensional representation of a 10 GeV e^+ incident perpendicular to the center of the detector. Not-to-scale separation among the longitudinal layers is added for visualization purposes.



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- **Diffusion Models**: text-to-image generation in industry (e.g. StableDiffusion, Midjourney, Dalle-2)

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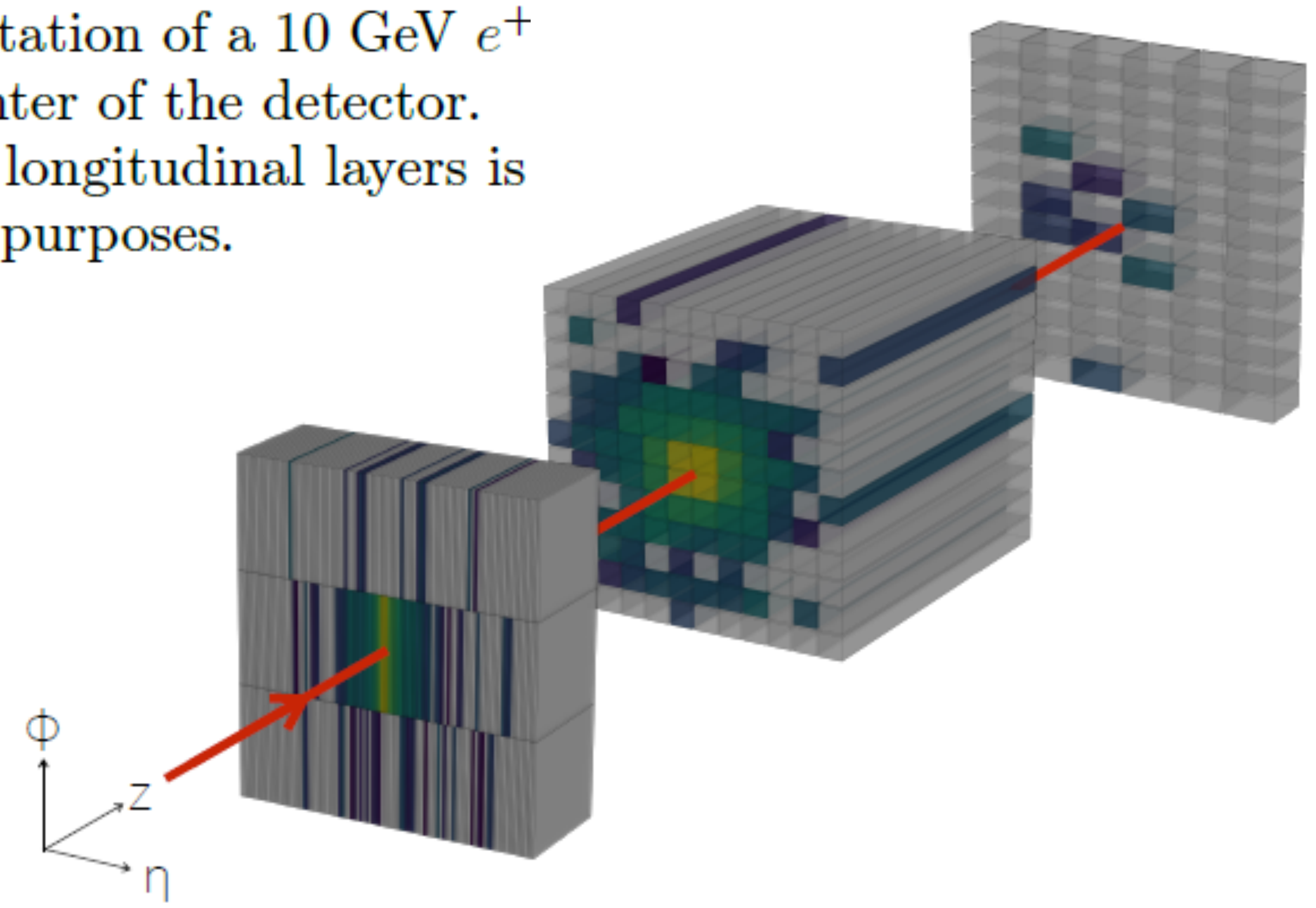
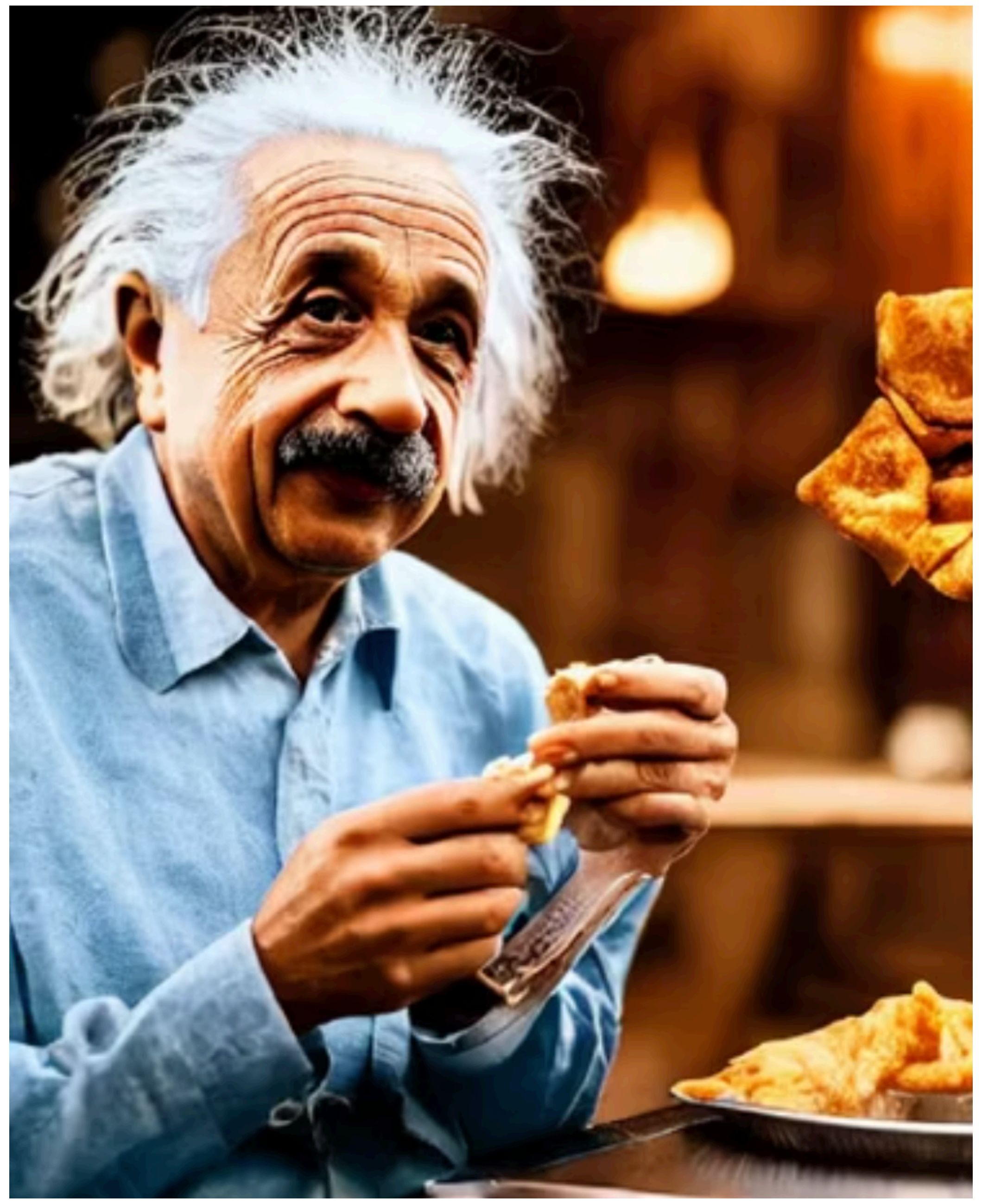
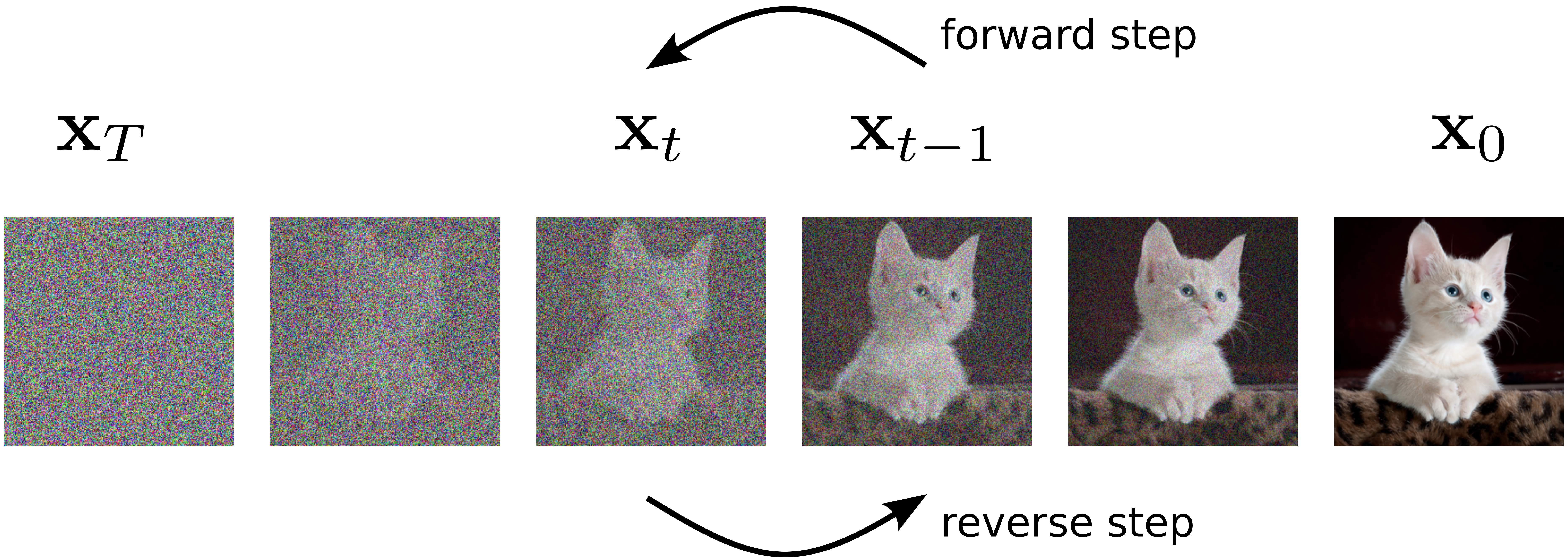




Denoising Diffusion Probabilistic Model (DDPM)

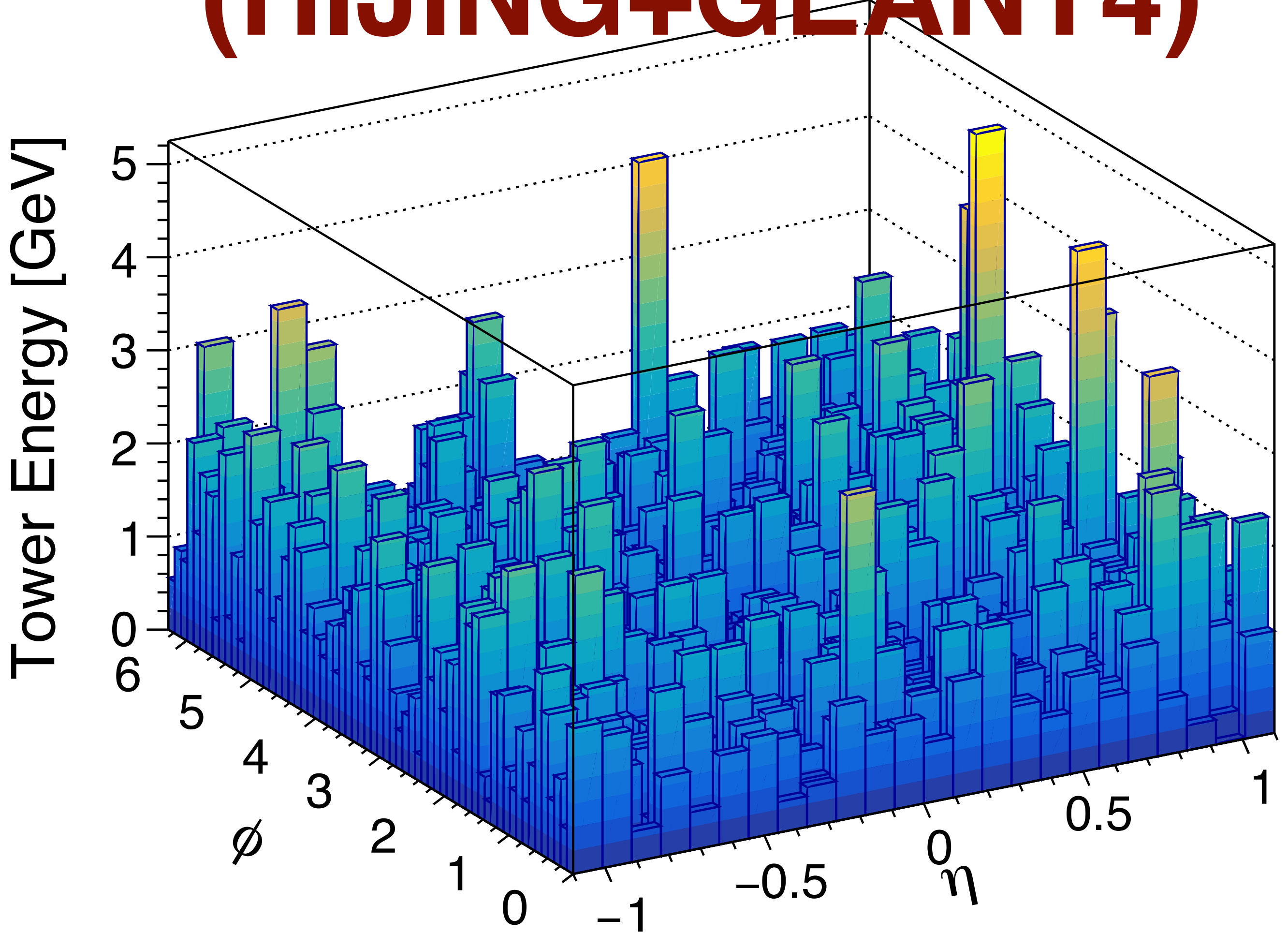
- DDPM provides ***high quality data from random noise***
- **Forward** process: add random gaussian noise
- **Reverse** process: use neural network and <u>generate data</u>
- In real application, O(1,000) steps are used



Display of Generated Events

Training sample (HIJING+GEANT4)

0-10% Centrality



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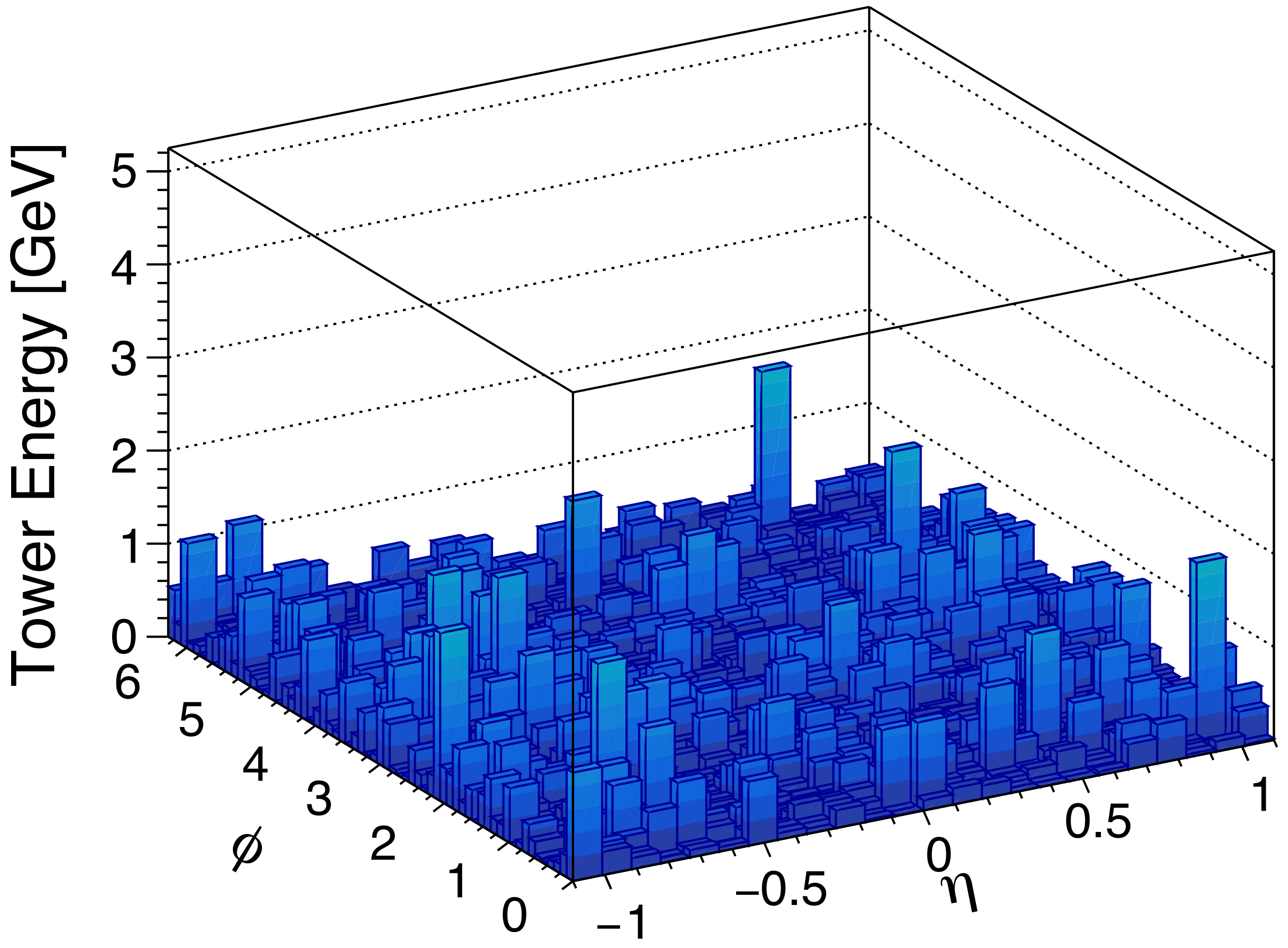
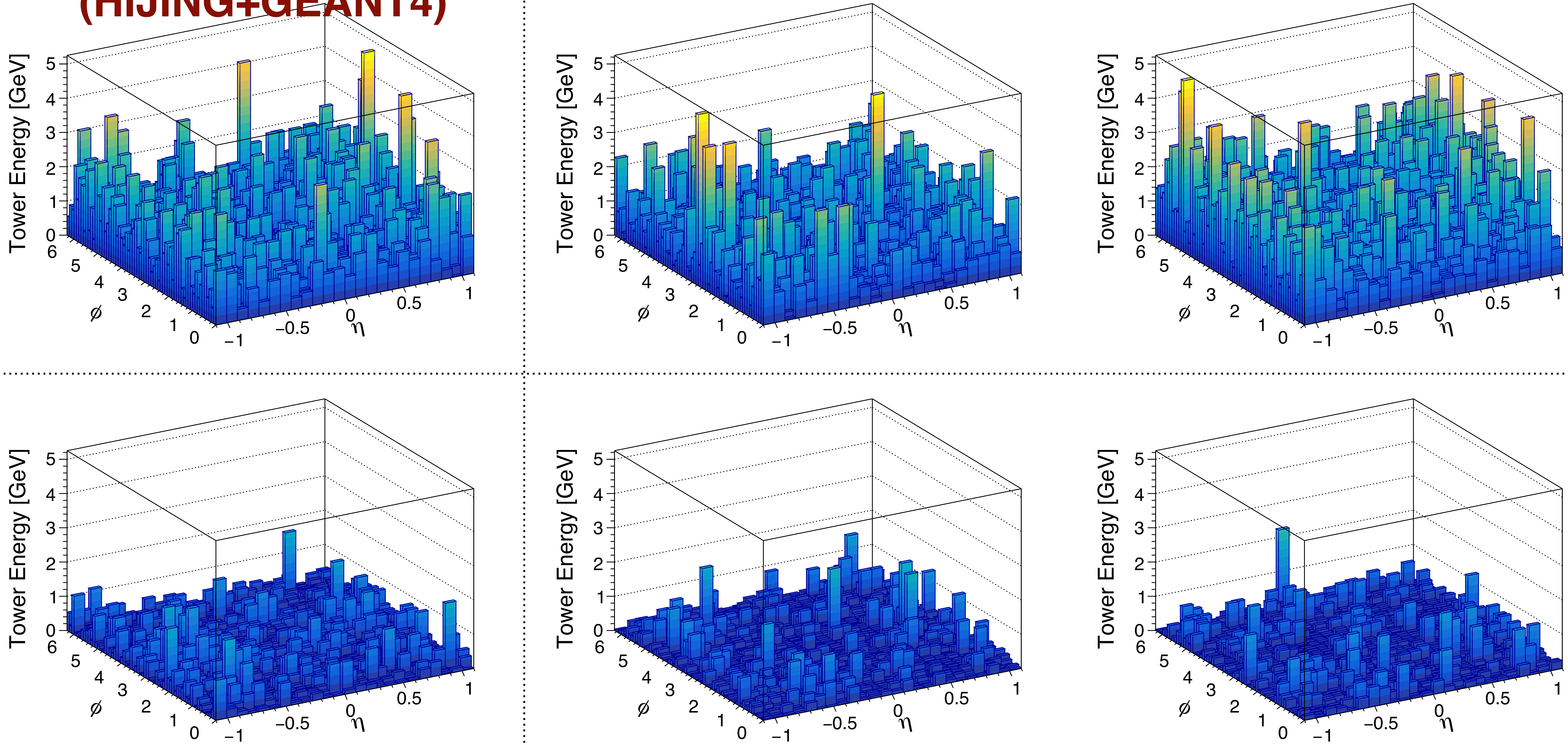


Display of Generated Events

Training sample (HIJING+GEANT4) | **Generated (DDPM)** | **Generated (GAN)**



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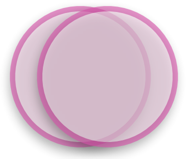

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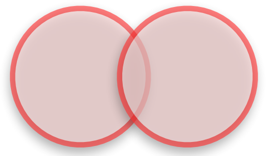
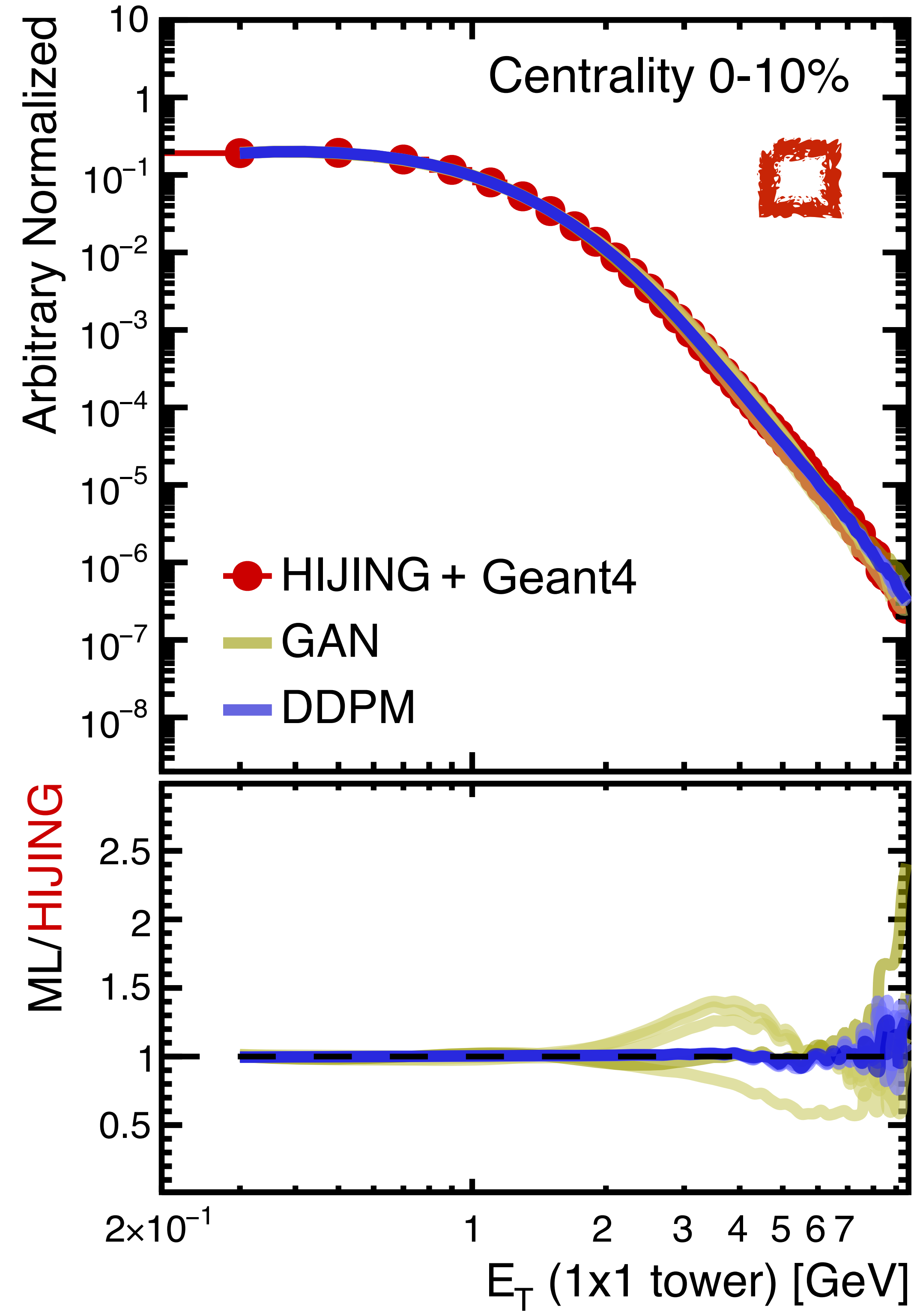
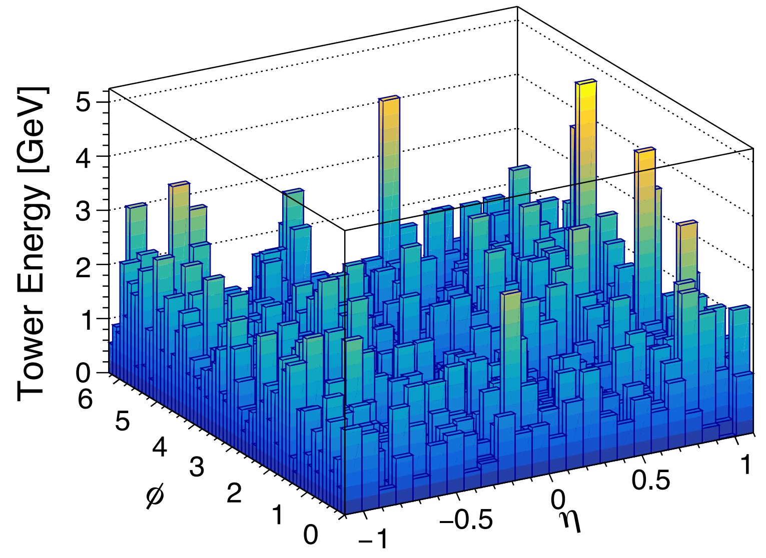


Performance: Transverse Energy (0-10%)

1x1 Tower | 4x4 Tower | 7x7 Tower | 11x11 Tower | All Towers



- Each model is retrained 5 times with different random seeds
- HIJING+Geant4 used as training data (600k events) and testing data (100k events)
- Both DDPM and GAN reproduce the data distribution where the data are abundant
- DDPM outperforms GAN in overall distribution w/ great stability and accuracy



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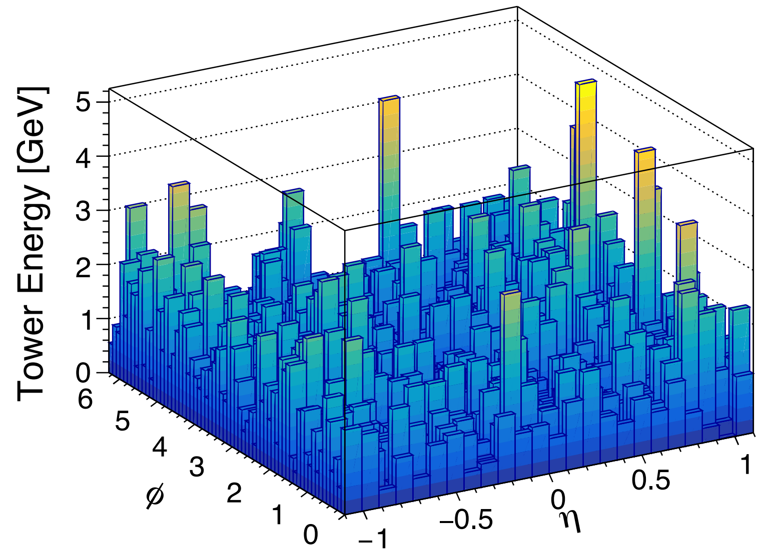

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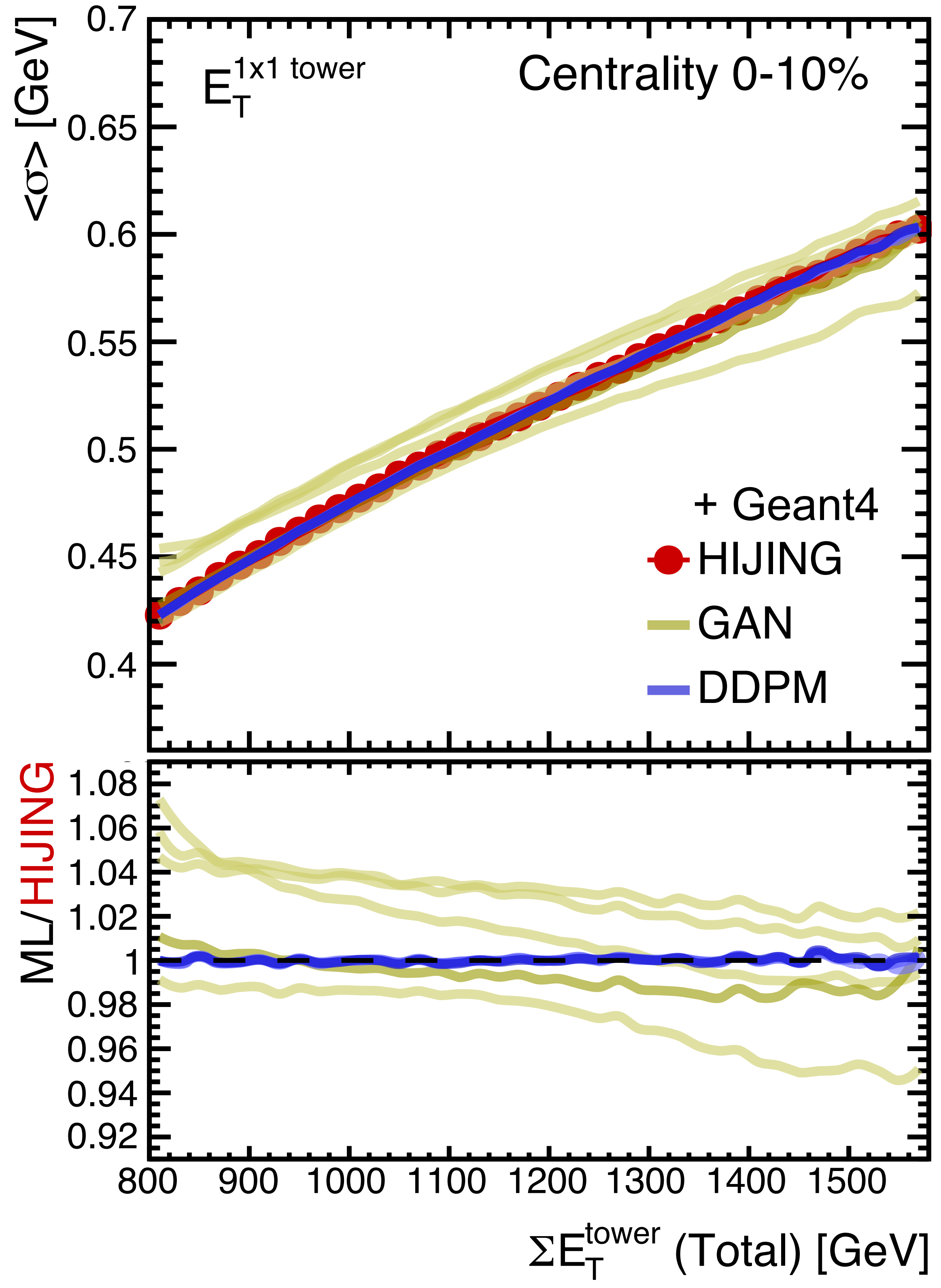
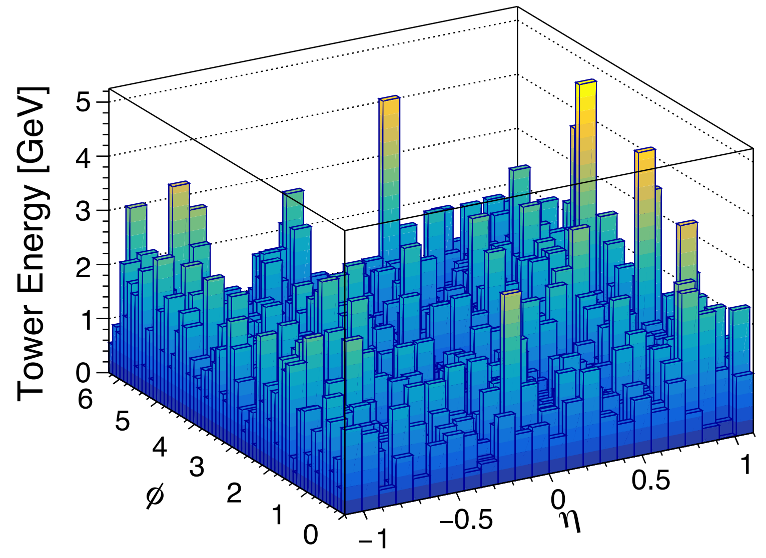


- GAN fails to describe fluctuation
- DDPM outperforms GAN w/ great stability, a few percent-level accuracy



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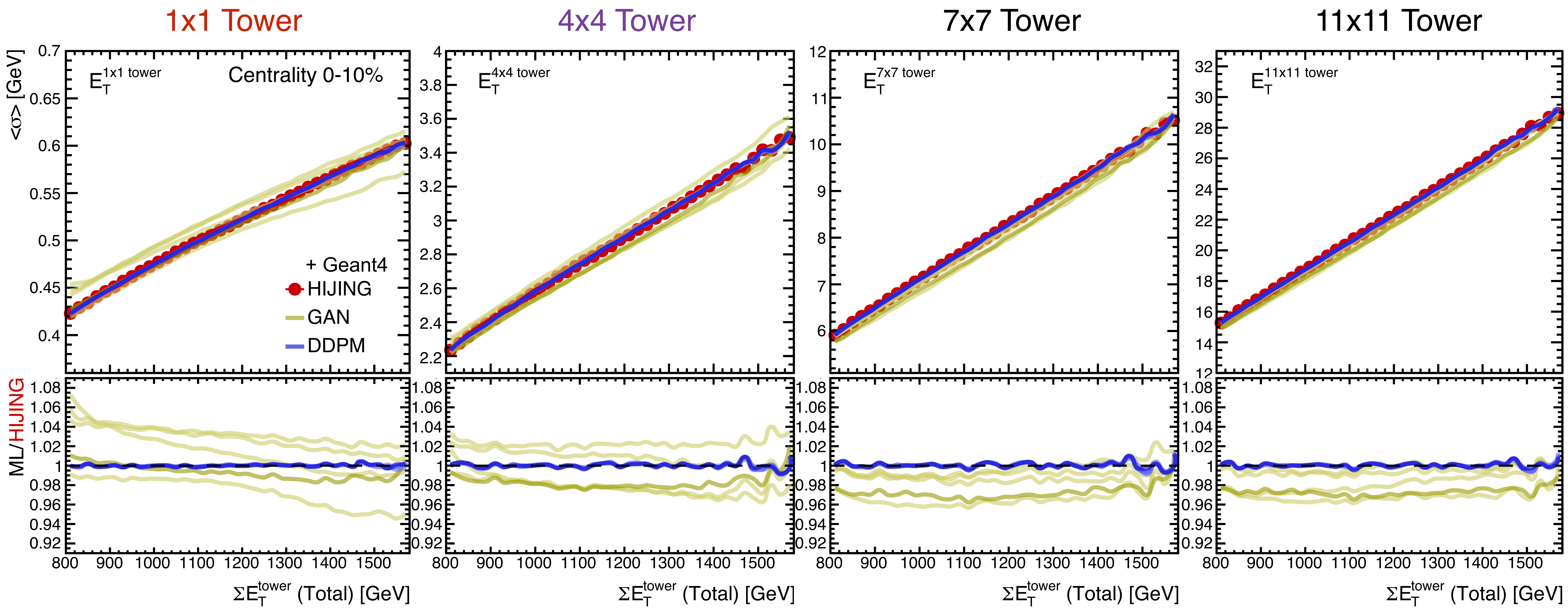

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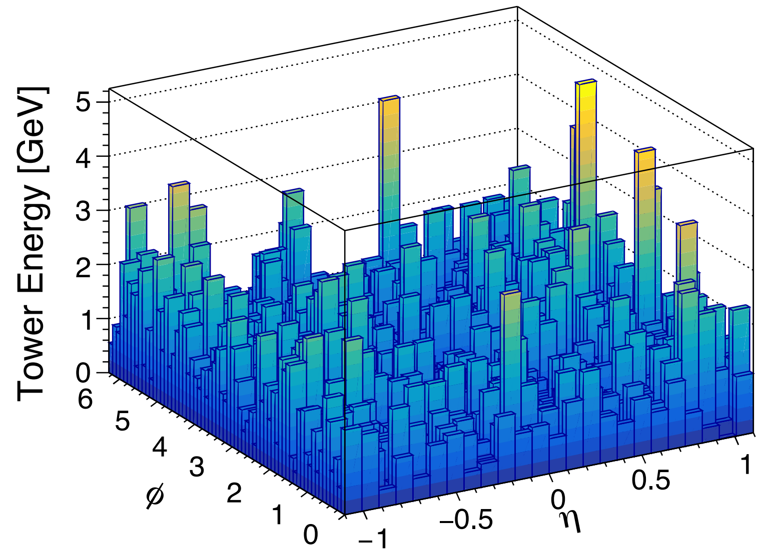

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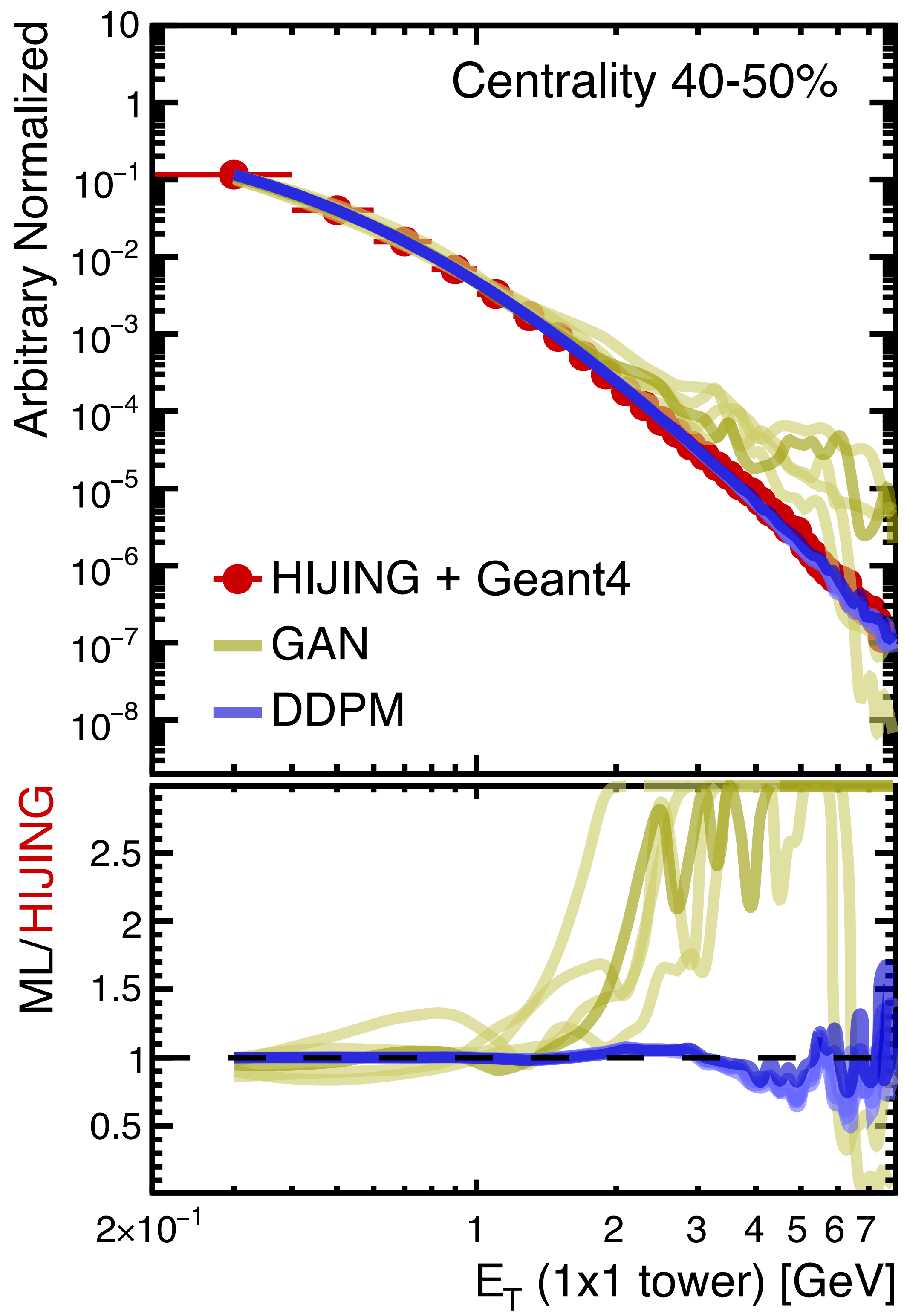

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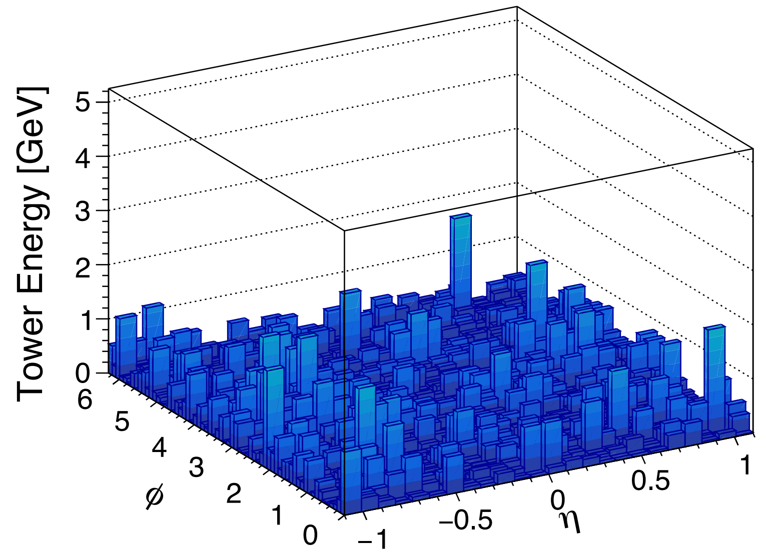
  - ➡ great stability, good agreement with HIJING+G4 at high probability region



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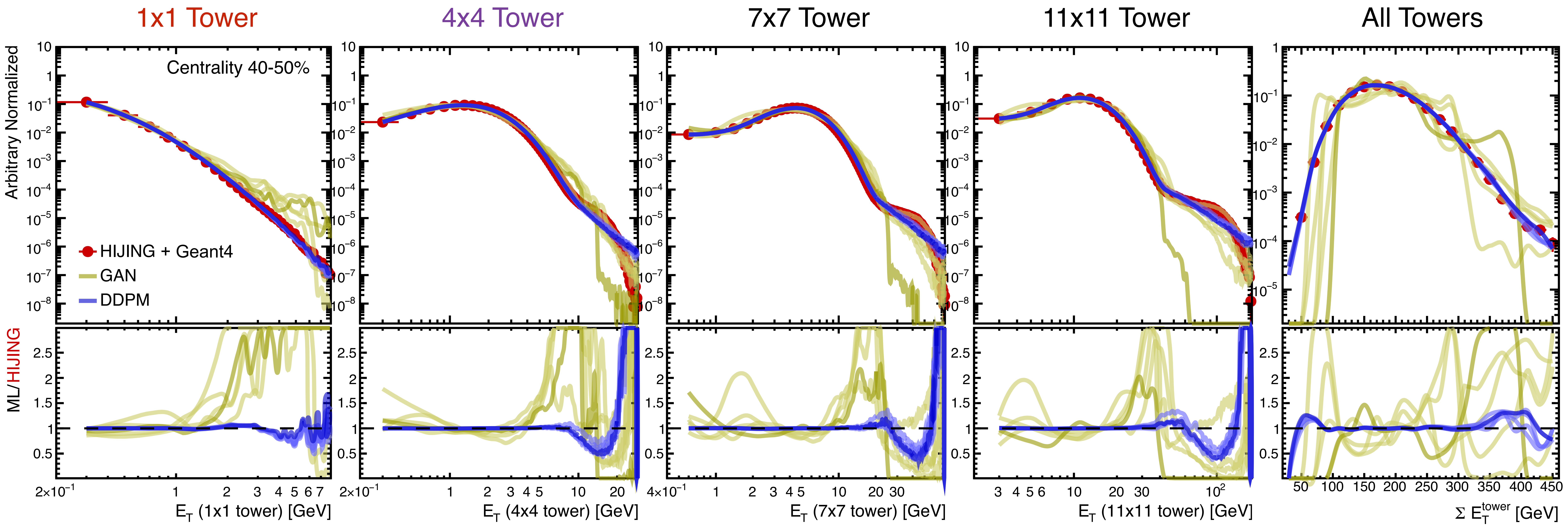

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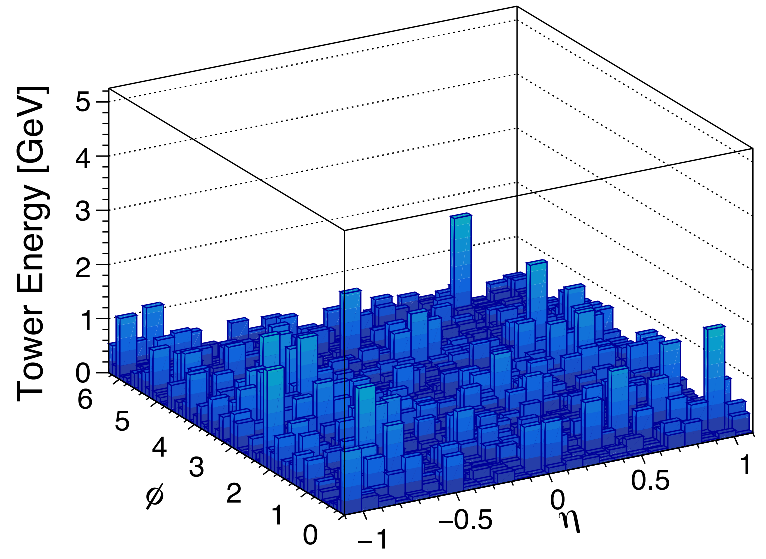

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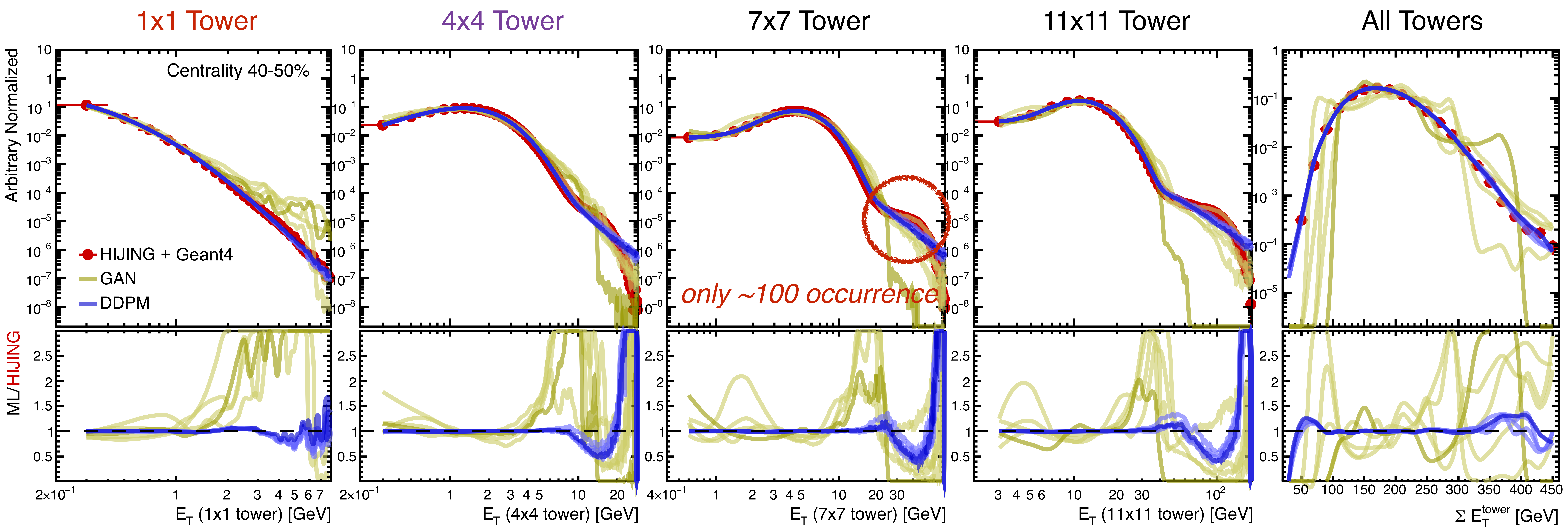

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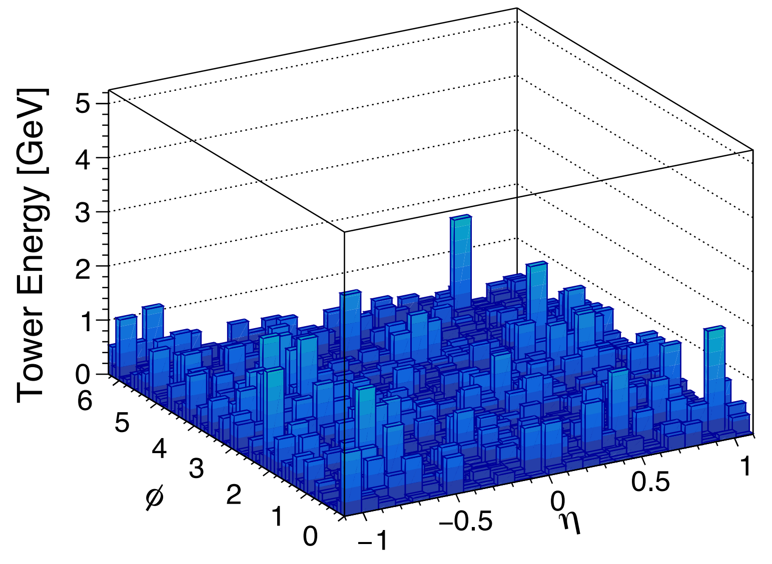
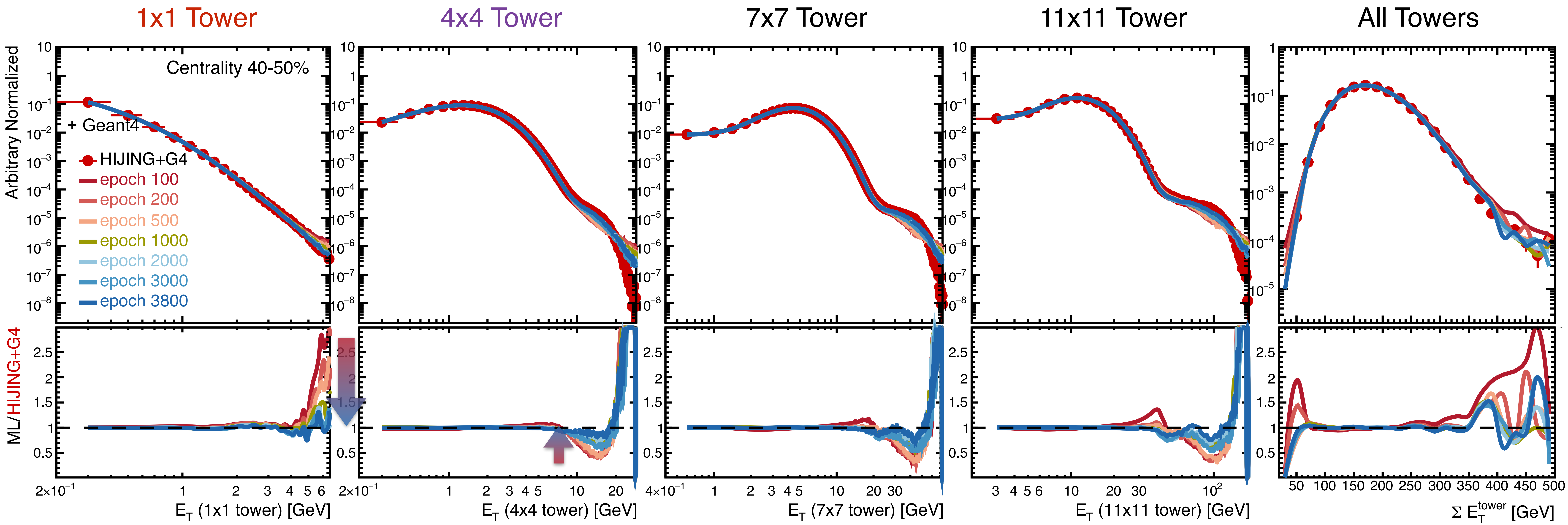
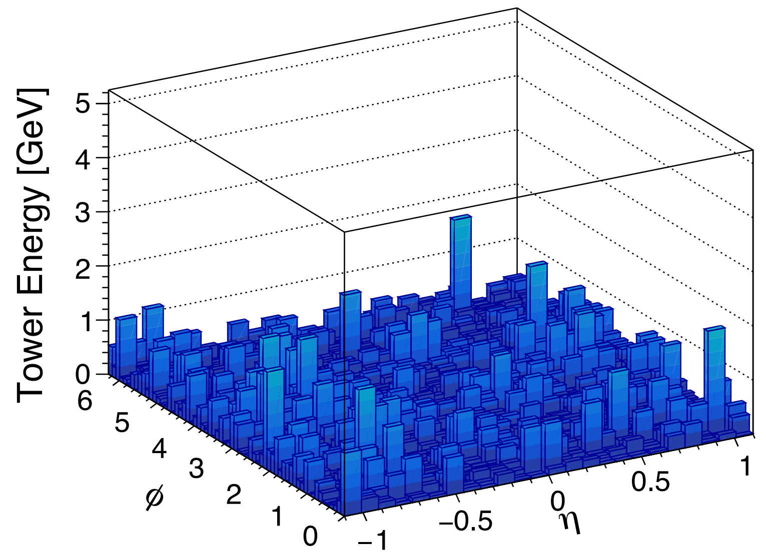


- Non-gaussian rare tail at the high energy region → challenge to reproduce

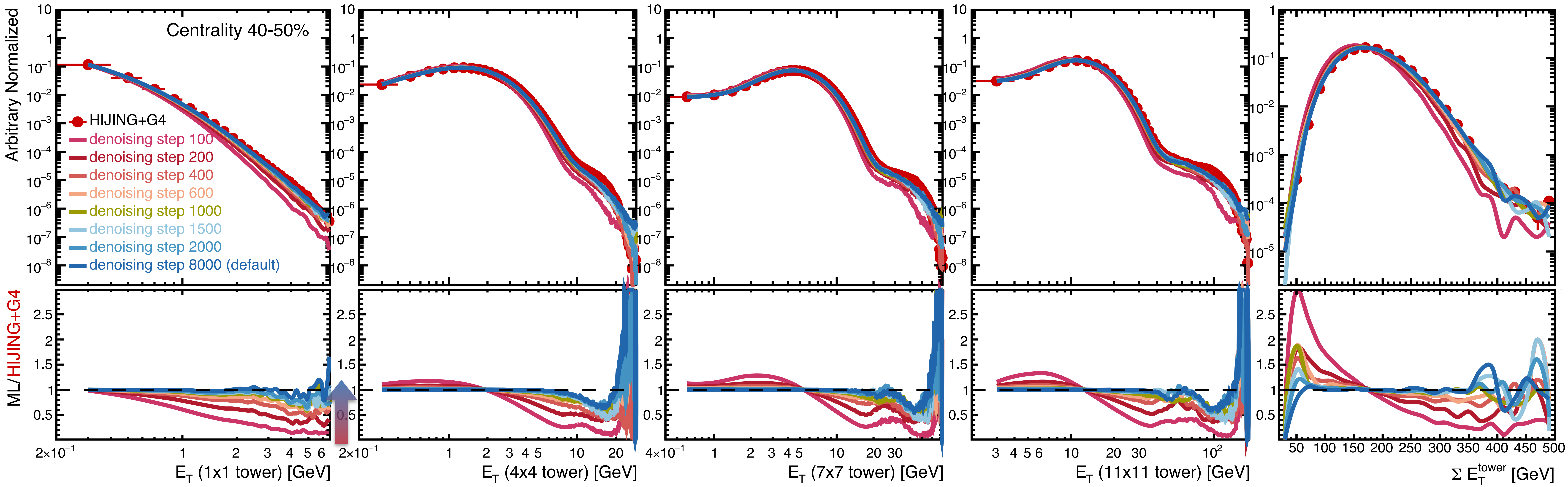
Trade-off between Training time and Fidelity



- epoch ~ training duration
- **DDPM** models with the higher epochs give **better performance**!
  ➡ but, the higher the epochs, the *longer the training time*



Trade-off between Generation time and Fidelity



- **DDPM** models with the higher de-noising steps give **better performance**!
  ➡ but, the higher the de-noising, the *longer the generation time*

How long does it take to simulate a large sample?

	Generating time	Speedup	CPU/GPU
HIJING + GEANT4 (Conventional)	40 minutes / event	1	Single CPU
DDPM	1.34 s / event	~1,800X	NVIDIA RTX A6000
GAN	0.42 ms / event	~5,700,000X	NVIDIA RTX A6000

- GAN is faster, but the DDPM exhibits high fidelity in describing the truth ground (HIJING+GEANT4)
- DDPM provide a speedup of O(100), considering a 32-core CPU equivalent to a GPU

Conclusion and Future work

- Simulations of high energy nuclear experiments
  ➡ **highly complex** and **computationally intensive**
  ➡ *both fidelity and speed is important*

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  ➡ GAN used as a reference
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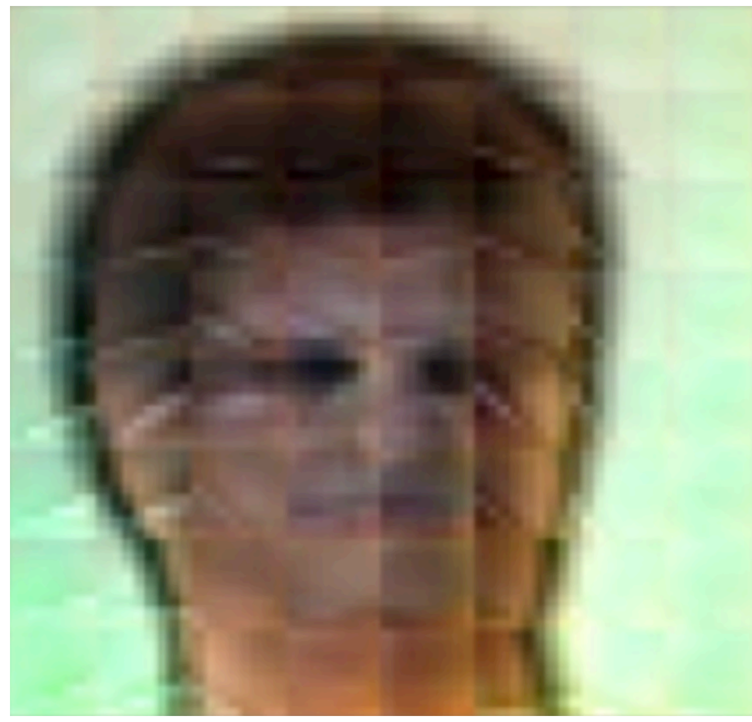
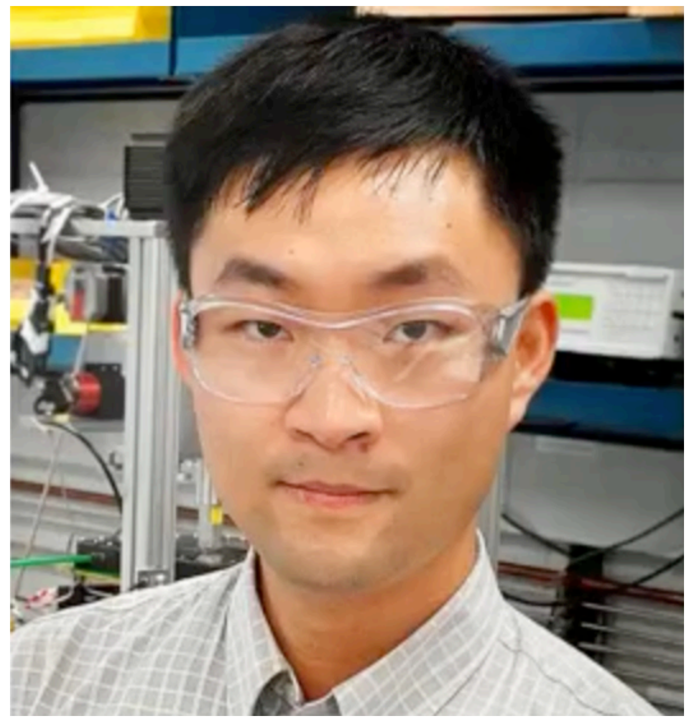
- **Outlook**
  ➡ future work includes improvement of performance in the region where data are rare
  ➡ using diffusion model to study rare probes (e.g. jets) in heavy ion collisions

Our Team

Yeonju Go



Dmitrii Torbunov



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Acknowledgement

- The LDRD Program at Brookhaven National Laboratory, sponsored by DOE's Office of Science under Contract DE-SC0012704, supported this work.

- We acknowledge sPHENIX. Its simulation data was used to demonstrate our algorithms.

BACKUP

DDPM Configuration

- number of diffusion steps T: default 8000 / variation [1000, 16000]
- variance schedule β_t: default 0.1 / variation [0.02, 0.2]
- training batch size: default 128 / variation [100, 12500]
- training steps per epoch: default 2000
- epoch: default 4000 / variation [100, 4000]
- training with the Adam optimizer with learning rate 10^{-4}
- trained with 600,000 events per each centrality bin
- tested with 100,000 events per each centrality bin
- neural network architecture (U-ResNet + Attention)
- depth/width of the model
  ➡ U-Net encoder-decoder stage, channels per stage: 32, 64, 128
  each of which comprised of two ResNet blocks

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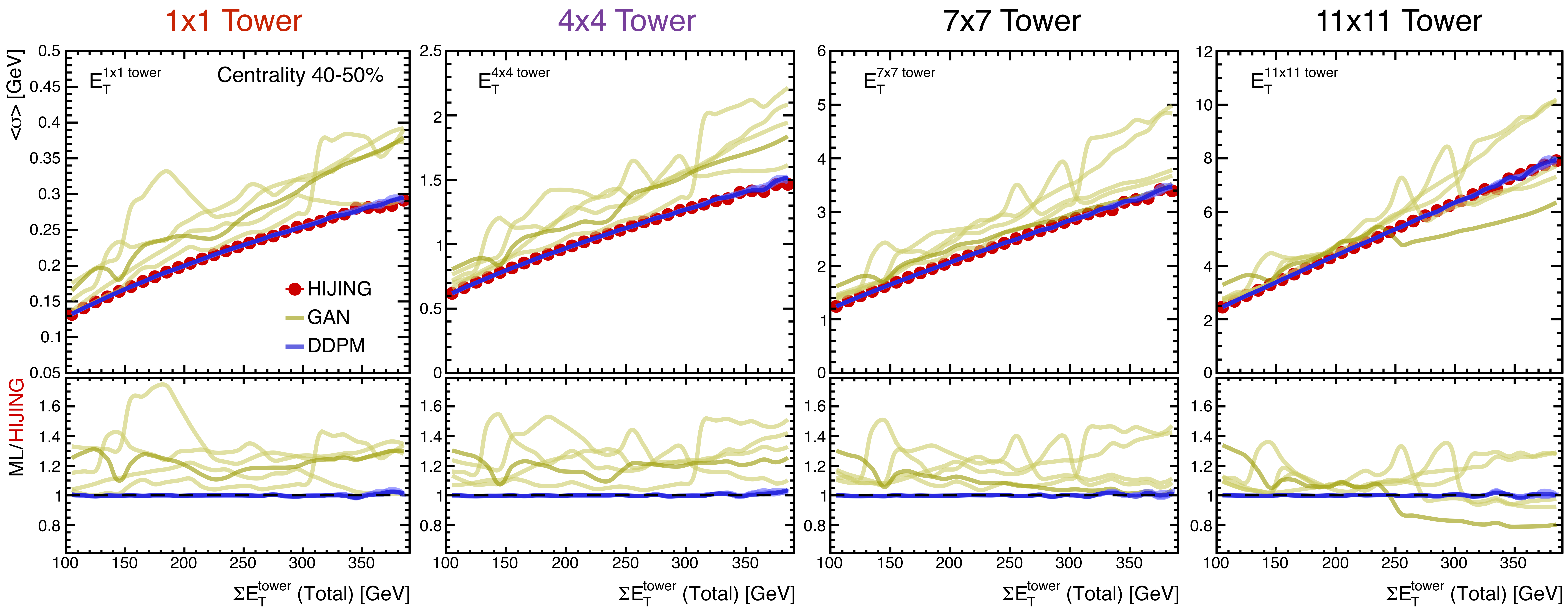

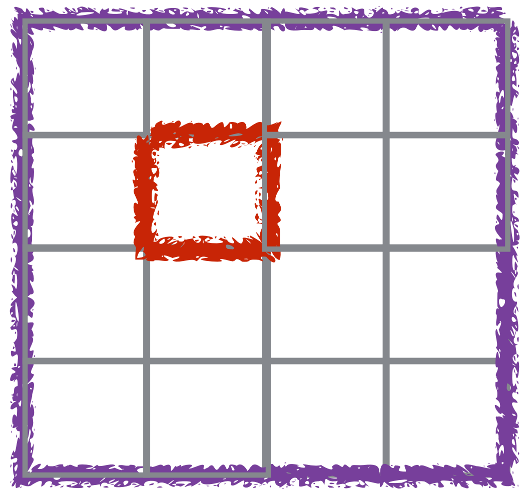

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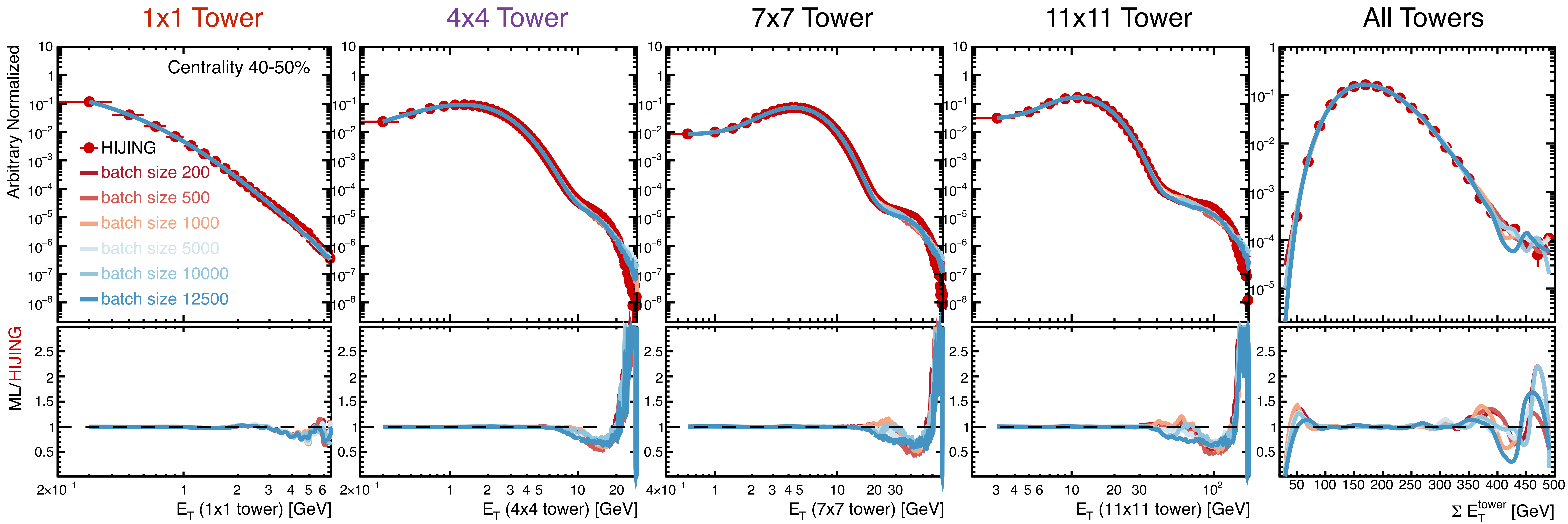
Batch Size Dependence



- Batch size not only introduces different random seeds and but also changes variance schedule (β_t)