PROCEEDINGS OF SCIENCE

Energy Reconstruction Method for LHAASO-KM2A Detector Based on Graph Neural Networks

Tian Xie,[a] **Xiaopeng Zhang,**[b,c] **Jia Liu,**[b,c] **Qingwen Tang**[a] **and Sha Wu**[b,c,*]

[a] *Nanchang University,*
330036 NanChang, JiangXi, China

[b] *Key Laboratory of Particle Astrophyics, Institute of High Energy Physics, CAS,*
100049 Beijing, china

[c] *TIANFU Cosmic Ray Research Center,*
610213 Chengdu, Sichuan, china

E-mail: xietian@ihep.ac.cn, zhangxp@ihep.ac.cn

The measurement of high-energy cosmic ray spectra is important for understanding extreme astrophysical processes and the origins of cosmic rays, representing one of the core scientific objectives of the LHAASO-KM2A experiment. This study employs deep learning algorithms to directly extract event features from extensive raw data. Within the energy range of the "knee" region .This research employs ParticleNet, a graph-based neural network model that achieves markedly improved energy resolution and reduced bias compared to traditional parametric methods.

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*Speaker

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1. Introduction

The Large High-Altitude Air Shower Observatory (LHAASO) is located in Daocheng, Sichuan, China at an elevation of 4410 m[9]. This altitude corresponds to an atmospheric depth of approximately $600 g/\mathrm{cm}^2$. LHAASO is a composite detection array whose key component, the KM2A array, covers one square kilometer and comprises an Electromagnetic Detector (ED) array paired with a Muon Detector (MD) array. This configuration enables precise measurement of 1×10^{13} eV to 1×10^{17} eV cosmic ray energy spectra in the energy range. KM2A uniquely features simultaneous detection of electromagnetic particles and muons from cosmic-ray-induced air showers. Notably, its muon detector array currently holds distinction as the world's largest high-altitude muon detection system. This observatory enables precise, all-weather observations of ultra-high-energy cosmic rays through the collaborative work of its multi-level detectors. Its unique "center-periphery" gradient layout design significantly enhances particle discrimination capability and spatial resolution.

The energy spectra and chemical composition of cosmic rays provide critical clues for elucidating the origin, acceleration mechanisms, and propagation processes of ultra-high-energy particles in the Universe. Cosmic rays below the knee feature (3 PeV) are predominantly attributed to Galactic sources, making precise measurement of the knee essential for understanding cosmic-ray acceleration and transport mechanisms within the Milky Way. However, spectral measurements face significant challenges: ground-based observations above 10 TeV rely on indirect detection via extensive air showers (EAS), wherein inherent degeneracies between the reconstructed energy spectrum, primary composition, and hadronic interaction models prevent definitive disentanglement. Consequently, developing a composition- and model-independent energy reconstruction method is imperative for advancing spectral studies of the knee region. Traditional energy reconstruction methods primarily rely on simple predictions using a few characteristic variables or classical multivariate analysis techniques. With the advancement and maturation of artificial intelligence, an increasing number of cosmic ray experiments are exploring deep learning applications in data analysis.

Graph Neural Networks (GNN) represent a graph-theory-based machine learning paradigm where data is structured as node-edge graphs, enabling information propagation through message-passing mechanisms that iteratively exchange features between connected nodes. This study adopts the ParticleNet architecture with EdgeConv blocks, which dynamically constructs edges via k-nearest neighbors aggregation and employs graph convolution to synthesize node-level information. Unlike traditional energy reconstruction methods—which rely on simplified regressions of limited handcrafted variables or classical multivariate analysis, thereby suffering from information loss due to human-driven feature engineering—our approach leverages raw detector-level data inputs to preserve event-level fidelity. The method's inherent adaptability to sparse, irregular spatial patterns (e.g., detector hits) provides distinct advantages over convolutional neural networks(CNN), which struggle with non-uniform geometries. By directly ingesting low-level features including detector coordinates(u, v, w), photoelectron counts, timing measurements, and detector type encodings (ED/MD), the model extracts intrinsic shower morphology characteristics inaccessible to conventional techniques. This paper is structured as follows: Section II details the experimental dataset; Section III evaluates established baseline methodologies and presents our energy reconstruction model. Section IV presents the energy reconstruction results, focusing on two key performance metrics: resolution (σ) and bias (μ). These quantities are formally defined as the standard deviation and mean, respectively, of the reconstructed energy residual distribution $(E_{\text{reco}} - E_{\text{true}})/E_{\text{true}}$.

2. Dataset

This study utilizes Monte Carlo simulations to generate training data for cosmic ray air shower events. The process is as follows: First, the CORSIKA software is used to simulate the atmospheric shower development[6], employing the QGSJETII model for hadronic interactions. Subsequently, a full physics simulation of the complete KM2A array detectors is performed based on the Geant4 software framework[4]. Approximately 2×10^7 cosmic ray shower event samples are generated. The simulated data covers an energy range from 10^{13} eV to 10^{16} eV[1], following a power-law spectrum with an index of -2. The simulated data is divided into two segments. Within the same segment, the data follows a -2 power-law distribution, thus ensuring sufficient statistics even in the last energy bin. The dataset for all primary particle species is uniformly mixed in a 1:1:1:1:1 ratio, comprising five types: Proton, He, CNO, MgAlSi, Fe. The zenith angle range is from 0° to 35°. The data selection criterion requires that the reconstructed core position lie within an annulus of 200-500 meters from the center of the KM2A array and the reconstructed zenith angle of 35 °. Following this selection, we obtained a total of over 400,000 simulated cosmic ray event samples. These events were then partitioned into datasets: Training Set (Train), Test Set (Test), and Evaluation Set (Eval), in a ratio of 3:1:1. The graph data structure of an exemplary input event to the graph neural network is depicted in Fig. 1.

3. Energy reconstruction method

3.1 Baseline Model

Hengying Zhang et al. published a paper in 2022 on the composition-independent energy reconstruction method for cosmic rays based on the LHAASO-KM2A detector[10]. In this report, this method is regarded as the baseline model and compared with the GNN method. The traditional method studies the energy reconstruction of cosmic rays based on the LHAASO-KM2A detector by combining parameters of muons and electromagnetic particles. Two methods are proposed: the $Ne{*}\mu$ method and the $Ne\mu$ method.

3.2 GNN Model

The Graph Neural Network (GNN) is a machine learning (ML) method based on graph theory[7], where data is represented as a graph composed of nodes connected by edges, and node information propagates across network layers through information exchange with neighboring nodes—a process known as message passing. The model input is the graph illustrated in Figure 1, which represents the response information of the KM2A detector array to a single event. The model used in this study is ParticleNet[5]. Its schematic diagram is shown in Figure 1, and the architecture adopted is the utilizing EdgeConv blocks[8], where edges are established based on each node's k-nearest neighbors, and node information is aggregated through dynamic graph convolution. During training, the learning rate is set to 0.001, with MSELoss employed as the loss

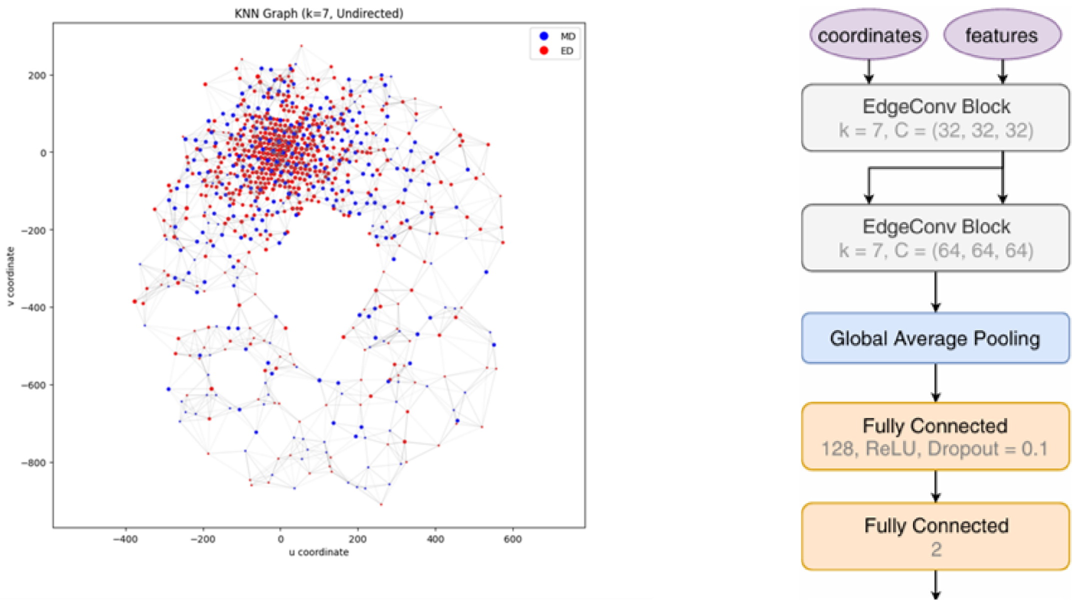

Figure 1: Illustrates an example input graph for the graph neural network. In the graph representation, red nodes denote ED (Electromagnetic Detector) stations while blue nodes represent MD (Muon Detector) stations. The size of each marker is proportional to the logarithm of the number of recorded photoelectrons at each detector station. The graph edges are constructed using the k-nearest neighbors algorithm with $k = 7$. The figure on the right illustrates the schematic structure of ParticleNet-Light.

function and the ranger optimizer used for parameter optimization[2]. The energy reconstruction procedure employs a structured three-stage approach initiated by transforming detector responses into graph-structured data where each node represents a physical detector unit characterized by spatial coordinates defining positions.The input coordinate information corresponds to the shower axis coordinates (u, v, w), which are obtained through coordinate transformation of the detector position coordinates (x, y, z). Particle features including detector type (ED or MD binary-encoded as 0/1), photoelectron count (pe) quantifying signal intensity, and precise hit timing (ns) for shower front reconstruction. To address inherent imbalance in simulation data generated with a power-law spectrum of index -2, we implement a weighted optimization model where training samples are weighted proportionally to the inverse spectral probability density, effectively prioritizing rare high-energy events. As shown in Figure 2.

The model runs for 100 epochs until convergence, with an early stopping mechanism terminating training when no performance improvement occurs for five consecutive epochs. Crucially, the GNN approach utilizes extensive raw detector-level data as input while implementing relaxed event selection criteria, this enables an order-of-magnitude increase in reconstructable events for energy reconstruction compared to baseline methods.

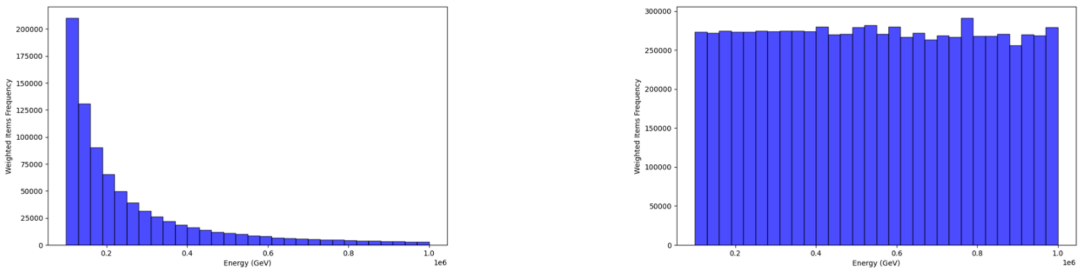

Figure 2: The left panel displays the energy spectrum distribution of simulated events, while the right panel shows the data distribution after weight application. The weighting scheme transforms the training data from an imbalanced state to a balanced distribution, thereby addressing the intrinsic data imbalance issue.

4. Performance analyses

To evaluate the performance of the Graph Neural Network (GNN), we examine the energy bias and energy resolution. These metrics are defined as the mean and standard deviation, respectively, of the distribution $(E_{\text{reco}} - E_{\text{true}})/E_{\text{true}}$. To address the necessity of distribution morphology validation, we performed a Kolmogorov-Smirnov test on the residual distribution $(E_{\text{reco}} - E_{\text{true}})/E_{\text{true}}$ for each energy bin and primary species. Results indicate that the distribution is consistent with a Gaussian profile, justifying the use of standard deviation and mean as robust metrics. We compare the this results with the performance of the $N_{e\mu}$ baseline method,show in 4. In Fig. 3, we present a comparison of the energy reconstruction performance. Within the 300 TeV–900 TeV energy range, the overall resolution decreases as the energy increases. Among the primary species[3], Fe achieves the best resolution, while proton nuclei exhibit the worst. Crucially, the overall resolution achieved by our method is significantly superior to that of the baseline approach. As shown in Fig. 4, the average energy resolution obtained via the this method is below 10% for this range. The bias of the this energy reconstruction also outperforms that of the traditional method. Fig. 3 illustrates that the reconstruction bias is predominantly negative across the spectrum. This systematic negative bias is likely attributed to boundary effects arising during the training procedure.

Furthermore, Figure 3 illustrates the bias performance of GNN-based reconstruction. The systematic bias remains consistently negative throughout the energy range, with absolute values confined within ±2%. We hypothesize that this negative bias trend may originate from boundary effects during model training. This issue is particularly pronounced because the training data were simulated according to a power-law distribution with exponent −2, and significant discontinuities exist in event counts at the energy boundaries. We extend our analysis to the broader spectrum of 300 TeV–9PeV as shown in Figure 5, where the boundary effects become pronounced near the junction between two independently simulated energy ranges due to data imbalance during model training. Comparative evaluation against baseline methods confirms the consistent superiority of GNN, demonstrating significantly reduced systematic bias and improved resolution across all primary particles (Proton, He, CNO, MgAlSi, and Fe), as quantitively validated in Figure 5. We also compared the results with those from the baseline model. Our method demonstrates

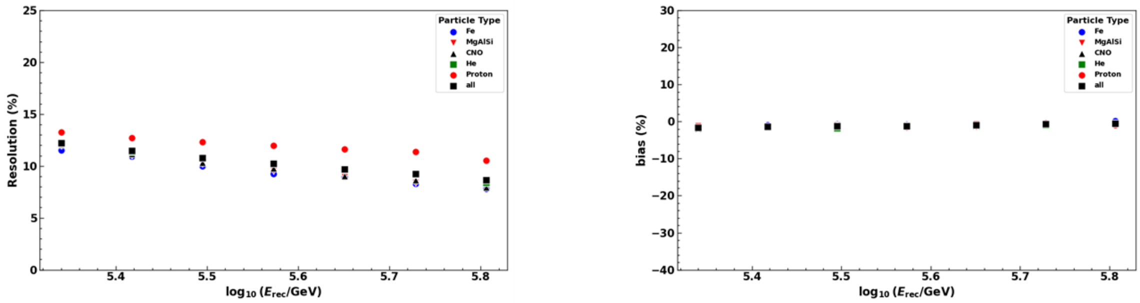

Figure 3: For the energy spectrum from 300 TeV to 900 TeV bias and resolution. The five primary compositions are distinguished using distinct colors and marker shapes. The black square represents the result for the all-particle spectrum. The left panel displays the energy reconstruction resolution, while the right panel shows the reconstruction bias. All species are plotted with identical abundance proportions in this representation.

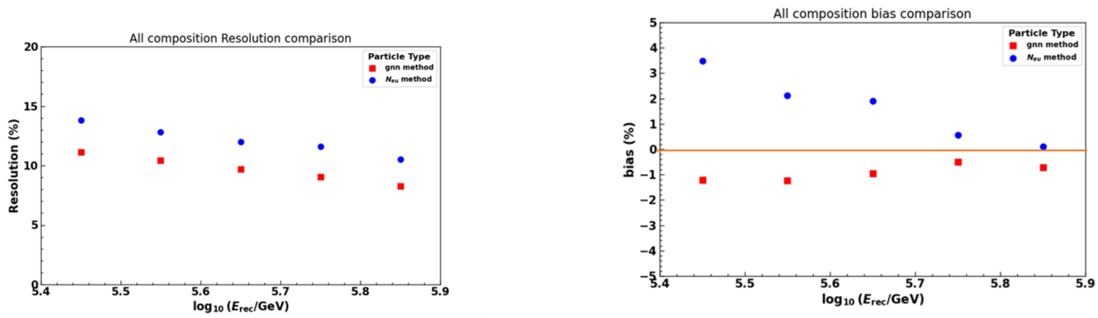

Figure 4: Comparison of energy reconstruction resolution and bias between the Graph Neural Network (GNN) method and the benchmark `Neu` method is presented. For the energy spectrum from 300 TeV to 900 TeV. The results (red points) correspond to events satisfying the selection criteria $\theta < 35°$ and $200\,\mathrm{m} < r < 500\,\mathrm{m}$, while the traditional method results (blue points) correspond to the stricter cuts $\theta < 18°$ and $320\,\mathrm{m} < r < 420\,\mathrm{m}$. Both resolution and bias are performance metrics where smaller values indicate superior reconstruction performance. Notably, the significantly looser selection requirements for the GNN method compared to the traditional $Ne\mu$ approach allow for substantially increased statistics while simultaneously delivering enhanced reconstruction performance.

better performance in both reconstruction bias and resolution compared to the baseline method, as illustrated in Fig. 6.

A current limitation of the this approach is its inherent inability to perform precise composition classification prior to energy reconstruction. Consequently, the energy reconstruction results exhibit a stronger dependence on cosmic-ray composition compared to traditional methods. This challenge can be addressed by implementing a two-stage procedure: first classifying cosmic-ray compositions and subsequently performing energy reconstruction based on the identified composition. This constitutes a key direction for our future work.

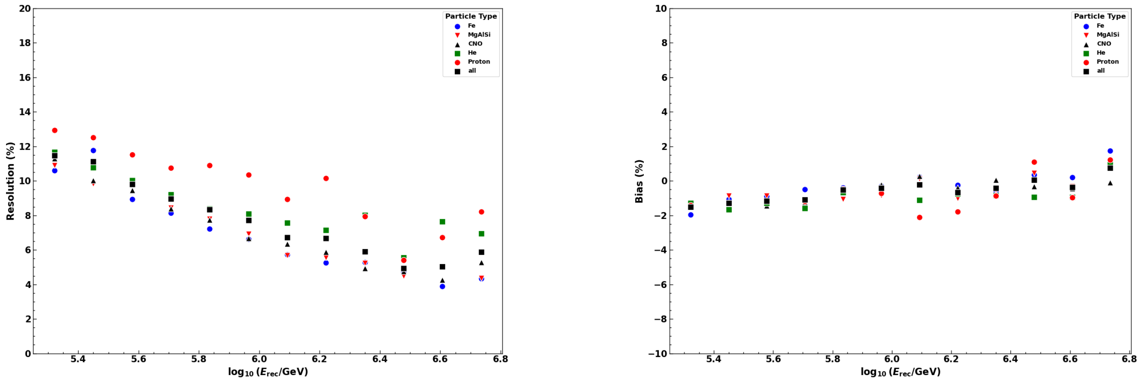

Figure 5: For the energy spectrum from 300 TeV to 9 PeV bias and resolution. The five primary compositions are distinguished using distinct colors and marker shapes. The black square represents the result for the all-particle spectrum. The left panel displays the energy reconstruction resolution, while the right panel shows the reconstruction bias. All species are plotted with identical abundance proportions in this representation.

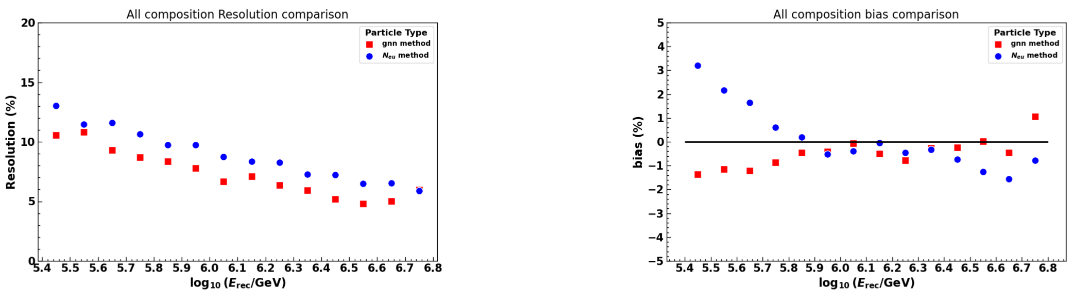

Figure 6: Comparison of energy reconstruction resolution and bias between the Graph Neural Network (GNN) method and the benchmark `Neu` method is presented. For the energy spectrum from 300 TeV to 9 PeV. The results (red points) correspond to events satisfying the selection criteria $\theta < 35^\circ$ and $200\,\text{m} < r < 500\,\text{m}$, while the traditional method results (blue points) correspond to the stricter cuts $\theta < 18^\circ$ and $320\,\text{m} < r < 420\,\text{m}$. Both resolution and bias are performance metrics where smaller values indicate superior reconstruction performance. Notably, the significantly looser selection requirements for our method compared to the traditional $Ne\mu$ approach allow for substantially increased statistics while simultaneously delivering enhanced reconstruction performance.

5. Conclusion

This study has used a graph neural network (ParticleNet) model for energy reconstruction of cosmic rays using the LHAASO-KM2A detector array, demonstrating measurable improvements over conventional parametric approaches. Particularly through significant expansion in the spatial acceptance for energy reconstruction events in handling large zenith-angle ($\theta < 35^\circ$) and peripheral events ($200\ \text{m} < r < 500\ \text{m}$).

While GNN models outperform traditional methods, the energy reconstruction bias is negative (approximately 1%) across most energy ranges.Furthermore, we will investigate the generalization capability by testing the model using hadronic interaction models beyond QGSJET as the test set.

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