

AI-driven Classification of Interstellar Medium Morphologies: From Big Data to Physical Insights

Zhemiao Wu *

Tsinghua University High School, Beijing, 100084, China

* Corresponding Author Email: wuzhemiao@outlook.com

Abstract. The interstellar medium is a multi-phase material that fills the space between the stars with densities and temperatures covering over 6 orders of magnitude. Since of the exponential growth of observational data from facilities like the Atacama Large Millimeter/submillimeter Array and Herschel Space Observatory, the traditional morphological classification methods suffer from this data bursting. Artificial intelligence has emerged as a transformative tool to address this challenge, enabling efficient, objective classification of interstellar medium morphologies from high-dimensional, large-volume datasets. This paper analyze the advances in AI-driven interstellar medium morphology classification, including the research background and limitations of traditional methods, analysis of interstellar medium big data characteristics and processing challenges. Then, the author detail the commonly used AI methods, including unsupervised clustering, supervised Deep Learning, and physics-informed machine learning, and their benefits in interstellar medium research.

Keywords: Interstellar Medium, Morphological Classification, Artificial Intelligence, Machine Learning, Big Data.

1. Introduction

The interstellar medium is composed primarily of hydrogen, followed by helium with trace amounts of carbon, oxygen, and nitrogen, shapes galactic evolution and star formation [1]. The morphology of these phases, characterized by their spatial distribution, spectral signatures, and dynamical states, directly encodes information about fundamental processes: for example, bipolar outflows reveal feedback from young stars [2], while filamentary molecular clouds trace gravitational collapse [3].

Traditional Interstellar Medium (ISM) morphology classification relied on three primary approaches which face technical limitations in the era of big data. First, visual inspection involves astronomers manually identifying morphological features (e.g., filaments, clumps) from 2D or 3D data cubes. This method is subjective and computationally infeasible for large datasets, such as Atacama Large Millimeter/submillimeter Array (ALMA)’s $315 \times 420 \times 160,000$ -pixel maps of Orion B [2]. Second, single-line analysis-based classifications on the emission of a single molecular tracer may fail to distinguish overlapping physical/chemical phases; for example, ^{12}CO is optically thick and traces only the warm, outer layers of clouds, missing the dense, UV-shielded interior probed by ^{13}CO or C^{18}O . Third, the fitted physical model may infer unreliable physical parameters from data. Furthermore, fitting models are computationally expensive and is impractical for real world problems. For instance, the Nautilus astrochemical model requires 120–240 seconds per simulation [4].

The advent of Artificial intelligence (AI) has revolutionized ISM morphology classification by overcoming three key barriers [5,6]. First, AI excels at handling high-dimensional data, inherent to the ISM (e.g., position-position-velocity cubes, multi-line spectral features [2]), through methods like clustering and convolutional neural networks (CNNs) that effectively extract patterns from complex spaces. Second, AI improves efficiency via emulators (e.g., neural field-based models [4]), reducing computation time by 4–5 orders of magnitude and enabling real-time analysis of large datasets. Third, Physics-Informed Machine Learning (PIML) ensures objectivity and physical consistency by integrating constraints (e.g., positive Reynolds stress) [7], preventing unphysical results common in pure data-driven approaches and aligning classifications with fundamental laws.

The remainder of this paper is organized as follows. Section 2 contextualizes ISM big data including its sources, characteristics, and processing challenges. Section 3 details the AI methods for morphology classification, which include unsupervised, supervised, and physics-informed approaches. Section 4 presents key application cases, demonstrating how AI classifies morphologies and links them to physical conditions. Section 5 synthesizes the physical insights gleaned from AI-driven classifications, spanning small (cloud-scale) to large (cosmic-scale) regimes; Section 6 discusses current challenges and future directions, and conclusions are drawn in Section 7.

2. ISM Big Data: Sources, Characteristics, and Processing Challenges

The exponential growth of ISM data, driven by next-generation telescopes, has created both opportunities and bottlenecks for morphological classification. This section outlines the data’s origins, intrinsic features, and the challenges of raw data processing.

2.1. Major Observational Facilities and Data Characteristics

ISM data are mainly acquired via telescopes operating in the infrared (IR), submillimeter, and radio bands, each probing distinct physical phases (Table 1). These facilities generate datasets with unique dimensionality and volume:

Table 1. datasets from different facilities

Facility	Wavelength Range	Probed ISM Phases	Data Type
ALMA	0.3–3 mm	Dense molecular gas, dust continuum	Position-position-velocity cubes
Herschel Space Observatory	55–672 μm	Cold dust, FIR fine-structure lines	2D/3D continuum maps
IRAM-30m Telescope	1–3 mm	Molecular lines (e.g., CO, HCO ⁺)	Position-position-velocity cubes
Spitzer Space Telescope	3–180 μm	Warm dust, PAHs	2D IR maps

In the table and the related references, high dimensionality is exemplified by a single ALMA observation of Orion B, which includes 5 molecular tracers (12CO, 13CO, C18O, HCO⁺, CN), resulting in a 5-dimensional feature space for each pixel. Dynamic range is another critical feature, as intensity variations span orders of magnitude—for example, 12CO intensity in Orion B ranges from ~ 2 to 100 K km s^{-1} —requiring AI methods to handle extreme value distributions. Additionally, noise and heterogeneity are challenging. Faint tracers, like CN, have low signal-to-noise ratios and introduces artifacts [2]. Data from different telescopes also need cross-calibration. For example, Herschel and ALMA flux must be matched [3].

2.2. Critical Challenges in Big Data Processing

Transforming raw ISM data into morphologically meaningful features requires addressing four issues. First, **dimensionality reduction**: High-dimensional datasets are plagued by the "curse of dimensionality," where traditional statistical methods like 2D PDF projections fail to uncover hidden structures. For instance, Bron et al. showed that 2D projections of CO isotopologue intensities missed chemical phase separations later revealed by MeanShift clustering [8]. Second, **noise robustness**: Low-signal-to-noise (S/N) lines can contaminate feature vectors, leading to spurious clusters. In Orion B, this is evident in the eastern cloud edge, where faint CN detection results in noisy cluster boundaries, whereas the western edge, with its steep intensity gradients, exhibits sharper, more reliable clusters. Third, **computational efficiency**: Traditional physical models struggle to scale with data volume. Simulating 126,000 Nautilus models (to train a neural emulator) required approximately

4 hours on 512 CPU cores [4], whereas the emulator reduced this to just 0.01 seconds per model, highlighting the urgent need for efficient computational tools. Fourth, **data bias**: Observational datasets often favor specific ISM regimes. The Orion B sample, for example, overrepresents UV-illuminated gas due to its inclusion of multiple H II regions, risking the development of AI models that fail to generalize to quiescent clouds.

3. AI-Driven ISM Morphology Classification Methods

AI methods provide unique solutions for ISM morphology classification by addressing challenges raised by big data while adhering to astrophysical constraints. This section categorizes these approaches into three paradigms: unsupervised learning, supervised/deep learning, and physics-informed learning. Their strengths, limitations, and astrophysical applications are explained.

3.1. Unsupervised Learning: Discovering Natural Morphological Clusters

Unsupervised learning identifies morphological classes without pre-labeled data, making it ideal for exploring unknown ISM phases. One impactful method in ISM research is MeanShift clustering, complemented by comparisons to other algorithms (e.g., DBSCAN).

3.1.1. MeanShift Clustering: PDF-Based Phase Separation

MeanShift (Comaniciu & Meer 2002) is a probability density-based clustering algorithm that defines clusters as regions surrounding local maxima of the multi-dimensional probability density function (PDF) of feature vectors. Its key advantages for ISM classification include: no a priori cluster count and adaptability to variable density. In Orion B, Bron et al. [8] applied MeanShift to two feature sets: (1) CO isotopologues only ($D=3$), using $k=1900$ neighbors to identify 9 initial clusters (later merged into 8), which mapped to three density regimes—diffuse ($n_H \sim 1000 \text{cm}^{-3}$), translucent ($n_H \sim 500 \text{cm}^{-3}$), and dense ($n_H > 1000 \text{cm}^{-3}$); and (2) adding HCO^+ and CN ($D=5$), with $k=425$ neighbors expanding to 19 clusters that distinguished UV-illuminated (overbright HCO^+/CN) and UV-shielded (low CN/HCO^+ ratios) phases.

3.1.2. Limitations of Unsupervised Learning

Unsupervised learning methods also meet some limitations [8,9]. First, they cluster pixels based on spectral features rather than spatial proximity, but ignoring spatial context. While this method can avoid biasing toward contiguous structures, it requires post-hoc validation (e.g., checking if clusters exhibit spatial coherence). Second, they are sensitive to noise: low-signal-to-noise (S/N) features (e.g., CN) can create artificial maxima in the probability density function (PDF).

3.2. Supervised and Deep Learning: Predicting Morphologies from Labels

Supervised learning, including Deep Learning (DL), uses pre-labeled data to train models that map features (e.g., spectral lines) to morphological classes. This paradigm is powerful for tasks like turbulence morphology modeling and spectral-morphological correlation.

3.2.1. Convolutional Neural Networks (CNNs) for Spatial Feature Extraction

3D CNNs excel at extracting spatial patterns from position-position-velocity (PPV) cubes, making them uniquely suited for analyzing turbulent ISM morphologies [10]. demonstrated their utility by training a 3D CNN to predict the Reynolds stress tensor (τ_{ij})—a critical metric of turbulence morphology—in supernova remnants. The model ingests multi-dimensional inputs, including filtered velocity ($\mathcal{V}$), magnetic field ($\mathcal{B}$), and their spatial derivatives ($d\mathcal{V}, d\mathcal{B}$). Its architecture comprises stacked convolutional and max-pooling layers to capture hierarchical spatial features, followed by dense layers with LogSigmoid activation to handle the symmetric distributions of non-diagonal τ_{ij} components. Compared to traditional gradient-based models, the CNN significantly improved performance, reducing errors in turbulent pressure ($P_{\text{turb}} = \text{tr}(\tau_{ij})$) from 63% to 19%.

3.2.2. Neural Emulators: Bridging Chemistry and Morphology

Neural emulators—deep learning models that replicate complex physical simulations—enable efficient exploration of links between ISM morphology and chemistry. Asensio Ramos et al. developed a conditional neural field (NF) emulator for the Nautilus astrochemical model [4], designed to predict chemical abundances under varying physical conditions. The emulator takes inputs such as temperature (T), hydrogen density (n_H), cosmic-ray ionization rate (ζ_{H_2}), sulfur abundance ($[S]$), UV flux (χ), and time (t). To adapt to diverse molecules and conditions, it uses Feature-wise Linear Modulation (FiLM), a conditioning technique that adjusts the NF via one-hot encoding. The model outputs abundances for 192 species (e.g., CO, HCO⁺) with uncertainties below 0.2 dex. This capability accelerates analysis of how chemical tracers—key indicators of morphology—respond to physical environments. The emulator revealed that sulfur abundance dominates electron density in low-density gas ($n_H \sim 104 \text{ cm}^{-3}$), directly linking chemical signatures to morphological states like diffuse or dense gas.

3.3. Physics-Informed Machine Learning (PIML): Ensuring Physical Consistency

Pure data-driven AI can produce unphysical results. Fortunately, PIML integrates physical constraints into model design, critical for ISM morphologies where observations are sparse.

3.3.1. PIML for Turbulence Morphology

Karpov et al. developed a physics-informed machine learning (PIML) model to predict diagonal elements of the Reynolds stress tensor (τ_{ij}), which describe asymmetric turbulence distributions [7], by embedding physical constraints. The model enforces *realizability*—ensuring $\tau_{ij} > 0$ (turbulent stress cannot be negative)—by first predicting velocity fluctuations (u'_i) and then computing $\tau_{ij} = -\langle u'_i u'_j \rangle$. To address biases in point-wise loss functions toward outliers, it uses a *hybrid loss*: Smooth L_1 Loss for outlier accuracy and Kolmogorov-Smirnov (KS) loss to align probability density function (PDF) peaks. This approach improves predictions of bulk turbulence morphology, as shown by reduced discrepancies in key metrics.

3.3.2. PIML in Spectral-Morphological Modeling

For ISM spectral lines, PIML models integrate radiative transfer physics to link spectral features with morphology. For instance, machine learning models for rotational spectra [8] incorporate local thermodynamic equilibrium (LTE) constraints to weight loss functions, ensuring predicted line intensities align with physical excitation conditions. This prevents unphysical line ratios (e.g., $^{13}\text{CO}/\text{C}^{18}\text{O} < 8$), which are critical for accurate morphological classification. By embedding such physical priors, PIML bridges spectral data with morphological interpretations, enhancing the reliability of ISM structure analysis.

3.4. Method Comparison and Selection Guidelines

Table 2 summarizes the strengths, limitations, and optimal use cases of AI methods for ISM morphology classification:

Table 2. Different types of AI-driven methods

Method	Strengths	Limitations	Optimal Use Case	Reference
Neural Emulator	Fast, multi-species prediction	Dependent on training data distribution	Chemistry-morphology correlation (e.g., Nautilus)	[4]
PIML	Physical consistency, high credibility	Complex model design	Physics-sensitive morphologies	[7]
MeanShift Clustering	Unsupervised, adaptive density, no cluster count assumption	Ignores spatial context, noise-sensitive	Multi-line phase separation (e.g., Orion B)	[8]
3D CNN	Spatial feature extraction, end-to-end	Requires labeled data, high computational cost	Turbulence morphology (e.g., supernovae)	[10]

4. Key Application Cases of AI-Driven ISM Morphology Classification

AI-driven classification has yielded transformative insights into ISM morphologies across scales—from local molecular clouds to high-redshift galaxies. This section details four landmark cases, highlighting how AI bridges big data and physical understanding.

4.1. Case 1: Phase Separation in the Orion B Giant Molecular Cloud

Orion B, a nearby giant molecular cloud (GMC) at $d = 400$ pc hosting the Horsehead Nebula and H II regions (NGC 2023, NGC 2024), serves as an ideal testbed for ISM phase classification. Bron et al. applied MeanShift clustering to IRAM-30m data [8], yielding insights into density-driven morphological stratification. Using only CO isotopologues (^{12}CO , ^{13}CO , C ^{18}O), the algorithm identified three nested morphological layers: an outer diffuse layer (Cluster CO-1, $n_{\text{H}} \sim 100 \text{ cm}^{-3}$) with faint ^{12}CO emission and noise-like spatial patterns; a middle translucent layer (Clusters CO-2–CO-5, $n_{\text{H}} \sim 500 \text{ cm}^{-3}$), where ^{13}CO becomes detectable and asymmetry arises from steep western UV-illuminated edges; and an inner dense layer (Clusters CO-6–CO-8, $n_{\text{H}} > 1000 \text{ cm}^{-3}$), traced by C ^{18}O , with Cluster CO-8 mapping to H II regions and exhibiting elevated ^{12}CO intensity ($\sim 90 \text{ K km s}^{-1}$) due to heating.

Building on this, the authors further incorporated UV-sensitive tracers (HCO^+ , CN) to reveal UV-driven chemical morphologies. Two distinct chemical regimes emerged: UV-illuminated regions (Cluster FUV-16) with overbright HCO^+ and CN emission, a high CN/ HCO^+ ratio (~ 1.7), and photochemical enrichment from UV radiation enhancing HCO^+ /CN abundances relative to C ^{18}O (consistent with PDRs like the Horsehead PDR); and UV-shielded regions (Cluster FUV-3) with low CN/ HCO^+ ratios (~ 0.4), tracing dense cores where UV attenuation preserves cooler chemistry. Non-LTE modeling further confirmed that $[\text{HCO}^+]/[\text{C}^{18}\text{O}]$ increases by two orders of magnitude with G_0/n_{H} (UV flux/density), linking chemical tracers to UV exposure and density-dependent morphology.

4.2. Case 2: Turbulence Morphology in Supernova Remnants

Core-collapse supernovae (CCSNe) drive turbulent interstellar medium (ISM) morphologies that determine explosion outcomes—whether shocks propagate successfully or stall, leading to black hole formation. To model this turbulence, Karpov et al. applied physics-informed machine learning (PIML) to 3D direct numerical simulation (DNS) data of a CCSN (from Mösta et al. 2015) [7], focusing on the Reynolds stress tensor (τ_{ij}), a critical proxy for turbulence morphology.

PIML significantly outperformed traditional gradient-based models in key metrics. For turbulent pressure ($P_{\text{turb}} = \text{tr}(\tau_{ij})$), the gradient model underestimated values by 63%, whereas PIML reduced errors to just 19%—a critical improvement, as P_{turb} contributes $\sim 30\%$ of the total pressure needed to re-energize stalled shocks. PIML also better captured high- τ_{ij} tails (intense turbulence), which the gradient model missed; these tails are vital for identifying magnetorotational instability (MRI)-driven turbulence, a key driver of CCSN explosions. Beyond performance, PIML uncovered a physical link: high- τ_{ij} regions (filamentary turbulence) correlated strongly with regions of enhanced magnetic fields ($B > 100 \mu\text{G}$), supporting the hypothesis that MRI amplifies turbulence, boosting P_{turb} and aiding shock propagation.

4.3. Case 3: Cosmic Evolution of ISM Morphologies

Analyzing large samples of galaxies helps to understand the characteristics of interstellar medium (ISM) morphologies as they evolve over cosmic time. Scoville et al. used an AI-assisted gas mass estimation method [3], combined with data from the Atacama Large Millimeter/submillimeter Array (ALMA) and the Herschel Space Observatory to study 708 star-forming galaxies (redshift $z=0.3\text{--}4.5$). Reference developed neural emulators [4], which significantly accelerated the calculation of chemical abundances. AI-driven analysis revealed two key trends.

First, gas masses in galaxies peak at redshift $z=2$. At this point, they dominate stellar masses. The gas mass fraction (f_{gas}) is about 0.6. By $z < 1.2$, stellar masses take over as the main baryonic component, surpassing gas. Second, main-sequence (MS) and starburst galaxies have distinct shapes. MS galaxies are extended and diffuse, with gas dominating their structure. For these galaxies, 70% of their star formation rate (SFR) evolution comes from increasing gas mass. Starburst galaxies, on the other hand, are compact and dense. For them, 70% of SFR growth stems from higher star formation efficiency (SFE) rather than gas mass growth.

These evolutionary patterns imply a physical mechanism tied to cosmic accretion. At high redshifts ($z > 2$), gas mass changes need accretion rates over $100 M_{\odot}\text{yr}^{-1}$. AI emulators [3] confirm this rate is enough to refill gas used up by star formation. This steady accretion explains why high-redshift main-sequence galaxies have extended, gas-rich shapes. It connects large-scale gas movements to the varied structures and evolution of ISM morphologies over cosmic time.

5. Physical Insights from AI-Driven Morphological Classification

AI does more than classify ISM morphologies—it reveals fundamental physical laws governing the ISM's structure and evolution. This section synthesizes these insights across three scales: cloud-scale phase coupling, turbulence-magnetic field interactions, and cosmic-scale evolution.

5.1. Cloud-Scale: Morphology-Density-Chemistry Coupling

AI clustering has clarified how ISM morphologies encode density and chemical state, resolving long-standing ambiguities in single-line analysis by revealing two key insights [8]: First, MeanShift clustering of CO isotopologues uncovers nested morphological structures tied to density, where ^{12}CO traces the warm, outer "skin" of clouds (optically thick, $\tau > 10$), ^{13}CO maps intermediate layers, and C^{18}O identifies dense cores (optically thin, $\tau < 1$), reflecting optical depth differences between tracers. Second, AI-driven separation of UV-illuminated and shielded regions demonstrates that chemistry acts as a critical morphological discriminant—non-LTE modeling confirms UV radiation enhances the $[\text{HCO}^+]/[\text{C}^{18}\text{O}]$ ratio by two orders of magnitude, creating a distinct chemical signature for photodissociation region (PDR) morphologies and linking chemical state directly to morphological structure.

5.2. Turbulence Scale: Morphology as a Tracer of Dynamical Processes

AI models, such as physics-informed machine learning (PIML) [5], have advanced our understanding of turbulence morphologies in core-collapse supernovae (CCSNe) by linking them to underlying dynamics, thereby addressing the longstanding "turbulence problem." Key insights include the identification of high Reynolds stress (τ_{ij}) filaments, which correspond to magnetorotational instability (MRI)-driven turbulence—where magnetic fields amplify velocity fluctuations—serving as a precursor to successful CCSN explosions by enhancing turbulent pressure (P_{turb}). Additionally, AI analysis of neutral hydrogen data from M82's outflow reveals a morphological transition: turbulence starts as filamentary in the inner outflow and becomes diffuse in the outer regions, indicating deceleration caused by interactions with the circumgalactic medium.

5.3. Cosmic Scale: Morphology Evolution as a Window into Galaxy Formation

An AI-powered analysis of a large dataset shows how interstellar medium (ISM) morphologies shift over cosmic time [3], offering key constraints for galaxy formation models. At high redshifts ($z = 2$), it uncovers extended, gas-dominated ISM structures with a high gas mass fraction ($f_{\text{gas}} \sim 0.6$)—a pattern that lines up with the rapid gas accretion rates predicted by hierarchical galaxy formation models, where galaxies bulk up by siphoning gas from the cosmic web. Also, AI clustering flags starburst galaxies—marked by compact, dense gas structures—as preferentially forming via galaxy mergers. This backs that gravitational tugs kickstart shape shifts: from sprawling, quiet disks to tight,

star-making systems. Together, these results tie big cosmic processes (like accretion, mergers) to the visible shape variety of ISMs over time, boosting our ability to model and decode galaxy evolution.

6. Current Challenges and Future Directions

There are some significant achievements in AI-driven ISM morphology classification. However, AI-driven solution also faces some challenges that must be addressed. This section outlines these challenges and potential future works.

6.1. Current Challenges

The data bias and limited generalization of AI prevent the application of AI-driven ISM morphology classification method. For instance, training datasets often prioritize nearby, bright ISM regions, leading to models that struggle to classify quiescent or high-redshift clouds. In reference [4], the neural emulator is trained on hydrogen number densities $n_H = 10^4 - 10^7 \text{cm}^{-3}$, fails to capture diffuse gas ($n_H < 10^4 \text{cm}^{-3}$), limiting its applicability to underrepresented regimes. To mitigate this, researchers are expanding training sets to include diverse environments (e.g., low-redshift dwarf galaxies) and employing data augmentation techniques, such as synthetically adding noise to simulate high-redshift signal-to-noise (S/N) conditions [3].

The second issue is model interpretability. For deep learning architectures [5], it functions as "black boxes," making it difficult to trace morphological classifications back to underlying physical mechanisms. For example, while an emulator can predict sulfur-driven electron density, it cannot inherently explain why sulfur dominates over other ions in specific regimes. To address this, interpretability tools like SHAP (SHapley Additive exPlanations) values are proposed to quantify feature importance [4].

Finally, multi-modal data fusion remains a barrier. ISM observations span diverse wavelengths (optical, infrared, submillimeter), currently proposed AI models rarely integrate these modalities. For instance, MeanShift clustering effectively identifies molecular line structures but overlooks dust continuum emissions, missing critical dust-gas correlations in [8].

6.2. Future Directions

The James Webb Space Telescope (JWST) is the largest telescope in space designed to conduct infrared astronomy. It is equipped with high-resolution and high-sensitivity instruments, allowing it to view objects too old, distant, or faint for the Hubble Space Telescope [11]. While, the Nancy Grace Roman Space Telescope is in development and scheduled to launch to a Sun–Earth L_2 orbit by May 2027 [12]. The Roman Space Telescope will carry Wide-Field Instrument (WFI). The WFI is a 300.8-megapixel multi-band visible and near-infrared camera, providing a sharpness of images comparable to that achieved by the Hubble Space Telescope over a 0.28 square degree field of view, 100 times larger than imaging cameras on the Hubble. They will generate petabytes of interstellar medium (ISM) data. To keep pace with this data deluge, AI models must be optimized for real-time analysis.

Data scarcity for extreme or unobserved physical conditions is another bottleneck in ISM research. Generative adversarial networks (GANs) are promising for addressing this issue. GANs can simulate realistic ISM morphologies for scenarios that are currently hard to observe. This capability not only fills gaps in existing datasets but also enables "what-if" experiments.

Finally, AI can revolutionize astrophysical discovery by automating the identification of new ISM morphological classes. Traditional manual inspection of large datasets—such as ALMA's Galactic Plane Survey, which covers thousands of square degrees but often misses rare or subtle structures (e.g., thin magnetic filaments or faint outflow shells). Physics-Informed Neural Networks (PINNs), embedding physical laws into Neural Networks training, can analyze these datasets to detect previously unrecognized morphological features.

7. Conclusion

Many AI-driven methods have been developed for the ISM morphology classification, which make ISM morphology classification evolving from a labor-intensive practice into a data-driven endeavor. First, the developed and applied methodologies can be roughly classified in to three types: unsupervised learning identifies natural phases, supervised deep learning extracts spatial features from complex datasets, and physics-informed machine learning ensures outputs align with astrophysical principles. Second, some application cases demonstrate significant benefits. For examples: AI-driven method can classify phases in nearby giant molecular clouds like Orion B, model turbulence in core-collapse supernovae, trac the cosmic evolution of the ISM.

There still exist several challenges hindering its further application to be addressed: mitigating data bias, enhancing model interpretability, and advancing multi-modal data fusion. Therefore, more research is need, for instance the transformer-based DL model accompanying Physics-informed machine Learning techniques in a promising solution, which can exploit the capability of large language model and physical principles. Eventually, with the deployment of next-generation missions such as the James Webb Space Telescope (JWST) and the Nancy Grace Roman Space Telescope, AI-driven classification is poised to play an increasingly critical role in unraveling the complexities of the interstellar medium (ISM), thereby deepening our understanding of star formation, galaxy evolution, and the cosmic baryon cycle.

References

- [1] Eric, Herbst. Chemistry in the interstellar medium. *Annual Review of Physical Chemistry*. 1995,46: 27-53
- [2] D. S. N. Rupke. A review of recent observations of galactic winds driven by star formation," *Galaxies*, 2018,6 (4) :1-24.
- [3] N. Scoville et al., Cosmic evolution of gas and star formation. *Astrophysical Journal*, 2023, 943 (82) :1-18.
- [4] A. A. Ramos et al. A fast neural emulator for interstellar chemistry. *Monthly Notices of the Royal Astronomical Society*, 2024, 531: 4930–4943.
- [5] P.Kovács, et al. Machine learning prediction of infrared spectra of interstellar polycyclic aromatic hydrocarbons. *The Astrophysical Journal*, 2020,902 (100):1-9.
- [6] P.Palud, et al. Neural network-based emulation of interstellar medium models. *Astronomy & Astrophysics*, 2023, 678 (A198):1-14.
- [7] P.I.Karpov et al. Physics-informed machine learning for modeling turbulence in supernovae. *Astrophysical Journal*, 2022, 940 (26) :1-13.
- [8] E. Bron et al. Clustering the Orion B giant molecular cloud based on its molecular emission. *Astronomy & Astrophysics*, 2018, 610 (A12) :1-26.
- [9] H. S. Samuel, et al. Machine learning of rotational spectra analysis in interstellar medium. *Communication in Physical Sciences*, 2023, 10 (1): 172-203.
- [10] J. E. G. Peek, et al. Do androids dream of magnetic fields-using neural networks to interpret the turbulent interstellar medium," *The Astrophysical Journal Letters*, 2018, 882 (L12) :1-8.
- [11] Clara Moskowitz. How JWST Is Changing Our View of the Universe—The James Webb Space Telescope has sparked a new era in astronomy". *Scientific American*. December 1,2022. online available: <https://www.scientificamerican.com/article/how-jwst-is-changing-our-view-of-the-universe/>
- [12] NASA Tool Gets Ready to Image Faraway Planets. May 21,2024. online available: <https://www.nasa.gov/missions/roman-space-telescope/nasa-tool-gets-ready-to-image-faraway-planets/>