A Physics-Informed Graph Neural Network for Unified Modeling of Anomalous Expansion in Ultracold Neutral Plasmas

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Abstract

Ultracold neutral plasmas (UNPs) exhibit anomalous expansion behavior at low temperatures that has resisted unified theoretical explanation for over two decades. We present a proof-of-concept physics-informed graph neural network, termed the Elemental Embedding Engine (E3), that successfully captures both the high-temperature hydrodynamic regime and the low-temperature anomalous regime within a single predictive framework. While limited by a small experimental dataset (N=10-15 data points across 4 elements), the model learns context-dependent elemental embeddings that naturally encode the crossover between elastic cooling and inelastic heating physics without explicit regime-switching logic. Training on experimental data from four chemical families (Noble Gases, Alkali Metals, Halogens, and Alkaline Earth Metals), the E3 achieves $R^2 = 0.82 \pm 0.15$ on leave-one-out cross-validation of original experimental data. The model identifies two characteristic timescales: a primary relaxation time (τ) and, for halogens, a secondary buffer time (t_{break}) that may correspond to instability growth. Analysis of the high-temperature regime reveals an empirical linear scaling between inverse relaxation time and temperature, with a proportionality constant $\kappa_{\text{eff}} = (1340 \pm 60) \times 10^{-6}$ $\text{K}^{-1}\text{s}^{-1}$. The model generates testable predictions for environmental modulation of relaxation dynamics and suggests ionization state may bridge

relaxation behaviors between chemical families. This work demonstrates the potential of physics-informed machine learning to resolve long-standing anomalies in plasma physics while generating hypotheses for future experimental investigation.

1 Introduction

Ultracold neutral plasmas (UNPs) represent a unique laboratory system at the intersection of atomic physics, plasma physics, and strongly correlated matter [1]. Created by photoionizing laser-cooled atoms, these systems can achieve electron temperatures ranging from 1 K to 1000 K while maintaining ion temperatures as low as millikelvin, accessing parameter regimes where the Coulomb coupling parameter $\Gamma = e^2/(4\pi\epsilon_0 a k_B T_e)$ exceeds unity [2]. This strong coupling regime, relevant to exotic astrophysical environments such as white dwarf interiors and neutron star crusts, exhibits dynamics that challenge conventional plasma theory.

A particularly puzzling aspect of UNP behavior is the anomalous expansion observed at low initial electron temperatures. Pioneering experiments by Killian and collaborators revealed that plasma expansion velocities at $T_e < 10$ K exceed hydrodynamic predictions by up to 50%, with the discrepancy increasing as temperature decreases [1, 3]. This anomaly has been attributed to the competition between adiabatic cooling and three-body recombination (TBR) heating, but existing theoretical models have struggled to provide a unified framework capturing both the high-temperature hydrodynamic behavior and the low-temperature anomalous regime within a single predictive scheme [4, 5].

The challenge of modeling this crossover behavior exemplifies a broader difficulty in plasma physics: capturing multi-scale, context-dependent phenomena where the dominant physical processes change dramatically with environmental conditions. Traditional approaches based on regime-specific models require explicit switching logic and often fail at transition boundaries. This motivates the exploration of data-driven approaches that can learn effective representations encoding the relevant physics across different regimes.

This paper introduces the Elemental Embedding Engine (E3), a physics-informed graph neural network designed to learn context-aware representations of elemental behavior in non-equilibrium plasmas. By processing plasma constituents as nodes in a dynamic graph, the E3 captures how atomic properties manifest differently under varying environmental conditions. Our approach builds on recent advances in graph neural networks for

molecular systems [6, 7] and physics-informed neural networks [8], extending these concepts to the challenging regime of strongly coupled plasmas.

The remainder of this paper is organized as follows: Section 2 reviews related work in plasma relaxation theory and machine learning applications. Section 3 details our methodology, including data curation, model architecture, and training procedures. Section 4 presents results on model performance and physical insights. Section 5 discusses implications, limitations, and future directions. Section 6 concludes.

2 Related Work and Theoretical Background

2.1 Plasma Relaxation Phenomena

Relaxation processes in plasmas encompass a hierarchy of timescales and mechanisms. The foundational Spitzer relaxation time describes electron-ion temperature equilibration through Coulomb collisions, scaling as $\tau_{\text{Spitzer}} \propto T_e^{3/2}/n_e$ where n_e is the electron density [9]. This $T^{3/2}$ dependence arises from the velocity dependence of the Coulomb cross-section and represents a cornerstone of classical plasma theory [10].

However, UNPs operate in regimes where classical theory breaks down. At strong coupling ($\Gamma > 1$), collective effects dominate over binary collisions, leading to phenomena such as disorder-induced heating and correlation-enhanced transport [11]. The relaxation dynamics become further complicated by the presence of neutral atoms, enabling three-body processes that are negligible in traditional plasmas.

The concept of staged or multi-timescale relaxation is well-established in plasma physics. In anisotropic systems, temperature equilibration between parallel and perpendicular degrees of freedom can proceed on different timescales [12]. Similarly, multi-component plasmas exhibit sequential relaxation: first within species, then between species [13]. These precedents suggest that the apparent "buffer time" we observe in some elements may reflect a known class of phenomena requiring proper contextualization.

2.2 Three-Body Recombination in UNPs

Three-body recombination, where two electrons and an ion combine to form a bound atom plus a free electron, plays a crucial role in UNP dynamics at low temperatures. The rate coefficient for this process in UNPs has been shown through kinetic modeling to scale as $k_3 \propto T_e^{-9/2}$, a much stronger temperature dependence than classical predictions [14]. This scaling arises from

the combined effects of the reaction cross-section and the thermal velocity distribution, with quantum mechanical corrections becoming important at the lowest temperatures. The application of this $T_e^{-9/2}$ scaling is consistent with experimental measurements, which use the accepted theory to interpret recombination rates in ultracold plasmas [15]. At temperatures below approximately 10 K, TBR heating can arrest or even reverse the adiabatic cooling expected from plasma expansion, leading to the observed anomalous behavior.

2.3 Machine Learning in Plasma Physics

The application of machine learning to plasma physics has accelerated in recent years, driven by the availability of large experimental datasets and the need for real-time control in fusion devices. Neural networks have been successfully deployed for disruption prediction in tokamaks [16], turbulence closure modeling [17], and optimization of plasma-facing materials [18].

Graph neural networks (GNNs) have emerged as particularly suitable for modeling systems with complex spatial relationships. In molecular systems, architectures like SchNet [6] and CGCNN [7] have demonstrated the ability to learn representations that respect physical symmetries while capturing many-body interactions. The extension of these concepts to plasma systems, where particles interact through long-range Coulomb forces and collective modes, presents both opportunities and challenges.

3 Methodology

3.1 Experimental Data and Feature Extraction

3.1.1 Data Sources

We compiled experimental data from published UNP expansion measurements, focusing on well-characterized systems with systematic temperature variation. Primary data sources included:

- Strontium (Sr): 8 experimental runs from Killian et al. [1, 3]
- Rubidium (Rb): 3 data points from literature surveys
- Iodine (I): 2 data points from halogen plasma studies
- Argon (Ar): 2 data points from noble gas experiments

This limited dataset (N=15 total experimental points) represents a fundamental constraint of this work and motivates our characterization of the E3 as a proof-of-concept rather than a production-ready model.

For each experimental run, we digitized the time-dependent expansion velocity $v(t)$ and fitted it to an exponential relaxation model:

$$v(t) = V_{\max} \cdot (1 - e^{-t/\tau}) \tag{1}$$

where $V_{\max}$ is the asymptotic expansion velocity and τ is the characteristic relaxation time.

3.1.2 Two-Regime Behavior

Analysis of the extracted relaxation times revealed distinct temperature-dependent behavior:

High-Temperature Regime ($T > 25$ K): We observed an approximately linear relationship between the inverse relaxation time and temperature:

$$\frac{1}{\tau} = \kappa_{\text{eff}} \cdot T \tag{2}$$

where linear regression yielded $\kappa_{\text{eff}} = (1340 \pm 60) \times 10^{-6}$ $\text{K}^{-1}\text{s}^{-1}$.

Low-Temperature Regime ($T < 10$ K): The linear relationship breaks down, with three-body recombination becoming dominant. The effective relaxation rate in this regime follows the expected TBR scaling [14].

3.2 Data Augmentation Strategy

The limited size of our experimental dataset necessitated a careful augmentation strategy to enable neural network training. We implemented a physics-constrained interpolation approach with the following principles:

1. **Regime-Specific Interpolation:**
   - High-T regime: Linear interpolation in $1/\tau$ vs T space
   - Low-T regime: Power-law interpolation respecting $T_e^{-9/2}$ scaling
   - Transition region (10-25 K): Smooth spline interpolation
2. **Constraint Enforcement:**
   - Monotonicity: τ decreases with increasing T
   - Continuity: Smooth transitions between regimes

- Physical bounds: $\tau > 0$, reasonable $V_{\max}$ limits

3. **Uncertainty Propagation:** Interpolated points carry larger uncertainty weights in the loss function

Critical Limitation: We acknowledge that this augmentation strategy introduces significant risk of overfitting and circular reasoning. The interpolation method embeds our assumptions about the underlying physics, potentially biasing the model toward "discovering" the relationships used in the interpolation. All performance metrics should be interpreted with this limitation in mind.

3.3 Model Architecture

The E3 employs a graph neural network architecture where:

Node Features:

- Element type (one-hot encoded, dimension: 4)
- Local electron temperature T_e (normalized)
- Local density n_0 (normalized)
- Coulomb coupling parameter $\Gamma = e^2/(4\pi\epsilon_0 a k_B T_e)$

Edge Construction:

- Edges connect all node pairs within cutoff radius $r_c = 10$ Debye lengths
- Edge weights: $w_{ij} = \exp(-r_{ij}/\lambda_D)$ where λ_D is the Debye screening length

Network Architecture:

1. Input embedding layer with MinMax normalization
2. Three graph convolutional layers:
    - Layer 1: 64 hidden units, ReLU activation
    - Layer 2: 32 hidden units, ReLU activation
    - Layer 3: 16 hidden units, ReLU activation
3. Two output heads:
    - Primary relaxation time τ

- Secondary buffer time t_{break}

The graph convolution operation follows the standard message-passing formulation:

$$h_i^{(l+1)} = \sigma\left(W^{(l)} \sum_{j \in \mathcal{N}(i)} w_{ij} h_j^{(l)} + b^{(l)}\right) \tag{3}$$

where $h_i^{(l)}$ is the hidden state of node i at layer l, $\mathcal{N}(i)$ denotes the neighbors of node i, and σ is the ReLU activation.

3.4 Training and Validation

3.4.1 Standard Training

We employed standard supervised learning with:

- Adam optimizer with learning rate $\alpha = 10^{-3}$
- Mean squared error loss: $\mathcal{L} = \frac{1}{N}\sum_{i=1}^{N}[(\tau_i - \hat{\tau}_i)^2 + (t_{\text{break},i} - \hat{t}_{\text{break},i})^2]$
- 80/20 train/validation split on augmented data
- Early stopping with patience of 50 epochs
- Total training epochs: typically 200-300 before convergence

3.4.2 Robust Validation Strategy

To provide a realistic assessment of model performance, we implemented leave-one-out cross-validation (LOOCV) exclusively on the original 15 experimental data points:

Algorithm 1 LOOCV on Original Data

for each original data point $i \in \{1, ..., 15\}$ **do**
  Remove point i and all interpolated points within $\Delta T = 5$ K
  Train model on remaining augmented dataset
  Evaluate model prediction on point i
  Record absolute error: $e_i = |\tau_i - \hat{\tau}_i|$
end for
Compute: $\bar{e} = \frac{1}{15}\sum_{i=1}^{15} e_i$ and $\sigma_e = \sqrt{\frac{1}{14}\sum_{i=1}^{15}(e_i - \bar{e})^2}$

This validation strategy provides our most honest estimate of generalization performance.

4 Results

4.1 Model Performance

Table 1 summarizes the model performance metrics:

Table 1: E3 Model Performance Metrics

Metric	Augmented Dataset	LOOCV (Original Data)
R^2 Score	0.9993	0.82 ± 0.15
Mean Absolute Error (τ)	0.15 μs	2.8 ± 1.2 μs
Mean Absolute Error (t_{break})	0.18 μs	3.1 ± 2.5 μs
Relative Error (τ)	0.8%	14.2 ± 8.3%

The stark difference between augmented and LOOCV performance highlights the model's limitations. The high performance on augmented data largely reflects the model learning the interpolation scheme rather than discovering new physics. The LOOCV results provide a more realistic assessment: the model achieves reasonable but not exceptional predictive accuracy on truly unseen data.

4.2 Chemical Family Differentiation

Despite the limited dataset, the model learned distinct relaxation signatures for different chemical families:

- **Noble Gases (Ar):** Moderate single-stage relaxation ($\tau = 15 \pm 5$ μs, $t_{\text{break}} \approx 0$)
- **Alkali Metals (Rb):** Fast single-stage relaxation ($\tau = 3.5 \pm 1.5$ μs, $t_{\text{break}} \approx 0$)
- **Alkaline Earths (Sr):** Slow single-stage relaxation ($\tau = 35 \pm 15$ μs, $t_{\text{break}} \approx 0$)
- **Halogens (I):** Two-stage relaxation ($\tau = 35 \pm 5$ μs, $t_{\text{break}} = 15 \pm 3$ μs)

The observation of non-zero t_{break} exclusively in halogens (based on only 2 data points) is intriguing but requires validation with additional halogen species before drawing strong conclusions.

4.3 Model-Generated Predictions

4.3.1 Environmental Modulation of Relaxation

The trained model generates predictions for how environmental conditions might alter relaxation behavior. For rubidium under modified conditions, the model predicts:

Table 2: Model Predictions for Rb Under Different Conditions

Condition	T (K)	n_0 (cm^{-3})	Predicted τ (μs)
Standard	10	10^9	2.28 ± 0.34
High-T, Low-n	100	0.5×10^9	57.68 ± 12.1
Low-T, High-n	5	5×10^9	0.83 ± 0.21

These predictions represent extrapolations beyond the training data and should be treated as hypotheses for experimental testing rather than validated results. The large uncertainty estimates reflect the model's limited confidence in these extrapolated regimes.

4.3.2 Cross-Family Relationships

Analysis of the learned embeddings revealed interesting patterns. When projecting the 16-dimensional final layer representations using t-SNE, we observed that Sr^+ embeddings cluster near neutral Rb embeddings. This observation led to the hypothesis that ionization state might provide a bridge between chemical families' relaxation behaviors. However, with only 15 original data points, this remains highly speculative.

5 Discussion

5.1 Physical Interpretation of Results

5.1.1 Empirical Scaling in the High-Temperature Regime

The observed linear relationship $1/\tau \propto T$ differs markedly from classical Spitzer scaling. Several interpretations are possible:

1. **Effective scaling in mixed systems:** The presence of both charged and neutral species may lead to an effective scaling that differs from pure plasma theory

2. **Limited parameter range:** Our data spans only 25-1000 K; the apparent linearity may break down outside this range

3. **Fortuitous cancellation:** Competing temperature dependencies in density and collision rates might coincidentally produce linear behavior

The empirical constant $\kappa_{\text{eff}} = (1340 \pm 60) \times 10^{-6}$ $\text{K}^{-1}\text{s}^{-1}$ provides a useful parameterization within the studied regime but should not be interpreted as a fundamental constant without theoretical justification.

5.1.2 Buffer Time Interpretation

The $t_{\text{break}} \approx 15$ μs observed in iodine plasmas suggests a two-stage relaxation process. Possible physical mechanisms include:

1. **Molecular ion formation:** I_2^+ formation could introduce a secondary timescale

2. **Electron attachment:** Halogens' high electron affinity might create negative ions, altering relaxation dynamics

3. **Instability growth:** The timescale matches expected growth rates for certain plasma instabilities

With only 2 halogen data points, these interpretations remain speculative.

5.2 Limitations and Caveats

This work has several fundamental limitations that must be acknowledged:

1. **Minimal dataset:** 15 experimental points across 4 elements is insufficient for robust machine learning. The model is severely undertrained by conventional standards.

2. **Circular validation:** The augmentation strategy embeds physical assumptions that the model then "rediscovers," limiting genuine insight generation.

3. **Limited chemical diversity:** Four elements cannot represent the full periodic table's behavior.

4. **Narrow parameter range:** Experiments span limited temperature and density ranges, restricting generalization.

5. **Single-author limitations:** As a solo project with limited resources, comprehensive validation was not feasible.

5.3 Future Directions

Despite limitations, this proof-of-concept suggests several promising research directions:

5.3.1 Immediate Experimental Priorities

1. **Expand the dataset:** Minimum 50-100 experimental points needed for reliable training
2. **Test specific predictions:** Validate the high-T/low-n Rb prediction as a model test
3. **Additional halogens:** Confirm whether $t_{\text{break}} > 0$ is universal for halogens
4. **Extended temperature range:** Test linear scaling beyond 25-1000 K

5.3.2 Model Enhancements

Future versions should incorporate:

- Uncertainty quantification using ensemble methods or Bayesian neural networks
- Physics constraints as regularization terms in the loss function
- Transfer learning from molecular dynamics simulations
- Attention mechanisms to identify dominant physical processes

5.3.3 Collaborative Opportunities

This single-author proof-of-concept would benefit from:

- Collaboration with experimental groups for data generation
- Partnership with plasma theorists for physical interpretation
- Open-source development to accelerate improvements

6 Conclusion

We have developed a proof-of-concept physics-informed graph neural network that demonstrates the potential for machine learning to address long-standing problems in plasma physics. Despite severe data limitations (N=15), the Elemental Embedding Engine (E3) successfully captures the qualitative transition between high-temperature hydrodynamic and low-temperature anomalous expansion regimes in ultracold neutral plasmas.

Key contributions include:

1. **Unified framework:** Single model capturing multiple physical regimes without explicit switching
2. **Empirical discovery:** Linear $1/\tau \propto T$ scaling in high-temperature regime
3. **Testable predictions:** Specific experimental conditions for validation
4. **Open-source tool:** Publicly available code for community development

Key limitations include:

1. **Minimal dataset:** Results based on only 15 experimental points
2. **Limited validation:** Cross-validation shows modest performance ($R^2 = 0.82 \pm 0.15$)
3. **Augmentation bias:** Model partially learns interpolation scheme rather than physics

This work represents an initial step toward physics-informed machine learning for plasma dynamics. While not ready for production use, it establishes a framework that, with additional data and development, could provide valuable insights into non-equilibrium plasma behavior. We hope this proof-of-concept stimulates both experimental work to expand the dataset and theoretical efforts to understand the empirical patterns observed.

Data and Code Availability

The complete dataset (clearly distinguishing original from augmented data), trained models, and analysis code are available at `https://github.com/ismpower/E3_Project` under MIT license. Version 1.0 corresponds to this publication. We encourage community contributions and collaborative development.

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Author Contributions

I.C. conceived the project, developed the model, performed all analyses, and wrote the manuscript.

Competing Interests

The author declares no competing financial or non-financial interests.

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