Physics-Guided Self-Supervised Graph Neural Networks for Power Grid Analysis: Transfer Learning Across Cascade Prediction, Power Flow, and Line Flow

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For Review

***Abstract*—Modern power grid operations require rapid computational methods for decision support, but traditional solvers face severe bottlenecks. We present a physics-guided self-supervised learning framework for graph neural networks that addresses labeled data scarcity in power system analysis. Our approach embeds admittance-weighted message passing into the encoder architecture and develops grid-specific pretext tasks (masked injection and parameter reconstruction) enabling representation learning from unlabeled operational data. Evaluated on the PowerGraph benchmark, our method achieves substantial improvements in low-label regimes: 29.1% power flow error reduction, 26.4% line flow error reduction, and 6.8% F1-score improvement for cascading failure prediction—all at 10% labeled data availability. On the IEEE 118-bus system under severe class imbalance, self-supervised pretraining dramatically reduces training instability (variance reduction from $\pm$0.243 to $\pm$0.051) while improving mean performance (ΔF1 = +0.61). We achieve 0.93 AUC-ROC explainability fidelity via Integrated Gradients, addressing a recognized gap in interpretable cascade prediction.**

***Index Terms*—Power systems, graph neural networks, self-supervised learning, cascading failures, power flow, optimal power flow, explainability, physics-informed machine learning**

I. Introduction

Modern power grid operations demand rapid decision-making capabilities that traditional computational methods struggle to provide. Optimal power flow (OPF) solvers—used to determine economically efficient generator dispatch while respecting physical and operational constraints—can require minutes to solve on utility-scale networks with thousands of buses [1], rendering them impractical for real-time control and contingency analysis. Cascading failure risk assessment presents an even greater challenge: comprehensive N-k security analysis requires evaluating thousands or millions of contingency scenarios, each necessitating a full power flow calculation [2]. These computational bottlenecks have motivated a shift toward machine learning surrogates that approximate complex power system computations at dramatically reduced cost. Recent supervised learning approaches have demonstrated remarkable speedups—ranging from 100$\times$ to 10,000$\times$ faster than conventional solvers [1], [3]—while maintaining solution quality within 0.2% of optimality. However, these methods rely fundamentally on labeled training data: typical implementations require 5,000 to 60,000 labeled samples per network [**?**], [3], where each label is itself the output of the computationally expensive solver the surrogate aims to replace. This chicken-and-egg problem—needing expensive simulations to train models meant to avoid expensive simulations—severely limits the practical deployment of learning-based power system analysis, particularly for networks with limited historical data or frequently changing topologies.

Self-supervised learning (SSL) offers a compelling solution to the labeled data bottleneck by leveraging abundant unlabeled operational data. In the broader machine learning community, graph SSL methods have demonstrated substantial performance gains in low-label regimes: GraphMAE2 achieves a 5.46 percentage point accuracy improvement using only 1% labeled data on molecular property prediction benchmarks [4], while contrastive learning frameworks enable effective transfer across diverse graph domains [5]. These successes suggest that self-supervised pretraining could similarly benefit power system applications, where operational measurements (bus voltages, line flows, injection patterns) are continuously recorded but corresponding "labels" (optimal solutions, failure classifications) are costly to obtain. However, a critical gap exists: among the extensive body of graph SSL research spanning molecular graphs [6], social networks [5], and traffic systems [7], applications to power grids remain remarkably scarce. Our comprehensive literature review identified only five to six papers applying SSL to power systems [**?**], [**?**], and critically, *none* of these methods incorporate physics-informed pretext tasks that leverage the fundamental electrical relationships governing grid behavior. This represents a significant missed opportunity: power systems are governed by well-understood physical laws—Kirchhoff's current and voltage laws, power flow equations, admittance relationships—that could serve as powerful self-supervisory signals for representation learning.

The graph structure of electrical networks naturally aligns with graph neural network (GNN) architectures, where message passing along edges can mirror the physical propagation of power flows along transmission lines [8]. Recent work has begun embedding power system physics into GNN designs:

impedance-weighted aggregation schemes [9], complex-valued representations preserving phase relationships [**?**], and hard Kirchhoff's law constraints enforced through architectural projections [**?**]. These physics-informed GNNs demonstrate improved accuracy and generalization compared to topology-agnostic baselines, particularly for out-of-distribution scenarios and N-1 contingencies [**?**]. However, existing physics-guided approaches remain tethered to supervised learning paradigms, requiring labeled power flow solutions or optimal dispatch setpoints for training. *No prior work has combined physics-guided GNN architectures with self-supervised pretraining*, leaving unexplored the question of whether physics-informed message passing can enable effective representation learning from unlabeled data alone.

This paper introduces a physics-guided self-supervised learning framework for power grid analysis that addresses these gaps. We make the following contributions:

- **Physics-Guided Graph Neural Network Architecture:** We design a message-passing encoder that incorporates admittance-weighted aggregation, where line conductance and susceptance values directly control information flow between connected buses, embedding the structure of the power system admittance matrix into the neural network computation graph.
- **Self-Supervised Pretraining Objective:** We develop grid-specific pretext tasks—masked injection reconstruction (predicting active and reactive power injections at randomly masked buses) and masked parameter reconstruction (predicting line impedance parameters at randomly masked edges)—that enable representation learning from unlabeled grid operational data without requiring solutions from conventional solvers. Critically, we ensure no label leakage by pretraining exclusively on the training partition, with validation and test sets never exposed during self-supervised learning.
- **Multi-Task Transfer Learning Evaluation:** We demonstrate that representations learned via physics-guided SSL transfer effectively to three downstream tasks: (1) power flow prediction (bus voltage magnitudes), (2) line flow prediction (active and reactive power flows on transmission lines), and (3) cascading failure classification (graph-level binary prediction of cascade occurrence). On the PowerGraph benchmark [10], our approach achieves 29.1% mean absolute error reduction for power flow, 26.4% reduction for line flow, and 6.8% F1-score improvement for cascade prediction—all measured at 10% labeled data availability relative to scratch training baselines.
- **Scalability and Variance Reduction:** On the larger IEEE 118-bus system under severe class imbalance conditions (5% cascade rate), self-supervised pretraining not only improves mean performance (ΔF1 = +0.61) but dramatically reduces training instability: scratch training exhibits $\pm$0.243 F1 variance across random seeds, while SSL-pretrained models achieve $\pm$0.051 variance—a stabilization effect critical for reliable deployment.
- **Explainability Validation:** Using ground-truth edge importance masks from the PowerGraph benchmark, we quantitatively evaluate explanation fidelity via Integrated Gradients, achieving 0.93 AUC-ROC compared to 0.72 for heuristic baselines. This addresses a recognized gap in cascading failure prediction, where current explainable AI methods have been reported to perform "suboptimally" [10].
- **Robustness Under Distribution Shift:** We evaluate model behavior under load stress conditions (1.0$\times$ to 1.3$\times$ nominal loading), demonstrating that SSL-pretrained representations exhibit superior robustness, maintaining 22% higher performance advantage at 1.3$\times$ load compared to scratch training.

The remainder of this paper is organized as follows. Section II reviews related work in power system machine learning, graph neural networks, self-supervised learning, physics-informed methods, and cascading failure prediction. Section III formulates the graph representation of power grids and defines the three downstream tasks. Section IV details our physics-guided encoder architecture and self-supervised pretraining objective. Section V describes the experimental setup, including datasets, baselines, and training protocols. Section VI presents comprehensive results across all tasks and grid scales, including ablation studies and robustness analysis. Section VII discusses implications for operational deployment, limitations, and future directions. Section VIII concludes.

II. Related Work

Traditional power flow and optimal power flow computations rely on iterative numerical methods such as Newton-Raphson and interior-point algorithms, which can require seconds to minutes per solve on large-scale grids [3]. To enable near-real-time decision support, researchers have developed machine learning surrogates that approximate these complex mappings from grid conditions (load demands, generation capacities, network topology) to power flow solutions or optimal dispatch setpoints. Fully-connected deep neural networks have demonstrated impressive results: Pan et al.'s DeepOPF framework achieves feasible OPF solutions with less than 0.2% optimality loss and up to 100$\times$ speedup over conventional solvers on benchmark IEEE test systems [3], while Huang et al.'s DeepOPF-V extends this approach to AC-OPF with reported speedups exceeding 10,000$\times$ on 2,000-bus networks [1]. Graph neural networks have emerged as a particularly promising architecture due to their ability to exploit grid topology and achieve greater scalability [11], [12]. For instance, PowerFlowNet demonstrated successful scaling to a 6,470-bus French transmission network with voltage magnitude prediction errors below 0.001 per-unit [11], while heterogeneous message-passing neural networks maintain constant parameter counts across grid sizes ranging from 14 to 2,000+ buses [**?**]. However, these supervised approaches face a critical limitation: they require extensive labeled training data. Typical implementations demand 5,000–60,000 OPF solutions per network [**?**], [3], and generating this labeled data via conventional solvers is computationally expensive—precisely

the bottleneck these methods aim to circumvent. This data scarcity challenge motivates unsupervised and self-supervised learning approaches that can leverage abundant unlabeled operational data.

The natural graph structure of electrical networks—with buses as nodes and transmission lines as edges—makes graph neural networks an ideal architecture for power system analysis. GNNs encode topological relationships through message passing, where each node aggregates information from its neighbors according to the grid's physical connectivity [8]. This inductive bias enables GNNs to handle topology changes (such as N-1 contingencies) without retraining, a critical advantage over fully-connected networks that treat grid states as fixed-dimensional vectors [**?**]. Empirical studies demonstrate that GNN-based approaches achieve substantially lower prediction errors than traditional neural networks: for example, an electrical-model-guided GNN for distribution system state estimation attained an order-of-magnitude lower error than standard feedforward networks, even with missing sensor measurements [13]. Recent work has begun incorporating power system physics more deeply into GNN architectures. Meta-PIGACN integrates impedance-weighted edge aggregation, where line admittance values directly control message-passing strength [9], while complex-valued spatial-temporal GCNs represent voltage phasors and impedance in their native complex form to preserve phase relationships inherent to AC power flow [**?**]. KCLNet enforces Kirchhoff's Current Law as hard architectural constraints via differentiable hyperplane projections, guaranteeing zero KCL violations by construction [**?**], and PINCO achieves zero inequality constraint violations through physics-informed hard constraints in an unsupervised learning framework [**?**]. The PowerGraph benchmark [10] provides standardized evaluation across GCN, GAT, GraphSAGE, and Graph Transformer architectures, establishing that topology-aware message passing consistently outperforms topology-agnostic baselines on both node-level (power flow, voltage estimation) and graph-level (cascading failure prediction) tasks.

Self-supervised learning has emerged as a powerful paradigm for learning graph representations without labeled data, with two dominant approaches: contrastive learning and generative masked reconstruction. Contrastive methods, exemplified by Deep Graph Infomax [14], InfoGraph [15], and GraphCL [16], maximize agreement between different augmented views of graphs through node dropping, edge perturbation, or subgraph sampling. More recent frameworks have reduced the complexity of these approaches: BGRL eliminates negative sampling through bootstrapped representation learning [17], achieving 2–10$\times$ memory reduction while matching state-of-the-art performance, and SimGRACE dispenses with manual graph augmentation entirely by perturbing encoder parameters to generate contrastive views [18]. In parallel, generative approaches have gained traction: GraphMAE employs masked feature reconstruction with a scaled cosine error loss and dedicated decoder architecture [19], demonstrating that carefully designed autoencoders can match or exceed contrastive methods (84.2% accuracy on Cora versus 82.7% for BGRL). GraphMAE2 extends this with multi-view random re-masking and latent representation prediction [4], scaling to graphs with over 100 million nodes. These graph SSL methods show substantial benefits in low-label regimes: GraphMAE2 achieves a 5.46 percentage point accuracy improvement with only 1% labeled data on large-scale molecular property prediction benchmarks [4], while GCC's cross-domain pretraining on diverse network types enables effective transfer to new graph tasks with minimal fine-tuning [5]. Applications to physical systems have proven successful in molecular graphs [6] and traffic networks [7], where graph structure naturally encodes physical relationships. However, a significant research gap exists for power grid applications: while SafePowerGraph [20] and recent work by Zhu et al. [**?**] introduced hybrid supervised-SSL approaches for power systems, no pure graph SSL method has been designed specifically for electrical networks with physics-informed constraints such as power flow equations, Kirchhoff's laws, or voltage-angle relationships.

Physics-informed neural networks embed domain knowledge—governing equations, conservation laws, or known constraints—into machine learning models to improve generalization and sample efficiency. The canonical PINN framework [**?**] encodes partial differential equations as soft regularization terms in the loss function, minimizing both data mismatch and PDE residuals at collocation points. This approach has proven effective for solving forward and inverse problems in fluid dynamics, solid mechanics, and heat transfer [**?**]. Alternative strategies include hard constraint enforcement, where physical laws are satisfied by construction through architectural design: Beucler et al. demonstrated that architecture-constrained networks can achieve energy and mass conservation to machine precision without loss penalties [**?**], while Hamiltonian Neural Networks embed symplectic structure to guarantee exact energy conservation in dynamical systems [**?**]. In power systems specifically, physics-informed approaches have addressed swing equation dynamics for transient stability [**?**], state estimation with admittance matrix constraints [**?**], and power flow prediction with Kirchhoff's law regularization [21]. These methods demonstrate compelling benefits: physics constraints act as inductive biases that limit the hypothesis space and improve out-of-distribution generalization, with physics-informed GNNs showing zero-shot generalizability to systems an order of magnitude larger than training configurations [**?**]. However, a critical gap remains: the vast majority of PINN research targets continuous PDE-governed domains where automatic differentiation naturally computes spatial and temporal derivatives. Discrete, graph-structured infrastructure networks like power grids present fundamentally different challenges—physical laws (KCL, KVL, power balance) operate directly on graph edges and nodes rather than as discretized continuous fields, and topological changes require handling discrete switching dynamics. While GraPhyR [**?**] demonstrated physics-informed GNNs with gated message passing for power system reconfiguration, graph-based power

system surrogates that combine self-supervised pretraining with physics-guided architectures remain unexplored.

Cascading failures—sequences of component outages that can escalate to widespread blackouts—represent a critical threat to power grid resilience, as evidenced by major disruptions including the 2003 Northeast blackout and the 2021 Texas winter storm [22]. Traditional simulation models such as OPA [23], DCSIMSEP [24], and the Manchester model [25] capture cascading dynamics through iterative power flow calculations coupled with protection system logic, revealing self-organized criticality in grid behavior. However, these physics-based simulators face computational limitations: DC cascade models provide two orders of magnitude speedup over AC models but sacrifice accuracy by ignoring voltage collapse mechanisms [**?**], while AC models are approximately 7× more computationally expensive and suffer convergence issues under high stress conditions. Machine learning approaches have achieved dramatic acceleration: deep convolutional neural networks enable 100× faster N-1 contingency screening [2], while graph neural networks leverage network topology to predict cascade outcomes with over 96% accuracy [**?**]. GNN-based methods demonstrate transfer learning capability across different grid topologies and operating conditions, addressing a key limitation of classical simulation approaches. However, explainability remains a significant gap. Post-mortem analyses of major blackouts still rely on manual timeline reconstruction and root cause analysis [22], and recent benchmarking reveals that current explainable AI methods perform "suboptimally" on cascade explanation tasks [10]. The PowerGraph benchmark explicitly identifies this gap, noting that "given the crucial role of explainability for power grid operators, this underscores the ongoing need for dedicated research and development in this field" [10]. While XAI techniques including SHAP, LIME, and attention mechanisms have been successfully applied to other power system tasks such as frequency stability prediction, cascading failure prediction lacks robust explainability frameworks that can identify critical transmission pathways and quantify failure propagation mechanisms in a way that operators can trust and act upon.

This work addresses the identified gaps by uniquely combining physics-guided graph neural network architectures with self-supervised pretraining for power grid analysis. Our physics-guided encoder embeds admittance-weighted message passing directly into the network architecture—drawing on the success of Meta-PIGACN [9] and KCLNet [**?**] but extending to a self-supervised learning paradigm. Unlike existing SSL approaches for graphs that ignore domain physics [17], [19], we design grid-specific pretext tasks (masked injection reconstruction, masked parameter reconstruction) that leverage power system structure without requiring labeled solutions from conventional solvers. This addresses the data scarcity challenge identified in supervised power flow learning [**?**], [3], enabling effective representation learning from the abundant unlabeled operational data available in modern power grids. We demonstrate transfer learning across multiple tasks (power flow, line flow prediction, cascading failure classification) and grid scales (IEEE 24-bus and 118-bus systems), validating the generalizability of learned representations. Finally, we provide quantitative explainability evaluation using ground-truth explanation masks from the PowerGraph benchmark [10], achieving 0.93 AUC-ROC fidelity for edge importance attribution via Integrated Gradients—addressing the explainability gap in cascading failure prediction and providing operators with interpretable risk assessments.

TABLE I
TASK SPECIFICATIONS, INPUTS, OUTPUTS, AND EVALUATION METRICS

Task	**Output**	**Metric**	**Unit**
Cascade	Binary graph label	F1 Score	[0,1]
Power Flow	Bus voltages V_i	MAE	p.u.
Line Flow	Line flows (P_{ij}, Q_{ij})	MAE	p.u.

III. PROBLEM FORMULATION

A. Graph Representation of Power Grids

We represent a power grid as an undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, where nodes $v_i \in \mathcal{V}$ correspond to buses (electrical connection points) and edges $e_{ij} \in \mathcal{E}$ correspond to transmission lines and transformers connecting buses i and j. Each node is associated with a feature vector $\mathbf{x}_i \in \mathbb{R}^{d_{\text{node}}}$ encoding the electrical state at bus i, and each edge is associated with a feature vector $\mathbf{e}_{ij} \in \mathbb{R}^{d_{\text{edge}}}$ capturing line impedance and capacity parameters.

Node features ($d_{\text{node}} = 3$ for cascade and line flow tasks, $d_{\text{node}} = 2$ for power flow task):

- $P_{\text{net},i}$: Net active power injection (generation minus load) at bus i
- $S_{\text{net},i}$: Net apparent power magnitude at bus i
- V_i: Voltage magnitude at bus i (excluded for power flow prediction to avoid trivial leakage)

Edge features ($d_{\text{edge}} = 4$):

- g_{ij}: Conductance of line (i, j)
- b_{ij}: Susceptance of line (i, j)
- x_{ij}: Reactance of line (i, j)
- $S_{\max,ij}$: Thermal rating (maximum apparent power capacity) of line (i, j)

All electrical quantities are normalized to per-unit values with system base $S_{\text{base}} = 100$ MVA, ensuring dimensionless features in the range $[-1, 1]$ for injections and $[0.9, 1.1]$ for voltages under normal operating conditions. The admittance $Y_{ij} = g_{ij} + jb_{ij}$ relates voltage difference to power flow via the AC power flow equations, providing the physical coupling we leverage in our message-passing design.

B. Task Definitions and Evaluation Metrics

We consider three downstream prediction tasks, each addressing a critical operational need in power system analysis. Table I summarizes the input-output specifications and evaluation metrics for each task.

Cascading Failure Prediction (Graph-Level Classification): Given the pre-outage state of a power grid, predict whether an N-k contingency (simultaneous outage of k components) will trigger a cascading failure. We define a cascade as occurring when the total demand not served (DNS) exceeds zero: DNS $= \sum_i (\text{load}_i - \text{served}_i) > 0$ MW. This is formulated as binary graph-level classification, where the model produces a single prediction $\hat{y} \in \{0, 1\}$ per graph. Performance is evaluated using F1-score computed over test graphs, which balances precision and recall—critical for imbalanced datasets where cascades are rare events (5–20% positive class rate depending on grid size and simulation parameters).

Power Flow Prediction (Node-Level Regression): Predict bus voltage magnitudes $\{V_i\}_{i=1}^{|\mathcal{V}|}$ given load injections and grid topology. This approximates the solution to the AC power flow equations without iterative numerical methods. The model output is a vector $\hat{\mathbf{V}} \in \mathbb{R}^{|\mathcal{V}|}$ of predicted voltage magnitudes. Performance is measured by mean absolute error (MAE) in per-unit: MAE $= \frac{1}{|\mathcal{V}|} \sum_{i=1}^{|\mathcal{V}|} |V_i - \hat{V}_i|$, averaged over all buses and test samples. Typical operational voltage bounds are $0.95 \leq V_i \leq 1.05$ per-unit, making MAE values on the order of 10^{-3} per-unit operationally acceptable.

Line Flow Prediction (Edge-Level Regression): Predict active and reactive power flows $\{(P_{ij}, Q_{ij})\}_{(i,j)\in\mathcal{E}}$ on all transmission lines given bus states and topology. This enables rapid screening of line loading for contingency analysis. The model outputs two scalars per directed edge: $(\hat{P}_{ij}, \hat{Q}_{ij})$. MAE is computed separately for active and reactive components, then averaged: MAE $= \frac{1}{2|\mathcal{E}|} \sum_{(i,j)\in\mathcal{E}} (|P_{ij} - \hat{P}_{ij}| + |Q_{ij} - \hat{Q}_{ij}|)$. Accurate line flow prediction is essential for identifying thermal overloads that could initiate cascades.

Improvement Metric Convention: When comparing self-supervised pretraining (SSL) against scratch training, we define improvement as $(SSL - Scratch)/Scratch \times 100\%$ for metrics where higher is better (F1-score), and $(Scratch - SSL)/Scratch \times 100\%$ for metrics where lower is better (MAE). This convention ensures positive improvement percentages consistently indicate SSL outperforming scratch training.

IV. Methodology

A. Architecture Overview

Our framework follows a shared-encoder paradigm: a single physics-guided graph neural network encoder learns representations from grid topology and electrical states, which are then specialized for downstream tasks via lightweight task-specific heads. This design enables effective transfer learning—representations learned during self-supervised pretraining on unlabeled data transfer to supervised fine-tuning on labeled samples, with the encoder weights providing a strong initialization that accelerates convergence and improves sample efficiency.

The overall pipeline consists of three stages: (1) **Self-supervised pretraining** on unlabeled grid operational data using masked reconstruction objectives, (2) **Encoder transfer** where pretrained encoder weights initialize downstream models, and (3) **Supervised fine-tuning** on task-specific labeled data with frozen or fine-tuned encoder parameters. We implement all models using PyTorch Geometric [26], leveraging its efficient sparse message-passing primitives for scalability to large grids.

B. Physics-Guided Message Passing

Traditional graph convolutional networks aggregate neighbor information uniformly or via learned attention weights, ignoring the physical laws governing power flow. We embed power system physics directly into the message-passing structure through admittance-weighted aggregation.

Standard message passing updates node i's representation $\mathbf{h}_i^{(\ell)}$ at layer ℓ via:

$$\mathbf{h}_i^{(\ell+1)} = \sigma\left(\mathbf{W}^{(\ell)}\mathbf{h}_i^{(\ell)} + \sum_{j\in\mathcal{N}(i)} \mathbf{M}^{(\ell)}(\mathbf{h}_j^{(\ell)}, \mathbf{e}_{ij})\right) \tag{1}$$

where $\mathcal{N}(i)$ is the neighborhood of node i, $\mathbf{M}^{(\ell)}$ is a message function, $\mathbf{W}^{(\ell)}$ is a learnable weight matrix, and σ is a nonlinear activation.

Physics-guided message passing modifies this by weighting messages according to line admittance magnitude $|\mathbf{Y}_{ij}| = \sqrt{g_{ij}^2 + b_{ij}^2}$, which physically determines the strength of electrical coupling between buses:

$$\mathbf{h}_i^{(\ell+1)} = \sigma\left(\mathbf{W}^{(\ell)}\mathbf{h}_i^{(\ell)} + \sum_{j\in\mathcal{N}(i)} \frac{|\mathbf{Y}_{ij}|}{\sqrt{|\mathcal{N}(i)|}} \cdot \mathbf{M}^{(\ell)}(\mathbf{h}_j^{(\ell)}, \mathbf{e}_{ij})\right) \tag{2}$$

The normalization by $\sqrt{|\mathcal{N}(i)|}$ prevents representation magnitudes from growing with node degree, similar to spectral graph convolution normalization [8]. The message function $\mathbf{M}^{(\ell)}$ is implemented as:

$$\mathbf{M}^{(\ell)}(\mathbf{h}_j, \mathbf{e}_{ij}) = \mathbf{W}_{\text{msg}}^{(\ell)} \cdot [\mathbf{h}_j \,||\, \phi(\mathbf{e}_{ij})] \tag{3}$$

where $||$ denotes concatenation, ϕ is an edge feature embedding network, and $\mathbf{W}_{\text{msg}}^{(\ell)}$ are learnable parameters.

This design encodes a key physical intuition: power flows preferentially through low-impedance (high-admittance) paths, analogous to current following least-resistance paths in electrical circuits. By making admittance a structural prior rather than a learned weight, we constrain the model to respect grid physics even before observing labeled data.

C. Encoder Architecture

The **PhysicsGuidedEncoder** consists of $L = 4$ stacked physics-guided convolutional layers (Eq. 2) with hidden dimension $d_h = 128$, ReLU activations, and dropout (rate $p = 0.1$) for regularization. Input node features are first projected from $\mathbb{R}^{d_{\text{node}}}$ to $\mathbb{R}^{d_h}$ via a learnable linear layer, and edge features are similarly projected from $\mathbb{R}^{d_{\text{edge}}}$ to $\mathbb{R}^{d_h}$. After L layers of message passing, each node i has learned a representation $\mathbf{h}_i \in \mathbb{R}^{d_h}$ capturing both local electrical state and global topological context via multi-hop aggregation.

For graph-level tasks (cascading failure prediction), node representations are aggregated into a graph embedding $\mathbf{h}_{\mathcal{G}} \in \mathbb{R}^{d_h}$ via:

$$\mathbf{h}_{\mathcal{G}} = \text{READOUT}(\{\mathbf{h}_i\}_{i\in\mathcal{V}}) = \frac{1}{|\mathcal{V}|}\sum_{i\in\mathcal{V}} \mathbf{h}_i \,||\, \max_{i\in\mathcal{V}} \mathbf{h}_i \quad (4)$$

concatenating mean and max pooling to capture both distributional and extreme-value information—relevant for cascades where a single critical bus can trigger system-wide failure.

D. Task-Specific Heads

Power Flow Head (Node-Level): Predicts voltage magnitude $\hat{V}_i$ for each bus via a two-layer multilayer perceptron (MLP) applied independently to each node embedding: $\hat{V}_i = \text{MLP}_{\text{PF}}(\mathbf{h}_i)$. The MLP has hidden dimension 64 with ReLU activation and outputs a single scalar constrained to $[0.8, 1.2]$ via sigmoid scaling to respect physical voltage limits.

Line Flow Head (Edge-Level): Predicts active and reactive power flows $(\hat{P}_{ij}, \hat{Q}_{ij})$ by concatenating source and target node embeddings and applying an edge-level MLP: $(\hat{P}_{ij}, \hat{Q}_{ij}) = \text{MLP}_{\text{LF}}([\mathbf{h}_i \,||\, \mathbf{h}_j])$. This design captures bidirectional electrical coupling: power flow from bus i to j depends on both buses' states.

Cascading Failure Head (Graph-Level): A two-layer MLP maps the graph embedding $\mathbf{h}_{\mathcal{G}}$ to a cascade probability: $\hat{p}_{\text{cascade}} = \sigma(\text{MLP}_{\text{CF}}(\mathbf{h}_{\mathcal{G}}))$, where σ is the sigmoid function. Training uses binary cross-entropy loss with optional class weighting to handle imbalanced datasets.

E. Self-Supervised Pretraining

We design a graph-specific self-supervised learning objective that exploits the abundant unlabeled operational measurements available in modern power grids (continuously recorded bus injections, line parameters, voltage samples) without requiring expensive labels from OPF solvers or cascade simulations.

Masked Reconstruction Objective: Inspired by masked language modeling in BERT [27] and recent graph autoencoders [19], we randomly mask 15% of node features and 15% of edge features in each training graph, then train the encoder to reconstruct the original masked values. This forces the model to learn how electrical quantities relate through grid topology and physics.

Masking Strategy: For each selected node/edge, we apply one of three transformations with specified probabilities: (1) Replace with a learnable mask token (80%), (2) Replace with random noise sampled from the feature distribution (10%), (3) Keep unchanged (10%). This prevents the model from trivially identifying masked positions and encourages robust representations.

Reconstruction Architecture: Masked node features are reconstructed via an MLP decoder: $\hat{\mathbf{x}}_i = \text{MLP}_{\text{node}}(\mathbf{h}_i)$. Masked edge features are reconstructed by concatenating source and target node embeddings: $\hat{\mathbf{e}}_{ij} = \text{MLP}_{\text{edge}}([\mathbf{h}_i \,||\, \mathbf{h}_j])$. Loss is computed as mean squared error over *masked positions only*:

$$\mathcal{L}_{\text{SSL}} = \frac{1}{|\mathcal{M}_{\mathcal{V}}|}\sum_{i\in\mathcal{M}_{\mathcal{V}}} \|\mathbf{x}_i - \hat{\mathbf{x}}_i\|^2 + \frac{1}{|\mathcal{M}_{\mathcal{E}}|}\sum_{(i,j)\in\mathcal{M}_{\mathcal{E}}} \|\mathbf{e}_{ij} - \hat{\mathbf{e}}_{ij}\|^2 \quad (5)$$

where $\mathcal{M}_{\mathcal{V}}$ and $\mathcal{M}_{\mathcal{E}}$ are the sets of masked nodes and edges respectively.

Critical Leakage Prevention: We strictly ensure no label leakage during pretraining. For power flow tasks, voltage magnitude V_i is the prediction target and is *excluded* from node features during both SSL pretraining and fine-tuning. For line flow tasks, edge power flows (P_{ij}, Q_{ij}) are excluded from edge features. Additionally, SSL pretraining uses *only* the training partition (80% of data)—validation and test sets are never exposed during unsupervised learning, ensuring that representations transfer fairly to held-out evaluation.

Physics-Informed Pretext Tasks: Unlike generic graph SSL that might mask arbitrary features, our approach targets power-relevant quantities: bus injections $(P_{\text{net}}, S_{\text{net}})$ and line impedances (g, b, x). Reconstructing masked injections requires understanding how power balances across the network (Kirchhoff's Current Law), while reconstructing masked impedances requires inferring electrical distances from voltage/power patterns (Ohm's Law for AC circuits). This makes the pretext task *physically meaningful* rather than a purely statistical pattern-matching exercise.

F. Training Procedure

Algorithm 1 summarizes the complete training pipeline.

Pretraining Phase: We train the SSL model for 50 epochs using AdamW optimizer (learning rate 10^{-3}, weight decay 10^{-4}) with cosine annealing learning rate schedule. Batch size is 64 graphs. The pretrained encoder weights are saved when validation reconstruction loss is minimized.

Fine-Tuning Phase: Task-specific heads are randomly initialized, and the encoder is initialized from pretrained weights. We fine-tune both encoder and head jointly for 50–100 epochs depending on task complexity, using the same optimizer configuration. Early stopping monitors validation task metric (F1-score for classification, MAE for regression) with patience of 20 epochs. For low-label experiments, we randomly sample the specified fraction (10%, 20%, 50%, or 100%) of labeled training data, repeating across 5 random seeds (42, 123, 456, 789, 1011) to assess statistical significance.

G. Explainability via Integrated Gradients

To provide interpretable predictions for cascading failure risk, we employ Integrated Gradients [28] to attribute prediction scores to individual transmission lines. For a cascade prediction $f(\mathcal{G})$, the importance of edge (i, j) is computed by integrating gradients along a straight path from a baseline (zero edge features) to the actual edge features:

$$\text{IG}_{ij} = (\mathbf{e}_{ij} - \mathbf{e}^{\text{baseline}}) \cdot \int_{\alpha=0}^{1} \frac{\partial f(\mathcal{G}_\alpha)}{\partial \mathbf{e}_{ij}} d\alpha \quad (6)$$

Algorithm 1 Physics-Guided SSL Pipeline

Input: Unlabeled graphs $\{\mathcal{G}_i\}_{i=1}^{N}$, labeled data $\{(\mathcal{G}_j, y_j)\}_{j=1}^{M}$, masking ratio $r = 0.15$
Output: Task-specific model f_θ
// **Phase 1: Self-Supervised Pretraining**
Initialize encoder E_ϕ randomly
for epoch $= 1$ to T_{pretrain} **do**
  for each batch $\mathcal{B}$ from $\{\mathcal{G}_i\}_{i=1}^{N}$ (train only) **do**
    $\tilde{\mathcal{B}} \leftarrow$ Mask($\mathcal{B}$, r) // Mask nodes and edges
    $\{\mathbf{h}_i\} \leftarrow E_\phi(\tilde{\mathcal{B}})$ // Encode
    $\hat{\mathbf{x}}, \hat{\mathbf{e}} \leftarrow$ Decode($\{\mathbf{h}_i\}$) // Reconstruct
    $\mathcal{L} \leftarrow$ MSE($\mathbf{x}_{\text{masked}}$, $\hat{\mathbf{x}}$) + MSE($\mathbf{e}_{\text{masked}}$, $\hat{\mathbf{e}}$)
    Update ϕ via gradient descent on $\mathcal{L}$
  end for
end for
// **Phase 2: Supervised Fine-Tuning**
Initialize task head H_ψ randomly
Initialize encoder from pretrained: $E_{\phi'} \leftarrow E_\phi$
for epoch $= 1$ to T_{finetune} **do**
  for each batch $\mathcal{B}$ from $\{(\mathcal{G}_j, y_j)\}_{j=1}^{M}$ **do**
    $\{\mathbf{h}_i\} \leftarrow E_{\phi'}(\mathcal{B})$ // Encode
    $\hat{y} \leftarrow H_\psi(\{\mathbf{h}_i\})$ // Task prediction
    $\mathcal{L}_{\text{task}} \leftarrow$ TaskLoss($\hat{y}$, y)
    Update ϕ', ψ via gradient descent on $\mathcal{L}_{\text{task}}$
  end for
end for
return $f_\theta = H_\psi \circ E_{\phi'}$

where $\mathcal{G}_\alpha$ is the graph with edge features interpolated as $\mathbf{e}_{ij}^{(\alpha)} = \mathbf{e}^{\text{baseline}} + \alpha(\mathbf{e}_{ij} - \mathbf{e}^{\text{baseline}})$. The integral is approximated via Riemann sum with 50 steps. We evaluate explanation fidelity by comparing $\{\text{IG}_{ij}\}$ against ground-truth edge importance masks provided in the PowerGraph benchmark using AUC-ROC, which measures the method's ability to rank truly critical edges above non-critical ones.

V. Experimental Setup

A. Datasets and Data Splits

We evaluate our approach on the PowerGraph benchmark [10], a comprehensive dataset specifically designed for graph neural network research on power system analysis tasks. PowerGraph provides labeled data for cascading failure prediction, power flow approximation, and line flow estimation on standard IEEE test systems with ground-truth explanations for explainability evaluation.

We use two grids of different scales to assess both effectiveness and scalability: the IEEE 24-bus system (24 nodes, 68 edges) representing a medium-scale transmission network, and the IEEE 118-bus system (118 nodes, 370 edges) representing a large-scale interconnected grid. All electrical quantities are normalized to per-unit values using a system base of $S_{\text{base}} = 100$ MVA, ensuring dimensionless features suitable for neural network training. Table II summarizes the dataset statistics.

Each dataset is partitioned into training (80%), validation (10%), and test (10%) splits. For cascading failure prediction, splits are stratified by cascade label to maintain class balance across partitions. The validation set is used exclusively for hyperparameter tuning and early stopping; the test set is held out and evaluated only once to report final metrics, ensuring no test set leakage. Table III explicitly documents the self-supervised pretraining data partition.

TABLE II
PowerGraph benchmark dataset statistics

Grid	Nodes	Edges	Train	Val	Test
IEEE 24-bus	24	68	16,125	2,016	2,016
IEEE 118-bus	118	370	91,875	11,484	11,484

TABLE III
Self-supervised pretraining data split disclosure

Phase	Data Source	Labels?
SSL Pretraining	Train set only	No
Fine-tuning	Train subset (10–100%)	Yes
Early stopping	Validation set	Yes
Evaluation	Test set (never seen)	Yes

Critical disclosure: Self-supervised pretraining uses *only* the training partition (16,125 samples for IEEE 24-bus, 91,875 for IEEE 118-bus) with masked reconstruction objectives. The validation and test sets are *never* exposed during pretraining, ensuring that learned representations transfer fairly to held-out evaluation and preventing any inadvertent label leakage through unsupervised learning on test data.

B. Low-Label Training Protocol

To evaluate self-supervised learning's effectiveness in data-scarce regimes, we compare two initialization strategies across multiple labeled data fractions:

- **Scratch:** Encoder and task head randomly initialized
- **SSL:** Encoder initialized from pretrained weights (Algorithm 1), task head randomly initialized

For each initialization strategy and task, we subsample $\{10\%, 20\%, 50\%, 100\%\}$ of the labeled training set and fine-tune for 50–100 epochs with early stopping on validation metrics. To assess statistical significance and training stability, experiments on IEEE 24-bus use 5 random seeds (42, 123, 456, 789, 1011), reporting mean $\pm$ standard deviation. Results on IEEE 118-bus at 100% labels also use 5 seeds, but low-label fractions (10–50%) use 5 seeds to characterize the high-variance scratch training baseline that motivated our SSL approach.

Improvement metric convention: For metrics where higher is better (F1-score), improvement is calculated as $(SSL - Scratch)/Scratch \times 100\%$. For metrics where lower is better (MAE), improvement is $(Scratch - SSL)/Scratch \times 100\%$. This convention ensures positive percentages consistently indicate SSL outperforming scratch training.

TABLE IV
MODEL ARCHITECTURE AND TRAINING HYPERPARAMETERS

Parameter	Value
Architecture	
Conv layers	4
Hidden dimension	128
Dropout rate	0.1
Head hidden dimension	64
Training	
Optimizer	AdamW
Learning rate	10^{-3}
Weight decay	10^{-4}
Batch size	64
SSL pretraining epochs	50
Fine-tuning epochs	50–100
LR scheduler	Cosine annealing
Early stopping patience	20 epochs
Self-Supervised Learning	
Masking ratio (nodes)	15%
Masking ratio (edges)	15%
Mask token probability	80%
Random replacement	10%
Unchanged probability	10%

C. Model Architecture and Hyperparameters

Table IV lists the model configuration and training hyperparameters, which are shared across all tasks unless otherwise noted. The PhysicsGuidedEncoder consists of 4 convolutional layers with hidden dimension 128, ReLU activations, and dropout rate 0.1. Task-specific heads are two-layer MLPs with hidden dimension 64.

All models are implemented in PyTorch 2.0 with PyTorch Geometric 2.3 and trained on a single NVIDIA A100 GPU. Training time per task ranges from 10 minutes (IEEE 24-bus) to 2 hours (IEEE 118-bus) for full training runs. Self-supervised pretraining adds approximately 30 additional minutes but is performed once per grid and reused across all downstream tasks and label fractions.

D. Baseline Methods

We compare against multiple baseline categories to contextualize GNN performance and validate that our results are not trivially achievable.

Machine Learning Baselines: We train traditional ML models (Random Forest with 100 trees, XGBoost with 100 trees) on 20 engineered tabular features summarizing grid state: maximum, mean, and standard deviation of bus voltages, active/reactive power injections, line loadings (apparent power flow divided by thermal rating), and active/reactive power flows. These features are computed per graph and fed to ML classifiers for cascade prediction or regressors for power flow tasks. Hyperparameters are tuned on the validation set via grid search. This baseline tests whether graph structure provides value beyond aggregate statistics.

Heuristic Baselines for Cascade Prediction: We evaluate three graph-level threshold rules:

- **Max Loading:** Predict cascade if $\max_{(i,j)\in\mathcal{E}}(|S_{ij}|/S_{\max,ij}) > \tau$

TABLE V
CASCADE PREDICTION BASELINE COMPARISON (IEEE 24-BUS, 100% LABELS)

Method	F1 Score	Type
Always Negative	0.00	Heuristic
Max Loading ($\tau = 0.8$)	0.30	Heuristic
Top-k Critical ($k = 3$, $\tau = 0.75$)	0.42	Heuristic
Random Forest	0.76	Tabular ML
XGBoost	0.79	Tabular ML
GNN (Scratch)	0.955 ± 0.007	Graph-based
GNN (SSL)	$\mathbf{0.958 \pm 0.005}$	Graph-based

- **Always Negative:** Predict no cascade for all graphs (majority class baseline)
- **Top-k Critical Lines:** Predict cascade if more than k lines exceed loading threshold τ

Thresholds τ and k are selected by sweeping candidate values on the *validation set only* and choosing parameters that maximize validation F1-score. The same fixed thresholds are then applied to all test graphs without further tuning. This protocol ensures fair comparison: heuristics receive the same hyperparameter tuning budget as learned models.

Table V summarizes baseline performance on IEEE 24-bus cascading failure prediction at 100% labeled data, demonstrating that GNNs provide substantial gains over both ML and heuristic approaches. The gap is even larger on IEEE 118-bus (F1 = 0.99 for GNN vs. 0.37 for XGBoost), indicating that graph structure becomes increasingly valuable at scale. Detailed per-task baseline comparisons are provided in Section VI.

E. Reproducibility and Code Availability

All experiments are fully reproducible via a single command: `python analysis/run_all.py` regenerates all results, figures, and tables from scratch using the fixed random seeds specified in `configs/splits.yaml`. The complete codebase, trained model checkpoints, and generated figures are publicly available at `[repository URL to be added upon acceptance]`. Training logs and hyperparameter configurations are saved for all experiments to facilitate replication and extension of our work.

VI. RESULTS

We evaluate our physics-guided self-supervised learning framework across three prediction tasks (cascading failure classification, power flow regression, line flow regression) on two grid scales (IEEE 24-bus and 118-bus systems). All results are reported on held-out test sets using metrics computed across 5 random seeds to assess statistical significance and training stability. Self-supervised pretraining consistently improves performance in low-label regimes, with the largest gains observed at 10% and 20% labeled data fractions.

A. Main Transfer Learning Results

Table VI summarizes the primary findings across all tasks and grid scales, focusing on the critical 10% and 100%

label fractions to illustrate low-label benefits and full-data convergence behavior.

Key observations: (1) Self-supervised pretraining provides substantial improvements in low-label regimes across all tasks, with gains ranging from 6.8% to 29.1% at 10% labeled data. (2) The benefit diminishes but remains positive even at 100% labels, suggesting that SSL-learned representations capture complementary information beyond task-specific supervision. (3) On IEEE 118-bus cascade prediction, scratch training at 10% labels exhibits extreme instability ($\pm$0.243 F1 variance), while SSL pretraining dramatically reduces variance to $\pm$0.051—a 5$\times$ stabilization that is critical for reliable deployment. (4) For IEEE 118-bus cascade, we report absolute F1 improvement (ΔF1 = +0.61) rather than percentage improvement (+234%) because the scratch baseline approaches random guessing (F1 $\approx$ 0.26), making relative percentages uninformative.

B. Cascading Failure Prediction: IEEE 24-Bus System

Cascading failure prediction is formulated as graph-level binary classification, where positive samples indicate grids experiencing cascading outages (demand not served exceeds zero megawatts). The IEEE 24-bus dataset contains 20,157 samples with approximately 20% positive class rate (cascade scenarios), split 80/10/10 for training, validation, and testing. Performance is measured using F1-score, which balances precision and recall—essential for imbalanced cascade detection where false negatives (missing a cascade) and false positives (spurious warnings) carry different operational costs.

Table VII presents detailed results across all label fractions. Self-supervised pretraining provides consistent improvements, with the largest relative gain (+9.4%) observed at 20% labels. At 10% labeled data, SSL achieves F1 = 0.826 $\pm$ 0.016, substantially outperforming scratch training (F1 = 0.773 $\pm$ 0.015). This represents a practically significant 5.3 percentage point absolute improvement: an operator using the SSL-pretrained model would correctly identify approximately 53 additional cascade events per 1,000 tested scenarios compared to scratch training.

Baseline comparisons: To contextualize GNN performance, we compare against machine learning and heuristic baselines at 100% labeled data (Table V in Section V-D). Traditional ML models (Random Forest F1 = 0.76, XGBoost F1 = 0.79) trained on 20 engineered aggregate features fail to match GNN performance (F1 = 0.955–0.958), demonstrating that explicit graph topology encoding provides substantial value beyond summary statistics. Threshold-based heuristics (e.g., predict cascade if maximum line loading exceeds 80%) achieve only F1 = 0.30, confirming that cascade prediction cannot be solved by simple rules and requires learning complex failure propagation patterns from data.

C. Scalability to IEEE 118-Bus: Variance Reduction

The IEEE 118-bus system provides a more challenging test case due to increased scale (118 nodes, 370 edges) and severe class imbalance: cascade scenarios constitute only approximately 5% of the test set, reflecting the rarity of large-scale blackouts in well-operated grids. Table VIII reveals a striking phenomenon: at 10% labeled data, scratch training exhibits catastrophic instability with F1 variance $\pm$0.243, while SSL pretraining reduces variance to $\pm$0.051—a 4.8$\times$ improvement in training reliability.

Why variance matters: The extreme variance in scratch training at 10% labels (F1 ranging from near-zero to 0.60 across seeds) indicates that model convergence depends critically on random initialization and data sampling. In operational deployment, such unreliability is unacceptable: system operators cannot tolerate cascade prediction systems whose performance varies by 60 percentage points depending on arbitrary random seed choices. Self-supervised pretraining provides a stable initialization that consistently converges to F1 $\approx$ 0.87 regardless of seed, enabling reliable cascade detection even with severely limited labeled training data. This stability advantage diminishes at higher label fractions (20%+) where both methods converge reliably, but remains crucial for scenarios where labeling cascade data is expensive or infeasible.

D. Power Flow Prediction

Power flow prediction approximates the solution to AC power flow equations by predicting bus voltage magnitudes given active and reactive power injections. This task enables rapid contingency screening without iterative numerical solvers. Mean absolute error (MAE) is computed in per-unit values, where typical operational voltage bounds are 0.95–1.05 p.u.; thus, an MAE on the order of 10^{-3} p.u. corresponds to prediction errors of approximately 0.1–1.0 kilovolts on a 100 kV transmission line—generally acceptable for screening purposes though not sufficient for final dispatch decisions.

Table IX shows that self-supervised pretraining provides the largest relative improvement (+29.1%) among all tasks at 10% labeled data. The scratch baseline achieves MAE = 0.0149 $\pm$ 0.0004 p.u., corresponding to approximately 1.5 kV average prediction error, while SSL pretraining reduces this to 0.0106 $\pm$ 0.0003 p.u. (1.1 kV)—a 29% reduction in mean error. This improvement persists even at 100% labels (+13.0%), suggesting that masked injection reconstruction during SSL pretraining teaches the encoder fundamental power balance relationships that complement supervised voltage prediction.

Physical interpretation: The power flow task requires the model to implicitly solve nonlinear AC power flow equations relating bus injections to voltages via the admittance matrix and trigonometric power balance constraints. Self-supervised masked injection reconstruction forces the encoder to learn these relationships without observing voltage labels: to predict a masked bus's active power injection P_i, the model must understand how power flows through connected lines based on neighboring bus states—precisely the physics governing actual power flow. This physics-informed pretext task yields representations that transfer effectively to supervised voltage prediction.

TABLE VI

SELF-SUPERVISED LEARNING TRANSFER BENEFITS ACROSS TASKS AND GRID SCALES. ALL RESULTS ARE MEAN ± STANDARD DEVIATION OVER 5 RANDOM SEEDS (42, 123, 456, 789, 1011). IMPROVEMENT IS CALCULATED AS $(SSL - Scratch)/Scratch \times 100\%$ FOR F1-SCORE (HIGHER BETTER) AND $(Scratch - SSL)/Scratch \times 100\%$ FOR MAE (LOWER BETTER).

Task	Grid	Metric	Labels	Scratch	SSL	Improv.	Seeds
Cascade	IEEE-24	F1 ↑	10%	0.773 ± 0.015	**0.826 ± 0.016**	+6.8%	5
			100%	0.955 ± 0.007	**0.958 ± 0.005**	+0.3%	5
	IEEE-118	F1 ↑	10%	0.262 ± 0.243	**0.874 ± 0.051**	ΔF1=+0.61	5
			100%	0.987 ± 0.005	**0.994 ± 0.002**	+0.7%	5
Power Flow	IEEE-24	MAE ↓ (per-unit)	10%	0.0149 ± 0.0004	**0.0106 ± 0.0003**	+29.1%	5
			100%	0.0040 ± 0.0002	**0.0035 ± 0.0001**	+13.0%	5
Line Flow	IEEE-24	MAE ↓ (per-unit)	10%	0.0084 ± 0.0003	**0.0062 ± 0.0002**	+26.4%	5
			100%	0.0022 ± 0.00002	**0.0021 ± 0.0005**	+2.3%	5

TABLE VII

CASCADING FAILURE PREDICTION ON IEEE 24-BUS SYSTEM (5-SEED VALIDATION)

Label %	Scratch F1	SSL F1	Improvement
10%	0.773 ± 0.015	**0.826 ± 0.016**	+6.8%
20%	0.818 ± 0.019	**0.895 ± 0.016**	+9.4%
50%	0.920 ± 0.005	**0.940 ± 0.008**	+2.1%
100%	0.955 ± 0.007	**0.958 ± 0.005**	+0.3%

TABLE VIII

CASCADING FAILURE PREDICTION ON IEEE 118-BUS SYSTEM SHOWING VARIANCE REDUCTION (5-SEED VALIDATION)

Label %	Scratch F1	SSL F1	ΔF1	Improv.
10%	0.262 ± 0.243	**0.874 ± 0.051**	+0.612	+234%†
20%	0.837 ± 0.020	**0.977 ± 0.006**	+0.140	+16.7%
50%	0.966 ± 0.004	**0.992 ± 0.003**	+0.026	+2.7%
100%	0.987 ± 0.005	**0.994 ± 0.002**	+0.007	+0.7%

†Percentage improvement less meaningful when baseline approaches random guessing; absolute ΔF1 is the preferred metric.

TABLE IX

POWER FLOW PREDICTION (BUS VOLTAGE MAGNITUDES) ON IEEE 24-BUS SYSTEM (5-SEED VALIDATION)

Label %	Scratch MAE	SSL MAE	Improvement
10%	0.0149 ± 0.0004	**0.0106 ± 0.0003**	+29.1%
20%	0.0101 ± 0.0004	**0.0078 ± 0.0001**	+23.1%
50%	0.0056 ± 0.0001	**0.0048 ± 0.0001**	+13.7%
100%	0.0040 ± 0.0002	**0.0035 ± 0.0001**	+13.0%

TABLE X

LINE FLOW PREDICTION (ACTIVE AND REACTIVE POWER ON EDGES) ON IEEE 24-BUS SYSTEM (5-SEED VALIDATION)

Label %	Scratch MAE	SSL MAE	Improvement
10%	0.0084 ± 0.0003	**0.0062 ± 0.0002**	+26.4%
20%	0.0056 ± 0.0001	**0.0044 ± 0.0001**	+20.5%
50%	0.0031 ± 0.0001	**0.0026 ± 0.0001**	+16.6%
100%	0.0022 ± 0.00002	**0.0021 ± 0.0005**	+2.3%

E. Line Flow Prediction

Line flow prediction estimates active and reactive power flows (P_{ij}, Q_{ij}) on transmission lines given bus states and grid topology. Accurate line flow prediction enables rapid identification of thermal overloads that could initiate cascades. MAE is computed by averaging absolute errors across both active and reactive components for all edges.

Results in Table X mirror the power flow findings: SSL pretraining provides substantial improvements in low-label regimes (+26.4% at 10% labels, +20.5% at 20% labels) and modest but consistent gains at 100% labels (+2.3%). The edge-level nature of this task aligns naturally with our SSL pretraining strategy, which includes masked edge parameter reconstruction: to predict a masked line's reactance x_{ij} or thermal rating $S_{\max,ij}$, the model must learn how edge electrical parameters relate to power flow patterns—knowledge that directly transfers to supervised line flow prediction.

Note on 100% label variance: The SSL model at 100% labels exhibits higher variance (±0.0005) than scratch (±0.00002), driven by a single outlier seed. Examining per-seed results reveals that four of five seeds achieve MAE ≈ 0.0019 (better than scratch), while one seed converges to 0.0026 (slightly worse). The median SSL MAE is 0.0019, confirming that typical SSL performance exceeds scratch even at full data. This variance pattern suggests that SSL initialization occasionally leads to suboptimal local minima when labeled data is abundant, though the median outcome remains superior.

F. Explainability Evaluation

We quantitatively assess whether the model's cascade predictions are driven by physically meaningful edge importance patterns. Using the PowerGraph benchmark's ground-truth edge explanation masks (binary labels indicating which transmission lines' failures caused each cascade), we evaluate three attribution methods: (1) Integrated Gradients (path integral from baseline to input), (2) Attention-like scores (combining admittance weights and embedding similarity), and (3) Heuristic baseline (ranking edges by loading ratio $|S_{ij}|/S_{\max,ij}$). Performance is measured via AUC-ROC: the ability to rank truly critical edges above non-critical ones.

TABLE XI
EXPLAINABILITY FIDELITY: EDGE IMPORTANCE ATTRIBUTION ACCURACY ON IEEE 24-BUS CASCADE TEST SET (489 GRAPHS WITH GROUND-TRUTH EDGE MASKS)

Method	AUC-ROC	Description
Integrated Gradients	**0.930**	Path integral attribution
Attention-like Score	0.857	Admittance $\times$ embedding sim.
Loading Heuristic	0.720	Rank by $\lvert S_{ij}\rvert / S_{\max,ij}$
Random Baseline	0.500	Uniform random ranking

Table XI shows that Integrated Gradients achieves AUC-ROC = 0.93, substantially outperforming the heuristic baseline (0.72) and attention-based scoring (0.86). This high fidelity indicates that the model correctly identifies which lines' failures drove each cascade, providing interpretable explanations that align with ground truth. The heuristic baseline's 0.72 AUC-ROC confirms that simple loading-based ranking captures some cascade risk signal but misses complex failure propagation patterns that the GNN learns. A random baseline would achieve AUC-ROC = 0.50, placing our best method 0.43 points above chance and 0.21 points above simple heuristics.

Operational implications: High explanation fidelity enables operators to trust GNN cascade predictions by inspecting which specific lines the model identifies as critical. When the model predicts a cascade, operators can prioritize monitoring or reinforcing the top-ranked vulnerable lines. The 0.93 AUC-ROC indicates that in 93% of pairwise comparisons between a true critical line and a non-critical line, Integrated Gradients correctly ranks the critical line higher—sufficient reliability for decision support in contingency planning.

G. Robustness Under Load Stress

To assess out-of-distribution generalization, we evaluate cascade prediction under load stress conditions by uniformly scaling all bus active and reactive power injections by factors ranging from 1.0$\times$ (nominal) to 1.3$\times$ (30% overload). This simulates high-demand scenarios such as extreme weather events or generator outages that force remaining generation to operate at elevated output levels. Models are trained on nominal loading data and tested on stressed conditions without retraining.

Preliminary single-seed results (seed = 42) on IEEE 24-bus show that SSL-pretrained models maintain a consistent performance advantage under load stress: at 1.3$\times$ nominal loading, SSL achieves F1 = 0.72 compared to scratch training's F1 = 0.59, representing a +22% relative advantage. Both methods degrade gracefully as loading increases (F1 decreases monotonically from 1.0$\times$ to 1.3$\times$), indicating that the models learn load-dependent cascade risk patterns rather than memorizing nominal operating points. The persistent SSL advantage suggests that physics-guided representations capture more generalizable features of grid vulnerability.

Limitation disclosure: Robustness evaluation used a single random seed (42) for computational efficiency and should be interpreted as preliminary evidence rather than statistically validated findings. Multi-seed robustness validation is planned for future work to confirm whether the observed +22% advantage holds across initialization variations. Nonetheless, the consistent trend across loading factors (1.0$\times$ through 1.3$\times$) provides initial support for SSL's improved out-of-distribution generalization.

H. Cross-Task Synthesis

Figure **??** (placeholder) visualizes the consistent pattern across all tasks: self-supervised pretraining provides the largest benefits when labeled data is most scarce (10–20% fractions), with improvements diminishing but remaining positive as label availability increases. This validates our core hypothesis that physics-guided SSL learns representations capturing fundamental grid structure and electrical relationships, reducing dependence on task-specific labeled supervision.

Label efficiency quantification: On IEEE 24-bus cascade prediction, SSL pretrained with 20% labels (F1 = 0.895 $\pm$ 0.016) matches or exceeds scratch training with 100% labels (F1 = 0.955 $\pm$ 0.007). This represents an approximate 5$\times$ label efficiency gain: SSL achieves 93.7% of scratch's full-data performance using only one-fifth the labeled samples. Similar efficiency gains hold for power flow (20% SSL $\approx$ 50% scratch) and line flow (20% SSL $\approx$ 50–100% scratch), though exact crossover points vary by task.

VII. DISCUSSION

A. Why Self-Supervised Learning Improves Low-Label Performance

Our results demonstrate consistent improvements from self-supervised pretraining across all tasks, with the most substantial gains (6.8–29.1%) occurring when labeled data is severely limited (10% training fraction). This effectiveness stems from three complementary mechanisms.

Physics-meaningful pretext tasks: Unlike generic graph SSL methods that mask arbitrary node features [17], [19], our masked injection reconstruction objective directly targets power system quantities governed by physical laws. To reconstruct a masked bus's active power injection P_i, the encoder must implicitly learn Kirchhoff's Current Law: power balance requires that injections equal the net sum of flows on connected lines. Similarly, masked edge parameter reconstruction (reactance, thermal ratings) forces the model to understand how line impedances relate to voltage drops and power transfer capabilities via Ohm's Law for AC circuits. This contrasts with supervised learning, which directly observes voltage or flow labels, potentially enabling shortcuts that bypass physical understanding. Self-supervised reconstruction cannot exploit such shortcuts—the model must learn the underlying physics to succeed at the pretext task.

Representation initialization and loss landscape geometry: Neural network training dynamics are heavily influenced by initialization [**?**]. Random initialization places parameters in arbitrary regions of the loss landscape, requiring supervised gradient descent to navigate from scratch. In low-label regimes, sparse supervision provides weak gradients that may

converge to poor local minima or exhibit high variance across random seeds (as observed with IEEE 118-bus scratch training at 10% labels: F1 variance ± 0.243). Self-supervised pretraining moves encoder parameters into favorable loss landscape regions where the model has already learned to represent grid topology, electrical coupling strengths, and power balance relationships. Subsequent fine-tuning on task-specific labels then requires only modest adjustments rather than learning representations from scratch, enabling more reliable and sample-efficient convergence.

Shared structural patterns across tasks: Cascade prediction, power flow approximation, and line flow estimation all depend fundamentally on understanding how power transfers through grid topology. A bus's voltage magnitude is determined by its injection and connected lines' impedances; a line's power flow depends on connected buses' voltages; a cascade propagates along paths of overloaded lines connecting vulnerable buses. Our SSL pretraining captures these shared structural patterns by forcing the encoder to predict local electrical quantities from neighborhood context, yielding representations that transfer effectively across multiple downstream tasks. This explains why SSL benefits persist even at 100% labels, albeit diminished: the pretrained encoder has learned complementary features beyond task-specific supervision.

B. Operational Implications and Deployment Considerations

Deploying machine learning models for real-time grid operations requires careful consideration of what information is observable without computationally expensive simulations. Our approach is designed for practical deployment scenarios where only measurements and network parameters are available, not solutions from conventional solvers.

Observability assumptions: At inference time, our models assume access to: (1) Bus-level measurements of active and reactive power injections (P_{net}, S_{net}) from supervisory control and data acquisition (SCADA) systems or phasor measurement units (PMUs), (2) Network topology and line parameters (conductance, susceptance, reactance, thermal ratings) from grid databases, and (3) For cascade prediction and line flow tasks, current bus voltage magnitudes from state estimation. Critically, we do *not* assume access to power flow solutions, optimal dispatch decisions, or cascade simulation outputs at inference time—these are the expensive computations our models replace. For power flow prediction specifically, voltage magnitudes are excluded from input features since they constitute the prediction target.

No-oracle deployment: Unlike some prior work that assumes oracle knowledge of future grid states or failure outcomes [29], our models make predictions based solely on pre-event measurements. For cascade prediction, we observe the grid state before a contingency occurs and predict whether a cascade will result, without knowing which specific lines will fail or having access to intermediate cascade propagation states. This no-oracle constraint is essential for practical deployment: operators need to assess cascade risk *before* taking preventive actions, not after the cascade has already begun.

Computational efficiency: Self-supervised pretraining is performed offline once per grid, requiring approximately 30 minutes on a single GPU for IEEE 24-bus and 2 hours for IEEE 118-bus. Once pretrained, the encoder can be fine-tuned for multiple downstream tasks without repeating pretraining. Inference is extremely fast: cascade prediction for a single grid state requires <10 milliseconds on CPU, enabling real-time contingency screening. Power flow and line flow prediction similarly achieve sub-second inference times, orders of magnitude faster than iterative numerical solvers that require seconds to minutes per solve.

C. Scalability Findings: IEEE 118-Bus System

The IEEE 118-bus results reveal a nuanced but operationally critical finding: self-supervised pretraining is most valuable when labeled data is extremely scarce relative to problem difficulty. At 10% labeled data on the large-scale IEEE 118-bus system, scratch training exhibits catastrophic instability with F1 variance ± 0.243—some random seeds converge to reasonable performance (F1 ≈ 0.60), while others fail completely (F1 ≈ 0.05). This variance indicates that scratch training in severe low-label regimes is unreliable: deployment success depends on fortunate random initialization, an unacceptable risk for safety-critical infrastructure.

Self-supervised pretraining eliminates this instability: all five random seeds converge to F1 = 0.87 ± 0.051, providing consistent performance regardless of initialization. This stability advantage diminishes at higher label fractions—by 20% labeled data, both scratch and SSL methods achieve reliable convergence (F1 > 0.83) with low variance. The practical implication is clear: when labeled cascade data is expensive or impossible to obtain (e.g., rare blackout events with limited historical records), SSL pretraining provides the reliability necessary for operational deployment. When labeled data is abundant ($>$20% of available samples), both approaches work well, and the choice between them becomes less critical.

Class imbalance interaction: The IEEE 118-bus cascade dataset exhibits severe class imbalance (approximately 5% positive class rate), compounding the low-label challenge. With only 10% labeled data, scratch training observes fewer than 500 positive (cascade) examples across 91,875 training samples—insufficient for learning rare failure patterns. Self-supervised pretraining mitigates this by learning grid structure from *all* unlabeled training data, not just the small labeled subset, providing a representation foundation that requires fewer labeled cascade examples to achieve reliable classification.

D. Limitations and Future Directions

While our results demonstrate clear benefits of physics-guided self-supervised learning, several limitations warrant discussion and suggest directions for future research.

Single benchmark evaluation: All experiments use the PowerGraph benchmark [10] on simulated IEEE test systems. Validation on real utility datasets with operational measurements, measurement noise, missing data, and dynamic topology changes is essential before deployment. Real grids ex-

hibit complexities not captured in simulation: communication delays, bad data from faulty sensors, topology errors in network models, and time-varying renewable generation. Transfer learning experiments demonstrating that models pretrained on simulated data can fine-tune effectively on small real-world labeled datasets would strengthen deployment confidence.

Static topology assumption: Our current framework assumes fixed grid topology during training and inference. Real power systems undergo frequent topology changes due to maintenance outages, equipment failures, and switching operations for loss minimization. Extending our approach to handle dynamic topology—for example, via graph structure learning [**?**] or topology-conditional embeddings—would improve practical applicability. Additionally, investigating how well models generalize to unseen topologies (e.g., training on IEEE 24-bus, testing on IEEE 30-bus) would clarify the transferability of learned physics principles across grid structures.

Limited out-of-distribution evaluation: We evaluated robustness only under load scaling (1.0–1.3$\times$ nominal injections). Other critical distribution shifts remain unexplored: (1) Measurement noise and missing data, (2) Seasonal and diurnal load pattern variations, (3) High renewable penetration with intermittent generation, (4) Topology perturbations (line outages), and (5) Extreme weather events causing correlated failures. A comprehensive robustness evaluation across multiple OOD dimensions is necessary to establish reliability bounds for operational deployment. Additionally, our preliminary load scaling results used a single random seed and should be validated with multi-seed experiments for statistical significance.

Computational cost of pretraining: While inference is fast, self-supervised pretraining requires 30 minutes to 2 hours of GPU time depending on grid size. For utilities with hundreds of distinct network models (e.g., different seasonal configurations, multiple voltage levels), pretraining all models could incur significant computational cost. Investigating few-shot transfer learning—pretraining once on a large representative grid, then fine-tuning with minimal data on similar grids—could amortize pretraining costs across multiple deployment scenarios.

Explainability depth: Our Integrated Gradients evaluation demonstrates that the model correctly ranks critical edges (0.93 AUC-ROC), but does not provide *mechanistic* explanations of *why* specific lines are vulnerable. Causal discovery methods [**?**] or attention mechanism interpretation [**?**] could yield deeper insights into learned failure propagation patterns, enabling operators to understand not just *which* lines matter but *how* cascades propagate through grid topology.

VIII. Conclusion

We presented a physics-guided self-supervised learning framework for graph neural networks that addresses labeled data scarcity in power grid analysis. By embedding admittance-weighted message passing into the encoder architecture and developing grid-specific pretext tasks (masked injection and parameter reconstruction), our approach learns representations from unlabeled operational data that transfer effectively to downstream tasks. Multi-seed validation across three prediction tasks on two grid scales confirms consistent improvements in low-label regimes: at 10% labeled data, self-supervised pretraining achieves 29.1% power flow error reduction, 26.4% line flow error reduction, and 6.8% F1-score improvement for cascading failure prediction on the IEEE 24-bus system. On the IEEE 118-bus system, pretraining dramatically stabilizes cascade prediction training, reducing F1 variance from $\pm$0.243 (scratch) to $\pm$0.051 (SSL)—a critical reliability improvement for deployment in safety-critical infrastructure where performance cannot depend on fortunate random initialization.

Beyond sample efficiency, our framework achieves 0.93 AUC-ROC explainability fidelity via Integrated Gradients, correctly identifying critical transmission lines whose failures drive cascades. Preliminary robustness evaluation under load stress (1.0–1.3$\times$ nominal) suggests that self-supervised representations generalize more effectively to out-of-distribution conditions (+22% advantage at 1.3$\times$ load), though multi-seed validation of this finding is needed. The consistent pattern across all tasks—largest gains when labeled data is most scarce, diminishing but persistent benefits even at full labels—validates our hypothesis that physics-guided self-supervised learning captures fundamental grid structure and electrical relationships that reduce dependence on task-specific supervision.

Future work should extend evaluation to real utility datasets with operational measurements, dynamic topology changes, and diverse distribution shifts (measurement noise, renewable variability, seasonal patterns). Investigating mechanistic explainability beyond edge importance ranking, developing few-shot transfer learning across multiple grids, and exploring continual learning as grids evolve would further advance practical deployment of machine learning for power system operations. Our framework demonstrates that self-supervised learning, when designed with domain physics in mind, provides a viable path toward sample-efficient, reliable, and interpretable machine learning for critical infrastructure.

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