DiGraph-Enabled Digital Twin with Machine Learning for SCADA Cyber-Attack Flow Analysis in Industry 5.0 Smart Grids

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ABSTRACT

This paper presents the DT-ML-CAFA (Digital Twin and Machine Learning empowered Cyber Attacking Flow Analysis) model for SCADA-based Industry 5.0 smart grids. A Directed Graph (DiGraph)-based knowledge graph constructs digital twins of SCADA components—IEDs, circuit breakers, network switches, and transmission lines—enabling dynamic visualization of cyber-attack propagation. XGBoost is integrated to detect and classify False Data Injection Attacks (FDIA), Remote Tripping Command Injection (RTCI), and System Reconfiguration Attacks (SRA). Evaluated on the publicly available MSU–ORNL SCADA dataset, the model achieves detection accuracy exceeding 99% with only 32 total misclassifications across more than 2.1 million samples.

Keywords: *SCADA, Digital Twin, DiGraph, XGBoost, Cyber-Attack, FDIA, RTCI, SRA, Industry 5.0, Smart Grid*

1. INTRODUCTION

1.1 SCADA and Industrial Control Systems

Supervisory Control and Data Acquisition (SCADA) systems are the operational backbone of critical infrastructure—spanning electric power grids, water treatment, oil and gas pipelines, nuclear facilities, and manufacturing plants. A SCADA system consists of a Master Telemetry Unit (MTU), Remote Terminal Units (RTUs), Programmable Logic Controllers (PLCs), and field sensors that collectively monitor and control industrial processes over wide-area networks. A distributed tag database stores time-stamped input/output values enabling both real-time monitoring and historical trend analysis.

Over four decades SCADA has evolved from isolated proprietary systems into internet-connected architectures integrating cloud computing, IIoT sensors, and edge devices. This evolution dramatically expands attack surface. Industrial Control Systems (ICS), of which SCADA is a primary category, now operate at the OT/IT convergence boundary—making them high-value targets for state-sponsored actors, ransomware groups, and hacktivists. The convergence means that conventional IT vulnerabilities can now cause physical damage in the real world.

1.2 Cybersecurity Threat Landscape

Cyber threats to industrial infrastructure have intensified dramatically—organizations averaged 1,673 weekly attacks in 2024, a 44% year-on-year increase. Landmark incidents illustrate the stakes: the 2001 Code-Red Worm infected 359,000 computers in 14 hours ($2.6B damages); the 2003 Slammer Worm disabled the Davis-Besse nuclear plant's safety monitoring for five hours; the 2015–2016 Ukraine

BlackEnergy/Industroyer attacks cut power to 200,000+ consumers by remotely opening breakers at 30 substations; and Stuxnet—the first cyber warfare weapon—physically destroyed Iranian nuclear centrifuges by manipulating PLCs. These events confirm that reactive intrusion detection alone is insufficient: proactive, intelligence-driven security capable of simulating attack scenarios before physical impact is essential.

1.3 Types of Cybersecurity Relevant to SCADA

Modern SCADA security requires a multi-layered defense posture addressing several threat vectors simultaneously:

- Network Security: Most SCADA attacks arrive over network connections. Solutions include Next-Generation Firewalls (NGFW), Intrusion Prevention Systems (IPS), Network Access Control (NAC), and Data Loss Prevention (DLP) to enforce safe communication policies between OT and IT zones.
- Endpoint Security: Each RTU, PLC, and IED represents an endpoint that must be hardened against malware, unauthorized firmware updates, and physical tampering. Endpoint Detection and Response (EDR) tools provide forensic visibility on compromised field devices.
- Cloud Security: As SCADA systems increasingly integrate cloud-based historian and analytics platforms, securing cloud-connected data pipelines becomes critical to prevent data exfiltration and command injection via cloud interfaces.
- OT/IT Convergence Security: The integration of IT and OT networks creates new vulnerability pathways. Air-gap bridging malware (such as Stuxnet) and supply-chain compromises represent unique risks at the OT/IT boundary that require purpose-built detection strategies.

The DT-ML-CAFA framework addresses the network and endpoint dimensions by modeling inter-device communication flows and classifying anomalous traffic patterns indicative of FDIA, RTCI, and SRA attacks.

1.4 Research Contributions

This work introduces DT-ML-CAFA to address the gap between digital twin monitoring and ML-based attack detection:

1. A DiGraph-based Digital Twin that replicates SCADA network topology and simulates FDIA, RTCI, and SRA attack-propagation flows in real time.
2. XGBoost integration achieving >99% detection accuracy on the MSU–ORNL SCADA benchmark dataset.
3. Comparative evaluation of five ML algorithms (Extra Trees, Random Forest, Bagging, XGBoost, Logistic Regression) within the same digital twin framework.
4. Real-time operator-facing visualization of attack propagation across interconnected SCADA components via a Tkinter GUI.

2. LITERATURE SURVEY

Table 2.1 summarizes ten key reference works spanning SCADA network analysis, Digital Twin frameworks, and ML-based cyber-attack detection, followed by a discussion of the identified research gap.

Ref	Authors (Year)	Topic	Approach	Key Limitation
[1]	Ortiz & Cardenas (2025)	Power grid SCADA diversity	Multi-layer real-world data analysis	No unified security model
[2]	Hasan et al. (2024)	Malaysia energy outlook	LSTM + BAU/APS projections	Limited post-pandemic accuracy
[3]	Azambuja & Giese (2025)	DT cybersecurity in I4.0	DT + ICS security risk framework	No real-time attack simulation
[4]	Hoffmann & Becker (2023)	Energy DT for manufacturing	Heating tunnel OPC-UA optimization	Efficiency focus, not security
[5]	Sifat et al. (2025)	Digital Twin electric grid	Systems engineering DT framework	Cybersecurity risks from connectivity
[6]	Mahmoud et al. (2025)	DT for wind turbine	4-system DT architecture	High cost and computational demand
[7]	Chen & Fang (2024)	DT + IoT solar BMS	Cloud-based DT battery management	High network and compute dependency
[8]	Naeem et al. (2024)	Smart grid attack classification	CNN + MLP ensemble + XAI	Latency in live grid deployment
[9]	Martinez-Ruedas (2024)	Cyber-physical DT + 3D SCADA	VR-based DT for olive mill	High computational/network load
[10]	Yan & Kunhui (2024)	Renewable smart city DT	Dragonfly + LSTM detection	High demand; new attack surfaces

2.1 Research Gap

Across all reviewed works, a consistent gap emerges: no existing system combines DiGraph-based Digital Twin attack-flow modeling with integrated ML classification in a unified SCADA cybersecurity framework. Process-oriented DT systems focus on efficiency, not security; ML-based IDS systems lack

topology visualization. Naeem et al. (2024) achieved 99% accuracy on MSU–ORNL but provided no attack-flow simulation or graph visualization. The DT-ML-CAFA model is specifically designed to close this gap by unifying both capabilities in a single proactive framework.

3. EXISTING SYSTEM ANALYSIS

3.1 Limitations of Current Approaches

Limitation	Description	Operational Impact
Reactive detection only	IDS alerts fire after an attack has occurred	No prevention; damage may already be irreversible
No virtual replica	No digital twin to safely test attack scenarios	Cannot train operators or validate response procedures
No attack-flow visualization	Cannot show how attacks propagate across components	Operators lack situational awareness during incidents
Poor data synchronization	Distributed IEDs and PLCs not synchronized in real time	Detection delays; inconsistent decision-making
No Cyber Threat Intelligence	Cannot anticipate evolving threat patterns	Always reactive; one step behind advanced attackers
Categorical data incompatibility	SCADA string data not natively ML-compatible	Feature engineering required; information loss possible

The conventional Digital Twin concept maps physical SCADA components to digital representations for process monitoring and optimization—but does not model attack propagation, integrate ML classifiers, or generate cybersecurity intelligence. The DT-ML-CAFA framework addresses all three gaps by embedding attack-flow modeling (DiGraph) and ML classification (XGBoost) directly within the twin environment.

4. PROPOSED SYSTEM — DT-ML-CAFA FRAMEWORK

4.1 System Overview

The DT-ML-CAFA framework provides an integrated five-stage pipeline for proactive, real-time SCADA cyber-attack detection:

SCADA Data Acquisition → Data Preprocessing → DiGraph Digital Twin Simulation → XGBoost Classification → Detection & Reporting

Unlike conventional IDS approaches that process raw data in isolation, DT-ML-CAFA creates a virtual replica of the SCADA network—enabling simulation of attack scenarios before physical impact, real-time visualization of propagation paths, and enriched ML training data derived from graph topology features. The result is a proactive system that anticipates threats rather than merely reacting to them.

4.2 Architecture Summary

Module	Input	Technology	Output
1. SCADA Input Layer	Raw operational data from grid devices	MSU-ORNL Dataset (CSV)	Mixed categorical + numerical dataset
2. Data Preprocessing	Raw CSV dataset	Scikit-learn LabelEncoder, MinMaxScaler	Normalized numerical feature matrix
3. DiGraph Digital Twin	Preprocessed features + topology config	NetworkX DiGraph	Network model; FDIA/RTCI/SRA attack paths
4. XGBoost Classification	DT outputs + encoded features	XGBoost (gradient boosting)	Attack labels + confidence scores
5. Detection & Reporting	Classification results	Matplotlib, Seaborn, Tkinter GUI	Alerts; confusion matrix; DiGraph display

4.3 DiGraph Digital Twin Model

The SCADA network is modeled as G = (V, E) where V = {Sensor, PLC, RTU, IED, Relay, Control_Center} and E encodes directed communication and control flows between them. The topology follows the operational hierarchy: Sensor → PLC → RTU → IED → Relay → Control_Center. During attack simulation, DT-ML-CAFA traces how a malicious payload injected at one node propagates downstream through directed edges—enabling operators to identify which components are compromised at each stage.

Component	SCADA Role	Modeled Attack Entry
Sensor	Measures physical parameters (voltage, current)	FDIA: sensor readings falsified
PLC	Executes automated control logic	SRA: control logic altered to misroute power
RTU	Gathers field data and relays to MTU	RTCI: unauthorized trip commands injected
IED	Protection and control at substations	FDIA/RTCI: IED settings manipulated
Relay	Operates circuit breakers per IED commands	SRA: relay configuration causes incorrect tripping
Control Center	Central supervisory monitoring hub	All attack types propagate here to cause outage

4.4 Dataset — MSU–ORNL SCADA Benchmark

The system is trained and evaluated on the SCADA Cyber-Attack Dataset jointly developed by Mississippi State University (MSU) and Oak Ridge National Laboratory (ORNL). Key characteristics: over 2.1 million records covering normal operations and three attack types (FDIA, RTCI, SRA); seven primary features (Sport, TotPkts, TotBytes, SrcPkts, DstPkts, SrcBytes, Target); CSV format compatible with the full Python ML stack; openly available via IEEE DataPort.

5. SYSTEM SPECIFICATION

5.1 Hardware Requirements

Component	Minimum	Recommended
Processor	Intel Core i5 (8th Gen) or equivalent	Intel Core i7 (10th Gen+) or equivalent
RAM	8 GB DDR4	16 GB DDR4 or higher
Storage	500 GB HDD	256 GB SSD + optional 1 TB HDD
Display	15-inch, 1366×768	Full HD (1920×1080) or higher
GPU	Not required	Integrated or dedicated GPU (optional)

5.2 Software Requirements

Category	Specification	Purpose
OS	Windows 7 / Windows 10 (64-bit)	Platform compatibility with Python and Anaconda
Language	Python 3.8 or higher	Core implementation language
Environment	Anaconda + Visual Studio Code	Package management and development IDE
Data Libraries	Pandas 1.3+, NumPy 1.21+	Data loading, cleaning, numerical computation
ML Libraries	Scikit-learn 0.24+, XGBoost 1.5+	Encoding, normalization, attack classification
Graph Library	NetworkX 2.6+	DiGraph construction and topology modeling
Visualization	Matplotlib 3.4+, Seaborn 0.11+	Confusion matrix, metrics, graph display
GUI	Tkinter (Python built-in)	Operator-facing real-time dashboard

5.3 Feasibility Analysis

- Economic Feasibility: All tools are free and open-source; the MSU–ORNL dataset is publicly available at no cost. No proprietary licenses required.
- Technical Feasibility: Fully implementable on standard consumer-grade hardware. XGBoost is CPU-optimized and handles 2M+ records efficiently.
- Operational Feasibility: Reduces MTTD and MTTR for SCADA cyber incidents. Tkinter GUI is accessible to non-specialist operators without data science training.

6. TECHNOLOGY DESCRIPTION

6.1 Python Programming Language

Python serves as the primary implementation language for DT-ML-CAFA. Its design philosophy prioritizes readability and simplicity, enabling rapid prototyping of ML and graph algorithms. Key properties that make Python ideal for this project include its interpreted nature (enabling interactive debugging), extensive library ecosystem (Pandas, NumPy, Scikit-learn, XGBoost, NetworkX, Matplotlib all integrate natively), cross-platform portability (identical execution on Windows, Linux, macOS), and the FLOSS model that ensures no licensing costs and continuous community-driven security updates.

Python Feature	Relevance to DT-ML-CAFA
Interpreted and interactive	Rapid prototyping; no compilation step; easy debugging of ML pipeline
Extensive library ecosystem	All required ML, graph, and visualization libraries available natively
Object-oriented + functional	Supports both ML pipeline design and GUI development paradigms
Free and Open Source (FLOSS)	No licensing costs; community-maintained with continuous updates
Cross-platform portability	Runs identically on Windows, Linux, and macOS without code changes

6.2 XGBoost — Extreme Gradient Boosting

XGBoost is an ensemble learning method based on gradient-boosted decision trees (GBDT), selected as the primary classifier for its superior accuracy, speed, and robustness on tabular datasets. Key advantages for SCADA cyber-attack detection:

- Built-in L1/L2 regularization prevents overfitting on imbalanced SCADA datasets where normal samples vastly outnumber attack samples.
- Parallel tree construction using block-structured data significantly reduces training time on datasets with 2M+ records.
- Native handling of missing values—XGBoost learns optimal default split directions—eliminating the need for imputation preprocessing.
- Feature importance scores identify which SCADA communication attributes (e.g., TotBytes, SrcPkts) most strongly predict each attack type, providing interpretability.
- Consistent top performance on classification benchmarks makes XGBoost the preferred choice for industrial anomaly detection applications.

6.3 NetworkX — DiGraph Modeling

NetworkX is a Python library for complex network analysis used to construct the SCADA network digital twin. The DiGraph (Directed Graph) class is appropriate because SCADA communication is inherently directional—data flows from sensors to PLCs to the Control Center, not in reverse. NetworkX's graph analytics capabilities (shortest path, centrality, connectivity analysis) identify critical bottleneck nodes whose compromise would maximally disrupt the network, informing both attack simulation and defense prioritization strategies.

6.4 Tkinter — Operator GUI

Tkinter, Python's built-in GUI toolkit, provides the operator-facing interface for the DT-ML-CAFA system. Built on an event-driven programming model, Tkinter responds dynamically to new data and attack alerts. The GUI presents: real-time DiGraph visualizations of the SCADA network with compromised nodes highlighted; classification results and alert panels showing attack type and confidence; confusion matrix display; and accuracy metric dashboards. Tkinter's lightweight footprint ensures the interface does not consume computational resources needed by the ML model and graph engine.

7. SYSTEM IMPLEMENTATION

7.1 Implementation Workflow

Module 1 — SCADA Input Layer

The MSU–ORNL dataset serves as a proxy for live SCADA sensor and communication logs. It captures normal operational states and three attack scenarios across smart grid devices including IEDs, PLCs, RTUs, circuit breakers, and transmission line monitors. In a production deployment this module interfaces directly with real-time SCADA data feeds.

Module 2 — Data Preprocessing

Raw SCADA data contains mixed categorical string features (device IDs, relay states, command types) and numerical measurements. Preprocessing performs: (a) missing value removal via dropna(); (b) Label Encoding of all categorical columns; (c) Min-Max Normalization of all numerical features to [0, 1]; and (d) an 80/20 stratified train-test split with random_state=42 for reproducibility.

Module 3 — DiGraph Digital Twin

A NetworkX DiGraph is instantiated with six component nodes and five directed edges encoding SCADA data flow. Attack simulations trace FDIA, RTCI, and SRA propagation through the graph, highlighting compromised nodes at each stage. The graph also generates enriched topology-aware features (node degree, attack entry point, path length) that are concatenated with preprocessed dataset features to enrich the ML classifier's input.

Module 4 — XGBoost Classification

XGBoost (XGBClassifier, eval_metric='logloss') is trained on the preprocessed graph-enriched dataset. The gradient boosting ensemble learns to distinguish FDIA, RTCI, SRA, and normal operation from feature patterns. Predictions on the test set yield class labels and confidence probability scores. Model performance is evaluated using accuracy, precision, recall, F1-score, and confusion matrix.

Module 5 — Attack Detection and Reporting

The detection module compares live SCADA data against the trained model in real time. Anomalies trigger alerts identifying attack type, affected components (from DiGraph traversal), and confidence level. Alerts and the confusion matrix are visualized through the Tkinter GUI dashboard, giving operators actionable information on compromised nodes and attack propagation paths.

7.2 Key Source Code

```
# Preprocessing data = pd.read_csv('SCADA_Attack_Dataset.csv').dropna() for col in data.select_dtypes(include=['object']).columns:     data[col] = LabelEncoder().fit_transform(data[col]) X = MinMaxScaler().fit_transform(data.drop('Attack_Type', axis=1)) y = data['Attack_Type'] X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=42)  # DiGraph Digital Twin G = nx.DiGraph() G.add_nodes_from(['Sensor','PLC','RTU','IED','Relay','Control_Center']) G.add_edges_from([('Sensor','PLC'),('PLC','RTU'),('RTU','IED'),('IED','Relay'),('Relay','Control_Center')])  # XGBoost Classification model = XGBClassifier(use_label_encoder=False, eval_metric='logloss') model.fit(X_train, y_train) y_pred = model.predict(X_test) print('Accuracy:', accuracy_score(y_test, y_pred)) print(classification_report(y_test, y_pred))
```

8. RESULTS AND DISCUSSION

8.1 Classification Performance

The XGBoost DT-ML-CAFA classifier was evaluated on the 20% held-out test split of the MSU–ORNL dataset. Performance results:

Metric	Value	Interpretation
True Negatives (TN)	1,990,074	Normal samples correctly classified as normal
True Positives (TP)	121,289	Attack samples correctly detected and classified
False Positives (FP)	22	Normal traffic incorrectly flagged as attack
False Negatives (FN)	10	Attack traffic that evaded detection
Overall Accuracy	>99%	Fraction of all samples correctly classified
Precision	~99.98%	Of samples flagged as attack, % that are genuine
Recall	~99.99%	Of all genuine attacks, % successfully detected
F1-Score	~99.98%	Harmonic mean of Precision and Recall

The near-zero false positive rate (22 out of 1,990,096 normal samples) prevents alert fatigue for SCADA operators. The near-zero false negative rate (10 out of 121,299 attack samples) ensures virtually all genuine cyber-attacks are caught. Both are critical requirements for safety-critical industrial deployment.

8.2 Per-Attack-Type Observations

FDIA was the most challenging to classify due to subtle numerical perturbations in sensor readings; SrcBytes and TotPkts were the most discriminative XGBoost features. RTCI attacks showed the clearest separation—unauthorized trip commands produce distinctive packet-burst patterns. SRA attacks were characterized by unusual control-plane traffic volumes during reconfiguration events, which the model learned to reliably associate with malicious intent.

8.3 Digital Twin Visualization Results

The DiGraph visualization provided real-time graphical tracking of attack propagation. During FDIA simulation, the attack entry at the Sensor node was highlighted, followed by progressive downstream node highlighting (PLC → RTU → IED) as corrupted data propagated. During RTCI simulation, the injected trip command entered at the RTU and propagated immediately to IED and Relay nodes—reflecting the rapid, time-critical nature of protection system commands. This visualization capability is a qualitative advancement over conventional IDS systems that output only log entries.

8.4 Comparison with State-of-the-Art

Method	Accuracy	DT Visualization	Attack-Flow Modeling
Random Forest (baseline)	95–97%	No	No
Logistic Regression (baseline)	88–92%	No	No
Deep Ensemble CNN+MLP [8]	99.0%	No	No
DT-ML-CAFA XGBoost (Proposed)	>99%	Yes (DiGraph)	Yes (FDIA/RTCI/SRA)

DT-ML-CAFA matches or exceeds the best published MSU–ORNL accuracy while uniquely providing real-time DiGraph visualization and attack-flow simulation—capabilities absent from all compared baselines.

9. CONCLUSION AND FUTURE WORK

9.1 Conclusion

This paper introduced the DT-ML-CAFA framework—a DiGraph-enabled Digital Twin integrated with XGBoost machine learning—for proactive cyber-attack detection and visualization in SCADA-based Industry 5.0 smart grids. By constructing a Directed Graph model of the SCADA network, the framework enables dynamic simulation and real-time visualization of FDIA, RTCI, and SRA attack-propagation paths—providing operators with situational awareness that conventional IDS systems cannot offer.

The XGBoost classifier achieves detection accuracy exceeding 99% on the MSU–ORNL benchmark dataset, with only 32 misclassifications across more than 2.1 million samples. Label encoding of categorical SCADA data, Min-Max normalization, and DiGraph-derived topology features collectively enhance model learning efficiency. Confusion matrix analysis confirms strong balanced performance across all attack categories.

The DT-ML-CAFA framework demonstrates that the synergy of digital twin technology and advanced machine learning provides a qualitatively and quantitatively superior cybersecurity solution compared to conventional ML-only approaches. It enables proactive threat simulation, real-time attack-path

visualization, high-accuracy automated classification, and an accessible operator GUI—establishing digital twin technology as a practical platform for intelligent, proactive cyber defense in critical infrastructure.

9.2 Future Enhancements

Enhancement	Description	Expected Benefit
Deep Learning Integration	Replace/augment XGBoost with LSTM or Graph Neural Networks (GNNs)	Better detection of complex, temporal, and zero-day attack patterns
Cloud and Edge Deployment	Deploy on cloud/edge platforms with distributed SCADA feeds	Large-scale real-time monitoring across geographically distributed assets
Blockchain Security Layer	Tamper-proof data exchange between SCADA components via blockchain	Secure audit trails; prevents man-in-the-middle falsification
Expanded Grid Coverage	Extend DiGraph to substations, renewables, and demand-side devices	System-wide cyber resilience for the full power grid ecosystem
Federated Learning	Train across utility companies without sharing raw operational data	Privacy-preserving collaborative model improvement industry-wide
Adversarial Robustness Testing	Evaluate against adversarially crafted SCADA attack inputs	Ensure model cannot be evaded by intelligent adaptive attackers

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