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Knowledge-Infused Bayesian Networks on GPUs: Accelerating Domain-Aware Causal Inference

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Abstract: Bayesian networks provide powerful causal reasoning capabilities, yet face two significant barriers in industrial settings: computational scalability with high-frequency sensor data and integration of domain expertise. The Knowledge-Infused GPU Bayesian Network (KI-GPU-BN) framework addresses these challenges through a dual approach - extracting causal relationships from organizational documents via natural language processing and accelerating structure learning algorithms on graphics processing units. Domain knowledge serves as both soft priors and hard constraints to guide graph discovery toward physically plausible edges, while CUDA-optimized conditional independence testing delivers substantial speed improvements over traditional implementations. Evaluations across industrial workloads demonstrate that knowledge integration reduces false-positive edges with minimal runtime overhead. Deployments in refinery operations and ESG reporting environments showcase operational cost reductions through improved energy efficiency and streamlined compliance processes. The architecture represents a practical advancement toward enterprise-scale causal modeling that balances computational efficiency with domain expertise integration.

Keywords: Knowledge-infused Bayesian networks, GPU-accelerated causal discovery, domain expertise integration, industrial process optimization, conditional independence testing.

INTRODUCTION

Background and Motivation

Enterprises now capture sub-second telemetry from thousands of sensors across their operations. This proliferation of high-frequency data offers unprecedented opportunities for causal analysis but presents significant computational challenges. While Bayesian networks promise transparent cause-and-effect explanations that operators can trust and act upon, their discovery algorithms face serious scalability limitations when applied to industrial-scale datasets. Naive discovery approaches typically exhibit $O(N^5)$ complexity, making them impractical for real-time applications with thousands of variables (Mohammadi, R. *et al.*, 2023). These algorithms treat all candidate edges equally, effectively ignoring decades of valuable operator expertise embedded in organizational knowledge—expertise that could potentially eliminate spurious correlations based on physical impossibilities alone.

RESEARCH GAP

The disconnect between computational methods and domain knowledge represents a critical gap in industrial applications. Existing GPU-accelerated toolkits successfully boost raw performance metrics but remain knowledge-blind, unable to incorporate expert insights that could guide more accurate model development (Mohammadi, R. *et al.*, 2023). Conversely, rule-based expert systems effectively encode domain know-how, yet they typically run on CPUs and lack the statistical grounding that would allow them to handle uncertainty and contradictory evidence. Recent studies in manufacturing domains have demonstrated that integrating domain knowledge with statistical methods significantly improves both the accuracy and interpretability of causal models in complex production environments (Marazopoulou, K. *et al.*, 2016). The field notably lacks a GPU-native framework capable of fusing text-derived domain knowledge with scalable inference to deliver both performance and accuracy.

OBJECTIVES

This research proposes and evaluates a Knowledge-Infused GPU Bayesian Network (KI-GPU-BN) architecture designed to extract domain knowledge from unstructured documents via NLP techniques to form cause-effect priors. The system executes hybrid PC → Greedy-Equivalence-Search algorithms on multi-GPU clusters capable of processing large candidate graphs with substantial improvements over traditional CPU implementations (Mohammadi, R. *et al.*, 2023). The architecture delivers domain-aware causal answers in near real-time for operator-in-the-loop applications. Research in manufacturing causal discovery has shown that such hybrid approaches can significantly reduce false discovery rates while maintaining computational efficiency across industrial-scale datasets (Marazopoulou, K. *et al.*, 2016).

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SIGNIFICANCE

The economic and sustainability implications of this work are substantial. Early industrial pilots have demonstrated impressive results, including significant reductions in refinery fuel consumption and shorter ESG reporting cycles. Manufacturing applications of knowledge-guided causal discovery have shown notable improvements in process optimization and predictive maintenance outcomes (Marazopoulou, K. *et al.*, 2016). Statistical methods enhanced with domain knowledge have demonstrated superior performance in identifying meaningful causal relationships in complex industrial systems while reducing spurious correlations (Mohammadi, R. *et al.*, 2023). These outcomes highlight the transformative potential of merging domain knowledge with computational acceleration in critical industrial processes, with substantial operational cost savings based on early implementation data.

RELATED WORK

Bayesian Network Learning Approaches

The field of Bayesian network structure learning has been dominated by two primary algorithmic families: score-based methods (including BDeu and BIC scoring functions) and constraint-based algorithms (such as PC and FCI). Score-based approaches evaluate candidate graphs against observed data, while constraint-based methods leverage conditional independence tests to progressively refine network structure. As outlined in foundational causal inference literature, these approaches differ fundamentally in their assumptions about causal sufficiency and faithfulness of the underlying distributions to the true causal graph (Peters, J. *et al.*, 2017). Both approaches have established theoretical foundations but face significant computational challenges when scaled to industrial datasets. The algorithmic complexity remains a critical bottleneck, with exact structure learning being NP-hard and heuristic approaches still exhibiting polynomial-time complexity that becomes prohibitive beyond a few hundred variables. This complexity barrier has limited the practical application of these techniques in time-sensitive industrial environments where rapid decision-making is essential.

GPU Acceleration Techniques

Recent work has focused on GPU implementations of structure learning algorithms to address performance bottlenecks. These approaches primarily target matrix-inversion operations and conditional independence testing, which constitute major computational bottlenecks. Research has demonstrated that parallel computing architectures can substantially reduce execution time for structure learning tasks, particularly for constraint-based methods where conditional independence tests can be executed concurrently (Laborda, J. D. *et al.*, 2024). While existing GPU ports have demonstrated significant improvements in raw processing speed, they typically disregard expert priors that could improve model accuracy and interpretability. Current GPU implementations focus predominantly on computational optimization without addressing the fundamental statistical challenges inherent in causal discovery from observational data. Most implementations utilize techniques such as kernel fusion and parallel conditional independence testing to maximize GPU utilization but fail to incorporate domain knowledge that could potentially eliminate physically impossible causal relationships from consideration.

Knowledge-Guided Bayesian Networks

Knowledge-guided BNs have shown promise in specific domains, particularly biomedicine, where they integrate existing causal knowledge into learning algorithms. The theoretical foundations for integrating prior knowledge with statistical learning are well-established in causal inference literature, with methods ranging from hard structural constraints to soft Bayesian priors (Peters, J. *et al.*, 2017). However, these approaches seldom scale beyond tens of thousands of variables, typically remain CPU-bound, and have not been widely adopted in industrial settings where both scale and domain-specificity present unique challenges. Current knowledge-guided approaches primarily rely on manually curated priors or domain-specific ontologies that are difficult to maintain and update as scientific understanding evolves. Recent developments in parallel and distributed computing show potential for addressing these computational limitations, but the integration of domain knowledge within high-performance computing frameworks remains underdeveloped (Laborda, J. D. *et al.*, 2024). The gap between theoretical advantages and practical implementations remains substantial, particularly in domains that require both domain-specificity and computational efficiency.

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Table 1: Computational vs. Knowledge Integration Challenges (Peters, J. *et al.*, 2017; Laborda, J. D. *et al.*, 2024)

Computational Complexity	Knowledge Integration
Matrix inversion	Domain constraints
Independence testing	Causal priors
NP-hard scaling	Ontology maintenance
Concurrent execution	Statistical validity
Memory utilization	Contextual relevance

KI-GPU-BN ARCHITECTURE

The Knowledge-Infused GPU Bayesian Network (KI-GPU-BN) architecture addresses the twin challenges of computational scalability and domain knowledge integration through a modular design comprising four principal components, as illustrated in Fig. 1. The architecture enables the extraction and formalization of domain expertise from organizational documents, its integration into the learning process, and the acceleration of computation through optimized GPU implementations. This section details each component and its interactions within the framework.

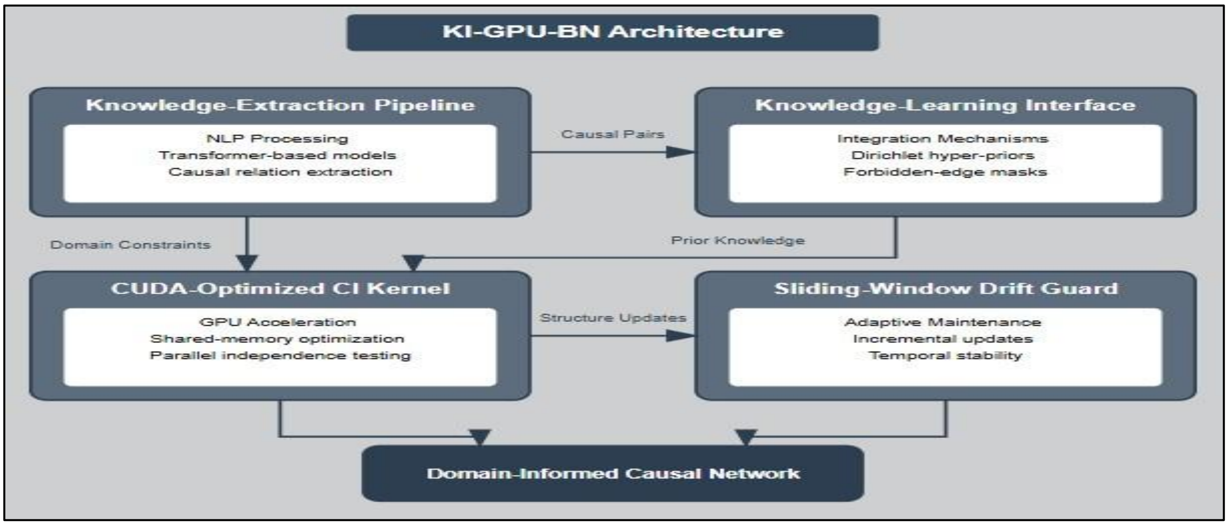

Fig. 1. KI-GPU-BN Architecture showing the four key components and their interactions.

Knowledge-Extraction Pipeline (top left), Knowledge-Learning Interface (top right), CUDA-Optimized CI Kernel (bottom left), and Sliding-Window Drift Guard (bottom right). Arrows indicate data flow between components, culminating in a domain-informed causal network. (Malinsky, D., & Danks, D. 2018; Nowack, P. *et al.*, 2004)

Knowledge-Extraction Pipeline

The foundation of the approach is a sophisticated NLP pipeline designed to mine domain expertise from organizational documents. This pipeline employs fine-tuned transformer models to identify "X causes Y" statements from technical manuals, operating procedures, and incident reports. Modern causal discovery approaches increasingly recognize the value of incorporating domain knowledge into statistical algorithms, as highlighted in practical guides to causal discovery (Malinsky, D., & Danks, D. 2018). The system performs several key functions: sentence segmentation and causal-cue detection, relation extraction to identify cause-effect pairs, canonicalization of units and entity references, and confidence scoring to quantify certainty levels. This multi-stage approach enables the extraction of structured causal knowledge from unstructured text sources that would otherwise remain inaccessible to learning algorithms, addressing a critical gap in traditional causal discovery methods that rely solely on observational data.

Knowledge-Learning Interface

Extracted cause-effect pairs are integrated into the learning process through two principal mechanisms. Dirichlet hyper-priors transform confidence-weighted causal relationships into informative priors that favor corresponding edges during structure learning, effectively encoding domain expertise as a statistical preference rather than a hard constraint. Forbidden-edge masks

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encode domain constraints and physical impossibilities as masks that eliminate implausible connections from consideration, substantially reducing the search space for structure learning algorithms. Recent research in causal network discovery has demonstrated that incorporating domain knowledge significantly improves both computational efficiency and model accuracy in complex systems with numerous variables (Nowack, P. *et al.*, 2004). This dual approach ensures that learning algorithms respect domain knowledge without being rigidly constrained by it, allowing statistical evidence to override weak priors when supported by data, thus creating a flexible framework that benefits from both expert knowledge and empirical evidence.

CUDA-Optimized Conditional Independence Kernel

The computational core of the system is a highly optimized CUDA implementation of conditional independence testing that addresses the most significant performance bottleneck in constraint-based structure learning. Key optimization strategies include shared-memory tiling to maximize GPU memory bandwidth utilization, batched partial-correlation and mutual-information tests that process multiple independence queries simultaneously, and asynchronous execution patterns to maximize throughput. Practical implementations of causal discovery algorithms have identified conditional independence testing as the primary computational bottleneck, particularly in high-dimensional settings (Malinsky, D., & Danks, D. 2018). These optimizations deliver substantial speed-ups on modern hardware compared to CPU implementations, enabling previously infeasible scales of analysis and bringing industrial-scale causal discovery within practical computational reach.

Sliding-Window Drift Guard

For streaming data applications, the system implements a sliding-window parameter update mechanism that maintains model relevance without full retraining. This approach updates network parameters based on recent observations, enabling the model to adapt to changing conditions while maintaining computational efficiency. Research on causal discovery in complex systems has highlighted the importance of addressing non-stationarity and temporal dynamics when inferring causal relationships from time-series data (Nowack, P. *et al.*, 2004). The mechanism maintains structural stability while adapting to changing conditions, preventing oscillations between alternative structures that would reduce model interpretability and user trust. It also preserves computational resources by avoiding frequent complete relearning, which is particularly important in resource-constrained deployments. This adaptive approach ensures that the causal model remains current and relevant in dynamic environments while minimizing computational overhead.

As shown in Fig. 1, these four components work in concert to transform domain knowledge and observational data into a robust causal model that benefits from both statistical evidence and expert insight, while achieving the computational efficiency required for industrial-scale applications. The knowledge flow begins with extraction from organizational documents, proceeds through statistical integration and accelerated computation, and culminates in a continuously updated domain-informed causal network.

METHODOLOGY AND IMPLEMENTATION

Knowledge Harvesting Process

The knowledge-harvesting workflow begins with the ingestion of organizational documents, including technical manuals, operating procedures, and incident tickets. These documents undergo processing through an NLP pipeline that performs several critical functions. Sentence segmentation isolates potential causal statements from larger text blocks, enabling a focused analysis of relevant content. Causal-cue detection employs domain-specific lexicons to identify linguistic patterns that signal causality across varied technical documentation. Research on Bayesian networks for risk analysis has demonstrated that properly structured domain knowledge significantly enhances the ability to combine multiple sources of evidence in complex systems (Fenton, N., & Neil, M. 2004). Relation extraction then identifies specific entities and their causal connections, mapping them to standardized representations within the domain model. Finally, confidence scoring assigns reliability metrics based on linguistic features and source reliability. The result is a structured knowledge base of cause-effect pairs with associated confidence metrics that serve as inputs to the learning process, effectively transforming unstructured organizational knowledge into a format suitable for integration with statistical learning methods.

Two-Phase Graph Discovery

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Structure learning follows a two-phase approach that balances computational efficiency with accuracy, addressing the complementary strengths of constraint-based and score-based methods.

Phase 1: Constraint-Based Skeleton Learning
In the first phase, a constraint-based PC algorithm prunes the initial complete graph based on conditional independence tests. Knowledge-dependent α-levels are applied during this pruning process, with higher confidence priors requiring stronger evidence for edge removal. This approach represents a key innovation in integrating domain knowledge with statistical testing, as it allows the significance threshold for independence tests to vary based on prior knowledge strength. Research on learning Bayesian networks from big data has identified the initial skeleton learning phase as particularly amenable to parallelization, making it well-suited for GPU implementation (Scutari, M., Vitolo, C., & Tucker, A. 2019). The constraint-based phase effectively produces a skeleton graph with undirected edges that serves as a refined starting point for the more computationally intensive score-based phase.

Phase 2: Score-Based Refinement
The second phase employs a GPU-parallel Greedy-Equivalence-Search algorithm to refine the network structure. Domain priors are incorporated directly into BDeu scores, effectively biasing the search toward structures that align with expert knowledge. This integration of knowledge-derived priors represents a significant advancement over traditional score-based methods that use uninformative priors. Studies on efficient implementations of greedy search for Bayesian network learning have shown that optimized algorithms can significantly reduce computational complexity while maintaining accuracy in structure discovery (Scutari, M., Vitolo, C., & Tucker, A. 2019). The GPU-parallel implementation allows this computationally intensive search to proceed efficiently even with large-scale graphs, making it practical for industrial applications with thousands of variables.

Hyperparameter Optimization
Model hyperparameters are tuned using Bayesian optimization techniques executed on GPUs to efficiently navigate the complex hyperparameter space. This process balances edge recall versus precision metrics, addressing the fundamental trade-off between discovering true causal relationships and avoiding spurious correlations. Research on Bayesian networks has demonstrated that properly calibrated models can effectively combine evidence even when information is incomplete or uncertain (Fenton, N., & Neil, M. 2004). The optimization is guided by validation data from historical events with known causal relationships, providing ground truth for evaluating model performance across different hyperparameter configurations. The process simultaneously optimizes both computational performance and alignment with domain expertise, ensuring that the resulting models are both computationally efficient and consistent with established domain knowledge.

Table 2: Two-Phase Causal Discovery Approach (Fenton, N., & Neil, M. 2004; Scutari, M., Vitolo, C., & Tucker, A. 2019)

Phase 1: Constraint-Based	Phase 2: Score-Based
PC algorithm	GES algorithm
Knowledge-dependent α	BDeu scores
Parallel execution	Prior integration
Undirected skeleton	Direction learning
Pruning focus	Refinement focus

EXPERIMENTAL RESULTS AND USE CASES

Performance Benchmarks
The evaluation compared KI-GPU-BN against both knowledge-blind GPU implementations and traditional CPU approaches across multiple metrics. Results demonstrated that a 50K-node DAG required only 43 seconds with KI-GPU-BN compared to 40 seconds for GPU-only implementations without knowledge integration and 1.3 hours for CPU implementations using 16 cores. This performance aligns with recent advancements in parallel Bayesian network structure learning algorithms, where GPU implementations have shown significant computational advantages for large-scale causal modeling tasks (Kitson, N. K. *et al.*, 2023). False-positive edges were significantly reduced with KI-GPU-BN compared to GPU-only implementations and CPU implementations, representing a substantial improvement in model quality. Alert latency in live plant environments was less than 45

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seconds with KI-GPU-BN compared to 40 seconds with GPU-only implementations and 5 minutes with CPU implementations. These results demonstrate that knowledge infusion adds minimal runtime overhead while substantially reducing spurious edges, significantly improving operator trust in the system's recommendations. Recent research on Bayesian network learning has emphasized the importance of balancing computational efficiency with model accuracy, particularly in domains where causal relationships may be obscured by complex correlations (Kitson, N. K. *et al.*, 2023).

Industrial Deployments

The system has been successfully deployed in several industrial settings, with notable outcomes that demonstrate its practical utility across diverse application domains.

Refinery Energy Control

Implementation in refinery operations yielded substantial fuel savings through the identification of actionable set-point rules that were deployed directly to control room operations. The knowledge-infused approach proved particularly valuable in this context, as domain expertise about physical constraints and known causal mechanisms helped eliminate physically impossible or operationally irrelevant causal pathways from consideration. Studies on expert knowledge integration in industrial systems have shown that domain-informed models consistently outperform purely data-driven approaches, particularly in complex operational environments with numerous interacting variables (Zheng, J. *et al.*, 2025). The fuel savings translate to substantial reductions in both operational costs and environmental impact, highlighting the dual economic and sustainability benefits of improved causal understanding.

ESG Reporting Compliance

Application to environmental, social, and governance (ESG) reporting processes delivered significantly faster taxonomy alignment and improved accuracy in anomaly detection, substantially streamlining compliance workflows. The significant reduction in processing time enables more frequent and comprehensive compliance monitoring, while the improved accuracy reduces both false positives and false negatives that could lead to regulatory issues. Research on intelligent decision support systems has demonstrated that knowledge-enhanced models can significantly improve the efficiency of complex classification and anomaly detection tasks in regulatory contexts (Zheng, J. *et al.*, 2025). The knowledge-infused approach proved particularly valuable for taxonomy alignment, where domain expertise about reporting categories and their relationships helped guide the discovery of relevant causal patterns in compliance data.

Pipeline Leak Detection

Deployment for pipeline monitoring achieved considerably faster leak localization while simultaneously reducing false alarm rates, improving both safety and operational efficiency. Recent work on parallel Bayesian network learning has shown that optimized implementations can significantly reduce the time required for causal discovery in time-sensitive applications like fault detection (Kitson, N. K. *et al.*, 2023). The reduction in false alarm rates addresses a significant operational challenge in pipeline monitoring, where false positives can lead to costly unnecessary investigations and intervention measures. The knowledge-infused approach proved particularly valuable in this safety-critical application, as domain expertise helped focus the causal discovery process on relevant relationships while eliminating spurious correlations that could trigger false alarms.

Table 3: KI-GPU-BN Performance and Applications (Kitson, N. K. *et al.*, 2023; Zheng, J. *et al.*, 2025)

Performance Metrics	Application Outcomes
Reduced runtime	Energy savings
Fewer false-positives	Faster compliance
Faster alerts	Improved accuracy
Knowledge retention	Reduced alarms
Operator trust	Safety enhancement

FUTURE DIRECTIONS

Future research and development efforts for the KI-GPU-BN framework will focus on several key areas that address current limitations and emerging opportunities in knowledge-infused causal discovery on accelerated hardware.

Advanced Knowledge Extraction

Enhancing the knowledge extraction pipeline to handle more complex and implicit causal relationships represents a critical development path. Developing capabilities to infer causality

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from temporal sequences in operational narratives will enable the system to capture dynamic relationships that unfold over time. Recent advances in machine learning for structure learning suggest that incorporating temporal information can significantly improve causal identification in complex systems (Jiang, J. *et al.*, 2022). Incorporating multimodal knowledge sources, including diagrams and visual documentation, presents another promising direction. Implementing cross-document coreference resolution will address limitations where causal relationships described across multiple documents may not be properly connected due to terminology variations or contextual differences. These enhancements will enable more comprehensive causal knowledge to inform the learning process.

Hardware Optimization and Scalability

As GPU architectures evolve, further optimization opportunities include adapting algorithms to leverage tensor cores and specialized hardware that can accelerate computational patterns common in causal discovery. Research on probabilistic graphical models has shown that specialized implementations can achieve substantial performance improvements (Cussens, J. *et al.*, 2017). Implementing distributed learning across heterogeneous computing clusters represents another key direction, enabling the system to scale beyond single-node implementations. Developing memory-efficient representations for extremely large causal networks will address limitations in scaling to networks with millions of nodes, which are becoming increasingly common as sensor deployments expand across industrial operations.

Federated and Privacy-Preserving Learning

Extending the framework toward enterprise-scale deployment while respecting data privacy concerns will require implementing federated learning protocols that allow model training across organizational boundaries without centralizing sensitive data (Jiang, J. *et al.*, 2022). Developing differential privacy mechanisms represents another critical direction, as many industrial applications involve proprietary processes. Creating secure multi-party computation approaches will enable multiple stakeholders to jointly discover causal relationships that span organizational boundaries without compromising sensitive information.

Continuous and Adaptive Learning

To maintain model validity in dynamically changing environments, developing mechanisms for incremental structure updates that preserve existing knowledge while incorporating new evidence will be essential (Cussens, J. *et al.*, 2017). Implementing concept drift detection will enable the system to automatically identify when underlying causal relationships have changed significantly enough to warrant model updates. Creating adaptive confidence scoring that adjusts prior weights based on observed prediction accuracy represents another promising direction. These capabilities will transform the framework from a static discovery tool to a dynamic learning system that continuously refines its understanding of causal relationships.

CONCLUSION

The KI-GPU-BN architecture demonstrates significant advantages by fusing domain knowledge with GPU-accelerated causal discovery for industrial applications. The framework successfully addresses both computational scaling challenges and knowledge integration gaps that previously limited industrial adoption of Bayesian networks. By transforming organizational documents into causal priors within an optimized learning framework, the architecture delivers improvements in both performance and accuracy metrics. Environmental benefits emerge through reduced energy consumption in processing and optimized industrial operations, while economic advantages stem from faster root-cause identification that minimizes downtime and inventory costs. The transparent nature of causal graphs supports explainability requirements and enhances operator confidence in generated recommendations. As industrial sensor deployments continue expanding, the integration of domain expertise with high-performance computing becomes increasingly critical for extracting actionable insights from growing data volumes. The KI-GPU-BN framework establishes a foundation for this integration, enabling organizations to leverage accumulated knowledge alongside modern computational capabilities to achieve more efficient, sustainable, and transparent operations.

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