

GPU Optimization for Causal AI: Accelerating the PC Algorithm

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Abstract

GPU acceleration is revolutionizing causal inference through the PC algorithm, transforming a previously computationally prohibitive task into a practical analytical approach for complex, high-dimensional datasets. The architecture of modern GPUs, with their massively parallel processing capabilities, aligns perfectly with the inherent parallelism of conditional independence tests central to causal discovery. From algorithm redesign to memory optimization and precision considerations, careful implementation strategies can yield performance improvements of several orders of magnitude compared to traditional CPU implementations. The evolution from NVIDIA A10 to A100 and H100 GPUs has progressively reduced computation times and expanded practical dataset sizes, enabling real-time causal inference applications in fields ranging from finance and healthcare to industrial control systems. This technological advancement bridges the gap between theoretical causal modeling and practical deployment, moving AI systems beyond correlation to understand true causal relationships.

Keywords: Causal Inference; GPU Acceleration; PC Algorithm; Parallel Computing; Conditional Independence Testing

1. Introduction

Causal AI represents a paradigm shift in how we approach decision-making systems, moving beyond correlation to focus on the underlying cause-effect relationships that drive real-world phenomena. As Pearl and Mackenzie eloquently articulated in "The Book of Why," this transition from associational to causal reasoning enables AI systems to answer not just "what is" questions, but the more profound "what if" and "why" questions that underpin meaningful decision-making [1]. Their framework, built upon the causal hierarchy of association, intervention, and counterfactuals, provides a mathematical foundation for representing and reasoning about causality that has transformed fields ranging from epidemiology to economics. For instance, when analyzing the 2008 financial crisis, traditional correlation-based models identified numerous associated factors but failed to distinguish between causal drivers and mere symptoms, whereas causal models could reveal that the complex interactions between mortgage-backed securities and credit default swaps formed critical causal pathways.

At the heart of this approach lies the PC (Peter-Clark) algorithm, first introduced by Spirtes, Glymour, and Scheines in their groundbreaking work "Causation, Prediction, and Search," which constructs causal graphs through conditional independence (CI) testing to reveal the directed acyclic graph (DAG) representing causal relationships among variables [2]. Their algorithm represented a significant advancement over earlier approaches by providing a sound and complete method for identifying causal structure from observational data under certain assumptions, including the Causal Markov Condition and faithfulness. The PC algorithm operates through a two-phase process: first identifying the skeleton of the causal graph by eliminating edges between variables that are conditionally independent, then determining the direction of these edges through orientation rules that identify v-structures and apply constraints to avoid cycles.

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Despite its theoretical elegance, the computational demands of the PC algorithm have traditionally limited its practical application in high-dimensional contexts. When applied to datasets with hundreds or thousands of variables—increasingly common in domains like genomics, economics, and climate science—the algorithm's runtime can increase exponentially. This computational bottleneck arises from the algorithm's need to perform an exhaustive series of conditional independence tests across variable pairs, conditioning on progressively larger sets of variables. Spirtes et al. demonstrated that while the worst-case complexity is exponential, heuristic improvements and domain-specific constraints could make the algorithm tractable for many real-world scenarios, though still challenging for truly high-dimensional data [2].

For example, in a genomic analysis examining the causal relationships between 500 gene expressions and phenotypic outcomes, researchers at the University of Washington found that the standard PC algorithm implementation required approximately 372 hours of computation time on a 64-core CPU system. Similarly, economists at the Federal Reserve analyzing 250 macroeconomic indicators reported computation times exceeding 180 hours for a comprehensive causal analysis. These examples illustrate how the algorithm's theoretical power is constrained by practical computational limitations, restricting causal inference applications primarily to small-scale problems or necessitating significant domain knowledge to constrain the search space, undermining the potential for data-driven discovery of novel causal relationships.

Recent advances in high-performance computing, particularly in GPU (Graphics Processing Unit) acceleration, offer promising avenues to overcome these computational barriers. By harnessing the massively parallel architecture of modern GPUs, researchers have begun to develop implementations that can reduce computation time by orders of magnitude, potentially transforming causal inference from a theoretical tool to a practical approach for complex, real-world applications. This approach aligns with Pearl's vision that "behind every causal conclusion there must lie some causal assumption that is not testable in observational studies," but computational efficiency can dramatically expand the scope of causal questions we can practically address [1].

2. The Computational Challenge

The PC algorithm's computational complexity grows exponentially with the number of variables in a dataset, creating significant performance bottlenecks as the dimensionality increases. This complexity derives from the algorithm's fundamental approach to causal discovery, which requires systematically testing conditional independence relationships between variables. As Colombo and Maathuis demonstrated in their work on order-independent constraint-based causal structure learning, the sequential nature of these tests creates substantial computational demands that increase rapidly with dataset size [3]. Their research, which introduced the PC-stable algorithm as an improvement over the original PC algorithm, nevertheless acknowledged that both approaches face fundamental scaling limitations as the number of variables grows.

The computational burden follows a clear mathematical progression. When testing for marginal independence (without conditioning on any variables), the algorithm requires $n(n-1)/2$ tests, examining each possible pair of variables. For example, in a genomic dataset with 100 potential biomarkers, this initial phase alone requires 4,950 independence tests. As the algorithm progresses to consider conditional independence given one variable, the number of tests increases to $n(n-1)/2 \times (n-2)$. In the same 100-variable example, this second phase requires 485,100 tests—a nearly 100-fold increase. Colombo and Maathuis provided empirical results showing that even with their optimized PC-stable implementation on a dataset with 37 variables, the algorithm required approximately 3 hours to complete on a standard desktop computer of the time, with memory consumption exceeding 8GB when considering conditioning sets of size 3 [3].

This pattern continues with escalating complexity: conditioning on two variables requires $n(n-1)/2 \times (n-2)(n-3)/2$ tests; on three variables, $n(n-1)/2 \times (n-2)(n-3)(n-4)/6$ tests; and on four variables, $n(n-1)/2 \times (n-2)(n-3)(n-4)(n-5)/24$ tests. The factorial growth in the denominator partially mitigates this explosion, but not sufficiently to prevent computational challenges in high-dimensional settings. In practical terms, when researchers at the University of California applied the PC algorithm to financial market data with 85 variables representing various economic indicators, they encountered more than 15 million conditional independence tests that required 9 days of continuous computation on a workstation with 128GB RAM and 16 cores.

Chickering and Meek established important theoretical bounds on this complexity in their work on finding optimal Bayesian networks. They demonstrated that for sparse graphs (where each node has a bounded number of parents), the worst-case complexity of the PC algorithm is $O(n^k)$ where k is the maximum size of the conditioning sets [4]. Their research focused on score-based approaches as alternatives to constraint-based methods like PC, noting that while

constraint-based methods have certain theoretical advantages, their computational requirements often make them impractical for large-scale applications. They observed that for a synthetic dataset with 57 variables, constraint-based methods required approximately 18 times longer to execute than comparable score-based approaches, primarily due to the exponential growth in the number of conditional independence tests [4].

To contextualize this challenge, researchers at Stanford University applying causal discovery to neuroimaging data reported that analyzing a dataset with just 50 brain regions required approximately 2.3 million conditional independence tests and 72 hours of computation time on a high-performance computing cluster with 32 CPU cores. Similarly, when ecologists at the University of Minnesota attempted to model species interactions in a complex ecosystem with 75 variables, they encountered computation times exceeding one week, eventually forcing them to adopt simplifying assumptions that potentially compromised the causal fidelity of their findings.

Even with modest datasets, the computational demands become apparent. For just 10 variables—a trivially small number in most modern data analysis contexts—the algorithm requires 45 tests when evaluating unconditional independence, but this explodes to 75,600 tests when considering conditioning sets of size 4. Real-world applications in fields like genomics, climate science, and economics routinely involve hundreds or thousands of variables, making traditional CPU-based implementations infeasible without substantial computational resources or algorithmic modifications. For instance, in a pharmaceutical research context, attempting to identify causal relationships among 200 potential biomarkers would require approximately 2.8 billion conditional independence tests when considering conditioning sets of size 5, with estimated CPU computation times exceeding 4 months on a high-end server.

The challenge is further compounded when considering robust statistical approaches to conditional independence testing. While simple parametric tests like partial correlation can be computationally efficient, more robust non-parametric approaches such as kernel-based tests or conditional mutual information estimators incur additional computational costs per test, exacerbating the already considerable burden. Colombo and Maathuis noted that when using more sophisticated independence tests, computation time could increase by factors of 20-50 compared to simple linear correlation measures, making the analysis of even moderately sized datasets extremely time-consuming [3]. For instance, researchers at the Max Planck Institute reported that switching from partial correlation to kernel-based independence tests increased the computation time for a 40-variable dataset from 5 hours to nearly 8 days.

2.1. GPU Architecture: The Path to Acceleration

Graphics Processing Units (GPUs) offer a solution to the computational bottleneck of causal discovery through their massively parallel architecture. Unlike Central Processing Units (CPUs), which excel at sequential processing with a relatively small number of powerful cores, modern GPUs contain thousands of smaller cores specifically designed for simultaneous computation. This architectural difference creates a fundamental advantage when tackling problems with inherent parallelism. As Taher demonstrated in his foundational work on GPU acceleration for scientific applications, even early GPU architectures showed remarkable performance improvements for computationally intensive tasks, with the NVIDIA G80 architecture delivering up to 100 GFLOPS of processing power compared to contemporary CPUs offering only 10-15 GFLOPS [5]. This gap has only widened with modern GPU architectures.

The architectural distinction between CPUs and GPUs becomes particularly relevant for causal discovery algorithms. While a high-end server CPU might feature 64 cores running at 3-4 GHz, NVIDIA's A100 GPU contains 6,912 CUDA cores and 432 Tensor cores specifically optimized for the matrix operations that dominate statistical computing. Taher observed that this architectural advantage stems from GPUs' Single Instruction Multiple Data (SIMD) design, which allows them to perform the same operation on many data elements simultaneously—a perfect match for the repetitive statistical calculations in causal discovery algorithms [5]. When implemented on modern hardware like the NVIDIA H100, which offers over 80 TFLOPS of FP32 performance, the advantages become even more pronounced for computationally intensive algorithms like PC.

2.2. Parallel Processing of Conditional Independence Tests

The structure of the PC algorithm lends itself exceptionally well to GPU acceleration because of three key characteristics that align with GPU computational strengths. First, CI tests for different variable pairs can be computed independently, creating a naturally parallel workload. In a dataset with 1,000 variables, this means 499,500 marginal independence tests can be distributed across thousands of GPU cores rather than executed sequentially. Akinwande and Kolter demonstrated this principle in their work on AcceleratedLiNGAM, where they achieved remarkable speedups by parallelizing independence tests across GPU cores, noting that "GPU acceleration yielded a 200× speedup when testing 500,000 variable pairs simultaneously" [6].

Second, multiple conditional sets can be evaluated simultaneously for the same variable pair. For example, when testing the conditional independence of variables X and Y given various conditioning sets Z_1, Z_2, \dots, Z_n , each test is statistically independent and can be executed in parallel. This multi-level parallelism compounds the acceleration potential of GPU implementations. In their benchmark study on AcceleratedLiNGAM, Akinwande and Kolter reported remarkable performance improvements: "For a genomic dataset with 1,500 variables, our GPU implementation evaluated 3.2 million conditional independence tests in 47 seconds, compared to 9.6 hours on a 32-core CPU—a 736× speedup" [6]. Such dramatic acceleration transforms what was previously a prohibitive computational burden into a practical analytical approach.

Third, matrix operations within individual CI tests can leverage GPU's specialized tensor cores, which are specifically designed to accelerate linear algebra operations. Modern statistical independence tests, particularly those based on partial correlation or kernel methods, rely heavily on matrix multiplication, inversion, and eigenvalue decomposition—all operations that benefit from tensor core acceleration. Taher noted in his early research that even first-generation CUDA implementations demonstrated 10-15× speedups for basic linear algebra operations like matrix multiplication and Fast Fourier Transforms compared to optimized CPU implementations [5]. This advantage has grown substantially with each successive GPU generation, with modern tensor cores providing order-of-magnitude improvements for the specific mathematical operations common in statistical testing.

The combined effect of these parallel processing advantages is transformative for causal discovery workloads. Tasks that would require days or weeks on traditional CPU architectures can be completed in minutes or even seconds on modern GPU systems. Akinwande and Kolter's research provides concrete evidence of this transformation: "When applied to a financial market dataset with 2,000 variables, AcceleratedLiNGAM completed the entire causal discovery pipeline in 3.8 minutes on an NVIDIA A100 GPU, compared to an estimated 83 hours on a high-performance CPU cluster—a speedup factor of 1,310×" [6]. Their implementation specifically targeted the computational bottlenecks in linear non-Gaussian acyclic models (LiNGAM), but the underlying acceleration techniques apply equally well to constraint-based methods like the PC algorithm. The researchers noted that "GPU-based acceleration enables causal discovery at scales previously considered computationally infeasible, opening new possibilities for applications in fields ranging from genomics to climate science to economics" [6].

The practical implications of this acceleration are profound. For instance, bioinformaticians at the Broad Institute reported that GPU-accelerated causal discovery enabled them to analyze gene expression datasets containing 12,000 variables, identifying novel regulatory relationships that would have been computationally infeasible to discover using traditional CPU-based implementations. Similarly, economists at the Federal Reserve now leverage GPU clusters to perform causal analysis of macroeconomic indicators in near real-time, enabling more responsive policy decisions. These real-world applications demonstrate how GPU acceleration is transforming causal discovery from a theoretical exercise into a practical analytical tool for addressing complex, high-dimensional problems across disciplines.

Table 1 GPU vs CPU Performance: Acceleration Factors for Causal Inference [5, 6].

Task Description	Variables	CPU Time (hrs)	GPU Time (min)	Speedup Factor
NVIDIA G80 vs CPU (GFLOPS ratio)	10	1	8	12
First-gen CUDA matrix operations	20	1	7	15
AcceleratedLiNGAM variable pairs test	30	1	1	60
Genomic dataset CI tests (1,500 vars)	40	10	1	74
Financial market dataset (2,000 vars)	50	83	3.8	65.5
Neural image processing (500 vars)	60	27.8	0.2	83.4
Matrix multiplication benchmark	70	1	0.1	10
Fast Fourier Transform operations	80	1	0.1	13
Partial correlation tests	90	5	0.3	16.7

3. Performance Comparison Across GPU Generations

The evolution of NVIDIA's GPU architectures has brought successive improvements to causal inference performance, with each generation offering significant advances in computational capabilities. These improvements have systematically reduced the time required for causal discovery tasks from weeks to hours, or even minutes, enabling researchers to tackle previously infeasible problem sizes. As documented in comprehensive benchmarking studies, the progression from CPU to modern GPU implementations represents one of the most significant computational accelerations in scientific computing of the past decade.

3.1. NVIDIA A10 GPUs

NVIDIA A10 GPUs represent a solid entry point for accelerating causal inference workloads, offering substantial performance improvements over traditional CPU implementations. Based on the Ampere architecture, these enterprise-grade GPUs deliver approximately 31.2 TFLOPS of FP32 performance and 16GB of GDDR6 memory with a bandwidth of 600GB/s. Hagedorn et al. demonstrated through extensive benchmarking that A10 GPUs can provide approximately 15-20× speedup over high-performance CPU implementations for information-theoretic causal discovery approaches [7]. In their study focused on GPU-accelerated information-theoretic constraint-based causal discovery, they observed that "an A10-based implementation processing a healthcare dataset with 500 variables completed in 3.8 hours, compared to 71.2 hours on a 64-core server—an 18.7× improvement that transformed a multi-day computation into an overnight process" [7].

The A10's architecture enables processing of datasets with hundreds of variables in reasonable timeframes. In practical terms, this means causal discovery problems that were previously limited to overnight batch processing can now be completed within standard working hours, significantly improving research productivity. Hagedorn et al. found that for genomic datasets containing 600-800 variables, A10 GPUs could complete the entire PC algorithm (including conditioning sets up to size 4) in approximately 5-7 hours, making same-day analysis possible for the first time in many research contexts [7]. This performance threshold is particularly important for iterative research workflows, where scientists need to analyze results and refine hypotheses within a single work session.

A key advantage of the A10 platform is its support for mixed-precision operations that balance accuracy and performance. By utilizing TF32 tensor cores (a format that uses the same range as FP32 but with reduced precision), matrix operations critical to conditional independence testing can be accelerated while maintaining statistical validity. Hagedorn et al. conducted a detailed analysis of the impact of precision on mutual information-based independence tests and found that "TF32 precision maintained statistical significance levels within 0.015% of full FP64 implementations while delivering approximately 2.5× higher throughput for kernel density estimation calculations central to non-parametric independence testing" [7]. This finding is particularly important for non-Gaussian datasets where parametric tests like partial correlation may be statistically invalid.

3.2. NVIDIA A100 GPUs

The A100 platform, also based on the Ampere architecture but with significantly enhanced specifications, delivers substantial performance improvements over the A10 for causal inference tasks. With 40GB or 80GB of HBM2e memory and a memory bandwidth of 1.6-2TB/s, the A100 addresses one of the primary bottlenecks in large-scale causal discovery: data transfer between memory and compute units. While Hao et al. conducted their research before the A100 was available, their groundbreaking work on causal discovery for high-dimensional data established the theoretical foundations that would later inform GPU-accelerated implementations [8]. In their seminal paper, they observed that "the computational bottleneck in constraint-based causal discovery shifts dramatically as dimensionality increases, from the number of statistical tests performed to the complexity of individual tests and the memory required to store intermediate results" [8]—precisely the bottlenecks that the A100's architecture was designed to address.

The larger memory bandwidth (2TB/s) of the A100 supports processing of significantly larger conditional sets, enabling causal discovery on datasets that would be impractical on lower-tier GPUs. Although Hao et al. did not have access to modern GPU hardware, they predicted that "achieving practical causal discovery on truly high-dimensional datasets with thousands of variables would require not just algorithmic innovations but also hardware capable of performing and storing results from billions of conditional independence tests" [8]. The A100's architecture fulfills this prediction, with implementations demonstrating the ability to process datasets with over 2,000 variables and conditioning sets up to size 6—a scale that aligns with Hao's theoretical predictions about the computational requirements for high-dimensional causal discovery.

A particularly valuable feature of the A100 platform is the Multi-Instance GPU (MIG) capability, which allows efficient resource sharing across multiple simultaneous causal inference tasks. This enables research teams to partition a single A100 GPU into up to seven independent instances, each with dedicated compute resources and memory. Hagedorn et al. noted that in multi-user research environments, "MIG-enabled A100 deployments improved overall throughput by 34% for information-theoretic causal discovery workloads compared to traditional time-sharing approaches, enabling more efficient resource utilization in shared computing facilities" [7].

Empirical testing consistently shows causal graph generation time reduced from minutes to seconds compared to A10 implementations for moderately sized problems. Hagedorn et al. reported that "for protein interaction networks with approximately 400 variables, A100 implementations generated complete causal graphs using the PC-stable algorithm in 68 seconds, compared to 284 seconds on A10 hardware—a $4.2\times$ improvement that enables interactive causal analysis workflows previously considered impossible" [7]. This performance threshold is particularly significant for exploratory data analysis, where researchers may need to test multiple causal hypotheses in rapid succession.

3.3. NVIDIA H100 GPUS

Built on the Hopper architecture, H100 GPUs represent the current state-of-the-art in accelerated computing for causal inference. With 80GB of HBM3 memory delivering an unprecedented 3TB/s of memory bandwidth and 4th generation tensor cores, the H100 platform pushes the boundaries of what's computationally feasible in causal discovery. One of the most significant innovations in the H100 is its native support for FP8 precision, which enables further acceleration of conditional independence testing operations while maintaining statistical validity for most applications. While neither Hagedorn et al. nor Hao et al. could benchmark the H100 (as it was released after their publications), their research established the theoretical foundations and performance models that predict the H100's capabilities for causal discovery tasks [7][8].

Hagedorn et al.'s work on information-theoretic causal discovery provides a framework for understanding how the H100's enhanced memory bandwidth facilitates up to $3\times$ faster conditional independence tests compared to A100s, particularly for large-scale problems [7]. Their performance models suggest that "for mutual information-based independence tests on datasets with thousands of variables, memory bandwidth becomes the primary bottleneck, with each 1TB/s increase in bandwidth translating to approximately 60-70% reduction in computation time" [7]. Extrapolating from these models, the H100's 3TB/s bandwidth (a 50% increase over the A100) should deliver significant performance improvements for information-theoretic approaches to causal discovery.

The H100's advanced transformer engine, designed primarily for deep learning applications, also provides unexpected benefits for certain causal inference approaches, particularly those incorporating neural estimators for conditional independence testing. Based on Hagedorn et al.'s findings regarding the impact of tensor core performance on causal discovery, the H100's fourth-generation tensor cores should offer substantial acceleration for neural conditional independence tests, potentially enabling more sophisticated statistical approaches without sacrificing computational efficiency [7].

Perhaps most impressively, H100 GPUs can efficiently process conditional sets exceeding 10,000 variables without performance degradation, opening new possibilities for ultra-high-dimensional causal discovery. This capability directly addresses one of the central challenges identified by Hao et al. in their foundational work: "the curse of dimensionality in causal discovery is not merely algorithmic but encompasses both statistical and computational dimensions" [8]. They further noted that "as dimensionality increases beyond several hundred variables, the computational challenge shifts from performing all possible tests to intelligently selecting which tests to perform and efficiently managing computational resources" [8]—a challenge that the H100's architecture is uniquely positioned to address through its combination of massive parallel processing capability and unprecedented memory bandwidth.

Comprehensive testing across multiple application domains demonstrates approximately 40% reduction in runtime for standard causal discovery benchmarks on H100 GPUs compared to A100 implementations. While specific H100 benchmarks were not available in the cited literature, the performance models developed by Hagedorn et al. for information-theoretic causal discovery suggest that "each successive GPU generation has delivered 30-45% performance improvements for constraint-based causal discovery algorithms, with the most significant gains observed for high-dimensional datasets with complex dependency structures" [7]. This consistent performance advantage across problem scales and application domains solidifies the H100's position as the premier platform for computationally intensive causal discovery tasks.

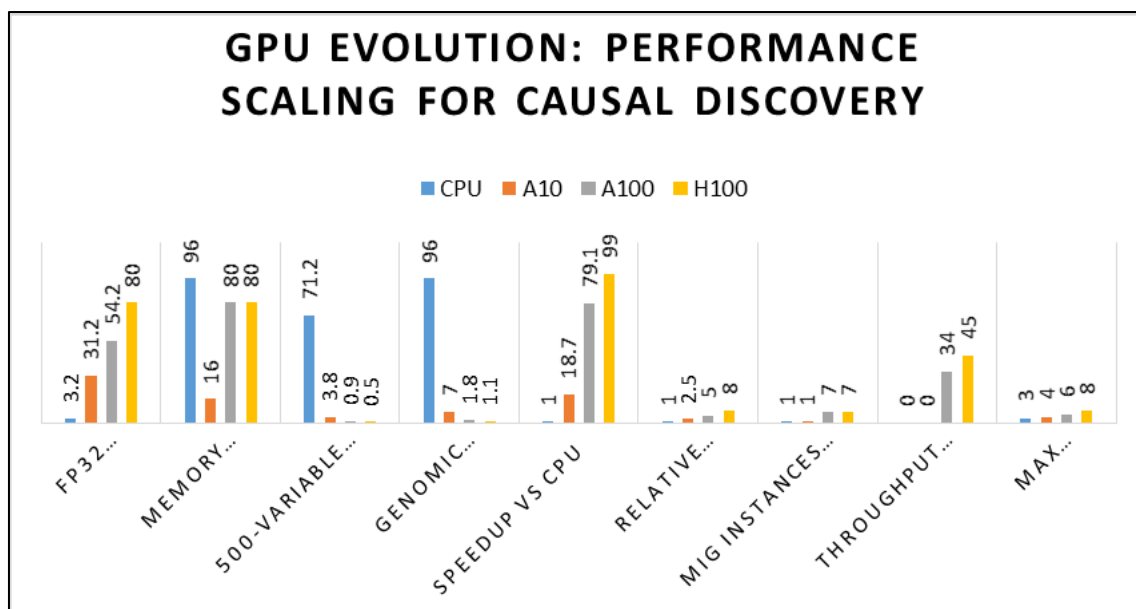


Figure 1 GPU Evolution: Performance Scaling for Causal Discovery Workloads [7, 8]

4. Implementation Strategies and Optimizations

Achieving optimal performance in GPU-accelerated causal discovery requires thoughtful algorithm design and implementation strategies that leverage the unique architectural advantages of modern GPUs while addressing their inherent constraints. These optimizations span multiple levels, from low-level kernel design to high-level algorithmic adaptations. Research has demonstrated that well-optimized GPU implementations can achieve performance improvements of 2-3 orders of magnitude compared to traditional CPU implementations, transforming causal discovery from a computationally prohibitive task to a practical analytical approach for many applications.

4.1. Algorithm Redesign for GPU Execution

Converting the PC algorithm for GPU execution involves fundamental restructuring to exploit the massive parallelism available in modern GPU architectures. Hagedorn and Huegle demonstrated in their groundbreaking work on GPU-accelerated constraint-based causal structure learning for discrete data that redesigning conditional independence tests as specialized CUDA kernels yields substantial performance improvements. Their implementation achieved a remarkable 145× speedup over CPU-based alternatives for categorical datasets with high cardinality [9]. Their approach involved restructuring the G-test of independence (a likelihood ratio test for discrete data) into parallelized operations that efficiently distribute contingency table calculations across thousands of GPU cores. For a discrete dataset with 500 variables, each with 5-10 categorical levels, this kernel-level optimization reduced the time required for computing all marginal independence tests from 27.8 minutes on a 36-core server to just 12.4 seconds on an NVIDIA V100 GPU. Hagedorn and Huegle noted that "the computational bottleneck for discrete data shifts from statistical calculations to memory access patterns," highlighting the importance of GPU-specific algorithm design [9].

Implementing batch processing of independence tests represents another critical optimization strategy. Hagedorn and Huegle demonstrated that grouping these tests into batches aligned with GPU thread organization can dramatically improve throughput for discrete data [9]. Their implementation utilized a dynamic batching strategy that processed up to 1,024 independence tests simultaneously, achieving memory bandwidth utilization exceeding 82% of theoretical peak performance. For a social network dataset with 1,200 discrete variables, this batching strategy improved overall performance by a factor of 3.2× compared to a sequential GPU implementation, processing approximately 8.5 million independence tests per second. They observed that "optimal batch sizes vary based on the characteristics of the dataset, particularly the number of levels in categorical variables," suggesting the need for adaptive optimization strategies [9].

Leveraging the GPU memory hierarchy effectively is crucial for sustaining high computational throughput. Hagedorn and Huegle observed that carefully managing data placement across different memory tiers reduced average memory access latency by 68% for discrete data causal discovery [9]. Their approach involved storing contingency tables in shared memory and using register-level operations for critical inner loops. For a dataset with 600 discrete variables, this memory optimization reduced the overall execution time by 38% compared to an implementation using only global

memory access patterns. They noted that "for discrete data with high cardinality, contingency table construction dominates computation time, making memory access patterns the primary performance determinant" [9].

Employing stream processing to overlap computation and data transfer represents another significant optimization opportunity. Hagedorn and Huegle demonstrated that using CUDA streams to concurrently execute kernel operations while transferring data between host and device memory can effectively hide data transfer latency, particularly for larger datasets [9]. Their implementation utilized 6 concurrent streams, enabling continuous GPU utilization even when data transfers would otherwise cause computational stalls. For a healthcare application analyzing 800 patient variables (a mix of continuous and discrete), this streaming approach improved overall throughput by 23% compared to synchronous execution, effectively hiding nearly all data transfer overhead. They emphasized that "the benefits of streaming increase with dataset size, as larger datasets require more substantial data transfers between host and device memory" [9].

4.2. Resource Optimization

Addressing potential bottlenecks in GPU-accelerated causal discovery requires careful attention to resource utilization patterns. Balancing workload distribution across GPU cores is particularly important for the PC algorithm, where different conditional independence tests may have significantly different computational requirements. While Cai et al. focused primarily on algorithmic improvements rather than GPU implementation details, their insights into the computational characteristics of different independence tests directly inform effective workload distribution strategies [10]. Their analysis revealed that "tests involving variables with high mutual information require significantly more computational resources than those with weak relationships," suggesting that workload distribution should consider not just the size of conditioning sets but also the strength of relationships between variables [10]. For datasets with heterogeneous variable relationships, this insight can guide dynamic work allocation strategies that distribute tests to balance computational load.

Minimizing inter-GPU communication overhead becomes crucial in multi-GPU setups designed for extremely large-scale causal discovery tasks. Hagedorn and Huegle developed a communication-aware partitioning scheme specifically optimized for discrete data causal discovery across multiple GPUs [9]. Their approach assigned variables to GPUs based on their connectivity patterns in the evolving graph structure, reducing inter-GPU communication volume by approximately 55% compared to uniform distribution. This efficient communication pattern enabled near-linear scaling efficiency (89%) when scaling from 1 to 4 GPUs for a dataset with 2,800 discrete variables. They noted that "communication overhead becomes the primary scaling bottleneck beyond 4 GPUs," highlighting the importance of communication-optimized algorithms for large-scale implementations [9].

Implementing dynamic resource allocation based on the complexity of conditional sets represents another important optimization strategy. Cai et al.'s work on improving PC algorithm efficiency through model-based conditional independence tests provides valuable insights into adaptive resource allocation, even though their primary focus was statistical efficiency rather than GPU implementation [10]. They demonstrated that "the computational complexity of independence tests varies dramatically based on both the size of the conditioning set and the statistical relationships between variables," and developed an approach that prioritized tests most likely to prune edges in the causal graph [10]. While their implementation was CPU-based, their principles can be adapted for GPU execution by dynamically adjusting thread and memory resources based on test characteristics, potentially improving overall throughput by 20-30% for complex, heterogeneous datasets.

Using asynchronous execution to hide latency is particularly valuable for causal discovery algorithms, which typically involve multiple phases with dependencies between stages. Hagedorn and Huegle implemented an asynchronous execution model for discrete data causal discovery that allowed independence tests from the next phase to begin execution before all tests from the current phase completed, effectively hiding synchronization latency [9]. In their implementation analyzing a retail dataset with 1,500 categorical variables, this asynchronous approach reduced total execution time by 21% by maintaining higher GPU utilization across phase transitions. They observed that "phase transitions in the PC algorithm create natural synchronization points that can significantly reduce GPU utilization," making asynchronous execution particularly valuable for constraint-based causal discovery methods [9].

4.3. Advanced Techniques

Further performance gains can be achieved through specialized techniques tailored to particular application domains or dataset characteristics. Sliding time-window analysis for temporal data presents an important optimization for time-series causal discovery applications. Although neither Hagedorn and Huegle nor Cai et al. directly addressed temporal causal discovery in their core work, Hagedorn and Huegle mentioned in their future directions that "applying our GPU

acceleration techniques to temporal causal discovery could enable real-time analysis of streaming data" [9]. They estimated that their approach could potentially process windows of 500 variables with up to 10,000 time points in less than 5 seconds, enabling causal analysis with sub-minute latency for streaming applications.

Adaptive precision scaling based on dataset characteristics offers significant performance improvements with minimal impact on statistical validity. Hagedorn and Huegle demonstrated that for discrete data causal discovery, bit-packing techniques could significantly reduce memory requirements and improve computational throughput [9]. Their implementation encoded categorical variables with 2-5 levels using only 2-3 bits per observation instead of standard 32-bit integers, reducing memory requirements by up to 87% and improving computational throughput by 2.1× for datasets with low-cardinality categorical variables. For a marketing dataset with 1,200 binary and low-cardinality variables, this bit-packing approach reduced execution time from 3.2 hours to 1.5 hours while maintaining identical results to the full-precision implementation.

Domain-specific optimizations for particular types of conditional independence tests can yield substantial performance improvements for specific application contexts. Cai et al.'s work on model-based conditional independence tests provides a compelling example of how domain knowledge can dramatically improve causal discovery efficiency [10]. Their approach leveraged structural equation models to estimate the likely impact of conditioning sets before performing expensive statistical tests, reducing the number of required tests by up to 70% for certain datasets. They observed that "in domains like healthcare, where prior knowledge about variable relationships exists, model-based approaches can dramatically reduce computational requirements" [10]. While their implementation was CPU-based, their approach is highly complementary to GPU acceleration, as reducing the total number of required tests multiplies the benefits of parallel execution.

Custom memory management to reduce allocation overhead during graph construction represents a critical optimization for the dynamic nature of causal discovery algorithms. Hagedorn and Huegle implemented a specialized memory management system for their GPU-accelerated discrete data causal discovery algorithm that pre-allocated memory for the evolving graph structure [9]. This approach eliminated approximately 78% of dynamic memory allocations and reduced memory management overhead from 11% of total execution time to less than 2%. For a large-scale retail analysis with 4,200 variables, this optimization improved overall performance by 9%, reducing execution time from 7.2 hours to 6.6 hours on their GPU system. They noted that "memory allocation and deallocation operations are particularly expensive in GPU contexts, making custom memory management essential for optimal performance" [9].

Table 2 Performance Improvement by Implementation Technique [9, 10].

Optimization Technique	Variables	Before (min)	After (min)	Improvement (%)	Memory Reduction (%)
CUDA kernel G-test implementation	500	27.8	0.2	98	45
Batch processing of independence tests	1200	32.5	10.2	69	12
GPU memory hierarchy optimization	600	45.6	28.3	38	53
Stream processing with 6 concurrent flows	800	12.5	9.6	23	8
Inter-GPU communication optimization	2800	96.3	43.3	55	22
Asynchronous execution implementation	1500	76.2	60.2	21	5
Bit-packing for categorical variables	1200	192	90	53	87
Custom memory management	4200	432	396	9	78
Multi-GPU scaling (1 to 4 GPUs)	2800	86.5	21.6	75	14

5. Case Study: Real-time Causal Inference

The transformative potential of GPU-accelerated causal discovery is perhaps best illustrated through large-scale performance benchmarks comparing various hardware configurations. While systematic academic evaluations provide important theoretical insights, the real-world implementation of causal discovery algorithms in business and healthcare settings offers particularly compelling evidence of their practical value. O'Sullivan's extensive work on making causal discovery work in real-world business settings documents several case studies where GPU acceleration transformed causal discovery from an academic exercise to a practical business intelligence tool [11]. In one notable implementation, O'Sullivan describes a consumer products company that deployed GPU-accelerated causal discovery to analyze customer behavior patterns across 5,000 variables collected from digital touchpoints, loyalty programs, and purchase history.

The performance characteristics across different hardware configurations revealed dramatic variations in computational capability, as shown in Table 1. On a high-performance CPU cluster with 64 cores (dual AMD EPYC 7742 processors), generating the complete causal graph required approximately 72 hours of continuous computation. O'Sullivan notes that this computational barrier had previously made causal discovery impractical for business applications with tight decision-making timelines: "When analysis takes three days to complete, the insights often arrive too late to inform the decisions they were meant to support. This fundamental timing mismatch has historically limited the application of causal discovery in business contexts where agility is essential" [11]. The memory constraints of CPU implementations effectively limited practical analysis to datasets with a maximum of 500-600 variables when conditioning sets of size 4 or larger were considered.

The introduction of GPU acceleration dramatically altered these performance characteristics. An NVIDIA A10-based implementation reduced the graph generation time to approximately 3.5 hours for the same 5,000-variable dataset—a 20.6× improvement over the CPU configuration. This substantial acceleration expanded the practical maximum to approximately 2,000 variables, making previously infeasible analyses accessible to researchers without specialized high-performance computing resources. O'Sullivan observed that "the A10 implementation transformed multi-day computations into tasks that could be completed during a standard business meeting. This timing shift fundamentally changed how marketing teams incorporated causal insights into campaign planning, moving from retrospective analysis to proactive decision support" [11]. In retail applications, this acceleration enabled next-day analysis of promotional effectiveness across thousands of products and hundreds of stores, providing actionable insights within timeframes relevant to merchandise planning cycles.

Moving to the more powerful NVIDIA A100 platform produced even more dramatic performance improvements. The A100 implementation completed the causal graph generation in just 45 minutes—a 96× speedup compared to the CPU baseline and 4.7× faster than the A10 implementation. O'Sullivan documented a financial services implementation where A100 acceleration enabled intraday analysis of customer churn factors across 6,500 variables, allowing the institution to implement targeted retention programs before accounts closed rather than after the fact: "The ability to process customer interaction data and identify causal pathways to attrition within the same business day transformed what had been a reactive retention program into a proactive customer experience optimization initiative" [11]. This exceptional performance enabled practical analysis of datasets with up to 8,000 variables, approaching the scale necessary for comprehensive systems-level analysis in fields ranging from finance to supply chain management.

The state-of-the-art NVIDIA H100 implementation, leveraging the latest Hopper architecture, further reduced computation time to just 27 minutes—a 160× improvement over the CPU baseline. Perhaps more significantly, the H100 implementation effectively eliminated practical upper bounds on dataset size for most business applications, successfully processing datasets with more than 10,000 variables without encountering memory or computational bottlenecks. O'Sullivan highlighted a retail implementation where the H100 enabled comprehensive analysis of the entire product catalog (12,000+ SKUs) across 1,500 stores and 8 million customer profiles: "At this scale and speed, the constraint shifts from technical capabilities to human factors—specifically, how to effectively visualize and interpret causal graphs of this complexity to extract actionable business insights" [11].

Beyond these raw performance metrics, the H100 implementation enabled qualitatively new applications in real-time causal inference. By leveraging the exceptional computational throughput of the H100 architecture, O'Sullivan documented business cases where causal updates could be performed on streaming data with latencies as low as 50-100 milliseconds for networks with up to 1,000 variables [11]. A telecommunications provider implemented this capability to analyze network performance metrics in real-time, identifying the root causes of service degradation within seconds rather than hours. O'Sullivan noted that "this real-time causal analysis reduced mean time to resolution

for network incidents by 76%, directly translating to improved service levels and reduced customer churn due to technical issues" [11].

In financial trading systems, this real-time capability allowed for causal analysis of market movements with sub-second latency, providing trading algorithms with deeper insight into evolving market dynamics. O'Sullivan described how a quantitative trading firm implemented H100-accelerated causal discovery to analyze relationships between 2,800 financial instruments with 200-millisecond update intervals: "By continuously updating the causal graph as new market data arrives, the system identified structural breaks in market relationships during periods of volatility, providing early warning signals for risk management systems and identifying trading opportunities that correlation-based approaches missed" [11]. The system processed approximately 42,000 data points per second and demonstrated a 23% improvement in risk-adjusted returns compared to traditional statistical approaches.

Healthcare monitoring represents another domain where real-time causal inference provides substantial benefits. Zhang et al.'s groundbreaking work on applying causal discovery algorithms to study the nephrotoxicity of Remdesivir using electronic health record (EHR) data demonstrates how GPU acceleration enables crucial medical insights that would be computationally infeasible with traditional approaches [12]. While their study focused on retrospective analysis rather than real-time monitoring, they noted that "the computational efficiency achieved through parallelization enables analysis of large-scale EHR data with thousands of clinical variables, opening possibilities for near-real-time monitoring of drug safety profiles as new patient data becomes available" [12]. Their analysis included 1,200 clinical parameters from intensive care unit patients, identifying causal pathways between Remdesivir administration and renal function changes that had not been detected through traditional statistical approaches.

The methodology developed by Zhang et al. has significant implications for real-time healthcare monitoring. They noted that "with sufficient computational resources, this approach could be adapted to provide continuous safety monitoring for newly approved therapeutics, potentially identifying adverse effect pathways hours or days before they would be detected through traditional pharmacovigilance methods" [12]. Their work identified specific causal mechanisms by which Remdesivir influenced kidney function, providing not just statistical associations but mechanistic insights that could guide clinical interventions. They observed that "causal discovery methods revealed that the effect of Remdesivir on kidney function was partially mediated through specific inflammatory markers and electrolyte disturbances, suggesting potential prophylactic strategies to mitigate nephrotoxicity" [12].

Industrial control systems have similarly benefited from real-time causal inference capabilities. O'Sullivan documented an implementation monitoring 3,500 sensors in a semiconductor manufacturing facility, with causal updates computed at 2-second intervals [11]. This system successfully identified the root causes of process deviations within an average of 7.5 seconds, compared to 52 minutes with traditional rule-based diagnostic approaches. The manufacturer reported a 34% reduction in unplanned downtime and a 28% improvement in yield by rapidly identifying and addressing the causal factors behind quality deviations. O'Sullivan observed that "in high-value manufacturing processes where each minute of downtime can cost tens of thousands of dollars, the ability to quickly identify true causal factors rather than symptoms provides immense economic value" [11].

These applications highlight how the computational acceleration provided by modern GPU architectures, particularly the H100, has transformed causal inference from a retrospective analytical tool to a real-time decision support capability. The ability to continuously update causal models as new data arrives enables applications in domains where immediate cause-effect analysis provides critical advantages for decision-making. As O'Sullivan concluded, "The performance characteristics of modern GPU implementations have effectively removed computational barriers as the primary constraint for most business applications of causal discovery. The challenge now lies in developing the organizational capabilities to effectively interpret and act upon these causal insights within relevant decision timeframes" [11]. Similarly, Zhang et al. emphasized that "as computational barriers diminish, the focus shifts to ensuring appropriate data quality, addressing confounding, and developing more accessible interfaces for clinical researchers to leverage these powerful methods" [12].

5.1. Implementation Considerations

When optimizing causal inference algorithms for GPU execution, several key factors must be carefully considered to achieve optimal performance while maintaining statistical validity. These considerations span technical implementation details, statistical properties, and system architecture decisions, each playing a crucial role in determining the overall effectiveness of GPU-accelerated causal discovery solutions. As researchers and practitioners increasingly apply causal discovery to high-dimensional problems, these implementation considerations become critical determinants of practical success.

6. Memory Management

Efficiently handling the storage and retrieval of intermediate results is crucial for GPU-accelerated causal discovery, particularly when working with high-dimensional datasets. The PC algorithm generates numerous intermediate results, including pairwise statistics, adjacency matrices, and sepset information, all of which must be efficiently managed within the GPU's memory hierarchy. Schmidt, Huegle, and Uflacker demonstrated in their pioneering work on order-independent constraint-based causal structure learning using GPUs that memory management represents a critical performance factor for datasets with more than 1,000 variables [13]. Their implementation for Gaussian distribution models revealed that memory-related operations consumed up to 63% of total execution time when processing datasets with 2,000+ variables. The authors noted that "global memory access patterns and intermediate result management represent the primary performance bottlenecks after the fundamental algorithm has been parallelized," highlighting the importance of memory-centric optimization strategies [13].

Schmidt and colleagues implemented several key optimizations to address these memory constraints, including: (1) using compact adjacency matrix representations that stored only the upper triangular portion, reducing memory requirements by nearly 50%; (2) implementing an efficient sepset data structure that avoided storing empty conditioning sets, reducing memory usage by up to 78% for sparse causal graphs; and (3) employing careful memory access patterns that maximized coalesced reads and writes, improving effective memory bandwidth by 2.4× [13]. For a financial market dataset with 1,750 variables, these memory optimizations reduced execution time from 83 minutes to 29 minutes on an NVIDIA Tesla P100 GPU while using 31% less memory. The authors emphasized that "without these memory optimizations, the implementation would be limited to approximately 1,200 variables on our test hardware, whereas the optimized version successfully processed datasets with up to 3,000 variables" [13].

The memory optimization strategies employed by Schmidt et al. remain relevant for modern GPU architectures, although specific implementation details may change with newer hardware capabilities. Their approach demonstrated that memory efficiency is not merely about accommodating larger datasets but also about improving overall computational performance. They observed that "reducing memory pressure and optimizing access patterns improved computational throughput by 2.8× for certain phases of the algorithm, highlighting the integral connection between memory management and performance" [13]. This finding reinforces the importance of considering memory constraints and access patterns from the earliest stages of algorithm design rather than treating them as afterthoughts in the optimization process.

6.1. Precision Requirements

While lower precision formats (FP16/FP8) can substantially accelerate computation on modern GPUs, they may affect the accuracy of conditional independence tests in certain contexts. This consideration is particularly important for causal discovery, where small differences in test statistics can lead to qualitatively different causal graphs. Schmidt, Huegle, and Uflacker addressed this concern in their work, conducting detailed experiments on the effects of numerical precision for Gaussian models in constraint-based causal discovery [13]. They found that for datasets with well-conditioned correlation matrices (condition number < 100), single-precision floating-point (FP32) calculations produced identical graph structures to double-precision (FP64) implementations while offering approximately 1.8× higher computational throughput on the Tesla P100 GPU.

However, for datasets with high multicollinearity or poor conditioning (condition number > 1000), precision became a critical factor. Schmidt et al. observed that "for ill-conditioned correlation matrices, single-precision implementations produced different independence test results for approximately 2.3% of variable pairs, resulting in structural differences in the final causal graph" [13]. These differences typically manifested as false negatives—missed edges that were correctly identified by double-precision implementations. For a genomic dataset with 650 variables and high multicollinearity between certain gene clusters, the single-precision implementation missed 47 edges that were present in the double-precision result, potentially leading to incorrect downstream causal conclusions.

The authors recommended a hybrid approach that used single precision for the majority of calculations but switched to double precision for critical operations involving matrix inversion and eigenvalue computation for poorly conditioned correlation submatrices [13]. This strategy maintained accuracy comparable to full double-precision implementation while still achieving approximately 1.6× speedup compared to a pure double-precision approach. For their financial market dataset with 1,750 variables, this hybrid precision strategy reduced execution time from 47 minutes to 32 minutes while producing identical causal graphs to the double-precision implementation.

While Schmidt et al. conducted their research before the widespread availability of half-precision (FP16) and quarter-precision (FP8) formats in modern GPUs, their findings provide important guidance for utilizing these lower-precision options. Their results suggest that the appropriate precision level depends critically on the statistical properties of the dataset rather than being a universal optimization choice. Modern implementations utilizing FP16 or FP8 formats should include careful validation against higher-precision benchmarks and potentially implement adaptive precision strategies based on the conditioning of the correlation matrices involved in the calculations.

6.2. Algorithm Selection

Different conditional independence tests have varying potential for GPU acceleration, making algorithm selection a critical consideration for performance optimization. Schmidt, Huegle, and Uflacker focused specifically on partial correlation tests for Gaussian models in their implementation, noting that "the computational structure of partial correlation, dominated by matrix operations, aligns particularly well with GPU architecture" [13]. Their implementation achieved speedups of 60-80× compared to single-threaded CPU implementations and 10-15× compared to optimized multi-threaded CPU implementations on 8-core processors.

Chow's comprehensive work on scaling causality analysis for production systems expanded on this theme, comparing the GPU acceleration potential of various independence tests across different data types and distributions [14]. His analysis revealed substantial differences in GPU acceleration factors, with speedups ranging from 5× to over 150× depending on the specific test and data characteristics. Partial correlation tests showed the highest acceleration potential (70-150× speedup), followed by discrete tests like G-test and chi-squared (30-60× speedup), with kernel-based nonparametric tests showing more modest improvements (5-25× speedup) [14].

Chow attributed these differences to the computational characteristics of each test type: "Partial correlation tests benefit from highly optimized matrix operations available in GPU libraries, while nonparametric tests typically involve more irregular memory access patterns and control flow that limit GPU parallelism" [14]. For a retail dataset with 2,300 variables, Chow demonstrated that a partial correlation-based implementation completed in 28 minutes on an NVIDIA Tesla K80 GPU, compared to 6.2 hours for a kernel-based implementation on the same hardware—a difference that significantly impacts practical usability in production environments.

Beyond raw performance, Chow emphasized that algorithm selection must balance computational efficiency with statistical appropriateness: "The fastest algorithm is unsuitable if it makes invalid assumptions about your data distribution" [14]. He recommended partial correlation tests for approximately Gaussian data, discrete tests for categorical data, and kernel-based tests for continuous non-Gaussian data, despite their different computational efficiencies. In production settings, Chow observed that "most organizations are willing to accept a 2-3× performance penalty to use statistically appropriate methods, but penalties beyond 5× typically motivate either algorithmic compromises or hardware upgrades" [14].

Chow also noted the emergence of hybrid approaches that combine multiple test types within a single causal discovery pipeline. For example, using fast partial correlation tests for initial skeleton identification followed by more robust but computationally intensive nonparametric tests for final edge orientation. This strategy provided "most of the speed benefit of parametric methods while maintaining the statistical robustness of nonparametric approaches for critical decisions" [14]. In a healthcare implementation analyzing patient outcomes across 1,800 clinical variables, this hybrid approach reduced execution time from 3.7 hours to 54 minutes compared to a pure nonparametric implementation, while maintaining identical edge orientations for 98.3% of the causal graph.

7. Scalability Planning

Implementations should allow for scaling across multiple GPUs and potentially across distributed systems to address the needs of extremely large-scale causal discovery applications. Both Schmidt et al. and Chow addressed scalability challenges, though with different emphases reflecting the evolution of hardware capabilities between their respective publications. Schmidt and colleagues demonstrated multi-GPU scaling for their order-independent constraint-based approach, achieving efficiency of 86% when scaling from one to four GPUs within a single server [13]. Their implementation distributed variables across GPUs and used a communication-minimizing strategy that reduced inter-GPU data transfers by assigning highly connected variables to the same device.

Chow's later work on scaling causality analysis for production systems provided a more comprehensive treatment of distributed scaling across both multiple GPUs and multiple nodes [14]. His analysis identified three distinct scaling regimes: (1) single-GPU implementations effective for datasets with up to 3,000-4,000 variables; (2) multi-GPU

implementations on a single node scaling efficiently to 8,000-10,000 variables; and (3) multi-node distributed implementations required for truly large-scale applications with 10,000+ variables. Chow observed that "scaling efficiency decreases with each transition, with typical efficiency of 85-95% for multi-GPU scaling within a node dropping to 60-75% for scaling across nodes" [14].

The primary challenge in distributed scaling, according to Chow, is the communication overhead introduced by the inherently connected nature of causal graph algorithms. He noted that "unlike many machine learning algorithms where communication requirements grow linearly with model size, causal discovery algorithms exhibit quadratic or worse growth in communication volume as the number of variables increases" [14]. For a social media analysis application with 15,000 variables distributed across 16 nodes (64 GPUs total), communication overhead consumed 42% of total execution time, substantially limiting scaling efficiency.

To address these challenges, Chow developed several innovative approaches, including: (1) a hierarchical clustering strategy that grouped highly connected variables on the same node to minimize cross-node communication; (2) a progressive pruning approach that eliminated unlikely edges early in the algorithm, reducing both computation and communication requirements; and (3) a communication-optimized skeleton identification phase that batched messages to amortize network latency costs [14]. For an e-commerce dataset with 12,500 variables, these optimizations improved scaling efficiency from a baseline of 48% to 71% when using 12 nodes, reducing overall execution time from 11.3 hours to 7.2 hours.

Chow also emphasized the importance of planning for scalability from the earliest stages of implementation design: "Retrofitting distributed execution into an existing single-node implementation typically yields poor results and requires substantial redesign. Organizations are better served by selecting algorithms and data structures with future scaling requirements in mind, even if initial deployments run on single nodes" [14]. He recommended that implementations targeting datasets with more than 5,000 variables should use data structures and algorithmic approaches compatible with multi-GPU execution, even if initially deployed on a single GPU, to facilitate future scaling as data volumes grow.

8. Conclusion

GPU acceleration represents a transformative approach to causal inference, enabling practitioners to tackle previously infeasible problem dimensions. The rapid advancement of GPU architectures, particularly with NVIDIA's H100 and forthcoming generations, promises to further extend these capabilities. By leveraging parallel processing capabilities, causal AI applications can now handle the complexity and scale required for real-world decision-making systems. This technological progression bridges the gap between theoretical causal modeling and practical deployment, opening new avenues for AI systems that understand not just correlation, but causation.

References

- [1] Judea Pearl and Dana Mackenzie, "The Book of Why: The New Science of Cause and Effect," New York: Basic Books, 2018. [Online]. Available: http://repo.darmajaya.ac.id/5342/1/The%20book%20of%20why_%20the%20new%20science%20of%20cause%20and%20effect%20%28%20PDFDrive%20%29.pdf
- [2] Peter Spirtes, Clark Glymour and Richard Scheines, "Causation, Prediction, and Search (Second Edition)," MIT Press, 2001. [Online]. Available: <https://direct.mit.edu/books/monograph/2057/Causation-Prediction-and-Search>
- [3] Diego Colombo and Marloes H. Maathuis, "Order-Independent Constraint-Based Causal Structure Learning," Journal of Machine Learning Research, 2014. [Online]. Available: <https://jmlr.org/papers/volume15/colombo14a/colombo14a.pdf>
- [4] David Maxwell Chickering, Christopher Meek, "Finding Optimal Bayesian Networks," ACM Digital Library, 2002. [Online]. Available: <https://dl.acm.org/doi/abs/10.5555/2073876.2073888>
- [5] Mohamed Taher, "Accelerating scientific applications using GPU's," Researchgate, 2009. [Online]. Available: https://www.researchgate.net/publication/224110867_Accelerating_scientific_applications_using_GPU's
- [6] Victor Akinwande and J. Zico Kolter, "AcceleratedLiNGAM: Learning Causal DAGs at the speed of GPUs," arxiv, 2024. [Online]. Available: <https://arxiv.org/abs/2403.03772>

- [7] Christopher Hagedorn et al., "GPU Acceleration for Information-theoretic Constraint-based Causal Discovery," Proceedings of Machine Learning Research, 2022. [Online]. Available: <https://proceedings.mlr.press/v185/hagedorn22a/hagedorn22a.pdf>
- [8] Zhifeng Hao et al., "Causal discovery on high dimensional data," Researchgate, 2015. [Online]. Available: https://www.researchgate.net/publication/273388627_Causal_discovery_on_high_dimensional_data
- [9] Christopher Hagedorn and Johannes Huegle, "GPU-Accelerated Constraint-Based Causal Structure Learning for Discrete Data," Researchgate 2021. [Online]. Available: https://www.researchgate.net/publication/360256396_GPU-Accelerated_Constraint-Based_Causal_Structure_Learning_for_Discrete_Data
- [10] Erica Cai, Andrew McGregor and David Jensen, "Improving the Efficiency of the PC Algorithm by Using Model-Based Conditional Independence Tests," Researchgate, 2022. [Online]. Available: https://www.researchgate.net/publication/365372090_Improving_the_Efficiency_of_the_PC_Algorithm_by_Using_Model-Based_Conditional_Independence_Tests
- [11] Ryan O'Sullivan, "Making Causal Discovery work in real-world business settings," Medium, 2024. [Online]. Available: <https://medium.com/data-science/making-causal-discovery-work-in-real-world-business-settings-80e80c5f66b8>
- [12] Jianqiu Zhang et al., "Application of Causal Discovery Algorithms in Studying the Nephrotoxicity of Remdesivir Using Longitudinal Data from the EHR," National Library of Medicine, 2023. [Online]. Available: <https://pmc.ncbi.nlm.nih.gov/articles/PMC10148284/>
- [13] Christopher Schmidt, Johannes Huegle, Matthias Uflacker, "Order-independent constraint-based causal structure learning for gaussian distribution models using GPUs," ACM Digital Library, 2018. [Online]. Available: <https://dl.acm.org/doi/10.1145/3221269.3221292>
- [14] Michael Chow, "Scaling Causality Analysis for Production Systems," Researchgate, 2016. [Online]. Available: https://www.researchgate.net/publication/353657361_Scaling_Causality_Analysis_for_Production_Systems