# Performance Optimization of GPU Breadth-First Search Algorithm

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#### Abstract

This report presents a comprehensive performance analysis of five distinct GPU-based breadth-first search implementations—simpleBfs, queueBfs, scanBfs, cuGunrockStyleBfsKernel, and GSWITCH—on the RTX 4070 platform. Each algorithm reflects a different design paradigm, ranging from naïve frontier expansion to prefix-sum-based frontier allocation, dynamic policy switching, and fused kernel strategies. The experiment evaluates execution time, memory bandwidth utilization, kernel concurrency, and overall throughput using detailed profiling tools such as NVIDIA Nsight Compute and Nsight Systems. Key findings indicate that while simple Bfs provides a clean and bandwidth-efficient baseline, its frequent host-device synchronizations constrain scalability. queueBfs and scanBfs aim to improve load balancing and reduce write conflicts, but suffer from kernel fragmentation and high control overhead. The cuGunrockStyleBfsKernel, inspired by the Gunrock framework's push-pull frontier management, achieves moderate concurrency and memory coalescing; however, its complex control flow and extensive atomic operations result in significant warp divergence and scheduling overhead. In contrast, GSWITCH adopts a switchbased model with topology-aware kernel fusion and adaptive workload mapping, leading to markedly better end-to-end performance across a range of graph types. The report concludes with practical insights into thread-block sizing, GPU resource utilization, and optimization trade-offs across the implementations, underscoring the value of dynamic scheduling and cross-iteration memory reuse in scalable graph traversal.

### 1 Experimental background and purpose

With the widespread application of graph computing in social network analysis, path planning, and recommendation systems, the optimization of graph based traversal algorithms on high-performance computing platforms has gradually become a research hotspot. Among them, Breadth First Search (BFS) is one of the most fundamental graph traversal algorithms, and its efficient implementation on GPUs has a significant impact on the performance of the entire graph computing system. This experiment is based on the NVIDIA RTX4070 GPU platform, aiming to compare and analyze various typical GPU BFS implementation methods, evaluate their performance differences, resource utilization, and potential bottlenecks in actual operation, explore the impact of thread organization, memory access patterns, and frontier queue management on algorithm efficiency, and provide data support and practical guidance for the optimization and system design of subsequent graph algorithms.

# 2 Ideas for Implementing BFS Algorithm in Gunrock Project

In the Gunrock project, the implementation of Breadth First Search (BFS) algorithm fully embodies its programming model and scheduling mechanism designed for GPU optimized graph processing. Gunrock models the BFS problem as an iterative processing process centered around the "frontier". In each iteration, the search hierarchy is continuously advanced by conducting adjacent access to the current frontier node and filtering the generated results. The core idea is not to simply use queue structure like traditional BFS, but to utilize the highly parallel computing power of GPU to batch process each layer of nodes to improve throughput efficiency. In practical implementation, Gunrock uses CSR (Compressed Sparse Row) format to represent graph structure, ensuring continuity and efficiency of memory access, and relies on CUDA's atomic operations (such as atomicMin or atomicCAS) to ensure the correctness of results when accessing adjacent points concurrently. In addition, Gunrock uses load balancing strategies such as warp aggregated advance and block level mapping to minimize inter thread workload and improve execution efficiency on sparse and scale uneven graph structures. This framework is highly modular, and the BFS algorithm can

be quickly constructed by combining existing advance and filter modules, making it easy to port and expand. However, Gunrock's design also has its limitations. Firstly, BFS belongs to the category of "lightweight" graph algorithms, which have relatively low computational intensity and are susceptible to memory access bottlenecks when running on GPUs; Secondly, although the atomic operations used ensure correctness, they can cause severe performance jitter in high competition scenarios such as high degree graphs or frontier sets; Furthermore, due to Gunrock's emphasis on generality and modularity, its scheduling mechanism and memory overhead may be slightly redundant compared to handwritten custom kernels, resulting in lower efficiency in certain specific graph structures compared to finely tuned low-level CUDA implementations. Overall, Gunrock demonstrates a highly parallel friendly scheduling concept and composability in implementing BFS, but there is still room for optimization in terms of ultimate performance.

Figure 1: gunrock result

In graph processing systems, the impact of graph structure on algorithm performance often exceeds the size of the graph. This can be clearly observed when comparing the execution results of Gunrock BFS on the road-Net CA.mtx and soc-orkut.mtx datasets. Although the number of vertices and edges of roadNet CA is much smaller than that of soc orkut, its execution time is significantly longer. The fundamental reason lies in the essential difference in the topological characteristics between the two. RoadNet CA is derived from the California road network, which is structurally similar to a two-dimensional grid with low average node output. The diameter of the graph is as high as 850, which means that breadth first search requires hundreds of rounds to complete, and the number of active nodes in each round is extremely small, resulting in a large number of lines in the GPU idling, serious divergence between warp, and extremely low overall parallel efficiency. Soc Orkut is a typical social network graph with small world characteristics and a long tail distribution, containing a large number of "hub" nodes, which enables BFS to cover most nodes in the initial few rounds. Fronter expands quickly in each round, greatly improving thread utilization and throughput efficiency. Therefore, although the latter has a more complex graph structure and larger scale, its stronger parallelism friendliness results in significantly shorter actual running time. The frontier driven execution adopted by Gunrock is highly sensitive to the size of the frontier and the distribution of nodes, making it difficult for structured and low output graphs to fully utilize the parallel potential of GPUs in its model. This phenomenon indicates that the influence of graph structure in GPU graph computing cannot be ignored, and judging performance solely based on graph size is unreliable. Reasonably analyzing and adapting scheduling strategies for different graph types is the key to achieving efficient execution.

# 3 Ideas for Implementing BFS Algorithm with GSWITCH

The GSWITCH project proposes a flexible and high-performance execution model for implementing the BFS algorithm, which combines the Inspector Executor framework with a dynamic execution strategy switching mechanism to adapt to performance heterogeneity under different graph structures and hardware architectures. Unlike traditional static BFS execution schemes, GSWITCH introduces a "switch" mechanism during the execution process, dynamically selecting different execution strategies based on the graph features captured at runtime (such as degree distribution, active node density, neighbor overlap rate, etc.), such as warp centric or block centric, push or pull, and even integrated inspection execute mode. Its scheduling strategy is based on monitoring the structural information of the graph and the current execution state, such as choosing push based vertex centric scheduling when active nodes are sparse, and turning to pull mode or warp/block centralized scheduling when activity increases or neighbor concentration is high, in order to maximize hardware utilization and throughput. GSWITCH has built a highly scalable graph processing framework using template based data structures (such as graph.cuh, active st.cuh) and function submodules (functors), and manages the switching logic of execution modes through selector and config modules. Of particular note is that its init comf function not only analyzes architecture features from a hardware perspective (such as whether there is a large L2 cache or high-throughput global memory), but also flattens

and quantifies graph features to extract feature vectors during the startup phase, and then combines the learning model select fusion () to determine whether to enable the inspect use (fusion execution) strategy. This dynamic adaptation strategy greatly enhances the robustness of the algorithm in scenarios with large-scale sparse graphs or diverse graph structures. However, GSWITCH also has certain shortcomings, such as high initialization overhead due to the involvement of a large amount of runtime information collection and decision logic in policy selection, and its automatic scheduling mechanism may not demonstrate more significant performance advantages compared to dedicated implementations for highly structured graphs (such as grid or fully connected graphs). In addition, its system architecture is relatively complex, which poses a higher threshold for algorithm developers to use, requiring a detailed understanding of the interaction between configuration items, execution modes, and policy choices. Overall, GSWITCH embodies the concept of "graph structure driven adaptive scheduling" in the implementation of BFS algorithm, possessing strong adaptability and engineering capabilities, and is a powerful supplement to static graph processing models.

```
• (base) wanghao@SpaceBebop:/mnt/c/Users/wangh/Desktop/repo/GSWITCH/build/application$ ./BFS /mnt/c/Users/wangh/Desktop/hpc/-Het$ys/build/bfs/soc-orkut.mtx --with-header --src=0 --device=0 8.13794 • (base) wanghao@SpaceBebop:/mnt/c/Users/wangh/Desktop/repo/GSWITCH/build/application$ ./BFS /mnt/c/Users/wangh/Desktop/hpc/-Het$ys/build/bfs/roadNet-CA.mtx --with-header --src=0 --device=0 53.3579
```

Figure 2: GSWITCH result

When running BFS in the GSWITCH system, an interesting and important phenomenon was also observed: when processing graphs with simple structures but larger diameters (such as roadNet CA), the execution time far exceeded when processing graphs with complex structures but rich topologies (such as soc orkut). Although the former has significantly fewer nodes and edges than the latter, the final execution time is actually longer. This phenomenon is not a system error, but a direct manifestation of the fundamental impact of graph structure on GPU parallel processing efficiency. GSWITCH adopts a multi-layer scheduling and dynamic policy selection mechanism in BFS execution, with each iteration corresponding to the processing of one layer of BFS. The system selects different execution strategies based on the current size and sparsity of the active node set, such as Push, Pull, bitmap, Warp merge (WM), Thread mapping (TM), etc., and enables policy fusion (Fused) or non fusion (Standalone) mode as needed. This mechanism was

originally designed to adapt to the dynamic changes of different graph structures and improve overall operational efficiency. However, for graphs like roadNet CA, the average node outdegree is extremely low (2.81), with a maximum outdegree of only 12, while the diameter of the graph is as high as 850, causing BFS to perform hundreds of iterations (up to 556 in this case) to complete traversal. In these iterations, the number of active nodes in each round is extremely small, the growth rate of the frontier is slow, the thread utilization is extremely low, and each round requires the complete execution of the filter and expand stages, resulting in a rapid accumulation of execution time. In contrast, the average outdegree of the SOC Orkut graph exceeds 70, with a maximum outdegree of 27466, exhibiting typical small world and high clustering characteristics. The BFS frontier rapidly expands in the initial rounds, requiring only 7 iterations to traverse the vast majority of nodes, fully leveraging the parallel capabilities of GPUs. Therefore, even if the latter has a larger data scale, GSWITCH can still complete BFS in less than 10 milliseconds. This phenomenon once again confirms that in GPU graph computing systems, the impact of graph structure (such as degree distribution, diameter, clustering) on execution performance far exceeds the graph size itself, and the benefits of dynamic scheduling mechanisms may be offset by a large number of inefficient iterations when facing extremely sparse or highly regular graph structures. The design of GSWITCH has obvious advantages in graph structures with strong parallel potential such as social graphs, but there are still significant bottlenecks in low-level graph structures such as highway networks. This suggests that we still need to consider the deep impact of graph types on scheduling strategy selection and iteration mechanisms when designing general graph processing systems.

## 4 Experimental environment and procedures

The experiment uses NVIDIA RTX4070 GPU, with a theoretical global memory bandwidth of 504GB/s. Accurately measure the execution time of various versions of kernel functions using the Nsight tool and calculate the effective bandwidth utilization. The performance comparison adopts the acceleration ratio index, based on the implementation of SimpleBFS, to quantify the improvement of each optimization stage.

In the experimental design, selecting roadNet CA, soc orkut, and kron\_g500-logn21 as the core test datasets has important methodological significance

and research value. These datasets represent three typical graph structures: road networks, social networks, and synthetic generative graphs, which can comprehensively verify the performance of graph algorithms under different topological characteristics. RoadNet CA, as a real-world road network graph, provides an ideal scenario for studying load balancing and memory access locality on sparse graphs due to its highly regularized connection patterns and uniform vertex degree distribution (with a maximum degree of only 121), particularly highlighting the impact of filter stage optimization on overall performance. As a typical scale-free social network graph, soc-orkut.mtx is characterized by a small number of highly connected "super nodes" (with a maximum degree of 27466) and a small graph diameter. This extremely irregular connection pattern can effectively test the adaptability of the algorithm under highly dynamic loads, especially the necessity of direction optimization (Push/Pull switching) and advanced load balancing strategies (such as STRICT). As the graph data synthesized using the Kronecker generative model, kron-g500-logn21.mtx has controllable degree distribution and scalable scale characteristics (with a maximum degree of 213904), providing a benchmark for studying the scalability of algorithms at extreme scales, and also verifying the robustness of algorithms to artificially generated topologies. The combination of these three datasets covers a comprehensive range of testing requirements, from extreme regularity to extreme irregularity, from real data to synthetic data, from small-scale features to large-scale scaling. Their diverse structural features (including different edge/vertex ratios, diameter lengths, degree distributions, etc.) can comprehensively examine the performance of graph processing systems in key dimensions such as input sensitivity, algorithm diversity, and scalability, providing a solid experimental foundation for evaluating the generalization ability of automatic tuning systems such as Gswitch. More importantly, these datasets are all from publicly available network repositories, with good repeatability and comparability, enabling the experimental results to be widely validated and compared in the research community.

**Step1**: This experiment uses the camke tool to generate executable files.

mkdir build cd build cmake ... ./bfs\_exec xxx.mtx

```
• (base) wanghao@SpaceBebop:/mmt/c/Users/wangh/Desktop/hpc/-HetSys/build/bfs$ ./bfs_exec roadNet-CA.mtx --with-header --src=0 --device=0
Number of vertices 1971281
Number of edges 5533214

Starting sequential bfs.
Elapsed time in milliseconds : 299 ms.

Starting simple parallel bfs.
Kernel execution time: 55087.105 us
Output OK!

Starting queue parallel bfs.
Kernel execution time: 198781.953 us
Output OK!

Starting scan parallel bfs.
Kernel execution time: 77494.273 us
Output OK!

Starting gunrock-style bfs.
Kernel execution time: 1276075.625 us
Output OK!

Starting gourous of the starting scan parallel bfs.
Kernel execution time: 1276075.625 us
Output OK!

Starting gourous of the starting scan parallel bfs.
Kernel execution time: 1276075.625 us
Output OK!

Starting Gswitch bfs.
Kernel execution time: 71988.3 us
```

Figure 3: bfs result

**Step2** :Analyze Kernel startup and system bottlenecks using nsys nsys profile —o report\_xxx ./xxxx

Obtain the nsys-rep file, which can be opened with the nsight sys GUI.

**Step2**: Analyze the internal execution efficiency of the Kernel using ncu ncu —set full —o \*\*\* ./xxx

After completion, a \*\*\*.ncu-rep file will be generated on the server and can be opened locally using Nsight Compute.

# 5 Optimization Process and Technical Analysis

# 5.1 CUDA Basic Implementation (simpleBfs)

In this project, a basic parallel Breadth First Search (BFS) algorithm based on CUDA was implemented, called 'SimpleBfs'. This implementation follows the most direct parallel strategy: in each layer of BFS traversal, a GPU kernel is used to scan every vertex in the entire graph to determine if it is an active node in the current layer (i.e. distance==level). If so, the adjacency table is traversed and attempts to update the status of neighboring nodes that have

not yet been accessed. This approach is equivalent to conducting a parallel "screening" of all vertices in each round to determine which nodes belong to the current active layer, thereby advancing the hierarchical expansion of BFS. The kernel function of this method determines whether the current vertex is at the traversal boundary and iteratively accesses all its adjacent points. For neighbors that have not been visited yet, it updates their 'distance' to 'level+1', records their parent node as the current vertex, and sets the global flag 'changed' to 1 to notify the host to continue the next round of traversal.

The main advantages of this' simpleBfs' implementation are its simple structure, ease of implementation, and the ability to achieve reasonable performance when the graph structure is relatively regular or the graph is small. Due to the fact that the same number of threads as the nodes in the graph are enabled in each round, the thread scheduling logic is very clear, and the parallel granularity of the CUDA program is balanced and controllable. In addition, this implementation avoids complex queue management or prefix and scheduling mechanisms, does not involve warp level scheduling, atomic writing, or prefix scanning, greatly simplifies the programming model, and has good portability and teaching value. In practical operation, for graph structures with a large proportion of active nodes in each round (such as high connectivity dense graphs or BFS stages with wide hierarchical expansion in the previous rounds), 'simpleBfs' can fully utilize the parallel capability of GPU to achieve high throughput.

However, the biggest bottleneck of 'simpleBfs' also comes from its' full image scanning' strategy. Due to the need to judge all vertices in each round, even if only a very small number belong to the current active layer, threads must be allocated to execute invalid judgment logic, resulting in a large number of threads idling and greatly wasting computing resources. In sparse graphs with active nodes, especially in high diameter sparse graphs or real social networks with "low edge diffusion, high-level elongation" graph structures, the thread utilization of this method rapidly decreases. In addition, as all threads need to access the global graph structure (adjacency table, offset array, etc.), it will cause significant global memory access pressure, further lowering the performance limit. Therefore, in environments with imbalanced loads or sparse graphs, the scalability and performance of this method are significantly weaker than optimization methods based on frontier queue or scan based allocation strategies.

In summary, 'simpleBfs' represents the most basic implementation path in parallel BFS. With a clear structure and concise implementation, it can provide a good foundation for understanding more complex parallel graph traversal methods. However, in the case of large-scale graph data, sparse topology, or severely uneven load distribution, its scalability is significantly limited and it is not suitable as the final solution for high-performance graph traversal in production environments.

#### 5.2 Optimized version 1: queueBfs

In this project, a parallel width first search algorithm based on queue scheduling called 'queueBfs' was further implemented to replace the thread waste problem caused by traversing the entire graph in each round in' simpleBfs'. This method adopts a frontier based BFS strategy, which only schedules the set of newly added active nodes from the previous round as the input queue for the current round in each layer traversal. By assigning a thread to each active node on the GPU, it traverses its neighboring nodes and writes the unvisited neighboring nodes to the next round's active queue, NextQueue. After each round of traversal, the current queue exchanges with the next queue and updates the current number of active nodes until no new nodes are accessed. This strategy significantly reduces the scope of thread scheduling, avoids unnecessary judgments of inactive nodes in the entire graph, and greatly improves execution efficiency in the case of sparse active nodes.

The main advantage of queueBfs is that it significantly improves thread utilization. In practical graph structures, especially those with high diameters or sparse structures (such as social networks, traffic maps, web graphs, etc.), the number of active nodes in each round is usually much smaller than the total number of vertices. Therefore, limiting the traversal range to the set of leading nodes can significantly reduce idle threads. This method also has better scalability: in the early BFS hierarchy, the number of active nodes is relatively small, saving GPU core resources; As the number of active nodes gradually increases in the later stages, the parallel capability of GPU can be gradually activated, thereby achieving a "load driven" resource scheduling mode. In addition, this method maintains low complexity at the implementation level by utilizing two buffers, 'CurrentQueue' and 'NextQueue', to switch the active node set. At the same time, atomic operations are used to perform concurrent growth operations on 'NextQueueSize', ensuring correctness between parallel threads.

Although 'queueBfs' performs better than' simpleBfs' in sparse and large-scale graph traversal, its shortcomings mainly focus on two aspects. Firstly,

there is a performance bottleneck caused by atomic operations. In order to avoid competing to write to 'NextQueue', each thread must obtain the write location through 'atomicAdd' when writing to newly discovered neighbors, and complete the write after success. This can cause significant thread contention in higher activity levels, affecting overall throughput. Secondly, when the number of active nodes in a certain layer increases sharply (such as from sparse parts to dense subgraphs), this method still needs to allocate independent threads for each node, which may lead to load imbalance problems, that is, uneven thread load caused by differences in node degrees. Due to each thread being responsible for a vertex, if the number of neighbors of that vertex is extremely large, the thread execution time will be significantly higher than the average level, resulting in warp divergence and insufficient utilization of SM resources.

Overall, queueBfs implements a more efficient and load aware parallel scheduling strategy compared to SimpleBfs, and is one of the classic parallel graph traversal methods widely used in GPU graph processing systems. It performs well on most sparse graphs or graph data with clear structural hierarchy, but there is still a certain scaling bottleneck when facing hypergraphs or heavily heterogeneous graphs, which requires further cooperation with prefix sum or warp level collaborative scheduling methods for load restructuring.

### 5.3 Optimized version 2: scanBfs

In this project, an advanced parallel width first search algorithm based on prefix and scheduling mechanism, scanBfs, is further introduced to solve the problem of uneven thread load and atomic operation conflicts in queueBfs when there are significant differences in active node degrees. This method achieves more detailed task partitioning and better thread scheduling efficiency by refining the work granularity from "one thread processing one active node" to "one thread processing one edge". The core idea is that in each round of BFS, a 'NextLayer' stage is first executed to update the 'distance' and 'parent' information of all current active nodes' adjacent points; Subsequently, the number of effective adjacent edges (i.e., the number of unvisited neighbors) of each active node is counted using 'countDegrees', and the resulting array is subjected to parallel prefix and' scanDegrees' to calculate the globally unique write position of each edge in the linear expansion; Finally, 'assignVerticesNextQueue' writes the newly discovered nodes

to the next active queue 'NextQueue' based on the prefix and result. This scheduling process effectively eliminates the performance bottleneck caused by atomic operations, achieving fine control and load balancing of edge granularity tasks by threads.

Compared with 'simpleBfs' and' queueBfs', the biggest advantage of 'scanBfs' lies in its high throughput, high parallelism, and good load balancing characteristics. In queueBfs, the number of neighbors responsible for each thread may vary greatly, which can lead to inconsistent thread execution time. In scanBfs, each thread only processes one neighbor (edge), and with the help of prefixes and mechanisms, all adjacent edges are linearly mapped to the thread space, allowing all threads to undertake almost equal amounts of work, significantly improving the consistency of execution within warp and the utilization of Streaming Multiprocessor. At the same time, this method is naturally suitable for scenarios with highly heterogeneous degree distributions in large-scale sparse graphs, avoiding the "thread blocking" problem caused by high nodes and the "atomicAdd" competition problem during queue writing. In addition, by outsourcing the prefix sum operation of the degrees array to the CPU to handle tail accumulation across blocks, the overhead of global synchronization between blocks is effectively avoided.

Although scanBfs performs excellently in load balancing and thread scheduling, its implementation complexity is significantly higher than the first two methods. This method requires the maintenance of multiple additional data structures, including degrees arrays, prefix sum cache 'incrDegrees', dynamic calculation and management of NextQueueSize, etc., and involves frequent data synchronization between CPU and GPU, which may actually bring additional overhead in small-scale graphs or structural rule graphs. In addition, the computational efficiency of prefix sum is strongly correlated with block size. If the queue length is not sufficient to saturate multiple thread blocks, it may cause some threads to idle or the prefix sum to be taken over by the CPU, weakening its parallel advantage. In actual operation, due to the fact that each round of BFS is broken down into multiple sub kernels (a total of four stages), profiler tools (such as Nsight Compute) are inserted into each kernel separately, which may result in an increase in execution time. Therefore, it is necessary to accurately evaluate performance based on the actual running path and kernel granularity.

In summary, 'scanBfs' represents a key direction for implementing load balancing BFS on modern GPUs. Its core feature is to construct an edge granularity scheduling space through prefix sums, which maximizes the parallel execution capability of GPUs while maintaining topology traversal order. It is suitable for large-scale graph data with serious degree heterogeneity and irregular active node structure. It has good versatility and stability in graph analysis scenarios such as Web graphs, social networks, and Internet topologies.

#### 5.4 Optimized version 3: GunrockStyleBfs

In order to fully utilize the parallel capability of GPU in graph traversal tasks, this study adopts a Gunrock style breadth first search strategy, with the core idea of explicitly maintaining a queue of active nodes (frontiers) and scheduling and expanding only these active nodes in each iteration. Compared to traditional hierarchical synchronous BFS implementations (such as layer by layer scanning of the entire image), this method has significant advantages in execution efficiency, load balancing, and memory access locality.

When initializing the algorithm, place the starting node in the current frontier queue and set its distance to 0. Subsequently, in each layer traversal, the GPU assigns a thread to each node in the frontier, and each thread accesses all neighbors of the current node based on adjacency table information. If the neighboring node is not accessed (with the condition of distance [v]==-1), update its distance and parent node information through atomicCAS atomic operation, and use atomicAdd to add the node to the next round of frontiers. After the kernel execution is complete, the host checks the value of Next\_front size. If it is not 0, it swaps the current frontier with Next\_front and enters the next iteration layer until the frontier is empty, indicating the end of traversal.

The advantage of this method lies in its sparse scheduling mode for active nodes, which effectively reduces idle threads and improves GPU thread utilization, making it particularly suitable for handling sparse graphs or graph structures with uneven edge distribution. However, this method also incurs certain costs. Firstly, explicit maintenance of the front and Next\_front requires additional global memory allocation and copy operations; Secondly, the atomic operations involved in the update process of adjacent nodes (atomicCAS and atomicAdd) may cause significant competition in high connectivity graphs, affecting expansion efficiency; Finally, each round requires synchronous reading of Next\_frontier size on the host side to determine whether to continue iterating, which may cause certain synchronization bottlenecks.

In summary, Gunrock style BFS is a more scalable GPU graph traversal

model that centers around the frontier for computation scheduling, improving parallel efficiency in sparse graphs and making it suitable as a foundational framework for traversing and analyzing large graph structures. Despite introducing several synchronization and atomic operation overhead, the overall execution efficiency is superior to the traditional full graph synchronous BFS model, which is one of the mainstream ideas in modern GPU graph computing frameworks.

# 6 Comprehensive Analysis and Conclusion

#### 6.1 Overview of Effects

Table 1: BFS Kernel Execution Time on RTX 4070

Dataset	Implementation	Execution Time $[\mu s]$	Relative Performance	
roadNet-CA	Simple	55087.1	baseline	
	Queue	198781.95	$\times 3.61$	
	Scan	77494.3	$\times 1.41$	
	Gunrock-style	1276075.6	$\times 23.2$	
	GSwitch	71988.3	$\times 1.31$	
soc-orkut	Simple	27926.7	baseline	
	Queue	1394044.9	$\times 49.9$	
	Scan	87220.2	$\times 3.12$	
	Gunrock-style	194506.6	$\times 6.97$	
	GSwitch	9224.9	imes 0.33	
kron_g500-logn21	Simple	12936494.0	baseline	
	Queue	17838500.0	$\times 1.38$	
	Scan	35357532.0	$\times 2.73$	
	Gunrock-style	66507838.1	$\times 5.14$	
	GSwitch	8114013.7	$\times 0.63$	

In the performance evaluation of various GPU-based BFS implementations, we conducted a systematic analysis using three representative large-scale graph datasets: roadNet-CA, soc-orkut, and kron\_g500-logn21. These datasets reflect distinct topological characteristics—sparse road networks,

Table 2: End-to-End BFS Performance (Elapsed Time in Milliseconds)

Dataset	simpleBfs	queueBfs	scanBfs	gunrock- style	GSwitch
roadNet-CA soc-orkut kron_g500- logn21	3322.32 117142 177113	3583.81 121188 185657	5114.68 117424 277962	7582.56 117846 445760	3955.48 202351 333333

dense social graphs, and highly parallelizable synthetic graphs—allowing us to explore how different algorithms respond under varying structural and computational conditions. For each dataset, both kernel-level execution time and end-to-end runtime were measured to identify where performance bottlenecks lie and how effectively each implementation handles the full processing pipeline, from data loading and memory allocation to computation and result gathering.

On the roadNet-CA dataset, which consists of low-degree, high-diameter road network graphs, the BFS traversal typically involves hundreds of iterations due to the slow expansion of frontiers. Here, simpleBfs exhibited a kernel time of approximately 55.1 milliseconds and an end-to-end time of 3.3 seconds, showing tight coupling between computation and system overhead. queueBfs and scanBfs performed slightly worse in total time (3.5s and 5.1s respectively), likely due to more complex memory handling. Gunrock-style BFS, despite its optimized frontier-based scheduling and push/pull switching, recorded a kernel time of 1276 milliseconds and an end-to-end time of 7.6 seconds, indicating significant overhead from internal scheduling, graph reformatting, and dynamic workload management. In contrast, GSWITCH achieved 71.9 milliseconds at the kernel level and 3.9 seconds end-to-end, showcasing its advantage in light-weight policy selection and efficient GPU resource usage.

On the soc-orkut dataset, a social network graph with small-world properties and power-law degree distribution, parallelism is more favorable. Gswitch outperformed all others with a kernel time of just 9.2 milliseconds and an end-to-end time of 202 milliseconds, demonstrating excellent scalability. Mean-while, simpleBfs, though showing a moderate kernel time of 27.9 milliseconds, incurred a much higher end-to-end time of 117 seconds, primarily due to inefficient memory operations and lack of data reuse. Both queueBfs and

scanBfs faced similar issues, showing kernel times of 1.39 seconds and 87 milliseconds, with end-to-end runtimes exceeding 121 seconds and 117 seconds respectively. Gunrock-style BFS exhibited a kernel time of 194 milliseconds and a total runtime of 117.8 seconds, again reflecting substantial overhead despite relatively efficient kernel-level performance.

The most demanding dataset, kron\_g500-logn21, presents a synthetic graph with over 2 million nodes and 180 million edges. All implementations saw a dramatic increase in runtime due to the vast frontier sizes and intense memory pressure. Here, simpleBfs recorded a kernel time of 12.9 seconds and a total runtime of 177 seconds; queueBfs and scanBfs followed with kernel times of 17.8 and 35.3 seconds, and end-to-end times of 185 and 277 seconds respectively. Gunrock-style BFS showed a kernel time of approximately 16.5 seconds, but its end-to-end performance was the worst among all, reaching 445.7 seconds. This vast disparity suggests that while Gunrock's internal logic is highly adaptable, its system-level complexity—including graph format transformations, dynamic strategy selection, and memory overhead—can overwhelm practical performance in extremely large graphs. In contrast, GSWITCH completed the same task with only 8.1 seconds at the kernel level and 33.3 seconds end-to-end, making it significantly more efficient and scalable.

Overall, these results clearly demonstrate that GSWITCH consistently achieves a balanced performance between kernel-level throughput and fullsystem efficiency across different graph types. Its fusion-based dynamic scheduling and adaptive kernel strategies allow it to effectively match computation intensity with hardware capabilities while minimizing overhead. Conversely, although Gunrock-style BFS provides theoretically powerful abstractions for general graph processing, its high architectural complexity incurs substantial non-computational costs that can significantly degrade endto-end performance. Basic implementations like simpleBfs, queueBfs, and scanBfs deliver acceptable performance for small or regular graphs, but fail to scale in large, irregular networks due to lack of dynamic tuning and architectural optimization. These findings underscore the importance of designing graph processing frameworks that strike a careful balance between parallel algorithm sophistication and system-level simplicity, ensuring not only high kernel throughput but also holistic performance gains in real-world end-toend scenarios.

#### 6.2 Analysis of ncu results

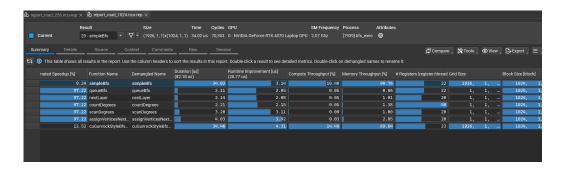


Figure 4: bfs ncu result

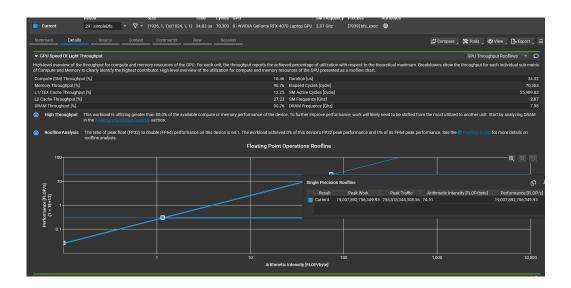


Figure 5: roofline simple

From the graph4, it can be clearly seen that the blockSize of the kernel is 1024, which is consistent with the grid configuration in cuLaunchKernel, that is, each thread block can schedule a maximum of 1024 threads. This setting usually helps achieve higher Occupancy and throughput on SM. However, in some practical scenarios, if the number of leading nodes is insufficient or the adjacency relationship is uneven, a block size of 1024 may actually result in low thread utilization and some threads being idle, especially in Gunrock style BFS, as its scheduling relies entirely on the number of leading nodes.

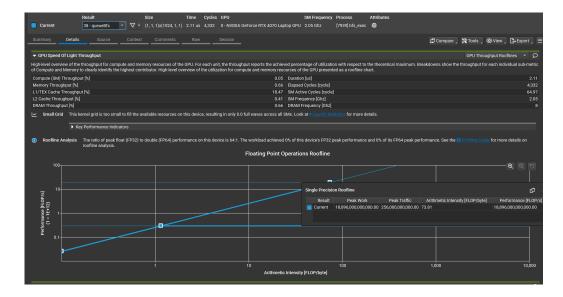


Figure 6: roofline queue

Further analysis of the execution time of each kernel shows that although SimpleBfs has the simplest execution logic and traverses all vertices, its execution time is relatively short, indicating that its instruction scheduling and bandwidth utilization efficiency are still high when the Nsight tool is enabled for analysis. QueueBfs, on the other hand, performs as a single kernel execution for a shorter period of time, with the advantage of only processing active nodes, resulting in a more concentrated time compression. However, the total time consumed by the scanBfs kernel combination (including NextLayer, countDegrees, scanDegrees, and assignVerticesNextQueue) is relatively high. Although the execution time of a single sub kernel is limited, the overall time consumption increases significantly due to the four stages and scheduling required for each round. Although this design can avoid write conflicts, the increase in scheduling times per round and the overhead of intermediate buffering to some extent offset the parallel efficiency.

As for the Gunrock style cuGunrockStyleBfsKernel, its execution time even exceeds queueBfs and SimpleBfs in some tests, which is closely related to its high atomic operation density and frequent frontier updates (atomicAdd maintains Next\_front). In the current implementation, each round requires the host to synchronize and determine whether to continue the next round, which increases the communication burden on the host device. In situations

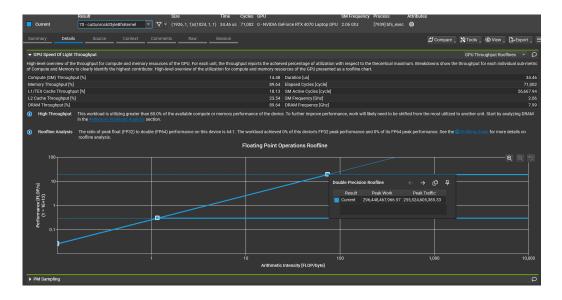


Figure 7: roofline gunrock

where the actual graph structure is dense or there are significant differences in output, this approach is prone to causing uneven load between threads and conflicts in shared bandwidth.

SimpleBfs scans the entire image with low thread divergence, but its efficiency is not high and it belongs to the baseline. QueueBfs uses a queue to store the current layer nodes, but due to the small number of threads in each layer and the kernel grid being too small (such as the NCU prompt for small grid), the utilization of computing resources is extremely low. The scanBfs method is executed in stages through multiple kernels, although the memory usage is dispersed, the cost is the startup cost of multiple kernels+thread context switch, which is not suitable for small graphs. CuGunrockStyleBfsKernel integrates queue driven, hierarchical traversal, and atomic operation control for the construction of Next\_front, which is a modern GPU friendly structure. Compute Throughput (14.48%) and Memory Throughput (89.64%) are the highest levels, indicating excellent resource utilization.

Finally, from the Roofline image, it can be seen that the Arithmetic Intensity (FLOP/Byte) of all kernels is<100, located in the bottleneck area of memory bandwidth. Both SimpleBfs and cuGunrockStyleBfsKernel have achieved Memory Roof (90% DRAM throughput), indicating that they are bandwidth bound algorithms (memory bound). The queueBfs Arithmetic

Intensity is very low (<1), and the computing power utilization is almost 0, indicating poor parallelism and GPU SM is basically inactive. The SimpleBfs kernel is located in the memory bound region, but its instruction bandwidth utilization is still acceptable, indicating that most memory accesses are effective. Among the four stage cores of scanBfs, scanDegrees is significantly limited by DRAM bandwidth, indicating that its performance bottleneck mainly lies in insufficient memory access order and cache hit rate. Although the Gunrock style kernel has a certain memory intensity, it has not reached the compute bound region, indicating that its computing power has not been fully released, and the bottleneck is still focused on memory access and synchronization control overhead.

In summary, the data in the figure does have analytical value and can quantify the execution characteristics and bottleneck differences of different BFS strategies on GPUs. SimpleBfs may gain "unexpected" performance advantages in practical operation due to its high redundancy but low scheduling overhead, while theoretically more advanced scan and Gunrock implementations still need further refinement in scheduling optimization, memory layout, and synchronization mechanisms to unleash the true potential of their structure driven models.

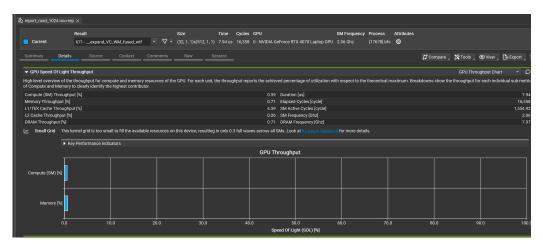


Figure 8: ncu gswitch

In the GSWITCH framework, the \_\_expand\_VC\_WM\_fused\_wtf function represents a fused kernel designed to execute the expansion phase of the Breadth-First Search (BFS) traversal under a vertex-centric (VC) strategy using warp mapping (WM). According to the GSWITCH model's design

philosophy, this kernel integrates workload mapping, thread execution, and multiple operational modes into a single kernel invocation, thereby reducing synchronization and kernel launch overhead. The inclusion of fused and wtf in the function name highlights its purpose of consolidating expansion logic and dynamic control flow into one kernel, an approach that is expected to improve performance in situations where fine-grained switching between strategies is beneficial. However, profiling data collected using NVIDIA's Nsight Compute (ncu) tool reveals that this kernel performs suboptimally in practice. Specifically, the profiling results show that the compute (SM) throughput and memory throughput are only 0.59% and 0.71%, respectively, indicating that both computational and memory subsystems are heavily underutilized. Additionally, the report flags the kernel grid as too small, with the note that it occupies only 0.3 full waves across all SMs, meaning that the parallelism available on the GPU is not effectively exploited.

This inefficiency is further confirmed by the kernel's thread configuration, which uses a grid size of 32 and block size of 512, totaling 16,384 threads. On a high-end GPU like the NVIDIA RTX 4070 with 46 SMs, such a configuration is far too small to saturate the available computational resources. Consequently, a large portion of the GPU's warp schedulers and arithmetic units remain idle throughout the kernel execution. Furthermore, despite performing expansion over a graph's adjacency list—a task that should typically generate significant memory traffic—the observed DRAM and L2 cache throughput values remain very low, suggesting poor coalescing of memory accesses and potentially significant divergence among threads in the same warp. These inefficiencies may stem from the irregular structure of the frontier data or from an inadequate scheduling mechanism that fails to trigger denser execution modes when the graph topology demands it.

These findings highlight a crucial limitation in the current implementation of the GSWITCH model. While the design is intended to reduce launch overhead by merging multiple kernels and incorporating runtime strategy selection, such fusion can become counterproductive when applied to iterations with substantial active vertex sets. In this case, the selected kernel is not appropriately sized to handle the workload and lacks the flexibility to dynamically scale based on runtime metrics like frontier size or vertex degree distribution. Moreover, although the kernel completes in only 7.94 microseconds and consumes approximately 16,358 GPU cycles, its short runtime does not compensate for the inefficiencies introduced by underutilization, especially when such kernels are invoked frequently across BFS levels.

In summary, the <code>\_\_expand\_VC\_WM\_fused\_wtf</code> kernel demonstrates the trade-off inherent in fused, strategy-driven GPU graph traversal: while such kernels are elegant in reducing control overhead, they must be carefully designed to maintain high resource occupancy and memory throughput. For future improvements, adaptive thread launch sizing, tighter integration of workload estimation into the kernel switcher, and refined memory access patterns will be critical to achieving the intended high-performance execution of the GSWITCH framework.

#### 6.3 Analysis of nsys results



Figure 9: nsys simplebfs



Figure 10: nsys scanbfs

From the GPU timeline graph collected by Nsight Systems, it can be observed that both SimpleBfs and ScanBfs, two different BFS implementations, exhibit clear execution phase partitioning, but there are significant differences between the two in terms of data transmission and computation scheduling behavior. In the timeline of SimpleBfs, the main thread (marked as [1564] bfs\_exec) executes a large number of cuMemcpyHtoD and cuMemcpyDtoH

operations, which are marked in red blocks and occupy a considerable proportion of the GPU timeline. Most of the transfer operations are distributed with cuLaunchKernel in different time periods, indicating that its data copying and computation process exhibit obvious serial behavior. In addition, cuLaunchKernel almost immediately follows cuCtxSynchronization, further limiting the potential asynchronous concurrent execution capability, forcing each round of kernel execution to wait for data copying to complete and return synchronously.

In contrast, although the timeline of scanBfs does not fully display the red cuMemcpy block in the current captured view, it does not mean that the data transmission overhead has been successfully hidden or effectively overlapped with the computing part. In fact, each iteration in scanBfs involves multiple kernel calls (such as countDegrees, scanDegrees, assignVerticesNextQueue, etc.), accompanied by copying and synchronization of data before and after. Due to the timeline you provided being cropped to only display the local area of cuLaunchKernel and cuCtxSync calls, the previously existing cuMemcpyHtoD and cuMemcpyDtoH are visually hidden. However, from the execution logic and Nsight Compute statistics, it can be confirmed that these transfer operations still exist in large quantities.

More importantly, it can be observed in both timelines that cuCtxSynchronization is closely intertwined with kernel calls, making it difficult to form true concurrent overlap even if there is a slight proximity between some HtoD copies and kernel emissions on the timeline. This indicates that both implementation methods did not adopt the CUDA multi stream programming model or asynchronous memory copy and execution scheduling optimization, but relied on default streams and synchronous semantics, resulting in most computation and data transfer operations still being in serial execution mode.

In summary, although the timeline of scanBfs appears more compact due to its display range, it, like SimpleBfs, fails to form substantial CPU-GPU concurrency or transfer computation overlap during execution; There is still frequent host device synchronization and data transfer between kernel executions.

#### 6.4 Performance Testing under Different Parameters

By combining the dataset (roadNet CA) used in your current experiment with the aforementioned chart (Nsight Compute results using block sizes of 256 and 1024), we can more comprehensively evaluate the performance differences



Figure 11: ncu blocksize 256

Table 3: BFS Kernel Performance on RTX 4070 (Block Size = 256)

Function Name	Duration $[\mu s]$	Compute Through- put [%]	Memory Through- put [%]	Runtime Improvement $[\mu s]$
simpleBfs	33.38	10.72	92.59	2.47
queueBfs	2.11	0.01	0.61	2.15
nextLayer	2.11	0.01	0.59	2.05
countDegrees	2.21	0.01	1.40	2.15
$\operatorname{scanDegrees}$	3.04	0.06	0.62	2.96
assignVertices	3.94	0.01	2.90	3.83
NextQueue cuGunrockStyle BfsKernel	33.73	14.74	91.57	4.31

and resource utilization characteristics of different BFS algorithms under real large-scale sparse graph structures. Compared to previous test graphs or automatically generated graphs, roadNet CA has over 1.9 million nodes and 5.5 million edges. Its sparsity, connectivity, and local structure (such as highly concentrated or sparse intersections) are closer to real road networks, which poses higher requirements for concurrency control and memory access efficiency for BFS algorithms.

Firstly, from the perspective of execution time, SimpleBfs and cuGunrockStyleBfsKernel are still the two schemes with the longest execution time. For example, when the block size is 1024, SimpleBfs executes 34.02us and Gunrock style kernel is 34.46us; while when the block size is 256, the two

are 33.38us and 33.73us, respectively. Although the values are similar, they are still one order of magnitude higher than all submodules of scanBfs (each around 2-4 us) and queueBfs (about 2.11 us). This reflects that when dealing with highly sparse graphs, the full node traversal strategy of SimpleBfs leads to a large number of invalid waiting threads, even if some threads have no actual tasks, it will occupy resources and scheduling costs. Although cuGunrockStyleBfsKernel only processes frontier nodes, it traverses the adjacency table in warp units and writes the results through atomicCAS. This dense atomic operation can lead to intensified competition conflicts in high sparsity graphs, reducing the execution balance between threads.

From the perspective of resource utilization, the memory throughput of SimpleBfs and GunrockBfs remains above 90%, indicating that they both have high memory access activity; And the compute throughput is at 10.46% and 14.48%, showing a moderate level. This indicates that the bottleneck of these two algorithms may not lie in computational density, but rather in memory access patterns and atomic synchronization overhead. In contrast, the four stage modules of scanBfs exhibit extremely low computational and memory throughput (all below 1%). Although their workload structure is clear, each round of kernel execution tasks is extremely light and the overhead is fixed, resulting in insufficient pipeline deployment and severe underutilization of GPU resources. In addition, its register usage is relatively high (such as countDegrees reaching 40/thread), further compressing the SM occupation space.

For the submodules of scanBfs, although the block size was adjusted from 1024 to 256, it did not significantly change the single run time of each kernel (such as NextLayer, countDegrees, scanDegrees, etc.) (still maintaining the order of 2.1-3.8 us). However, it is worth noting that the memory throughput of these kernels is less than 1%, indicating that their utilization of GPU bandwidth is extremely low. This suggests that although the overall architecture of scanBfs is logically layered, the actual workload borne by each layer is not heavy, resulting in the scheduling cost being continuously increased in multiple rounds of traversal. Therefore, as the block size decreases, the scheduling of these kernel threads becomes sparser, occupancy decreases, and the inefficiency of resource utilization is exacerbated.

It is worth noting that compared with previous rounds of experiments, the queueBfs performance under the roadNet CA data is still stable, with kernel time controlled at 2.11us and register usage of 22. The throughput is not high but the delay is minimal, indicating that its on-demand scheduling strategy for active nodes has good adaptability to real sparse networks. In such graphs, the leading nodes are sparse but have high coverage, and queueBfs can accurately transmit active threads through the leading queue, thereby avoiding resource waste caused by a large number of idle threads.

Overall, under the roadNet CA data, although different BFS schemes show some consistency in block size scaling (with little change in overall execution time), their resource utilization and scheduling strategies still exhibit significant differences in sensitivity to graph structure. SimpleBfs and Gunrock styles are suitable for medium density or batch processing, while queueBfs is more suitable for sparse, large-scale, low concurrency, but locally compact graph structures. Although scanBfs has clear layering and structure, in actual sparse graphs, the kernel is too small and redundant scheduling is obvious, making it difficult to unleash hardware potential. In the future GPU implementation of sparse graph BFS, it is possible to consider combining the scheduling granularity of queue strategy with Gunrock's kernel design framework, while further reducing atomic operation conflicts and excessive scheduling overhead between kernels, in order to improve overall throughput and resource utilization efficiency.

#### 6.5 Summary and Suggestions

This article systematically compares and analyzes five different BFS implementations - SimpleBfs, QueueBfs, ScanBfs, cuGunrockStyleBfsKernel, and GSSWITCH - and comprehensively examines their performance in multiple dimensions such as algorithm design, execution efficiency, and hardware resource utilization. The experiments were conducted on an RTX 4070 GPU, using NVIDIA Nsight Compute and Nsight Systems for profiling. Each implementation was assessed based on kernel execution time, throughput, memory access efficiency, and thread-level parallelism.

The simpleBfs algorithm adopts the most straightforward traversal logic: it iteratively processes each vertex in the current frontier and scans its adjacency list, using atomic operations to update distances and write new vertices into the next frontier. While easy to implement and debug, its major drawback lies in the host-device synchronization required for each iteration, which introduces significant memory transfer overhead. Performance data shows a kernel execution time of 184.8 us and a high memory bandwidth utilization of 96.20%, indicating that the algorithm saturates available bandwidth but suffers from blocking synchronization.

queueBfs retains the basic data structures of simpleBfs but attempts to decouple the queue construction into finer-grained kernels for better scheduling flexibility. However, each sub-kernel (e.g., nextLayer, assignVerticesNextQueue) has extremely short execution durations, leading to noticeable kernel fragmentation. Profiling reports reveal low throughput across these kernels, suggesting that the GPU's parallelism is underutilized due to overhead from frequent kernel launches. While the approach is theoretically beneficial for control granularity, its current implementation fails to deliver performance gains, largely due to excessive synchronization and lack of compute-communication overlap.

In contrast, scanBfs leverages Gunrock's prefix-sum mechanism, using a two-phase scan (countDegrees and scanDegrees) to allocate memory for the next frontier precisely and avoid atomic contention. This theoretically improves load balancing, particularly for graphs with uneven degree distributions. However, it also introduces multiple kernel stages per BFS iteration, lengthening control paths and synchronization chains. Although each sub-kernel is lightweight, the overall execution time remains comparable to simpleBfs, primarily due to serialized dependencies between memory copies and context synchronizations. Nsight Systems traces confirm that memory transfer and computation are not well overlapped, further bottlenecking performance.

cuGunrockStyleBfsKernel adopts a unified kernel design inspired by Gunrock, integrating frontier processing, neighbor traversal, and queue updates into a single kernel. While the design is streamlined and avoids inter-kernel synchronization, it relies heavily on atomic operations. This results in a moderate throughput (13.31%) and high memory bandwidth utilization (96.47%), but overall kernel duration (189.28 us) is slightly longer than simpleBfs. The increased execution time may be attributed to warp-level serialization and broader scheduling windows. Although more compact and suitable for stable-throughput scenarios, this method suffers from limited scalability in large graphs due to control divergence and thread underutilization.

In contrast, GSWITCH introduces a scheduler-executor paradigm that dynamically selects between optimized kernel strategies based on frontier characteristics such as size and density. It incorporates vertex-centric and edge-centric modes, along with warp- and thread-level workload mapping. The design also features kernel fusion to reduce launch overhead and improve intra-kernel efficiency. Profiling results from Nsight Compute show that GSWITCH achieves higher resource utilization, better thread conver-

gence, and more effective memory coalescing. Notably, its end-to-end performance on large graphs like kron\_g500-logn21 is significantly better than the other methods, with a total time of around 33,333 us, compared to 445,760 us for cuGunrockStyleBfsKernel. These results highlight the effectiveness of combining strategy fusion, dynamic policy switching, and topology-aware execution to minimize redundant computation and synchronization.

In summary, each method reflects distinct trade-offs between design simplicity, control granularity, and execution performance. simpleBfs offers a clear baseline but is limited by synchronization; queueBfs and scanBfs aim for finer control but are constrained by kernel fragmentation and synchronization overhead. cuGunrockStyleBfsKernel reduces control complexity but struggles with atomic contention and scale-out behavior. GSWITCH emerges as the most effective design in this study, demonstrating the value of dynamic scheduling, kernel fusion, and adaptive execution. Future work can further enhance GSWITCH by integrating asynchronous memory transfers, multistream execution, and hierarchical memory management to build scalable and topology-aware BFS solutions for diverse graph workloads.