Optimizing GPU-based Graph Sampling and Random Walk for Efficiency and Scalability

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Abstract—Graph sampling and random walk algorithms are playing increasingly important roles today because they can significantly reduce graph size while preserving structural information, thus enabling computationally intensive tasks on large-scale graphs. Current frameworks designed for graph sampling and random walk tasks are generally not efficient in terms of memory requirement and high-performance graph sampling and random walk framework on multiple GPUs supporting multiple algorithms. Skywalker+ makes four key contributions: First, it realizes highly paralleled alias method on GPUs. Second, it applies finely adjusted workload-balancing techniques and locality-aware execution modes to present a highly efficient execution engine. Third, it optimizes the GPU memory usage with efficient buffering and data compression schemes. Last, it scales to multi-GPU to further enhance the system throughput. Abundant experiments show that Skywalker+ exhibits significant advantage over the baselines both in performance and utility.

Index Terms—GPU graph sampling; graph random walk; scalability; throughput

1 INTRODUCTION

GRAPH has drawn great attention these years since graph can effectively model entities and their relations in the non-Euclidean space. Most of traditional graph processing algorithms mainly study the low-level information [1], [2], while graph learning algorithms adopt graph embedding to reduce target graphs to low-dimension vectors. The learned embedding can be used for the downstream tasks. It has been actively studied in recommendation system, e-commerce, and many other fields [3].

However, graph representation learning suffers time-consuming feature engineering. With multi-level optimizations, its overhead is still much higher than the cost of classical graph data traversal since graph learning requires capture graph features in multiple and deep levels. The ever-increasing size of graph data can be handled by graph sampling and random walk algorithms. These algorithms focus on local structural information and global information, respectively. Additionally, it enables the use of deeper and more intricate neural networks on massive graphs. Some graph learning algorithms (e.g., node2vec [4], DeepWalk [5] GraphSAGE [6], Para-GCN [7] and GraphSAINT [8]), which learn from sampled embedding, can approximate or even replace directly learning from the intact graph. The learned embedding can be used for the downstream tasks. It has been actively studied in recommendation system, e-commerce, and many other fields [3].

As sampling can be executed following the vertex-centric execution model [10], some works modified state-of-the-art graph processing frameworks to support sampling algorithms. For example, DrunkardMob [11] extends GraphChi [12] to support out-of-memory random walk capability while Deep Graph Library (DGL) [13] applies Gunrock [14] to perform graph sampling. While exhibiting some extent of utility and performance, these systems treat graph sampling same as traditional graph algorithms, ignoring its unique properties.

Specialized graph sampling frameworks have been proposed to maximize the overall sampling throughput both on CPU and GPU. KnightKing [15] is a distributed random walk system based on the alias method [16]. The system excels in graph sampling, but it requires building the alias table for all the vertices of the graph dataset. Recently, ThunderRW [17] introduces a step-interleaving technique, which switches among different walk queries to reduce the CPU pipeline stalls resulted from irregular memory access. Some works further apply CPU designs to GPU to leverage their massive computing power and high memory bandwidth. C-SAW applies inverse transform sampling (ITS) [18] method to select neighbours, while NextDoor adopts the rejection sampling technique from KnightKing. Although these frameworks shows superior performance compared with their CPU-based predecessors, they fail to implement most advanced sampling algorithms, having problems such as high time complexity and highly varied trial number.

Note that the above specialized system designs all have their limitations. While CPU-based frameworks manage to alleviate irregular memory usage, the overall performance is limited compared with GPU-based ones due to lack of parallelism. On the other hand, GPU-based systems stuck in the problem of insufficient GPU memory. Once using host
memory, low PCIe bandwidth can be a severe bottleneck. One may choose to neglect high-degree vertices to improve performance [19], but it ends up getting inexact results.

In this paper we aim to achieve high-quality sampling/walking in an efficient and scalable way. We thoroughly investigate existing algorithms, frameworks, and systems for sampling. Prior works [1], [19] believe that the alias method is not suitable for GPU execution. Nevertheless, we believe the alias method is underestimated and has shown great potential for performance optimization. Our goal is to execute low-complexity sampling while amortizing the high-complexity preprocessing cost and preserving the sampling quality.

We introduce Skywalker+, an high-performance solution specialized for graph sampling and random walks on multiple GPUs exploiting both intra- and inter-instance parallelism while optimizing memory access and data locality. It provides usable interfaces and comprehensive support for all kinds of algorithms We have further extended our design to multiple GPUs, using balanced workload partition and locality-aware data management strategies to optimize the sampling throughput. Extensive experiments show that Skywalker+ exhibits significant advantage over the baselines while maintaining robustness on handling large graphs. We have open-sourced Skywalker+, which can be accessed online 1.

This work highlights the following contributions:

- We realize highly paralleled alias table construction on GPUs, making it practical for efficient SIMD execution for the first time.
- We propose an efficient execution engine supporting various sampling algorithms. It is capable of determining the proper execution mode as well as balancing the workload.
- We exploit the data locality in graph sampling by leveraging a locality-aware asynchronous execution strategy. It reorganizes the execution order so that the cached data is more likely to be reused.
- We introduce efficient buffering and data compression schemes to optimize the GPU memory usage, accelerating the execution process while cutting down the memory footprint.
- We extend the graph-friendly versatile sampler and alias table optimization to the multi-GPU domain. We devise efficient graph partition and GPU communication methods, which can effectively utilize multiple GPUs for better scalability.
- We put the above techniques together and present Skywalker+, a novel system executing various graph sampling algorithms with high computing and memory efficiency. Abundant experiments show that Skywalker+ exhibits significant advantage over the baselines both in performance and utility.

2 BACKGROUND

2.1 Graph Sampling and Random Walk

We start from the terminology of graph sampling and random walk. Graph sampling and random walk are two algorithms widely used to extract small-size embedding form large graphs while preserving structural information. They can be considered as pro-processing processes for downstream graph learning tasks. Sampling and random walks can be regarded as embarrassingly parallel computing tasks, since they seldom update graph information. Specifically, sampling and random walks can be unbiased (unweighted) or biased (weighted). The former selects the neighbors uniformly, while the latter computes the transition probability according graph property.

Graph Sampling. In graph sampling, several samplers start from one given root vertex and repeatedly selects several neighbors to generate a small sample graph from the large graph dataset, thus aggregating the neighbor information of the root vertex. The selection process can be either uniform (unbiased sampling) or based on a specific transition probability distribution (biased) generally calculated based on the weight of edges. A fixed number of neighbors are chosen for each layer when performing Neighbor sampling, as Figure 1 shows. GraphSage [6] is an inductive algorithm to learn graph embedding using Neighbor sampling, sampling k-hop neighbours. Hop indicates the distance of the target vertex to the seed vertex.

Random Walk. The random walk algorithms work similarly to sampling. Walkers repeatedly select one neighbor and moves to the selected vertices from their residing vertices until satisfying certain conditions, as Figure 2 shows. Personalized PageRank (PPR) [20] is a optimized version of PageRank [21]. Deepwalk [5] is an unbiased walk algorithm, while a later work [22] extends it to a biased version. Some dynamic algorithms further use runtime information to make decision. Node2vec [4] introduces the 2nd order random walk and defines two hyperparameters for the walking states.

Summary. Random walk algorithms can be seen as special cases of graph sampling that only select (at most) one vertex per step. They both select vertices based on the connectivity of graphs, leaving the opportunity to optimize them at the same time. For conciseness, we use sampling to refer to both the two algorithms. We term the vertices whose neighbors are to be selected as transit vertices.

2.2 Sampling Operations

For unbiased sampling, we can directly generate an random integral number to select the neighbour to be sampled in the next step of the current vertex. On the other hand, there are multiple neighbouring selecting methods when it comes to biased sampling, which are introduced next. We use an example where \( v_1 \) to \( v_4 \) are the adjacent vertexes of \( v_0 \) and have edge weight of 1, 1, 1 and 2 respectively to demonstrate the workflow of these methods.
Rejection sampling

and execution are real number generates a uniform integer number process stage. The execution stage takes two steps: (1) generates a random number as 0.8, then uses binary search to determine the smallest index on its preprocess stage. Suppose a vertex uses its bias to help sampled vertex. The preprocess takes \( O(n) \) time and space while the execution takes \( O(\log n) \) time.

Rejection Sampling calculates \( p^* = \max p_i \) on its preprocess stage. The execution stage takes two steps: (1) generates a uniform integer number \( x \) in \([0, p_n^*]\) and a uniform real number \( y \) in \([0, p^*_n]\); and (2) if \( y < p_x \), then select \( v_x \); otherwise repeat step (1). The time complexity of preprocess and execution are \( O(n) \) and \( O(\log n) \), respectively. Since it only needs to store the max bias \( p^*_x \), the space complexity is \( O(1) \). As shown in Figure 3(b), the rectangle areas covering \((0,0)\) to \((3,1)\) and \((4,0)\) to \((4,2)\) is the envelope and the sampling is accepted as long as it falls into these areas.

Alias method builds two tables on its preprocess stage: a probability table \( P \) and an alias table \( A \). All biases are distributed into \( n \) groups of the same total bias. The vertices with biases above average fill up the gap of those with biases below average. As Figure 3(c) shows, \( v_4 \) uses its bias to help \( v_1, v_2, v_3 \) to form a normalized distribution. The normalized bias (i.e., \([0.8, 0.8, 0.8, 1]\)) is then recorded in the probability table while the alias table records \([v_4, v_4, v_3, v_4]\). We then need to produce two random numbers in order to select one sample. While the first one chooses an index, the second one chooses the vertex of that index or its alias vertex stored in the alias table. The complexity of building an alias table for a vertex is \( O(n) \); however, the cost of drawing sample once based on the table is \( O(1) \). The complete probability table and alias table both have \(|E|\) elements, where \( E \) is the number of edges in the target graph.

2.3 Limitations of the Prior Work

Multiple CPU-based frameworks have been proposed to accelerate graph sampling tasks. Knighting [15] leverages rejection sampling along with the alias method for lower sampling cost. ThunderRW [17] makes further optimization by alleviating irregular memory access. But the overall performances of these frameworks are limited compared to GPU-based frameworks, as GPUs far overwhelm CPUs in massive parallel computing.

While showing higher throughput, existing GPU-based frameworks fail to provide comprehensive support for graph sampling. For example, C-SAW (the latest work on GPU-based sampling) can easily produce biased results. It is because its open-sourced implementation [19] simply choose to skip the vertices with degrees over 8000 when computing Cumulative Transition Probability Space for the vertices. In addition, C-SAW applies simple binary search to draw samples, which leads to high time complexity compared with alias method \( O(\log n) \) vs. \( O(1) \). Furthermore, the C-SAW implementation fails to optimize the storage of intermediate data and sampling results, storing them in space-consuming data structure. According to our profiling results, it can only issue about 4000 in-memory random walkers at a time on a RTX 2080Ti with 11 GB memory.

Another key work is NextDoor [9]. It is based on rejection sampling, but it suffers from the problem of highly varied trial number. It can lead to severe slow down especially on large graphs. The biases of some hotspot vertices could be so large in this case that result in unexpectedly large average trial number.

2.4 Key Design Considerations

Once the alias table is built, the sampling process takes constant time as long as the graph bias does not change. This is significant as downstream CNN tasks always require multiple iterations of training, generating multiple sampling/walking queries on the same graph.

However, although alias methods shows superiority in execution stage, building the alias table appears to be the bottleneck especially for dynamic sampling algorithms such as node2vec. A natural way to speed up this procedure is leveraging parallel processors such as GPGPUs. However, alias table construction is considered to be problematic on GPUs [1], [19].

Wei et al. [23] found that their GPU implementation of alias method [1] performs even worse than the CPU version. Specifically, adopting the alias method on GPU platforms haves four challenges:

1) The alias method is hard to parallelize on GPU. Classical alias table construction method is executed largely in serial, making it non-trivial to map the alias table to SIMT-style GPUs. Unpredictable logical branching would result in warp divergence if the serial portion of the method were naively mapped to each GPU thread.

2) It is nontrivial to implement the application-aware execution engine. The irregularity of graphs leads to extremely unbalanced workload distribution, creating severe stragglers. Besides, samplers may visit any...
part of the graph, which leads to frequent thrashing in both cache and on-board memory.

3) It is difficult to effectively utilize the hybrid memory structure. While processing many sampling instances concurrently is preferable, constructing an alias table for each vertex requires large memory space (detailed in §3.4.1). Therefore memory can be a scarce resource for graph sampling workloads.

4) It is non-trivial to schedule workloads on multiple GPUs. Since graph tends to have skewed distribution, simply dividing workload according to vertex can lead to inefficiency on different GPUs. Besides, it would suffer from massive long-latency accesses to remote data without careful arrangement.

3 Skywalker+

In this paper, we aim to address the aforementioned challenges and unleash the potential of the alias-method-based sampling on GPUs.

We propose Skywalker+, a highly efficient framework for random walk and graph sampling algorithms on heterogeneous computing platform. The optimization strategies of our design are multi-pronged, leading to significantly improved efficiency and scalability with multiple GPUs.

3.1 Design Overview

As shown in Figure 4, Skywalker+ is optimized along multiple dimensions. We revisit the sampling/random walk algorithm, devise the parallel execution engine, fine-tune memory usage, and enable multi-GPU scheduling.

1) At the algorithm level, we separate the samplers of Skywalker+ so the construction process of the alias table and sampling process of the graph can be done in parallel.

2) In terms of computing engine, we leverage a new execution model that can fully utilize the parallelism of independent sampling instances. It not only utilizes the high computing power of the SIMD architecture, but also exploits data locality of graph applications.

3) For memory management, we build memory hierarchy aware scheme that can reduce memory requirement for large graphs. Doing so allow us to further accelerate the entire graph sampling process.

4) Finally, at the cluster level, our multi-GPU scheduler distributes workloads evenly based on interleaved indices and leverages a heuristic strategy to instruct the execution.

In total, Skywalker+ supports a number of different workloads and execution modes. For example, it can constructs the alias table as an offline procedure. It can also work in a realtime mode, which is necessary for dynamic sampling tasks that cannot build the entire table beforehand without runtime information.

3.2 Tapping into Intra-instance Parallelism

To effectively run the alias method on GPUs, we parallelize the alias-table constructing algorithm while taking load balancing into consideration.

3.2.1 Parallel Table Construction Algorithm

Skywalker+ assigns many threads to compute the alias table of a single vertex in order to make use of the parallelism of the GPU. A workgroup is a collection of threads that cooperate to process nearby vertexes within a single thread warp/block. We use atomic operations so that threads in a workgroup can simultaneously put vertices into Large and Small. Each thread in a workgroup handles one pair of large-/small- bias vertices individually.

If the proportion of vertices in Large or Small is uneven, the parallelism of the construction would be restricted. For example, we take into account a workgroup with eight threads in Figure 5(a). Only three vertices make up Large, but Small’s size is equal to or more than eight. Five threads will therefore be idle because only one large-bias vertex can be processed. Note that Large and Small do not necessarily have equal sizes, this circumstance occurs frequently.
process their low-bias vertices using atomic operations. In this way, the parallelism is improved. Algorithms 1 shows

\begin{algorithm}
\caption{Serial algorithm to construct alias table.}
\begin{algorithmic}[1]
\Require $B = \{b_1, b_2, \ldots, b_n\}$
\Ensure $\text{Prob}, \ldots$
\State If $\text{Prob}[v_l] > 1$ then
\State $\text{Large} = \text{Large} \cup v_l$;
\State Else if $\text{Prob}[v_l] < 1$ then
\State $\text{Small} = \text{Small} \cup v_l$;
\State End
\End
\end{algorithmic}
\end{algorithm}


\section{3.3 Tapping into Inter-instance Parallelism}

This section explains how Skywalker+ makes use of the graph sampling inter-instance parallelism.

\subsection{3.3.1 Versatile Sampler}

We propose versatile sampler, a new execution model which enables GPU threads to engage in various levels of collaboration for alias table creation with the minimal overhead.

Our design features a multi-level load balancing technique for assigning GPU resources for vertices with various degrees of skewness. Specifically, it uses two key parameters, the warp-processing threshold and the block-processing threshold, to decide the various sizes of workgroups for one transit vertex. For example, several threads working in the same warp are used to build the alias table for low-degree vertices whose degrees are below the warp-processing threshold. Threads within a block collaborate to process vertices with degrees greater than the block-processing threshold.

The jobs in a queue are processed by GPU kernel threads that remain active during execution until there are no job left. Threads contained within one block of execution can switch between different modes if necessary. We devise collective samplers at the sub-warp level, warp level, and block level. We use shared memory to store sampler context. In contrast to prior execution model \cite{25} where threads in one block independently complete the same task on several inputs, our versatile sampler allows threads in one block to switch between three working modes. As the burden of alias table formation varies greatly for each vertex, a distinct number of threads collaborate to process one task.

\subsection{3.3.2 Semi-asynchronous Execution}

The workload for each vertex is significantly skewed due to the irregularity of graphs, and therefore all the existing iterative-based GPU sampling frameworks can face significant performance overhead due to the straggler issue.

We use a semi-asynchronous \cite{26} execution model, other than conventional synchronous one. In particular, the samplers in Skywalker+ separately handle each job after continuously requesting it from a per-depth global queue. One sampler advances to process jobs for the next depth without waiting for other samplers when the current depth has no jobs in the queue and just one sampler is available.

The execution flow of Skywalker+ is depicted in Figure 6: ① A subwarp-collective sampler is executed by each thread warp. The sampler builds the alias table and draws samples for the low-degree transit vertex. ② A sampler adds a high-degree transit vertex to a queue that holds high-degree jobs whenever it receives one. Our design momentarily saves mid-degree transit vertices in a per-SM queue. ③ Subwarp-collective samplers can form one warp-collective sampler to process jobs in the per-SM queue when the global job queue for the current iteration is empty. ④ Warp-collective samplers in a thread block gather together and become a single block-collective sampler when the per-SM queue is empty. ⑤ The transit vertices in the high-degree queue are processed by the block-collective sampler. ⑥ For
the following iteration, the block-collective sampler changes back to subwarp-collective samplers.

3.3.3 Locality-aware Asynchronous Execution

When performing online sampling, the samplers need to access all the neighbors of transit vertices to construct alias tables. In this case, data locality is crucial for performance. Though the above semi-asynchronous execution style is efficient in load-balancing, it overlooks the locality existing in sampling just like other existing GPU-based method implementing the synchronous style. Vertices in large graphs are partitioned and processed successively, eliminating the chance of leveraging data locality. It can lead to frequent data thrashing, since data may be evicted from cache even it is to be used in the next iteration.

For example, suppose we need to sample vertex 0 and 4 in the example graph of Figure 7 in an iterative-based manner. The graph is divided into two parts so that each part can fit into a virtual cache. For the given sample results, the procedure is as follows: vertex 0 and 4 are in the frontier of the first iteration; to construct the alias table for vertex 0, Sampler0 loads partition A and then selects vertices 3 and 4; then, Sampler1 loads partition B and selects vertices 3 and 5; similarly, we construct the alias table and select neighbors for vertices 3, 4, and 5. In this way, we need to repetitively load graph partitions to process each sampling task in iterative execution order, which is highly inefficient.

To address the above problems, Skywalker+ further introduces a locality-aware asynchronous execution strategy to explicitly exploit the locality existing in sampling. The main idea is to rearrange the order in processing the transit vertices based on their position in the graph so that the cached data is more likely to be reused.

Specifically, we partition the graph into subgraphs virtually based on vertex indices. Then, a locality-aware sampler creates one sub-frontier for each subgraph. During execution, tasks in the same sub-frontier are processed successively while the newly-generated sampling tasks enqueue into their corresponding sub-frontiers. The tasks from different sampling depths can be processed together. In other words, once a warp- or block- sampler constructs the alias table and selects several samples, the newly-generated sampling tasks can be processed immediately as long as they belong to the same subgraph. For example, as shown in the locality-aware execution of Figure 7, instead of moving to vertex 4 stored in another partition, the sampler first sample on vertex 2, thus eliminating an unnecessary subgraph switching. In this way, the data loaded in the cache is more likely to be reused and the number of loading data in memory is reduced eventually. On the other hand, if thread blocks do not get valid tasks from the current sub-frontier, they will immediately move on to the next sub-frontier and do not wait for other blocks.

3.3.4 Selecting Vertices

Skywalker+ choose vertices depending on the constructed alias table. Sampling algorithms generally use *sampling without replacement*. In other words, there shouldn’t be any repetition in the vertices chosen for a single transit vertex. This leads to repeatedly sampling overhead, which stems from duplicate detection and resampling. Skywalker+ adopts several techniques to reduce this overhead for both offline and realtime workloads.

We use a bitmap for each transit vertex for duplicate detection. Each bit in the bitmap specifically specifies whether a certain vertex has been chosen. To avoid selecting the same vertex again when selecting, threads employ atomic compare-and-swap operations. Besides, Skywalker+ aggressively lets excessive threads atomically increase a counter. With twice or more threads than actually needed vertexes (depending on a pre-set expand factor) launched to select one neighbour using atomicCAS to generate unique results, the warp is more likely to succeed in one trial. For high-degree vertices, collisions would be rather rare. For low-degree vertexes smaller than the expand factor, Skywalker+ directly submits all its neighbors.

With already constructed alias table, we can perform resampling with a constant $O(1)$ overhead. No repetitive alias table construction is needed since the graph bias does not change. Thus, Skywalker+ has significant advantage over other frameworks such as C-SAW which requires $O(\log(d))$ operations to resample.

3.4 Memory-side Optimizations

This section explains how Skywalker+ optimizes memory access and lowers memory usage when creating alias tables.

3.4.1 Fast Alias Table Construction

To create the probability table and alias table ($Prob$ and $Alias$) for one vertex, we need to load all its neighbors in queues and process them with frequent enqueuing/dequeuing operations. Skywalker+ leverages shared memory of GPUs to further optimize the buffer. For example, each SM supports 1024 concurrent threads at most. Thus, each warp can be provisioned with around 1.5 KB shared memory. This means a warp-collective sampler can process nearly 100 elements using buffer shared memory, which is larger than a reasonable warp-processing threshold. For a block-collective sampler, shared memory in each SM alone is not sufficient for processing vertices with extremely high degrees. In this scenario, Skywalker+ splices shared memory and global memory for the buffer. In other words, the buffer falls back to global memory when the required buffer size is larger than the size of shared memory.
Graph partitioning with Multi-GPU. Skywalker+ partitions the workload by vertex indices instead of vertex number as table construction has \(O(d)\) complexity for each vertex. Skywalker+ inspects the vertex index offset first and then partitions the workload so that the partitions have similar edges for better load-balance.

Alias table partitioning with Multi-GPU. Alias table composes of an alias array and a probability array, which is stored corresponding to the input order. It requires extra space and time if we want to rearrange alias tables. The integral alias table is stored in the host memory and accessed through PCIe if there lacks enough space in GPU memory.

3.5.2 Balance-ensured Workload Distribution
Workload distribution is a key factor in Multiple GPU computing since straggler GPUs can severely lower the overall performance. Skywalker+ distributes the workload evenly for alias table construction and sampling in both realtime and offline sampling scenarios to alleviate this problem.

Alias table construction with Multi-GPU. Each GPU is distributed with certain partition of graph data. Based on these data, the GPU builds the partial alias table. When GPUs finish its partitioned table construction, those partitioned alias tables are assembled together for further usage. Depending on the size of the graph and GPU memory capacity, Skywalker+ either gathers the partial alias table in GPU memory for lower access latency or assemble the partial alias table in host memory to avoid exhausting the GPU memory.

Sampling with Multi-GPU. Skywalker+ distributes the sampling instances evenly to different GPUs. As the computing of instances is independent, there is no need for communication or synchronization. Each GPU processes its assigned sampling instances independently. Although graphs could have skewed edge distribution, the workload for the GPUs are generally evenly distributed. It’s because the time complexity for sampling is \(O(1)\) for each vertex and Skywalker+ ensures that each partition has a similar amount of vertices.

3.5.3 Latency-aware Data Management
Data management is crucial for multiple GPU computing as GPU has a limited memory capacity. Due to the irregularity of graphs, the sampler/walker may access any locations of the graph. Thus, each sampler/walker must be able to
access the whole graph data. Skywalker+ carefully places the necessary data to minimize the memory access latency.

*Design Space Analysis.* There are several options to allow GPU to access data larger than the GPU memory capacity, such as pinned host memory, Unified Memory (UM) and peer GPU memory. These options have different performance characteristics. Pinned host memory allows GPUs to directly access host memory through unified virtual address space, but fails to cache the hot pages. UM allows over-subscription of GPU memory, but can suffer from fault handing overhead [27]. Besides, directly applying UM among multi-GPU can lead to frequent data migration between host memory and devices, which further result in interface congestion. Peer-to-peer memory access enables GPUs to access remote graph data resident on other GPUs’ memory, but it is only supported by limited GPU types. Skywalker+ carefully weighs these options and adapts them to suitable scenarios.

*Heuristic Strategy.* Skywalker+ devises a heuristic strategy taking both graph data characteristics and hardware capability into consideration. The methodology is to leverage memory with lower latency as much as possible. Figure 9 presents our various execution modes. 1

![Image](image_url)

Fig. 9: Different execution modes on multiple GPUs.

Table 1: Evaluated walk & sampling strategies.

<table>
<thead>
<tr>
<th>Name</th>
<th>Sampling Method</th>
<th>Supported workload</th>
</tr>
</thead>
<tbody>
<tr>
<td>Graphwalker [28]</td>
<td>Unbiased sampling</td>
<td>Unbiased PPR</td>
</tr>
<tr>
<td>KnightKing [15]</td>
<td>offline Alias method</td>
<td>Based/unbiased random</td>
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<tr>
<td></td>
<td>for static sampling;</td>
<td>walks</td>
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<tr>
<td></td>
<td>rejection sampling</td>
<td></td>
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<tr>
<td></td>
<td>for dynamic sampling.</td>
<td></td>
</tr>
<tr>
<td>C-SAW [19]</td>
<td>Inverse transform (ITS) sampling</td>
<td>Biased sampling and DeepWalk</td>
</tr>
<tr>
<td>ThunderRW [17]</td>
<td>ITS, rejection, and</td>
<td>Biased/unbiased</td>
</tr>
<tr>
<td></td>
<td>Alias method</td>
<td></td>
</tr>
</tbody>
</table>

Our platform is well equipped with four RTX 2080Ti graphics cards. Each GPU has 4352 CUDA cores in total and 11GB of GDDR6 memory. We install Ubuntu with Linux kernel 4.15.0. We compile all programs using NVCC compiler version 11.0.167 (g++ version 7.5.0). For evaluation, we use nisght system v2021.5.2 and nisght compute v2022.1.1 to collect runtime information.

For CPU-based baselines, we let them use all 40 physical CPU cores to compute. The distributed systems KnightKing [15] is also executed on a single machine. For comparison with the GPU-based framework, we use only one GPU.

*Baseline Frameworks.* To verify the superiority of Skywalker+ over existing approaches, we compare it to the most representative baselines as summarized in Table 1.

1. **GraphWalker** [28] is a CPU-based random walk system targeting single node. To maximize data access efficiency, it gives priority to the loaded subgraphs.

2. **KnightKing** [15] targets distributed system. For algorithms with static deviations, it uses the aliasing method, while for algorithms with dynamic deviations, it uses the rejection sampling method.

3. **Nextdoor** [9] is another representative GPU-based graph sampling approach. Its rejection sampling technique is the same as KnightKing.

4. **C-SAW** [19] is one of the most representative graph sampling and random walk system for GPU. It represents the ones that utilize the Inverse Transform Sampling method.

5. **ThunderRW** [29] represents the latest CPU-based graph walk engine. It supports multiple sampling methods on both biased and unbiased workloads.

4 EXPERIMENTAL METHODOLOGIES

In this section, we show the experimental methodologies to verify the superiority of Skywalker+.

*Platform.* We use a Linux server that has two 2.4 GHz Intel Xeon 6148 CPUs (20×2 physical cores in total) as the evaluation platform. Each CPU has 27.5 MB of L3 cache and 256 GB of main memory.
GraphWalker only supports unbiased walk while the open-sourced C-SAW do not support PPR and unbiased sampling. Additionally, because C-SAW only supports pre-allocating a fixed size buffer for each thread block, it ignores all vertices with degrees greater than 8000.

Workloads. We have selected three types of workloads that can represent the most common sampling and random walk algorithms in a wide range of application domains. This helps to verify the performance and effectiveness of Skywalker+ in various settings. To be specific, we use these algorithms including Deepwalk, PPR, node2vec and NeighborSampling. As we mentioned above, some baselines may not support a portion of these algorithms due to their limited processing capabilities. We extend and improve them as much as possible to support more algorithms. Taking NeighborSampling as an example, we adopt the configuration from GraphSAGE [6] with the sampling depth as 2 and expansion factor (the number of neighbors to be sampled for one vertex) as $S_1 = 25$ and $S_2 = 10$. For PPR, we use 15% as determination probability. For node2vec, we set the hyper-parameters $p = 2.0$ and $q = 0.5$. We set 100 as the maximum length as adopted in previous works. For all algorithms, we perform sampling with batch size 40000, which is enough for most downstream applications. For our method Skywalker+, we evaluate the sampling algorithms in all possible execution modes and both unbiased/biased.

Graph Dataset. As shown in Table 2, we use a variety of state-of-the-art datasets in our experiments. We totally consider 7 datasets used in two representative graph applications, i.e., social networks and web graph snapshots. Among them, LiveJournal (LJ), Orkut (OK) and Friendster (FS) are commonly used in social networks, and Web-Google (GG), UK-2005 (UK), Arabic-2005 (AB) and SK-2005 (SK) are the SOTA datasets used in web graph snapshot applications. We also manually create a 67GB rmat graph to evaluate our scalability for large graphs.

Implementation Details. Node2vec uses dynamic bias and is executed in online mode for Skywalker+ and Knightking. Other algorithms are executed in offline mode unless otherwise stated. To be mentioned, C-SAW simply skips all the vertices with degrees higher than 8000, resulting in biased result. Skywalker+ and other baselines follow the standard sampling method, which guarantees the quality of the results. We use a factor of the sampled edges directly in ThunderRW’s source code since it samples on all vertices by default, which is less flexible.

Metrics. We collect and demonstrate the runtime information for most of the tests. We do not include the time to initialize and load data from the disk. All datasets that are available can be loaded into the main memory entirely except for Graphwalker, which uses only host memory. We do not include the processing time for Graphwalker to repeatedly load graph segments. Although different input formats are fetched from disk, all frameworks eventually store graph data in memory in the same CSR format. Skywalker+ and other frameworks that utilize the alias method require additional space same to the size of graph data as the alias table for offline workloads. As for the GPU-based baselines, we collect their kernel execution time on GPU. Unless otherwise noted, we include the time to create the entire alias table as part of the preprocessing overhead for KnightKing and Skywalker+.

5 Results and Evaluations

In this section, we demonstrate the results and evaluate the performance of Skywalker+ from four aspects: 1) How fast can unbiased workloads run with Skywalker+? 2) How does Skywalker+ perform when dealing with workloads with static or dynamic biases? 3) How do the new optimizations affect performance? 4) How scalable is Skywalker+ when using multiple GPUs?

5.1 Performance on Unbiased Workload

We begin with validating the performance of different methods i.e., Graphwalker, KnightKing, NextDoor, ThunderRW and Skywalker+ on the unbiased workload. The results are shown in Table 3. According to our observation, Skywalker+ outperforms all baselines in all test cases and can be adapted to a wide range of scenarios. To be fair, we only compare Skywalker+ with the baselines that support the unbiased model. In our comparison experiments, we do not use uniform bias as the unbiased workload. The unbiased model simply picks a random neighboring vertex, while the uniform bias must go through a complex preprocessing process, such as alias table construction.

Skywalker+ speeds up the execution time on Deepwalk by three orders of magnitude compared to Graphwalker; the result is two orders of magnitude on PPR. The key reason behind the performance improvement is that Graphwalker uses random walks to statically partition the graph, which involves significant additional coordination overhead. Instead, Skywalker+ is fully optimized for load balancing, data locality, memory access efficiency, and other factors.

Skywalker+ also respectively shows 641×, 142× and 4157× average speedup of improvement than knightking on Deepwalk, PPR and node2vec. Particularly, Skywalker+ achieves higher speedup on node2vec than the other algorithms. This is because the node2vec algorithm needs time to verify the connectivity of recently sampled vertices with previously sampled vertices. In this situation, the straggler thread would prevent all other threads from running. This problem is not present in Skywalker+ since different SMs are scheduled to work independently.

<table>
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<tr>
<th>Algorithms</th>
<th>Frameworks</th>
<th>GG</th>
<th>LJ</th>
<th>OK</th>
<th>AB</th>
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<th>SK</th>
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<th>Avg. Speedup of Skywalker+</th>
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Fig. 10: Results of biased graph sampling (normalized to Skywalker+’s runtime).

Due to its high memory needs, NextDoor cannot process graphs larger than UK. Therefore, we only compare Skywalker+ to NextDoor on UK and NeighborSampling. The result shows that Skywalker+ speeds up UK and NeighborSampling respectively by 49.8× and 5.2× on average compared with NextDoor.

To compare with ThunderRW, we set the thread number as 20. It shows that Skywalker+ outperforms ThunderRW by 101×, 94× and 143× on Deepwalk, PPR and node2vec respectively. It is notable that the throughput improvement declines from 3× to 10× when ThunderRW samples a batch of vertices rather than all vertices. This is because ThunderRW’s interleaving technique works well when the batch size is large. Its relatively constant start-up and shutdown time can surpass actual execution time when handling a small number of queries.

5.2 Performance on Biased Workloads.

In Figure 10, we demonstrate the result of the biased workloads. Compared with KnightKing, Skywalker+ achieves 3.6~21×, 1.7~38× and 2~190× of performance improvement on DeepWalk, PPR and node2vec, respectively.

Skywalker+ achieves 10~93× speedup on DeepWalk and 483~5878× speedup on NeighborSampling compared with C-SAW. The reason behind the significant improvement is that Skywalker+ can utilize the CPU’s main memory through the UM mechanism along with space-efficient designs. Therefore, well-designed UM has great potential in increasing the performance of graph sampling and random walk. Skywalker+ beats C-SAW mainly because Skywalker+ can utilize the precomputed alias tables.

Skywalker+ has a lower overhead for sampling multiple items without replacement. Firstly, sampling by aliasing is more efficient because it takes constant time. Secondly, Skywalker+ has lower selection collision cost. On Skywalker+, collision detection and resampling are substantially less expensive than they are on C-SAW. Thus, Skywalker+ shows higher speedup on NeighborSampling than DeepWalk.

When it comes to Nextdoor, the latest sampling framework on GPU, Skywalker+ achieves 2.6~35× speedup on DeepWalk and 2.5~40× speedup on PPR. Besides, Skywalker+ show more comprehensive support for different sampling algorithms and large graphs.

5.3 Impact of Different Schemes

In Table 4, we validate the effectiveness of the core optimizations of Skywalker+. We conduct this experiment by analyzing the normalized results on Deepwalk with or without the proposed optimizations. We have the following observations. 1) Speculative Execution. Skywalker+ uses speculative execution to speed up Deepwalk and Neighbor sampling by a factor of up to 3.1 and 1.6 times, respectively. 2) Semi-asynchronous Execution. Using semi-asynchronous execution, Skywalker+ has up to 3.6× and 5.2× speedup on
node2vec and Deepwalk, respectively. 3) **Data Locality-aware Execution.** Through data locality-aware execution, Skywalker+ achieves a speedup of $2.2 \sim 2.9 \times$ on Neighbor sampling in online mode, respectively. 4) **Compressed Alias Table.** On the evaluated graphs, the compressed alias array allows saving about 66% more spaces than the original ones. In this regard, Skywalker+ can handle large graphs with almost no overhead.

### 5.4 Data Locality-aware Execution Breakdown

In Figure 11, we evaluate the hardware characteristic of Skywalker+ and Skywalker. We validate the effectiveness of the locality-aware asynchronous execution technique. Compared with Skywalker, the normalized DRAM throughput of Skywalker+ increases up to $2.9 \times$; global throughput improves to 2.6 to 3.0; L1 cache hit rate improves up to 2.1 except for SK; IPC improves to 2.5 to 3.3; On the other hand, normalized DRAM utilization ratio ranges from 0.05 to 0.66; the number of stalls due to memory dependency reduces down to 0.65; DRAM transactions reduces to 0.42 to 0.97 except for LJ and SK; As a result, the normalized sampling throughput is improved from 1.9 to 2.8. All the above results illustrate that the locality-aware asynchronous execution can effectively harness the locality while reducing the pressure on the GPU memory subsystem, thus improving the overall sampling throughput.

### 5.5 Multi-GPU Scalability

Figure 12 shows the overall sampling throughput achieved by Skywalker+ using 1 to 4 GPUs. Skywalker+ delivers up to 520 and 3226 million SEPS of throughput on Deepwalk and Neighbor Sampling for real-time workloads, respectively. The large difference in throughput on Deepwalk and neighbor sampling is due to the fact that Deepwalk needs to compute the alias table once for each newly sampled vertex while neighbor sampling samples 20 vertices using each computed alias table. For offline workloads, Skywalker+ respectively achieves up to 5.7 and 5.6 GSEPS (billions sampled edge per second) throughput on Deepwalk and neighbor sampling. As for unbiased workloads, Skywalker+ achieves up to 14.2 and 59.3 GSEPS throughput on Deepwalk and Neighbor Sampling.

6 RELATED WORKS

To the best of our knowledge, this paper provides the first extensive analysis of graph sampling and random walk on multiple GPUs. We adopt a multi-pronged approach
and implement a highly efficient and scalable GPU graph sampling and random walk framework. The relevant prior work are summarized as bellow.

**CPU-based Random Walk Systems.** Similar to graph computing frameworks, DrunkardMob [11], leverages the popular vertex-centric computational model. KnightKing [15] is a distributed random walk system implementing on multi-core CPU. It applies alias method for static sampling algorithms, while implementing rejection sampling for dynamic sampling algorithms which are less suitable for alias method. We observe that the performance of the above designs are largely affected by the bias distribution. Similarly, GraphWalker [28] leverages GraphChi’s out-of-core processing capability. While only supporting unbiased random walk, it features an asynchronous walk updating technique to optimize I/O. ThunderRW [17] is a framework that supports diverse graph sampling workloads. It reduces the CPU pipeline stall resulting from irregular memory access in graph processing with a step interleaving technique. This technique switches between different walk queries to hide the memory latency.

**GPU-based Sampling Systems.** There are several GPU-based graph sampling and random walk frameworks. For example, C-SAW [19] introduces a parallel scan algorithm [32] to implement ITS to select neighbours. Unfortunately, its open-source implementation does not demonstrate how it is optimized for out-of-memory and multi-GPU sampling. Different from C-SAW, NextDoor [9] applies KnightKing’s rejection sampling technique to GPU, achieving higher throughput. It introduces a parallel paradigm called transit-parallelism. It assigns transit vertices to thread blocks and assigns samples to threads. It also optimizes for memory coalescing.

**Memory-constrained GPU Graph Computing.** GPU has very limited memory for handling large graph dataset. Therefore, prior studies propose to divide large graphs into subgraphs and process them in a streaming manner [33]. Garaph [34] takes advantage of both CPU and GPU to process large graphs. Recently, a few works [2], [35] start to adopt NVIDIA’s unified memory (UM) technique to oversubscribe GPU memory capacity, but often suffer from the problem of frequent page faults. HALO [36] introduces a graph reordering algorithm to speed up graph traversal with UM. Chen et.al [37] further applies a unified-memory-based hybrid processing for partition-oriented subgraph matching on GPU. Hum [38] tries to optimize the execution on unified memory. Subway [39] smartly chooses and transfers the subgraphs to process on the GPU.

**Graph partitioning.** Since it’s common practice to first divide large graphs into subgraphs, extensive researches have been conducted on efficient and effective graph partitioning. Multiple works [40], [41] have leveraged both heuristic and machine learning methods to provide communication-efficient and workload-balanced partitions so that multiple workers such as GPUs can handle these partitions with less memory thrashing and performance straggler. Partition-centric processing model has also been applied [42] to take advantage of data-locality of the partitions and accelerate the whole processing. Hep [43] proposes a new partitioning algorithm which flexibly adapts its memory overhead by separating the edge set of the graph into two sub-sets and achieves improvements in both in-memory partitioning and streaming partitioning.

**Multi-GPU.** An application can be accelerated by multiple GPUs to achieve higher speedup. Groute [44] introduces asynchronous multi-GPU programming in a thin runtime environment. cuTS [45] develops a GPU-friendly trie-based data structure and a distributed sub-graph isomorphism algorithm to leverage the computing power of multiple GPUs. Case [46] constructs GPU tasks from CUDA programs in the compilation to guide task assignments.

**Graph Compression.** Besides the general lossless and lossy data compression techniques [47], [48], graph compression techniques [49], [50] compress the graph structure data. POCLib [51] proposes a near orthogonal processing method for compression. It mainly targets data analysis tasks such as search and count which require to scan or traversal the whole data region. However, alias tables are only looked up randomly for a few specific elements in a fine-grained granularity, which is significantly different.

### 7 Conclusion
We present Skywalker+, an novel and powerful system that supports various key random walk and graph sampling algorithms. We introduce a parallel algorithm for alias table construction on GPU and design an efficient locality-aware execution engine. We also apply specialized buffer and storage optimizations and further extend the system to multiple GPUs. Our design exhibits notable performance advantage over the state-of-the-art baseline systems on a variety of scenarios. Importantly, it shows strong robustness and capability on handling large graphs and provides comprehensive support for all kinds of algorithms and execution modes. It also presents satisfactory scalability on multiple GPUs.

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