ABSTRACT

We present a multi-GPU graph processing library that allows programmers to easily extend single-GPU graph algorithms to achieve scalable performance on large graph datasets with billions of edges. Our design only requires users to specify a few algorithm-dependent blocks, hiding most multi-GPU related implementation details. Our design effectively overlaps computation and data transfer and implements a just-enough memory allocation scheme that allows memory usage to scale with more GPUs. We achieve $\sim 20$ GTEPS peak performance for BFS, demonstrating a $\sim 6X$ speed-up with $\sim 2X$ total GPU memory consumption on 8 GPUs. We identify synchronization/data communication patterns, graph topologies, and partitioning algorithms as limiting factors to further scalability.

Keywords

GPU, multi GPU, parallel graph processing

1. INTRODUCTION

Graphs are models of complex networks which map relationships among high volumes of highly connected data. Graph analytics includes traversal, query, matching, community and anomaly detection, and structural characterization (vertex ranking, centrality computation, shortest path computation, etc.). It serves as a fundamental tool for various domains from social network analysis to airline routing to computational biology. During the past few years, large-scale graph analytics has gained significant attention in supercomputing community as well. Several specialized supercomputing graph analytics systems focus on graph algorithms such as traversal [26], betweenness centrality [22], shortest path [4], personalized PageRank [19], and strongly connected components [15]. Other interesting applications use large-scale graphs on HPC systems, including genome assembly [12], video filtering and co-segmentation [20], and fraud detection in health-care systems [6].

Recently, the potential advantages in performance, price-performance, and power-performance of the modern graphics processing unit (GPU) over the traditional CPU has led to research on using GPUs for graph analytics [9, 11, 18, 31, 32]. The work we present here uses our “Gunrock” [31] graph-processing library for GPUs. While the conclusions in this paper apply broadly to GPU graph frameworks rather than just Gunrock, we summarize Gunrock’s programming model in Section 2.1. Gunrock provides an excellent foundation for developing GPU-based graph primitives. However, prior to this work, Gunrock was limited to single-GPU computation and graphs that fit into GPU memory.

We originally envisioned this work targeting traditional one-GPU-per-node clusters as the proper building block for multi-GPU (“mGPU”) graph analytics. In the course of this work, however, we turned to multiple GPUs on one node (“mGPU-1node”) instead as the right building block, and found numerous research challenges that we address in this paper. We found that multiple GPUs on one node offers ample optimization opportunities—including using shared CPU memory to exchange small amounts of data (e.g., GPU error-checking status, frontier sizes, and the stream statuses of peer GPUs to enable non-blocking inter-GPU cooperation)—and that we could build mGPU-1node programs with only small modifications of existing single-GPU programs.

The goal of our multi-GPU graph analytic system is to deliver high performance and scalability while maintaining programmability and compatibility. More specifically, we want:

a. Programmability: easy to write or transform graph primitives to support mGPU;

b. Algorithm generality: can support a wide range of graph algorithms;

c. Hardware compatibility: usable on most GPU systems;

d. Performance: low runtime, and leverages the underlying hardware well;

e. Scalability: scalable in terms of both performance and memory usage across GPUs.

To achieve these targets, we need to address several key issues:

- How do we distribute graphs across GPUs?
generates a new frontier by choosing a subset of the vertices or edges that are actively participating in the computation. We currently support three ways to manipulate the current frontier:

- **Advance** generates a new frontier by visiting the neighbors of the current frontier;
- **Filter** generates a new frontier by choosing a subset of the current frontier based on programmer-specified criteria;
- **Computation** executes an operation on all elements in the current frontier and can be combined for efficiency with advance or filter.

Gurock programs define graph algorithms as a sequence of the above three steps, beginning with an initial frontier and running to convergence (e.g., an empty frontier, a maximum number of iterations, or a volatile flag value that can be updated by a Gurock “computation” step).

### 2.2 Large-Scale Graph Libraries

The supercomputing community has spawned several large-scale distributed or shared-memory CPU-based graph libraries [14, 21, 24, 29] and BFS-specific frameworks [3, 7, 26]. They achieve performance and scalability at the cost of using much heavier machines and much more power.

There are also several existing mGPU graph processing frameworks, and each of them has their advantages and shortcomings. The following listed shortcomings refer to the full list at the end of this section.

Merrill et al. [24] presented the first notable linear parallelization of the Breadth-First Search (BFS) algorithm on the GPU. Their mGPU-Inode strategy distributes the vertices to GPUs; data related to remote vertices are fetched by GPU peers via pointer dereferencing in a unified virtual memory space. Their approach is focused only on BFS and adversely affects: a. programmability, as users must handle cross-GPU data access within main computation steps; c. hardware compatibility, by requiring GPUs with peer memory access capability; and d. performance, as accessing both local and remote vertices within the computation kernels introduces load imbalance.

Medusa [32] was the pioneering mGPU graph library, taking a more general approach. It partitions the graph using Metis [15], makes replications for neighbor vertices within n hops, and updates vertex-associated values every n iterations. Its shortcomings include: b. algorithm generality, because it cannot handle algorithms that jump beyond the n-hop limit, such as Soman et al.’s connected component algorithm [39]; d. performance, as reported performance values were low; and e. memory scalability, due to the replication caused by a large number of vertices within n hops of a partition boundary.

The parallel BFS work by Fu et al. [11] extends the expand-contract BFS algorithm by Merrill et al. to GPU clusters. They propose a 2D partitioning method, and use MPI to contract columns on the edge frontiers after each expand step. Their method has several disadvantages: b. algorithm generality, as it only works with graph algorithms with no data access beyond direct neighbors; c. hardware compatibility, because of its limitation to n^2 GPUs; and e. scalability, because of the large edge frontiers transmitted between GPUs, leading to heavy communication overheads.

Totem [13] is a graph processing engine for GPU+CPU hybrid systems. It either processes the workload on the CPU or transmits it to the GPU according to a performance estimation model. This approach has the potential to solve the long-tail problem on GPUs. However, it has limits in: b. algorithm generality, as it can only work with algorithms that only accesses direct neighbors; and d. scalability, as moving portions of the graph to GPU is a costly operation.

McLaughlin and Bader [22] targeted betweenness centrality (BC) on GPU clusters, which distributed BFS work for different source vertices to different nodes. It scales well in terms of performance, but still has limitations in: b. algorithm generality, as it only targets BC, which can utilize task parallelism in a way that other algorithms do not; and e. scalability, because it duplicates the graph on all GPUs, and cannot handle graphs bigger than the memory size of a single GPU.

To summarize, all existing multi-GPU graph analytics frameworks have at least one of the following shortcomings:

- **a Programmmability**: supporting multiple GPUs involves significant changes to a single-GPU implementation;
- **b Algorithm generality**: support for graph algorithms beyond a single algorithm or class of algorithms is limited...
or impossible;

c Hardware compatibility: requires peer accessible GPU memory, or \( n^2 \) GPUs;

d Performance: requires either a large amount of GPU memory and/or data communication between GPUs;

e Scalability: both performance and memory usage across GPUs; and

f Partitioner: requires either a simple method or Metis, and cannot be changed.

The multi-GPU graph analytics framework we present in this paper targets these goals.

3. MULTI-GPU GRAPH PROGRAMMING ABSTRACTION

Our philosophy in this work is to allow users to focus on specifying a broad range of high-level algorithms and let the implementation take care of the underlying parallelization and communication details. Thus we made the following design decisions:

1. The graph partitioner should be changeable, and the rest of the library should work regardless of how the graph is partitioned. We observe that no suitable partitioner targets all graph algorithms well, and wish to allow users to select any existing partitioner or implement their own.

2. The mGPU related implementation should be transparent to the computation kernels, which should work as they do on a single GPU. This isolation not only simplifies the 1GPU to mGPU transformation, but also allows optimizations to benefit both single and multiple GPU environments.

The mGPU layer of Gunrock uses a block design, which is illustrated in Fig. 1. A block here is a group of operations for a specific purpose, and it is often implemented as a function in practice. During each iteration, we unpackaged the received data package (except on iteration 1), pass the input frontiers though sub-queue or full-queue kernels, and split the output frontier into local and remote ones used for the next iteration. A user of the library only needs to formulate a graph primitive into one or more iteration loops, specify the following inputs, and the framework handles the rest.

Partitioner Selected by the user from the list in Section[5,6] If appropriate, users can also pass some parameters to the partitioner.

Computation kernels The implementation of graph algorithms, such as a group of advance, filter or computation kernels; this is the core of the graph algorithm, and is identical to Gunrock’s single-GPU implementation. Users set kernels to be either full-queue (applicable to all algorithms) or sub-queue (only applicable if a local/remote input frontier can be processed regardless of whether other local/remote input frontiers are ready).

Data packaging Which values associated with vertices need to communicate across GPUs?

Data unpackaging How should received data be combined with local values?

![Figure 1: Block design of the mGPU layer.](image)

**Convergence condition** When should the iteration loop stop? Normally it stops when errors occur at any GPU, or there is no more work to do for all GPUs.

For example, assuming the distance from the source vertex is stored as label values for all vertices, the mGPU BFS is:

**Algorithm 1 Multi-GPU Breadth-First-Search**

1. **Partitioner**: graph partition with any partitioner
2. **Computation kernels**: an advance and a filter step, identical to the single-GPU implementation, to serve as the “sub-queue kernels” block;
3. **Data packaging**: combine the label together with the remote vertices when pushing to peers;
4. **Data unpackaging**: for a vertex, if the received label is smaller than the local one, update the local label; otherwise mark the vertex as “do not process” in the remote input frontier;
5. **Convergence condition**: stop if errors occur on any GPU, or if there are no more vertices in any input frontier and there is no data package in preparation, transmission or waiting for unpackaging.

We describe the implementation details of the framework in the next section.

4. IMPLEMENTATION

We present the implementation details of the mGPU layer in this section, including graph partitioning, the iteration loop, a multi-threads/streams optimization, and a just-enough automatic memory reallocation scheme.

4.1 Partitioning of Input Graphs

At the beginning of the block design, a user-selected graph partitioner assigns the vertices to different GPUs, and
processes local vertex \( v \) of the original graph. The initial step converts it to sub-graphs. Suppose the source vertex is \( v \) on GPU0. BFS illustrates how an algorithm runs using the vertices and their labels. In iteration 1, GPU0 processes local vertex \( v_0 \), and marks labels of \( v_3 \), \( v_4 \), and \( v_5 \) as 1; since these vertices are all hosted on GPU1, they are converted to \( v_3 \), \( v_4 \) and \( v_5 \), and transmitted to GPU1, together with their labels. In iteration 2, GPU1 processes local vertices \( v_0 \), \( v_1 \), and \( v_2 \), and marks the labels for \( v_4 \), \( v_5 \), \( v_6 \) and \( v_3 \) as 2; \( v_2 \), \( v_3 \) and \( v_6 \) then get converted to \( v_0 \), \( v_1 \), \( v_2 \), and transmitted to GPU0 with labels 2. However, since the label for \( v_0 \) on GPU0 is 0, it will not be updated to 2, and \( v_0 \) will not appear in the input frontier for the next iteration. Iterations continue until all frontiers are empty.

### 4.2 The Iteration Loop

The key component of the block design is an iteration loop. Gunrock uses a bulk synchronous parallel model, and processes graph algorithms in iterations. For most algorithms, the mGPU BFS algorithm follows the iteration loop and computation kernels are placed in sub-queue or full-queue kernel blocks. At the beginning of each iteration, local and remote input frontiers will go through the sub-queue kernels in parallel. The output sub-frontiers are then merged, and go through the full-queue kernels.

At this point, the algorithm will check the convergence condition to decide whether the iteration loop should stop. Users can specify their own stop conditions. The stop condition is slightly more complex compared to the single GPU case. On a single GPU, an empty frontier means there is no more work to do, and the loop should stop. But for mGPU, peer GPUs may push new frontier elements to a GPU that has empty frontiers. The stop condition hence needs to guarantee there is no current or future workload on any GPU or in transmission. Generally, an algorithm stops if an error is reported by any GPU; and it continues if 1) any GPU has ongoing work or an non-empty input queue, 2) any GPU has outgoing data package to its peers, or 3) any GPU has received but not yet processed a data package.

If the loop continues, it will separate the local and remote vertices in the output frontier according to the local partition tables. The default separation process first marks a table to indicate whether each vertex in the output frontier is hosted on individual GPUs, then performs a multiple prefix sum on that table to get the positions of vertices in their corresponding remote output or local input frontiers, and finally writes the vertices to those frontiers. Local input frontiers will be used for the next iteration, and the remote ones will go through the data packaging process for vertex ID conversion and user-specified value attachment before being pushed to peer GPUs. Users can create their own separate blocks as well, such as PageRank’s block to put all vertices in the remote output frontiers by default.

At the other end, the peer GPU will check whether data packages have been received, and unpack them if they have. The unpackaging step is algorithm-specific: for BFS-like algorithms, it will update the local copy of vertex associated values, and output the frontier received from the peer GPU to the sub-queue kernel; for some other algorithms, like connected component, it will only update the vertex associated values, and output an empty frontier.

As mentioned before, the main computation steps can be placed at the sub-queue or the full-queue kernel blocks. It is always safe to use the full-queue option, since that will force the framework to wait for updates from all peers before proceeding with the computation. However, if the computation on local input frontiers does not depend on updated values from peers, then it can be placed in the sub-queue kernels block to expose more concurrency. For instance, the BFS algorithm can proceed on the local frontier without updates from peer GPUs. A vertex will only need to go through the computation again if a smaller label value for it is received from peer GPUs. A vertex will only need to go through the data packaging process for vertex ID conversion and user-specified value attachment before being pushed to peer GPUs. Users can create their own separate blocks as well, such as PageRank’s block to put all vertices in the remote output frontiers by default.

This guarantees the smaller values are the only effective ones after the merge step at the price of slightly more workload.

### 4.3 Multiple Threads, Multiple Streams and Synchronization

Gunrock uses dedicated CPU threads to control each GPU. Within the iteration loop, CPU threads monitor the status of all GPU operations, including API calls and kernel launches. Once an error occurs on any GPU, all CPU threads will break from their loop and the whole program exits. This mechanism effectively prevents locking caused by GPUs waiting on peers that encounter errors. The CPU threads also monitor the lengths of all frontiers, to provide them as parameters for GPU operations, and to judge whether the loop has finished.

Gunrock utilizes GPU streams to overlap computation and data movement. In Fig. 4, each column above the merge block is assigned to a dedicated GPU stream. All GPU operators in these columns are asynchronous, and there is no synchronization point in these blocks. This makes the GPU execution of each column independent, and enables the over-
GPU communication, the size is bounded by the number of vertices adjacent to the cross GPU edges, because mGPU Gunrock currently only communicates vertex frontiers, and no duplication can appear in the output frontiers.

Memory reallocation on GPU is expensive, because it needs to wait for all current tasks on the GPU to finish before performing the allocation/deallocation in a blocking manner, and only then re-enable the GPU for other operations. Knowing roughly how much memory is needed and providing this information to the library can reduce the number of reallocations. We notice that for a given algorithm, the memory requirement patterns are similar for graphs of the same kind. For instance, the required frontier sizes are \( \sim 8.2 \) times of the vertex count for BFS on road networks using 6 GPUs. The just-enough memory reallocation can make use of this information and do a preallocation at the initialization step. During the execution, if the preallocated size is not enough, auto-reallocation takes place, to guarantee the size of allocated memory is always enough.

In cases when the required memory sizes are known beforehand, the memory will be preallocated accordingly, and the size checking feature will be turned off, guaranteeing no reallocation will occur. Disabling size checking also enables some optimizations for better performance, such as removing the synchronization used to get the required frontier size on the CPU.

5. EVALUATION

We evaluate five graph primitives on our system: BFS, single-source shortest path (SSSP), single-source BC, connected components (CC), and PageRank. This set of primitives covers the most common basic graph analytic types mentioned in Section 4. The main purpose of the evaluation is to explore the performance and scalability of our graph analytics system, and analyze the factors affecting scalability.

Because primitives for BFS, SSSP and BC share a similar structure (all three are traversal-based primitives), and PageRank and CC are non-traversal-based graph primitives with a frontier of all vertices at the start, we use BFS to represent the former and CC to represent the latter in some analyses.

5.1 Testing Environment and Datasets

We run most tests on nodes with 6 NVIDIA Tesla K40 cards, a 10-core Intel Xeon E5-2690 v2, and 128 GB CPU memory, running on CentOS 6.4 with CUDA 7.0 (both driver and runtime) and gcc 4.7.3. We complete a small portion of the tests with 4 NVIDIA Tesla K80 cards (which feature two GPUs on one board, so 8 GPUs in total). We indicate which tests are performed on the latter. All programs are compiled with -O3 flag and set to target the actual streaming multiprocessor generation of the GPU hardware.

The dataset information is listed in Table 1 in six groups. Each contains graphs of a specific topology with various sizes. The real-world graphs are from the UF sparse matrix collection and the Network Data Repository. The “soc”, “web” and “road” groups are online social networks, web crawls of different domains, and road networks respectively. For SSSP, edge values are randomly generated from \([0, 64]\). We also include two types of synthesized graphs: R-MAT and random geometric graphs (RGG). We implement a R-MAT graph generator on top of the R-MAT generator in the GTgraph library, replacing the sprng
random number generator with the drand48 function. The R-MAT parameters are \( A = 0.57, B = 0.19, C = 0.19 \) and \( D = 0.05 \). Edge factors for the rmat_48 group is 48, the same as the Kronecker graphs commonly used. Edge factors for the rmat_2B group are selected to generate just under 2 billion edges (before self-loop and multiple edge removal). For RGG graphs, the vertices are randomly distributed points in the unit square. A pair of vertices are considered connected if the Euclidean distance is less than 0.55\( \sqrt{\log n/n} \), where \( n \) is the number of vertices in the graph. This threshold is chosen in order to ensure that the graph is almost connected [8]. Graphs in the “soc”, “web” and rmat groups follow the power-law distribution. Road networks and RGG graphs are more mesh-like with high diameters; here we call them high-diameter graphs.

All graphs we use in testing are converted to undirected graphs. Self-loops and duplicates of the same edge are removed from the graphs. Tests exceeding the single GPU memory limit are excluded from comparisons that use single-GPU results as the baseline. Our implementation does support graphs larger than a single GPU’s memory size, such as the \( ~15 \) GB rmat_n48 group as previous work for the single-node cases.

As shown in Fig. 3, we achieve 10.7 GTEPS when running mGPU Gunrock on 6 K40 GPUs for BFS, using rmat_n32_48. Our performance increases to 22.3 GTEPS using rmat_n20_1023. Our edge traversal rate outperforms all previous work on GPU BFS within a single node and is comparable to work on GPU clusters using more GPUs (Table 2). For comparison purposes, we use the same number of GPUs as previous work for the single-node cases.

PageRank in mGPU Gunrock shows linear scalability in both runtime and memory consumption on tests with 8 K80 GPUs (Fig. 4). For rmat_n22_48, it achieves 5.56x speedup.
with only 1.69x GPU memory usage as compared to a single GPU.

Strong and weak scaling are presented in Fig. 5. For
strong scaling, we use rmat_n22_48; for weak scaling, we use
R-MAT graphs with edge factor 48, and keep 180M edges on
each GPU. Comparing Fig. 4 and 5, we can see rmat_n22_48
still does not have enough work to saturate more than 4 K40s
for BFS (49.8% and 34.4% strong scaling factor for 4 and
6 K40s), and rmat_n20_1023 shows a better strong scaling
factor with 82.0%. Our BFS achieves a 40.6% weak scaling
factor, while PageRank shows 81.4% and 40.8% for strong
and weak scaling factors respectively.

Why does PageRank have a better strong scaling factor
than weak scaling factor? The cross-GPU communication
data package size is proportional to the number of vertices
in the graph, and the algorithm has both all-vertices and
all-edges operations. For strong scaling test cases, the number
of vertices is constant, so the communication overhead and
the time taken for all-vertices computation stays the same,
which helps PR scale well when the number of edges on each
GPU decreases. But for weak scaling tests, the number of
vertices increases, which not only increases the edge count
and all-edges computation workload, but also increases the
communication overhead and workload for all-vertices com-
putation.

In the rest of this section, we will analyze the test results
from different perspectives and identify the factors affecting
scalability, and discuss improvements that can be done to
further increase performance and scalability.

5.3 Impacts from Primitives

Communication latency is an issue with any distributed
system. GPUs are no exception: to achieve speedup, GPUs
require a large amount of data to hide latency. For this rea-
son, mGPU will generally show a performance gain for very
large frontiers with small overhead in mGPU-specific oper-
ations, such as data packaging, exchange, and unpackaging.

Fig. 6 shows the average speedup with error bars indicat-
ing the minima and the maxima for the five primitives. Four
primitives get 3 to 5 times speedup for the best cases (using
the R-MAT graphs), while SSSP gets 2. We also observe
that the speedup is primitive- and dataset-specific, and the
average performance improvement is only a few tens of per-
cent, except for PageRank. This low average is attributed
to results from high-diameter graphs, which we will discuss
in the next subsection. We compare BFS and PageRank to
show the difference in Fig. 7.

PageRank outperforms BFS on both power-law and high-
diameter graphs in terms of performance scalability (Fig. 7).
We believe the reasons are 1) the main body of PageRank-
based algorithms are operations on all vertices or all edges,
and this guarantees the working frontiers are always large,
even after distribution onto mGPUs; 2) the data commu-
Figure 8: Speedup of R-MAT (top) and RGG (bottom) graphs for five algorithms, with error bars indicating minima and maxima from different datasets of the same graph types.

The communication pattern is simple, because GPUs only need to push an associated value for each remote vertex to its hosting GPU. Given the frontiers are the same for all iterations in PageRank, the data communication can be achieved by a simple table lookup and a data movement operation.

On the contrary, BFS-based algorithms work on moving frontiers, and the frontier sizes are data-dependent. For datasets that can provide large frontiers most of the time, like rmat_48 and rmat_2B, enough workload can be sent to the GPUs to keep them fully occupied; but for datasets that generate small frontiers, GPUs are underutilized. The data communication pattern is more complex for this class of algorithms, as stated in Section 4.2—it requires marking, multiple prefix-sum computation, vertex ID conversion, and associated value packaging—before sending the remote output frontiers to peer GPUs. For small frontiers, the overhead of these operations is significant. These two factors together can make performance suffer on mGPU, as shown by the four primitives on the RGG dataset.

To overcome these two limits, a primitive needs to have large frontiers in most iterations, and simple operations for data exchange. The former is data-dependent, and can be achieved by either algorithm design or being able to guarantee there is enough data to saturate all the GPUs for most iterations. The latter may be achieved by sending the whole output frontier to all peer GPUs, but the tradeoff between computation and communication needs to be carefully studied.

5.4 Impacts from Datasets

Graph topologies also affect the frontier sizes and mGPU operation overhead. Fig. 8 shows the speedup of all primitives for R-MAT and RGG graphs, while Fig. 9 shows the frontier sizes per BFS iteration. Vertices in R-MAT graphs have high average out-degrees. This leads to huge frontiers for all GPUs in certain iterations, and those iterations account for most of the computation time. GPUs in these iterations are fully utilized. Diameters for R-MAT graphs are small, so the number of iterations for BFS-based algorithms are limited. This helps in reducing the total overhead of mGPU operations. Social networks, web graphs and other power-law graphs are similar to R-MAT graphs in these aspects. For web graphs, the diameters are about twice as high as social networks and R-MAT graphs; the mGPU operation overhead can be more significant, which may bring speedups down when more GPUs are used.

On the other hand, RGG graphs, as well as other high-diameter graphs like road networks, have a low average edge-to-vertex ratio. This means frontier sizes increase slowly, stay at around the same level, then come down slowly. The frontier never reaches a large enough size to fully utilize even a single GPU, so the utilization for mGPU is even worse. The high diameter also means high iteration counts for BFS-based algorithms, which amplifies the effect of mGPU operation overhead. Since frontiers are small, single-GPU computation is fast, so we see poor scalability on these graphs.

The average speedups are mostly close to the maxima in Fig. 8, which indicates the effect of dataset sizes. Only one or two datasets with small sizes in each group get about half of the average speedup; all other datasets have similar results. This shows that after some threshold, the speedup only has small variance for the same kind of graphs regardless of scale.

We considered that GPU-GPU communication bandwidth could be a bottleneck for good scalability. This is true if entire edge frontiers are transmitted, because their size can be extremely large (several hundred million for rmat_n23 and rmat_n24). However, if communication is only used on vertex frontiers, as in our mGPU framework, the transmitted frontier size is small (at most a few millions). Together with their associated values, the size of all data transmitted to/from one GPU at any iteration is generally under 100 MB, which only takes a few ms to pass through the PCIe 3.0 x 16 links. This constitutes a small portion of total computation time. But within a GPU cluster, the communication bandwidth is a more significant issue, as multiple GPUs on a node need to share the inter-node network, which has lower bandwidth and higher latency than PCIe links. We certainly anticipate that high-bandwidth, low-latency inter-node communication for GPUs is vital for good scalability on GPU clusters.

Exchange of a very small amount of data between GPU and CPU is a common occurrence for keeping track of GPU operation status and the resulted frontier sizes. It often happens that these frontier sizes are parameters to subsequent GPU operations, which imposes a synchronization requirement to get those sizes to the CPU. The cross-GPU data packages can also be small, for BFS-like algorithms on high-diameter graphs, as well as the first and last few
iterations of other graphs. It is not the bandwidth but instead the latency that plays the important role here. The NVLink CPU-GPU interface proposed for next generation GPUs, which has much less inter-GPU and CPU-GPU communication latency, is promising for alleviating these issues.

Graph topologies are not a factor that can be “solved” for better scalability. Nevertheless, techniques like hybrid CPU-GPU computing that only brings the GPU into action when the frontier size crosses a certain threshold may help.

5.5 Impacts from Memory Allocation Methods

Memory is another important aspect of mGPU scalability. Ideally, the total GPU memory consumption should be close to that on single GPU, but in practice extra memory is allocated for duplicated information, the partition table, transmission data package, etc. It is desirable that this additional memory usage is small, so that mGPU can deal with larger graphs. Graph problems impose a significant challenge on memory: the frontier sizes are unknown a priori. We implement a just-enough memory allocation scheme to deal with this issue. The effect of the scheme on BFS is shown in Fig. 10. We run tests under two conditions: 1) using minimum preallocation and auto-reallocation, and 2) using suitable preallocation size (as reported by the previous iteration) and turning off size-checking. The upper graph shows the speedup under testing condition 2 vs. 1, and the lower graph shows the respective memory usage comparison.

We can see that runtime improves significantly if no reallocation is required, but at the cost of using more memory. It gets about 2x speedup for power-law graphs when reallocation does not occur, but high-diameter graphs gain almost no benefit in performance. This is because the frontier sizes keep increasing for the first half of iterations on power-law graphs, which means reallocation happens for half of the iterations; but for high-diameter graphs, frontier size are mostly within a range, and reallocation only happens for a small number of iterations. The speedup is more significant if more GPUs are used, because a higher GPU count results in more arrays used, leading to more resizing for condition 1. The high speeds are contributed by the small datasets in each group, because the total runtime is small and the reallocation time can be a large fraction of that.

Currently we only profile the memory usage using two main factors: how much memory is required for frontiers and communication, both with respect to the number of vertices in the sub-graphs. Extra preallocation happens when these two factors are different across GPUs, and we will select the maximum. We cannot and should not compute different memory sizes for each individual GPU, because there is no guarantee from the partitioner that the same portion of graph will be assigned to the same GPU each time. What can be guaranteed is that these factors are similar for graphs of the same kind and can be used for the same primitives.

The results in other parts of this section are all taken with suitable size memory preallocated and size checking turned off. To our knowledge, no previous work has explored similar features like just-enough allocation.

Figure 11 shows the minimum memory usage as compared to using a single GPU. The average total usage is about 2 times for 6 GPUs. The large maxima are mostly for RGG graphs and road networks, which have low edge-to-vertex ratios. mGPU Gunrock duplicates vertices and associated values; these make up most of the additional memory usage on the aforementioned two graph types. But since the original single-GPU memory consumption is not high for these graphs (∼2.6GB for rgg_25), the high memory usage increase for these particular datasets is not a problem.

5.6 Impacts from Partitioner

We try different graph partitioning strategies to analyze their partitioning time as well as the impacts on algorithm runtime, workload redundancy, and memory usage. The partitioners are:

- **rand** Random partitioner: vertices are randomly assigned to GPUs;
- **static** Static partitioner: vertex v is assigned to GPUv mod #GPUs;
- **metis** the Metis partitioner with default settings;
- **brp** Bias random partitioner: the assignment is biased by how many neighbors have already been assigned to the GPUs, and it tends to put neighbors together. The par-
5.7 Discussion

From the above evaluations, we offer two general insights on evaluating multi-GPU graph analytics frameworks.

On Graph Primitives We see very different results regarding performance and scalability on different types of graph algorithms. PageRank, as a representative of non-traversal-based graph algorithms with dense computation, achieves high performance and approaches linear scalability on all datasets. This is because of its cross-iteration and cross-GPU load balancing and predictable memory access and control flow (the PageRank computation always visits all neighbors of an element). PageRank is a best-case scenario for scalability, and thus we submit that a full evaluation of a framework should also include graph algorithms with more workload irregularity and cross-GPU load imbalance.

On Graph Datasets Among the many synthesized and real-world datasets that we used for evaluation, we note that R-MAT graphs always yield the best peak performance and approach linear scalability. Although R-MAT was designed to represent the structure of scale-free graphs, our results suggest that it actually performs quite differently from other datasets, including real-world scale-free graphs, on which we achieve less ideal scalability, or even fail to scale at all. We submit that while R-MAT results can be used to show impressive numbers, graph analytics frameworks must demonstrate performance on a wide range of datasets for a proper evaluation.

6. CONCLUSIONS & FUTURE WORKS

Increasing graph sizes and a need to make graph processing faster provided the motivation to explore graph analytics on multiple GPUs. The size concern is particularly pressing for the limited memory space available in current GPUs. Our chief goals were generality (can target many graph algorithms), programmability (particularly a simple extension from single-GPU programs to the multi-GPU case), and scalability in performance and memory usage.

The most helpful decision we made was our unified framework for authoring a range of graph primitives, with high-level programmability for expressing the primitives and common components to extend these primitives to multiple GPUs. One challenge was the design of our abstraction that allowed both multi-GPU generality/programmability and scalable performance, but doing so both allowed straightforward extension from single to multiple GPUs as well as a higher level view of the key building blocks of a mGPU implementation, which operations are common to multiple algorithms, and what optimizations can be done at the framework level. As a result, improvements we make to the core of our framework apply to all graph primitives.

We see two key next steps. First, while we achieve good scalability on many graphs, many others do not scale well. How can we tackle these graphs from a systems perspective, whether that be GPU/platform hardware, system software, or our platform software? Second, can we achieve further scalability (scale-out) with multiple nodes, and given the increased latency and decreased bandwidth of those nodes, is it profitable to do so?
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