A Commodity Performance Baseline for HIVE Graph Applications:
Year 1 Report

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Chapter 1

HIVE Year 1 Report: Executive Summary

This report is located online at the following URL: https://gunrock.github.io/docs/hive_year1_summary.html.

Herein UC Davis produces the following three deliverables that it promised to deliver in Year 1:

1. **7–9 kernels running on a single GPU on DGX-1**. The PM had indicated that the application targets are the graph-specific kernels of larger applications, and that our effort should target these kernels. These kernels run on one GPU of the DGX-1. These kernels are in Gunrock's GitHub repository as standalone kernels. While we committed to delivering 7–9 kernels, we deliver 10 v0 kernels. Scan statistics is substantially done but the report is not complete and so we do not deliver it. Sparse graph lasso works on some inputs but requires more optimization in its maxflow component; we do include its report.
2. **(High-level) performance analysis of these kernels**. In this report we analyze the performance of these kernels.
3. **Separable communication benchmark predicting latency and throughput for a multi-GPU implementation**. This report (and associated code, also in the Gunrock GitHub repository) analyzes the DGX-1's communication capabilities and projects how single-GPU benchmarks will scale on this machine to 8 GPUs.

Specific notes on applications and scaling follow:

Application Classification

Application Classification Application classification involves a number of dense-matrix operations, which did not make it an obvious candidate for

implementation in Gunrock. However, our GPU implementation using the CUDA CUB library shows substantial speedups (10-50x) over the multi-threaded OpenMP implementations.

However, there are two neighbor reduce operations that may benefit from the kind of load balancing implemented in Gunrock. Thus, it would be useful to either expose lightweight wrappers of high-performance Gunrock primitives for easy intergration into outside projects *or* come up with a workflow inside of Gunrock that makes programming applications with lots of non-graph operations straightforward.

Geolocation

Geolocation Geolocation or geotagging is an interesting parallel problem, because it is among the few that exhibits the dynamic parallism pattern within the compute. The pattern is as follows; there is parallel compute across nodes, each node has some serial work and within the serial work there are sveral parallel math operations. Even without leveraging dynamic parallelism within CUDA (kernel launches within a kernel), Geolocation performs well on the GPU environment because it mainly requires simple math operations, instead of complicated memory movement schemes.

However, the challenge within the application is load balancing this simple compute, such that each processor has roughly the same amount of work. Currently, in gunrock, we map Geolocation using the `ForAll()` compute operator with optimizations to exit early (performing less work and fewer reads). Even without addressing load balancing issue with a complicated balancing scheme, on the HIVE datasets we achieve a 100x speedup with respect to the CPU reference code, implemented using C++ and OpenMP, and ~533x speedup with respect to the GTUSC implementation. We improve upon the algorithm by avoiding a global gather and a global synchronize, and using 3x less memory than the GTUSC reference implementation.

GraphSAGE

GraphSAGE The vertex embedding part of the GraphSAGE algorithm is implemented in the Gunrock framework using custom CUDA kernels, utilizing block-level parallelism, that allow a shorter running time. For the embedding part alone, the GPU implementation is 7.5X to 15X on P100, and 20X to 30X on V100, faster than an OpenMP implementation using 32 threads. The GPU hardware, especially the memory system, has high utilizations from these custom kernels. It is still unclear how to expose block-level parallelism for more general usage in other applications in Gunrock.

Connecting the vertex embedding with the neural network training part, and making the GraphSAGE workflow complete, would be an interesting task for

year 2. Testing on the complete workflow for prediction accuracy and running speed will be more meaningful.

GraphSearch

GraphSearch Graph search is a relatively minor modification to Gunrock's random walk application, and was straightforward to implement. Though random walks are a "worst case scenario" for GPU memory bandwidth, we still achieve 3–5x speedup over a modified version of the OpenMP reference implementation.

The original OpenMP reference implementation actually ran slower with more threads – we fixed the bugs, but the benchmarking experience highlights the need for performant and hardened CPU baselines.

Until recently, Gunrock did not support parallelism *within* the lambda functions run by the `advance` operator, so neighbor selection for a given step in the walk is done sequentially. Methods for exposing more parallelism to the programmer are currently being developed via parallel neighbor reduce functions.

In an end-to-end graph search application, we'd need to implement the scoring function as well as the graph walk component. For performance, we'd likely want to implement the scoring function on the GPU as well, which makes this a good example of a "Gunrock+X" app, where we'd need to integrate the high-performance graph processing component with arbitrary user code.

Community Detection (Louvain)

Community Detection (Louvain) The Gunrock implementation uses sort and segmented reduce to implement the Louvain algorithm, different from the commonly used hash table mapping. The GPU implementation is about ~1.5X faster than the OpenMP implementation, and also faster than previous GPU works. It is still unknown whether the sort and segmented reduce formulation map the problem better than hash table on the GPU. The modularities resulting from the GPU implementation are within small differences as the serial implementation, and are better when the graph is larger. A custom hash table can potentially improve the running time. The GPU Louvain implementation should have moderate scalability across multiple GPUs in an DGX-1.

Local Graph Clustering (LGC)

Local Graph Clustering (LGC) This variant of local graph clustering (L1 regularized PageRank via FISTA) is a natural fit for Gunrock's frontier-based programming paradigm. We observe speedups of 2-3 orders of magnitude over the HIVE reference implementation.

The reference implementation of the algorithm was not explicitly written as `advance`/`filter`/`compute` operations, but we were able to quickly determine how to map the operations by using a lightweight Python implementation of the Gunrock programming API as a development environment. Thus, LGC was a good exercise in implementing a non-trivial end-to-end application in Gunrock from scratch.

Graph Projections

Graph Projections Because it has a natural representation in terms of sparse matrix operations, graph projections gave us an opportunity to compare ease of implementation and performance between Gunrock and another UC-Davis project, GPU GraphBLAS.

Overall, we found that Gunrock was more flexible and more performant than GraphBLAS, likely due to better load balancing. However, in this case, the GraphBLAS application was substantially easier to program than Gunrock, and also allowed us to take advantage of some more sophisticated memory allocation methods available in the GraphBLAS cuSPARSE backend. These findings suggest that addition of certain commonly used API functions to Gunrock could be a fruitful direction for further work.

Seeded Graph Matching (SGM)

Seeded Graph Matching (SGM) SGM is a fruitful workflow to optimize, because the existing implementations were not written with performance in mind. By making minor modifications to the algorithm that allow use of sparse data structures, we enable scaling to larger datasets than previously possible.

The application involves solving a linear assignment problem (LSAP) as a subproblem. Solving these problems on the GPU is an active area of research – though papers have been written describing high-performance parallel LSAP solvers, reference implementations are not available. We implement a GPU LSAP solver via Bertsekas' auction algorithm, and make it available as a standalone library.

SGM is an approximate algorithm that minimizes graph adjacency disagreements via the Frank-Wolfe algorithm. Certain uses of the auction algorithm can introduce additional approximation in the gradients of the Frank-Wolfe iterations. An interesting direction for future work would be a rigorous study of the effects of this kind of approximation on a variety of different graph tolopogies. Understanding of those dynamics could allow further scaling beyond what our current implementations can handle.

Sparse Fused Lasso

Sparse Fused Lasso The SFL problem is mainly divided into two parts, computing residual graphs from maxflow and renormalizing the weights of the vertices. Maxflow is parallelizable with the push-relabel algorithm, so we adopt this algorithm in Gunrock's implementation. Moreover, each vertex has its own work to compute which communities it belongs to, and normalize the weights with other vertices in the same community. This renormalization requires global synchronization. SFL iterates by calling maxflow and renormalization several times before it converges. We notice that the overall runtime is mostly spent in maxflow, and thus improving the maxflow implementation will bring substantial speedup in the SFL.

Because of the current state of our maxflow implementation, we notice a 30x slowdown of Gunrock's GPU SFL with respect to the benchmark implementation. This slowdown is mainly caused by the parallel push-relabel implementation taking too many iterations to converge, and making SFL kernel launching overhead-bound. We are looking into algorithmic optimizations to reduce the number of iterations maxflow takes, and also engineering optimizations to reduce the effects of kernel overheads in computation time.

Vertex Nomination

Vertex Nomination The term "vertex nomination" covers a variety of different node ranking schemes that fuse "content" and "context" information. The HIVE reference code implements a "multiple-source shortest path" context scoring function, but uses a very suboptimal algorithm. By using a more efficient algorithm, our serial CPU implementation achieves 1-2 orders of magnitude speedup over the HIVE implementation and our GPU implementation achieves another 1-2 orders of magnitude on top of that. Implementation was straightforward, involving only a small modification to the existing Gunrock SSSP app.

Scaling analysis for HIVE applications

Scaling analysis for HIVE applications

Application	Computation to communication ratio	Scalability	Implementation diff.
Louvain	E/p : 2V	Okay	Hard
Graph SAGE	~ CF : min(C, 2p)x4	Good	Easy
Random walk	Duplicated graph: infinity	Perfect	Trivial
Random walk	Distrib. graph: 1 : 24	Very poor	Easy
Graph search: Uniform	1 : 24	Very poor	Easy
Graph search: Greedy	Straightforward: d : 24	Poor	Easy
Graph search: Greedy	Pre-visit: 1:24	Very poor	Easy

Application	Computation to communication ratio	Scalability	Implementation diff.
G.S.: Stochastic greedy	Straightforward: d : 24	Poor	Easy
G.S.: Stochastic greedy	Pre-visit: log(d) : 24	Very poor	Easy
Geolocation	Explicit movement: 25E/p : 4V	Okay	Easy
Geolocation	UVM or peer access: 25 : 1	Good	Easy
Vertex nomination	E : 8V x min(d, p)	Okay	Easy
Scan statistics	Duplicated graph: infinity	Perfect	Trivial
Scan statistics	Distrib. graph: ~ (d + a * log(d)) : 12	Okay	Easy
Sparse fused lasso	~ a:8	Less than okay	Hard
Graph projection	Duplicated graph : infinity	Perfect	Easy
Graph projection	Distrib. graph : dE/p + E' : 6E'	Okay	Easy
Local graph clustering	(6 + d)/p : 4	Good	Easy

Seeded graph matching and application classification are matrix-operation-based and not covered in this table.

From the scaling analysis, we can see these workflows can be roughly grouped into three categories, by their scalabilities:

Good scalability GraphSAGE, geolocation using UVM or peer accesses, and local graph clustering belong to this group. They share some algorithmic signatures: the whole graph needs to be visited at least once in every iteration, and visiting each edge involves nontrivial computation. The communication costs are roughly at the level of V. As a result, the computation vs. communication ratio is larger than E : V. PageRank is a standard graph algorithm that falls in this group.

Moderate scalability This group includes Louvain, geolocation using explicit movement, vertex nomination, scan statistics, and graph projection. They either only visit part of the graph in an iteration, have only trivial computation during an edge visit, or communicate a little more data than V. The computation vs. communication is less than E : V, but still larger than 1 (or 1 operation : 4 bytes). They are still scalable on the DGX-1 system, but not as well as the previous group. Single source shortest path (SSSP) is an typical example for this group.

Poor scalability Random walk, graph search, and sparse fused lasso belong to this group. They need to send out some data for each vertex or edge visit. As a result, the computation vs communication ratio is less than 1 (or 1 operation : 4 bytes). They are very hard to scale across multiple GPUs. Random walk is an typical example.

Chapter 2

Application Classification

The application classification (AC) workflow is an implementation of probabalistic graph matching via belief propagation. The workflow takes two node- and edge-attributed graphs as input – a data graph `G = (U_G, E_G)` and a pattern graph `P = (U_P, E_P)`. The goal is to find a subgraph `S` of `G` such that the dissimilarity between the node/edge features of `P` and `S` is minimized. The matching is optimized via loopy belief propagation, which consists of iteratively passing messages between nodes then updating beliefs about the optimal match.

Summary of Results

Application classification involves a number of dense-matrix operations, which did not make it an obvious candidate for implementation in Gunrock. However, our GPU implementation using the CUDA CUB library shows substantial speedups (10-50x) over the multi-threaded OpenMP implementations.

However, there are two neighbor reduce operations that may benefit from the kind of load balancing implemented in Gunrock. Thus, it would be useful to either expose lightweight wrappers of high-performance Gunrock primitives for easy intergration into outside projects *or* come up with a workflow inside of Gunrock that makes programming applications with lots of non-graph operations straightforward.

Summary of CUDA Implementation

We implement application classification from scratch in CUDA using CUB rather than Gunrock. Application classification requires the following kernels:

- compute pairwise distance between rows of dense matrices
- normalize the columns of a dense matrix
- compute maximum of columns in a dense matrix
- gather/scatter rows of dense matrix

- sum/max neighborhood reduce on the data/pattern graphs

Apart from the last one, these kernels do not obviously map to Gunrock's advance/filter model.

Pseudocode for the core belief propagation algorithm is as follows:

```
for iteration in range(num_iterations):

    # Update edge messages
    edge_msg_f = diff_r[data_edges.srcs] - edge_distances # data.num_edges x pattern.num_ed
    edge_msg_r = diff_f[data_edges.srcs] - edge_distances # data.num_edges x pattern.num_ed

    # Normalize edge messages
    edge_msg_f = normprob(edge_msg_f)
    edge_msg_r = normprob(edge_msg_r)

    # Max of forward/backward messages
    f_null = columnwise_max(diff_f)                          # 1 x pattern.num_edges
    r_null = columnwise_max(diff_r)                          # 1 x pattern.num_edges
    for edge_idx, (src, dst) in enumerate(data_edges):
        max_r[src] = max(max_r[src], edge_msg_r[edge_idx], f_null)
        max_f[dst] = max(max_f[dst], edge_msg_f[edge_idx], r_null)

    # Update beliefs
    belief = - node_distances                                # data.num_nodes x patt.num_node
    for edge_idx, (src, dst) in enumerate(pattern_edges):
        belief[:,dst] += max_f[:,edge_idx]
        belief[:,src] += max_r[:,edge_idx]

    # Normalize beliefs
    belief = normprob(belief)

    diff_f = belief[:,pattern_edges.dsts] - max_f          # data.num_nodes x pattern.num_e
    diff_r = belief[:,pattern_edges.srcs] - max_r          # data.num_nodes x pattern.num_e
```

where `normprob` is the column-wise log-softmax function. That is, since `belief` is `data.num_nodes x patt.num_nodes`, each node in the `pattern` graph gets assigned a probability distribution over nodes in the `data` graph.

Our implementation is based on the PNNL implementation rather than the distributed GraphX reference implementation. On all of the graphs we've tested, the output of our implementation exactly matches the output of the PNNL code. According to PNNL, their implementation may give different results than the HIVE reference implementation (due to e.g., different normalization schemes).

How To Run This Application on DARPA's DGX-1

Prereqs/input

```
git clone --recursive \
        https://github.com/owensgroup/application_classification
cd application_classification
make clean
make
```

Running the application

Example Command

```
mkdir -p results
./main \
    ./data/georgiyData.Vertex.csv \
    ./data/georgiyData.Edges.csv \
    ./data/georgiyPattern.Vertex.csv \
    ./data/georgiyPattern.Edges.csv > results/georgiy
```

Example output

```
$ head -n 5 results/georgiy
-8.985810e+00
-3.859019e+01
-4.470994e+01
-1.673157e+01
-1.730952e+01
$ tail -n 5 results/georgiy
-2.886186e+01
-1.499165e+01
-4.034595e+01
-1.060496e+01
-7.684015e+00
$ cat results/georgiy | openssl md5
(stdin)= bd57a5126d5f943ad5c15408d410790d
```

Expected Output

The output of the program is a `data.num_nodes x pattern.num_nodes` matrix, where each column represents a log-probability distribution of assignments of pattern node `j` to data node `i`. This matrix is printed in row major order as a file with `data.num_nodes x pattern.num_nodes` lines.

In python, you could inspect the output like:

```
import numpy as np

# load results
x = open('./results/georgiy').read().splitlines()
x = [float(xx) for xx in x]

# reshape to (data.num_nodes, pattern.num_nodes)
x = np.reshape(x, (1000, 10))

# exponentiate
x = np.exp(x)

# columns should sum to 1
x.sum(axis=0)
# array([1.0000001 , 1.00000001, 1.00000004, 0.99999999, 0.99999988,
       # 0.99999994, 0.99999985, 1.00000001, 1.        , 0.99999988])
```

As previously mentioned, our output exactly matches the output of the PNNL implementation on all of the graphs we have tested.

Performance and Analysis

We measure performance by runtime of the algorithm given

- a node- and edge-attributed data graph
- a node- and edge-attributed pattern graph

Though AC computes probabilities of matches between data and pattern nodes, this is a deterministic and parameterless algorithm, so we do not measure performance in terms of accuracy. Further, runtime does not depend on the *values* of the node/edge attributes, so we can reasonably run experiments using randomly generated values.

Implementation limitations

As currently implemented, the algorithm allocates a number of arrays of floats:

- 3 arrays of size `data.num_edges * pattern.num_edges`
- 3 arrays of size `data.num_nodes * pattern.num_edges`
- 2 arrays of size `data.num_nodes * pattern.num_nodes`

The combined memory usage of these arrays will be the primary bottleneck for scaling. For example, if

- data.num_nodes = 6M
- data.num_edges = 18M
- pattern.num_nodes = 10
- pattern.num_edges = 20

then the memory footprint will be on the order of 13 GB. (*Note:* It's likely that reordering of operations could reduce the number of intermediate data structures required.)

AC is only applicable to graphs with node and edge features. However, the runtime of the algorithm is only dependent on the *dimension* of these features, rather than the values. Thus, for benchmarking purposes, we can pick a `node_feature_dim` and `edge_feature_dim` and use randomly generated features. This is helpful becaus we do not have a good real-world dataset for benchmarking.

The algorithm requires both a data graph and a smaller pattern graph. Both the size and topology of the pattern graph may affect the runtime of the algorithm. However, we do not have examples of actual pattern graphs apart from `georgiyPattern`, so we are forced to generate them synthetically. Specifically, we do this by sampling a node `q`, sampling up to `max_pattern_nodes` number of `u` to form set `Q`, and using the subgraph induced by `Q + q` as the pattern graph.

We suspect the PNNL implementation may have a couple of minor bugs:

- the `CV` matrix is log-softmax normalized in the initialization phase, updated with values from `FMax` and `RMax`, and log-softmax normalized again. This kind of double normalization seems strange, and is perhaps incorrect.
- In our `RepeatColumnsByDataEdges`, `FE` and `RE` both use the `src` of an edge, which conflicts with the algorithm description in the paper. One of these should probably be using the `src` and the other the `dst`.

These bugs are easy to fix, but we left them "as is" because a) we have no easy way to verify which is correct and b) we'd like consistency of results w/ the PNNL implementation.

Comparison against existing implementations

The original reference implementation consisted of a large amount of distributed Spark and GraphX Scala code. For ease of implementation, and to make sure performance comparisons are meaningful, we instead based our implementation on the PNNL ApplicationClassification OpenMP code.

Overall, the CUDA implementation is between 10x and 100x faster than the best run of the PNNL OpenMP code.

We compare our CUDA implementation to PNNL's C++ OpenMP implementation on several different graphs:

georgiyData

- a small graph included w/ real (source unknown) node/edge features (included in PNNL repo)
- `|U|=1000 |E|=20135 node_feat_dim=13 edge_feat_dim=17`

rmat18

- a scale 18 RMAT synthetic graph w/ random node/edge features (included in PNNL repo)
- `|U|=262145 |E|=2008660 node_feat_dim=13 edge_feat_dim=17`

JohnsHopkins_random

- Social network graph w/ random node/edge features
- `|U|=5157 |E|=186572 node_feat_dim=12 edge_feat_dim=16`

For the first two, we use the `georgiyPattern` pattern graph included in the PNNL repo. For the latter, we generate a pattern graph using the neighborhood induction mentioned above.

georgiyData

implementation	threads	elapsed_ms
PNNL OpenMP	1	1635.774136
PNNL OpenMP	2	1405.072927
PNNL OpenMP	4	1005.914927
PNNL OpenMP	8	831.342936
PNNL OpenMP	16	793.069839
PNNL OpenMP	32	546.305180
PNNL OpenMP	64	706.761122
Our CUDA	1xP100	**42.533**

Takeaway: Our CUDA implementation is approximately 12.8x faster than the fastest OpenMP run (32 threads). However, this problem is quite small and both implementations run in under 1 second.

rmat18

implementation	threads	elapsed_ms
PNNL OpenMP	1	113337.949038
PNNL OpenMP	2	142036.607981
PNNL OpenMP	4	109564.634800
PNNL OpenMP	8	95680.689096
PNNL OpenMP	16	87083.579063
PNNL OpenMP	32	88772.798061
PNNL OpenMP	64	82495.028973
Our CUDA	1xP100	**827.573**

Takeaway: Our CUDA implementation is approximately 99x faster than the fastest PNNL run (64 threads). The absolute magnitude of the differences is much more substantial here – the CUDA implementation runs in < 1 second while the OpenMP version runs in ~ 1.5 minutes.

JohnsHopkins_random

implementation	threads	elapsed_ms
PNNL OpenMP	1	71190.566063
PNNL OpenMP	2	44293.390989
PNNL OpenMP	4	31736.392021
PNNL OpenMP	8	24292.662144
PNNL OpenMP	16	21556.239128
PNNL OpenMP	32	17082.650900
PNNL OpenMP	64	19473.608017
Our CUDA	1xP100	**450.897**

Takeaway: Our CUDA implementation is approximately 37x faster than the fastest PNNL run (32 threads). Again, the absolute difference in runtimes is more substantial, with our code running in < 1 second vs. ~ 20 seconds.

Performance limitations

Profiling (on the RMAT graph) reveals that the distribution of runtime over kernels is flatter in AC than for many applications – often, a single kernel will account for $> 80\%$ of runtime, but here the most expensive kernel only accounts for 12.8% of compute time.

- 12.8% of time spent in `__reorderColumns`, which is a gather/scatter operation (memory bandwidth = 281 GB/s)
- 10.5% of time spent in `__transpose`
- 12.1% of time spend in `__rowSubLog`, an edgewise arithmetic operation

- 9.5% of time computing `data.num_edges x pattern.num_edges` similarity matrix
- 8.1% of time doing neighborhood reductions (293 GB/s)

All of these are memory bound operations.

As mentioned above, the memory use of the app could be reduced (if need be) by reducing the number of intermediate data structures. This would come at the cost of increased (re)computation time.

Next Steps

Alternate approaches + Gunrock implications

In the CUDA implementation, there are a number of places where we could take advantage of multiple streams to reduce runtimes. For example, in the initialization phase, we compute the pairwise distance between a) data/pattern node features and b) data/pattern edge features. These operations are completely independent of one another, and so could happen asynchronously on different streams.

The application was implemented outside of the Gunrock framework because it had a large number of (dense matrix) operations that are not explicitly supported by Gunrock, and a relatively small number of kernels that map well to Gunrock's advance/filter paradigm. However, the code uses CUB's `DeviceSegmentedReduce` a number of times – Gunrock recently added a similar operator that is load-balanced for better performance. In the future, it would be worthwhile to see what kind of speedup we could get from the Gunrock version, which should roughly be a drop-in replacement.

Notes on multi-GPU parallelization

Most of the kernels are either row or column operations (reductions) over dense matrices, and thus relatively easy to partition over multiple nodes. They would either end up being embarrassingly parallel or would require a per-node reduction and then a reduction across nodes. Replacing CUB's `DeviceSegmentedReduce` with Gunrock's implementation would give us multi-GPU support for the remaining kernel.

Alternatively, depending on the topology of the graph, we may be able to partition the data graph so that we can duplicate the pattern graph across nodes and run an independent instance of application classification on each partition. The partition would need to be constructed in a way that ensures that every subgraph is intact on *some* GPU, which implies some partial duplication of the data graph. If the data graph has a large diameter, or the pattern graph has a small diameter, this may be possible without excessive duplication. If the data graph has a small diameter, we may still be able to partition the graph by

e.g. removing edges that are particularly dissimilar from edges in the pattern graph. This kind of approach is clearly very application specific, and may not be possible at all in some cases.

Notes on dynamic graphs

In practice, it's likely that practitioners would like to run application classification on a dynamic graph (e.g., the HIVE use case was for detecting certain suspicious patterns of communication in a cybersecurity graph). However, it is not obvious how the current algorithm would be applied in a streaming fashion without relatively major modifications. It's more likely that the current AC algorithm would be applied to a dynamic graph via some kind of sliding window.

Notes on larger datasets

We may be able to use a partitioning scheme like the one described in the multi-GPU section above to handle data graphs that are larger than GPU memory.

Notes on other pieces of this workload

The documentation on the wiki includes discussion of the various featurization methods used to produce the node/edge attributes. These are beyond the scope of this work, but do include things such as computing degree, number of triangles, betweenness centrality, etc. If we wanted to build a high-performance end-to-end application classification system, we would want to implement some of these featurization methods in Gunrock as well.

Chapter 3

Geolocation

Infers user locations using the location (latitude, longitude) of friends through spatial label propagation. Given a graph `G`, geolocation examines each vertex `v`'s neighbors and computes the spatial median of the neighbors' location list. The output is a list of predicted locations for all vertices with unknown locations.

Summary of Results

Geolocation or geotagging is an interesting parallel problem, because it is among the few that exhibits the dynamic parallism pattern within the compute. The pattern is as follows; there is parallel compute across nodes, each node has some serial work and within the serial work there are sveral parallel math operations. Even without leveraging dynamic parallelism within CUDA (kernel launches within a kernel), Geolocation performs well on the GPU environment because it mainly requires simple math operations, instead of complicated memory movement schemes.

However, the challenge within the application is load balancing this simple compute, such that each processor has roughly the same amount of work. Currently, in gunrock, we map Geolocation using the `ForAll()` compute operator with optimizations to exit early (performing less work and fewer reads). Even without addressing load balancing issue with a complicated balancing scheme, on the HIVE datasets we achieve a 100x speedup with respect to the CPU reference code, implemented using C++ and OpenMP, and ~533x speedup with respect to the GTUSC implementation. We improve upon the algorithm by avoiding a global gather and a global synchronize, and using 3x less memory than the GTUSC reference implementation.

Summary of Gunrock Implementation

There are two approaches we took to implement Geolocation within gunrock:

- [**Fewer Reads**] **Global Gather:** uses two `compute` operators as `ForAll()`. The first `ForAll()` is a `gather` operation, gathering all the values of neighbors with known locations for an active vertex `v`, and the second `ForAll()` uses those values to compute the `spatial_center` where the spatial center of a list's points is the center of those points on the earth's surface.

```
def gather_op(Vertex v):
    for neighbor in G.neighbors(v):
        if isValid(neighbor.location):
            locations_list[v].append(neighbor.location)

def compute_op(Vertex v):
    if !isValid(v.location):
        v.location = spatial_center(locations_list[v])
```

- [**Less Memory**] **Repeated Compute:** skips the global gather and uses only one `compute` operator as a `ForAll()` to find the spatial center of every vertex. During the spatial center computation, instead of iterating over all valid neighbors (where valid neighbor is a neighbor with a known location), we iterate over all neighbors for each vertex, doing more random reads than the global gather approach, but using `3x` less memory.

```
def spatial_center(Vertex v):
    if !isValid(v.location):
        v.location = spatial_median(neighbors_list[v])
```

- [**Optimization**] **Early Exit:** fuses the global gather approach with the repeated compute, by performing one local gather for every vertex within the spatial center operator (without a costly device barrier), and exiting early if a vertex `v` has only one or two valid neighbors:

```
def spatial_center(Vertex v):
    if !isValid(v.location):
        if v.valid_locations == 1:
            v.location = valid_neighbor[v].location:
            exit
        else if v.valid_locations == 2:
            v.location = mid_point(valid_neighbors[v].location)
        else:
            v.location = spatial_median(neighbors_list[v])
```

Comparing Global Gather vs. Repeated Compute

Approach	Memory Usage	Memory Reads/Vertex	Device Barriers	Largest Dataset (P100)
Global Gather	O(3x[E])	# of valid locations	1	~160M Edges
Repeated Compute	O([E])	degree of vertex	0	~500M Edges

Note: `spatial_median()` is defined as center of points on earth's surface – given a set of points `Q`, the function computes the point `p` such that: `sum([haversine_distance(p, q) for q in Q])` is minimized. See `gunrock/app/geo/geo_spatial.cuh` for details on the spatial median implementation.

How To Run This Application on DARPA's DGX-1

Prerequisites

```
git clone --recursive https://github.com/gunrock/gunrock -b dev-refactor
cd gunrock
mkdir build
ctest ..
cd ../tests/geo/
make clean && make
```

HIVE Data Preparation

Prepare the data, skip this step if you are just running the sample dataset. Assuming we are in `tests/geo` directory:

```
export TOKEN= # get this Authentication TOKEN from
              # https://api-token.hiveprogram.com/#!/user
wget --header "Authorization:$TOKEN" \
  https://hiveprogram.com/data/_v0/geotagging/instagram/instagram.tar.gz
tar -xzvf instagram.tar.gz && rm instagram.tar.gz
cd instagram/graph
cp ../../generate-data.py ./
python generate-data.py
```

This will generate two files, `instagram.mtx` and `instagram.labels`, which can be used as an input to the geolocation app.

Running the application

Application specific parameters:

```
--labels-file
    file name containing node ids and their locations.
```

```
--geo-iter
    number of iterations to run geolocation or (stop condition).
    (default = 3)

--spatial-iter
    number of iterations for spatial median computation.
    (default = 1000)

--geo-complete
    runs geolocation for as many iterations as required
    to find locations for all nodes.
    (default = false because it uses atomics)

--debug
    Debug label values, this prints out the entire labels
    array (longitude, latitude).
    (default = false)
```

Example command-line:

```
# geolocation.mtx is a graph based on chesapeake.mtx dataset
./bin/test_geo_10.0_x86_64 --graph-type=market --graph-file=./geolocation.mtx \
  --labels-file=./locations.labels --geo-iter=2 --geo-complete=false
```

Sample input (labels):

```
% Nodes Latitude Longitude
39 2 2
1 37.7449063493 -122.009432884
2 37.8668048274 -122.257973253
4 37.869112506 -122.25910604
6 37.6431858915 -121.816156983
11 37.8652346572 -122.250634008
19 38.2043433677 -114.300341275
21 36.7582225593 -118.167916598
22 33.9774659389 -114.886512278
30 39.2598884729 -106.804662071
31 37.880443573 -122.230147039
39 9.4276164485 -110.640705659
```

Sample output:

```
Loading Matrix-market coordinate-formatted graph ...
Reading from ./geolocation.mtx:
  Parsing MARKET COO format edge-value-seed = 1539674096
 (39 nodes, 340 directed edges)...
Done parsing (0 s).
  Converting 39 vertices, 340 directed edges ( ordered tuples) to CSR format...
Done converting (0s).
Labels File Input: ./locations.labels
Loading Labels into an array ...
Reading from ./locations.labels:
  Parsing LABELS
 (39 nodes)
Done parsing (0 s).
Debugging Labels -------------
 (nans represent unknown locations)
    locations[ 0 ] = < 37.744907 , -122.009430 >
    locations[ 1 ] = < 37.866806 , -122.257973 >
    locations[ 2 ] = < nan , nan >
    locations[ 3 ] = < 37.869114 , -122.259109 >
     ...
    locations[ 35 ] = < nan , nan >
    locations[ 36 ] = < nan , nan >
    locations[ 37 ] = < nan , nan >
    locations[ 38 ] = < 9.427616 , -110.640709 >

---------------------------
______ CPU Reference _____
---------------------------
 Elapsed: 0.267029
Initializing problem ...
Number of nodes for allocation: 39
Initializing enactor ...
Using advance mode LB
Using filter mode CULL
nodes=39

---------------------------
0        0       0       queue3          oversize :      234 ->  342
0        0       0       queue3          oversize :      234 ->  342
---------------------------
Run 0 elapsed: 11.322021, #iterations = 2
Node [ 0 ]: Predicted = < 37.744907 , -122.009430 > Reference = < 37.744907 , -122.009430 >
Node [ 1 ]: Predicted = < 37.866806 , -122.257973 > Reference = < 37.866806 , -122.257973 >
Node [ 2 ]: Predicted = < 9.427616 , -110.640709 > Reference = < 9.427616 , -110.640709 >
Node [ 3 ]: Predicted = < 37.869114 , -122.259109 > Reference = < 37.869114 , -122.259109 >
...
Node [ 35 ]: Predicted = < 37.864429 , -122.199409 > Reference = < 37.864429 , -122.199409
Node [ 36 ]: Predicted = < 23.755602 , -115.803055 > Reference = < 37.807079 , -122.134163
```

```
Node [ 37 ]: Predicted = < 37.053715 , -115.913658 > Reference = < 37.053719 , -115.913628
Node [ 38 ]: Predicted = < 9.427616 , -110.640709 > Reference = < 9.427616 , -110.640709 >
0 errors occurred.
[geolocation] finished.
 avg. elapsed: 11.322021 ms
 iterations: 2
 min. elapsed: 11.322021 ms
 max. elapsed: 11.322021 ms
 load time: 68.671 ms
 preprocess time: 496.136000 ms
 postprocess time: 0.463009 ms
 total time: 508.110046 ms
```

Output

When `quick` mode is disabled, the application performs the CPU reference implementation, which is used to validate the results from the GPU implementation by comparing the predicted latitudes and longitudes of each vertex with the CPU reference implementation. Further correctness checking was performed by comparing results to the HIVE reference implementation.

Geolocation application also supports the `quiet` mode, which allows the user to skip the output and just report the performance metrics (note, this will run the CPU implementation in the background without any output).

Performance and Analysis

Runtime is the key metric for measuring performance for Geolocation. We also check for prediction accuracy of the labels, but that is a threshold for correctness. If a certain threshold is not met (while comparing results to the CPU reference code), the output is considered incorrect and that run is invalid. Therefore, for the report we just focus on runtime.

Implementation limitations

Geolocation is also one of the few applications that exhibits a dynamic parallelism pattern:

- Parallel compute across the nodes,
- Serial compute per node, and
- Parallel compute within the serial compute per node.

One way to implement this will use the `ForAll()` operator for the parallel compute across the nodes, a simple while loop for the serial compute per node, and finally multiple `neighbor_reduce()` operators for the parallel work within

the serial while loop. Currently, we do not have a way to support this within Gunrock, but moving forward we can potentially leverage kernel launch within a kernel ("dynamic parallelism") to address this limitation.

Comparison against existing implementations

GPU	Dataset	[V]	[E]	Iterations	Spatial Iters	GTUSC (16 threads)	Gunrock (CF
P100	sample	39	170	10	1000	N/A	0.144005
P100	instagram	23731995	82711740	10	1000	8009.491 ms	1589.884033
V100	twitter	50190344	488078602	10	1000	N/A	9216.666016

On a workload that fills the GPU, gunrock outperforms GT's OpenMP C++ implementation by ~533x. Comparing gunrock's GPU vs. CPU performance, we see that gunrock's GPU version outperforms the CPU implementation by 100x. There is a lack of available datasets against which we can compare performance, so we use only the provided instagram and twitter datasets, and a toy sample for a sanity check on NVIDIA's P100 with 16GB of global memory and V100 with 32GB of global memory. All tested implementations meet the criteria of accuracy, which is validated against the output of the original python implementation.

- HIVE reference implementation uses distributed PySpark.
- GTUSC implementation uses C++ OpenMP.

Performance limitations

As discussed later in the "Alternate approaches" section, the current implementation of geolocation uses a compute operator with minimal load balancing. In cases where the graph is not so nicely distributed (where there is a great deal of difference in the degrees of vertices), the entire application will suffer significantly from load imbalance.

Profiling the application shows 98.78% of the compute time in GPU activities is in the `spatial_median` kernel, which gives us a good direction to focus our efforts on load-balancing the workloads within the operator. Specifically, we must target the `for` loops iterating over the neighbor list for spatial center calculations.

Next Steps

Alternate approaches

- **Neighborhood Reduce w/ Spatial Center:** We can perform better load balancing by leveraging a neighbor-reduce (`advance` operator +

`cub::DeviceSegmentedReduce`) instead of using a compute operator. In graphs where the degrees of nodes vary a lot, the compute operator will be significantly slower than a load-balanced advance + segmented reduce.

- **Push Based Approach:** Instead of gathering all the locations from all the neighbors of an active vertex, we could instead perform a scatter of valid locations of all active vertices to their neighbors; this is a push approach vs. our current implementation's pull. Similar to the global gather approach, a push-based geolocation could also suffer from load imbalance, where some vertices will have to broadcast their valid locations to a long list of neighbors, while others will only have few neighbors to update. A push-based approach will also require a device synchronize before the spatial center computation, but may perform better by using an `advance_op` with an atomic update (note, pull is done using a `ForAll()`).

Gunrock implications

- **The `predicted` atomic:** Geolocation and some other applications exhibit the same behavior where the algorithm stops when all vertices' labels are predicted or determined. In Geolocation's case, when a location for all nodes is predicted, geolocation converges. We currently implement this with a loop and an atomic. This needs to be more of a core operation (mini-operator) such that when `isValidCount(labels|V|) == |V|`, a stop condition is met. Currently, we sidestep this issue by using a number-of-iterations parameter to determine the stop condition.

- **Parallel -> Serial -> Parallel:** As discussed earlier, gunrock currently doesn't have a way to address the dynamic parallelism problem, or even a kernel launch within a kernel. In geolocation's case, these minor parallel work inside the serial loop need to be multiple neighbor reduce.

Notes on multi-GPU parallelization

The challenging part for a multi-GPU Geolocation would be to obtain the updated node location from a separate device if the two vertices on different devices share an edge. An interesting approach here would be leveraging the P2P memory bandwidth with the new NVLink connectors to exchange a small amount of updates across the NVLink's memory lane; other ways are simply using direct accesses or explicit data movement. This is detailed more in the scaling documentation, but the communication model for multi-gpu geolocation could be done in the following way:

```
do
    Local geo location updates on local vertices;
    Broadcast local vertices' updates;
while no more update.
```

Notes on dynamic graphs

Streaming graphs is an interesting problem for the Geolocation application, because when predicting the location of a certain node, if another edge is introduced, the location of the vertex has to be recomputed entirely. This can still be done in an iterative manner, where if a node was inserted as a neighbor to a vertex, that vertex's predicted location will be marked invalid and during the next iteration it will be computed again along with all the other invalid vertices (locations).

Notes on larger datasets

If the datasets are larger than a single or multi-GPU's aggregate memory, the straightforward solution would be to let Unified Virtual Memory (UVM) in CUDA automatically handle memory movement.

Notes on other pieces of this workload

Geolocation calls a lot of CUDA math functions (`sin`, `cos`, `atan`, `atan2`, `median`, `mean`, `fminf`, `fmaxf`, etc.). Some of these micro-workloads can also leverage the GPU's parallelism; for example, a mean could be implemented using `reduce-mean/sum`. We currently don't have these math operators exposed within Gunrock in such a way they can be used in graph applications.

Research Potential

Further research is required to study Geolocation's dynamic parallelism pattern, it's memory access behavior, compute resource utilization, implementation details (API and core) and load balancing startegies for dynamic parallelism on the GPUs. Studying and understanding this pattern can allow us to create a more generalized approach for load balancing `parallel -> serial -> parallel` type of problems. It further invokes the question of studying when dynamic parallelism is better than mapping an alogirthm to a more conventional static approach (if possible).

Chapter 4

GraphSAGE

GraphSAGE is a way to fit graphs into a neural network: instead of getting the embedding of a vertex from all its neighbors' features as in conventional implementations, GraphSAGE selects some 1-hop neighbors, some 2-hop neighbors connected to those 1-hop neighbors, and computes the embedding based on the features of the 1-hop and 2-hop neighbors. The embedding can be considered as a vector containing hash values describing the interesting properties of a vertex.

During the training process, the adjacency matrix and features of the nodes in the graph are fed into a neural network. The parameters (the `W` arrays in the algorithm) are updated after each batch by the difference between the predicted labels and the real labels. The per-vertex features won't change, but the parameters will, so the GraphSAGE computation needs to be performed for each batch. Ultimately it should connect to the training process to complete a workflow. However, the training part is pure matrix operations, and the year 1 deliverable only focuses on the graph related portion, which is the GraphSAGE implementation.

Summary of Results

The vertex embedding part of the GraphSAGE algorithm is implemented in the Gunrock framework using custom CUDA kernels, utilizing block-level parallelism, that allow a shorter running time. For the embedding part alone, the GPU implementation is 7.5X to 15X on P100, and 20X to 30X on V100, faster than an OpenMP implementation using 32 threads. The GPU hardware, especially the memory system, has high utilizations from these custom kernels. It is still unclear how to expose block-level parallelism for more general usage in other applications in Gunrock.

Connecting the vertex embedding with the neural network training part, and making the GraphSAGE workflow complete, would be an interesting task for year 2. Testing on the complete workflow for prediction accuracy and running speed will be more meaningful.

Summary of Gunrock Implementation

Gunrock's implementation for the 1st year is only the embedding / inferencing phase, without the training phase. It is based on Algorithm 2 with K=2 of the GraphSAGE paper ("Inductive Representation Learning on Large Graphs", https://arxiv.org/abs/1706.02216).

Given a graph G, the inputs are per-vertex features, weight matrices W^k, and a non-linear activation function (ReLu); the output from GraphSAGE is the embedding vector of each vertex. The current Gunrock implementation randomly selects neighbors from the neighborhood, and simple changes to the code can enable other selection methods, such as weighted uniform, importance sampling (used by FaseGCN), or a random walk probability like DeepWalk or Node2Vec (used by PinSage). An aggregator is a function to accumulate data from the selected neighbors; the current implementation uses the Mean aggregator, and it can be changed to other accumulation functions easily.

The pseudocode of Gunrock's implementation follows. The current implementation uses custom CUDA kernels, because block-level parallelism is critical for faster running speed; all other functions, such as memory management, load and store routines, block level parallel reduction, and graph accesses (get degree, get neighbors, etc.) are provided by the framework or the utility functions of Gunrock. The GraphSAGE algorithm uses B2, B1 and B0 for the sources, the 1-hop neighbors and the 2-hop neighbors; for easier understanding of the code, we use `sources`, `children` and `leafs` for these three groups of vertices instead. To manage the memory usage of intermediate data, batches of source vertices are processed one by one, with each of size B.

```
source_start := 0;
While (source_source < V)
    num_sources := (source_start + B > V) ? V - source_start : B;

    // Kernel1: pick children and leafs
    For children# from 0 to num_children_per_source x num_sources:
        source := source_start + (children# / num_children_per_source);
        child := SelectNeighbor(source);
        leafs_feature := {0};
        For i from 1 to num_leafs_per_child:
            leaf := SelectNeighbor(child);
            leafs_feature += feature[leaf];

        children[children#] := child;
        leafs_features[children#] := leafs_feature;

    // Kernel2: Child-centric computation
    For children# from 0 to num_children_per_source x num_sources:
        child_temp := ReLu(concatenate(
```

```
            feature[children[children#]] x Wf1,
            Mean(leafs_features[children#]) x Wa1));
        child_temp /= sqrt(sum(child_temp));
        children_temp    [children# / num_children_per_source] += child_temp;
        children_features[children# / num_children_per_source] += feature[child];

    // Kernel3: Source-centric computation
    For source# from 0 to num_sources - 1:
        source := source_start + source#;
        source_temp := ReLu(concatenate(
            feature[source] x Wf1,
            Mean(children_features[source#] x Wa1)));
        source_temp /= sqrt(sum(source_temp));

        result := ReLu(concatenate(
            source_temp x Wf2,
            Mean(children_temp[source#]) x Wa2));
        result /= sqrt(sum(result));
        source_embedding[source#] := result;

    Move source_embedding from GPU to CPU;
    source_start += B;
```

How To Run This Application on DARPA's DGX-1

Prereqs/input

CUDA should have been installed; `$PATH` and `$LD_LIBRARY_PATH` should have been set correctly to use CUDA. The current Gunrock configuration assumes boost (1.58.0 or 1.59.0) and Metis are installed; if not, changes need to be made in the Makefiles. DARPA's DGX-1 has both installed when the tests are performed.

```
git clone --recursive https://github.com/gunrock/gunrock/ \
  -b dev-refactor
cd gunrock
git submodule init
git submodule update
mkdir build
cd build
cmake ..
cd ../tests/sage
make
```

At this point, there should be an executable `test_sage_<CUDA version>_x86_64` in `tests/sage/bin`.

The datasets are assumed to have been placed in `/raid/data/hive`, and converted to proper matrix market format (`.mtx`). At the time of testing, `pokec`, `amazon`, `flickr`, `twitter` and `cit-Patents` are available in that directory.

Note that GraphSage is an inductive representation learning algorithm, so it reasonable to assume that there is no dangling vertices in the graph. **Before running GraphSAGE, please remove the dangling vertices from the graph.** In the case when dangling vertices are present, the dangling vertices themselves will be treated as their neighbors.

The testing is done with Gunrock using `dev-refactor` branch at commit `0ed72d5` (Oct. 25, 2018), using CUDA 9.2 with NVIDIA driver 390.30 on a Tesla P100 GPU in the DGX-1 machine, and using CUDA 10.0 with NVIDIA driver 410.66 on a Tesla V100 GPU in Bowser (an machine used by the Gunrock team in UC Davis).

Running the application

Application specific parameters

The W arrays used by GraphSAGE should be produced by the training process; without the training part at the moment, we use some given datasets or randomly generate them if not available. The array input files are floating-point values in plain text format; examples can be found in the `gunrock/app/sage` directory of the gunrock repo.

```
--Wa1 : std::string, default =
        <weight matrix for W^1 matrix in algorithm 2, aggregation part>
         dimension 64 by 128 for pokec;
         It should be leaf feature length by a value you want for W2 layer
--Wa1-dim1 : int, default = 128
        Wa1 matrix column dimension
--Wa2 : std::string, default =
        <weight matrix for W^2 matrix in algorithm 2, aggregation part>
         dimension 256 by 128 for pokec;
         It should be child_temp length by output length
--Wa2-dim1 : int, default = 128
        Wa2 matrix column dimension
--Wf1 : std::string, default =
        <weight matrix for W^1 matrix in algorithm 2, feature part>
         dimension 64 by 128 for pokec;
         It should be child feature length by a value you want for W2 layer
--Wf1-dim1 : int, default = 128
        Wf1 matrix column dimension
--Wf2 : std::string, default =
        <weight matrix for W^2 matrix in algorithm 2, feature part>
         dimension 256 by 128 for pokec;
```

```
         It should be source_temp length by output length
--Wf2-dim1 : int, default = 128
        Wf2 matrix column dimension
--feature-column : std::vector<int>, default = 64
        feature column dimension
--features : std::string, default =
        <features matrix>
    dimension |V| by 64 for pokec;
--omp-threads : int, default = 32
    number of threads to run CPU reference
--num-children-per-source : std::vector<int>, default = 10
        number of sampled children per source
--num-leafs-per-child : std::vector<int>, default = -1
        number of sampled leafs per child; default is the same as num-children-per-source
--batch-size : std::vector<int>, default = 65536
        number of source vertex to process in one iteration
```

Example Command

```
./bin/test_sage_9.2_x86_64 \
 market /raid/data/hive/pokec/pokec.mtx  --undirected \
 --Wf1 ../../gunrock/app/sage/wf1.txt \
 --Wa1 ../../gunrock/app/sage/wa1.txt \
 --Wf2 ../../gunrock/app/sage/wf2.txt \
 --Wa2 ../../gunrock/app/sage/wa2.txt \
 --features ../../gunrock/app/sage/features.txt \
 --num-runs=10 \
 --batch-size=16384
```

When `Wf1`, `Wa1`, `Wf2`, `Wa2`, or `features` are not available, random values are used. The embeddings may be not useful at all, but the memory access patterns and the computation workload are the same, regardless of whether the random inputs are used. Using the random inputs enable us to test on any graph without requiring the associative arrays.

Output

The outputs are in the `sage` directory; look for the .txt files. An example is shown below for the `pokec` dataset:

```
Loading Matrix-market coordinate-formatted graph ...
  ... Loading progress ...
Converting 1632803 vertices, 44603928 directed edges ( ordered tuples) to CSR format...Done
Degree Histogram (1632803 vertices, 44603928 edges):
    Degree 0: 0 (0.000000 %)
    Degree 2^0: 163971 (10.042301 %)
```

```
    Degree 2^1: 201604 (12.347111 %)
    Degree 2^2: 238757 (14.622523 %)
    Degree 2^3: 273268 (16.736128 %)
    Degree 2^4: 298404 (18.275567 %)
    Degree 2^5: 265002 (16.229882 %)
    Degree 2^6: 148637 (9.103180 %)
    Degree 2^7: 38621 (2.365319 %)
    Degree 2^8: 4089 (0.250428 %)
    Degree 2^9: 418 (0.025600 %)
    Degree 2^10: 23 (0.001409 %)
    Degree 2^11: 3 (0.000184 %)
    Degree 2^12: 3 (0.000184 %)
    Degree 2^13: 3 (0.000184 %)

============================================
 feature-column=64 num-children-per-source=10 num-leafs-per-child=-1
Computing reference value ...
============================================
rand-seed = 1540498523
============================================
CPU Reference elapsed: 25242.941406 ms.
Embedding validation: PASS
============================================
 batch-size=512
Using randomly generated Wf1
Using randomly generated Wa1
Using randomly generated Wf2
Using randomly generated Wa2
Using randomly generated features
Using advance mode LB
Using filter mode CULL
rand-seed = 1540498553
============================================
============================================
Run 0 elapsed: 2047.366858 ms, #iterations = 3190
... More runs
============================================
============================================
Run 9 elapsed: 2013.216972 ms, #iterations = 3190
Embedding validation: PASS
[Sage] finished.
 avg. elapsed: 2042.503190 ms
 iterations: 3190
 min. elapsed: 2009.524107 ms
 max. elapsed: 2243.710995 ms
 load time: 1600.46 ms
```

```
preprocess time: 3997.880000 ms
postprocess time: 2106.487989 ms
total time: 26634.360075 ms
```

There is 1 OMP reference run on the CPU for each combination of {`feature-column`, `num-children-per-source`, `num-leafs-per-child`}, with the timing reported after `CPU Reference elapsed`. There are 10 GPU runs for each combination of the previous three parameters, plus `batch-size`. The computation workload of the GPU runs are the same as the reference CPU run, with different batch sizes. The GPU timing is reported after `Run x elapsed:`, and the average running time of the 10 GPUs is reported after `avg. elapsed`.

The mathematical formula of the GraphSAGE algorithm is relatively simple and repeats itself three times in the form of `Normalize(C x Wf + Mean(D) x Wa)`. Because of this simplicity, it is still possible to verify the implementation by visually inspecting the code. The resulted embeddings are also checked for the L2 norm, which should be close to 1 for every vertex. Because the neighbor selection process is inherently random, it would be very difficult to do a number-by-number checking with other implementations, including the reference. A more meaningful regression test will look at the training or validation accuracy when the full workflow is completed, which is a possibility for future work in year 2.

Performance and Analysis

The OpenMP and GPU implementations are measured for runtime. It would be additionally useful to validate the successful rate of the whole pipeline with the training process in place (perhaps in year 2).

The datasets used for experiments are:

Dataset	V	E
flickr	105938	4633896
amazon	548551	1851744
pokec	1632803	44603928
cit-Patents	3774768	33037894
twitter	7199978	43483326
europe-osm	50912018	108109320

The running times in milliseconds are listed below, for both machines. F stands for the length of features, C stands for the number of children per source, the same as the number of leafs per child, and B notes the batch size that produces the shortest running time on GPU among {512, 1024, 2048, 4096, 8192, 16384}.

The running time on DGX-1 with Tesla P100 GPU:

Dataset	F	C	B	Gunrock GPU	OpenMP	Speedup
flickr	64	10	16384	113.431	1607.468	14.17
flickr	64	25	16384	248.523	2630.659	10.59
flickr	64	100	2048	1139.007	10702.981	9.40
flickr	128	10	16384	192.916	1800.150	9.33
flickr	128	25	8192	442.226	4022.799	9.10
flickr	128	100	2048	2116.955	20655.732	9.76
amazon	64	10	16384	579.342	8905.530	15.37
amazon	64	25	16384	1235.168	18034.229	14.60
amazon	64	100	4096	5486.910	45337.011	8.26
amazon	128	10	16384	976.759	9418.961	9.64
amazon	128	25	16384	2193.159	29645.709	13.52
amazon	128	100	4096	10112.228	80677.594	7.98
pokec	64	10	16384	1744.602	25242.941	14.47
pokec	64	25	16384	3806.404	34517.180	9.07
pokec	64	100	2048	17486.692	133920.000	7.66
pokec	128	10	16384	2950.606	41414.535	14.04
pokec	128	25	8192	6791.829	74983.391	11.04
pokec	128	100	2048	32000.378	297979.438	9.31
cit-Patents	64	10	16384	4005.860	52094.125	13.00
cit-Patents	64	25	16384	8541.500	93715.789	10.97
cit-Patents	64	100	4096	38494.688	293333.781	7.62
cit-Patents	128	10	16384	6784.752	95639.117	14.10
cit-Patents	128	25	8192	15250.170	146539.250	9.61
cit-Patents	128	100	4096	70074.883	530910.375	7.58
twitter	64	10	16384	7594.364	103753.961	13.66
twitter	64	25	16384	16212.790	162819.531	10.04
twitter	64	100	4096	73488.745	636224.625	8.66
twitter	128	10	16384	12753.125	147705.375	11.58
twitter	128	25	16384	28827.354	282497.438	9.80
twitter	128	100	4096	134027.966	1105741.500	8.25
europe_osm	64	10	16384	53521.982	611449.625	11.42
europe_osm	64	25	16384	113740.739	1016479.938	8.94
europe_osm	64	100	4096	509313.472	4441408.500	8.72

The running time on Bowser with a Tesla V100 GPU

Dataset	F	C	B	Gunrock GPU	OpenMP	Speedup vs. CPU	Speedup vs. P100
flickr	64	10	16384	39.894	1094.377	27.43	2.90
flickr	64	25	8192	91.810	2177.953	23.72	2.76
flickr	64	100	1024	448.888	8641.063	19.25	2.57
flickr	128	10	16384	65.131	1849.658	28.40	2.95
flickr	128	25	4096	156.965	3981.435	25.37	2.84
flickr	128	100	512	802.966	16471.338	20.51	2.70

Dataset	F	C	B	Gunrock GPU	OpenMP	Speedup vs. CPU	Speedup vs. P100
amazon	64	10	16384	196.079	6142.780	31.33	2.95
amazon	64	25	8192	423.145	12674.514	29.95	2.92
amazon	64	100	2048	1963.691	49205.359	25.06	2.79
amazon	128	10	16384	324.067	9978.198	30.79	3.10
amazon	128	25	8192	733.181	21726.697	29.63	2.99
amazon	128	100	2048	3361.894	86967.164	25.87	3.01
pokec	64	10	16384	602.116	17111.664	28.42	2.84
pokec	64	25	8192	1379.450	35887.129	26.02	2.71
pokec	64	100	1024	6793.011	140751.234	20.72	2.54
pokec	128	10	16384	1000.310	28987.953	28.98	2.96
pokec	128	25	4096	2366.202	63863.352	26.99	2.82
pokec	128	100	512	11859.789	265325.281	22.37	2.64
cit-Patents	64	10	16384	1374.782	38803.195	28.22	2.95
cit-Patents	64	25	8192	3006.717	78112.516	25.98	2.87
cit-Patents	64	100	2048	13910.529	291278.125	20.94	2.78
cit-Patents	128	10	16384	2276.261	65735.234	28.88	2.99
cit-Patents	128	25	8192	5201.184	141957.922	27.29	2.96
cit-Patents	128	100	2048	23922.527	560321.438	23.42	2.94
twitter	64	10	16384	2575.303	72372.484	28.10	2.91
twitter	64	25	8192	5658.345	148938.422	26.32	2.84
twitter	64	100	2048	26468.915	569925.500	21.53	2.77
twitter	128	10	16384	4270.454	125431.766	29.37	2.98
twitter	128	25	8192	9744.686	267841.563	27.49	2.93
twitter	128	100	2048	45604.444	1098039.375	24.08	2.93
europe_osm	64	10	16384	18440.253	497153.969	26.96	2.90
europe_osm	64	25	16384	39883.421	1008675.500	25.29	2.85
europe_osm	64	100	4096	184128.123	3825227.500	20.77	2.77

Implementation limitations

- **Memory usage** Gunrock's GPU implementation uses `B x (C x (Wf2.x + F + 1) + 2Wf2.x + 2R.x) x 4` bytes in additional to the features that takes up `VF x 4` bytes and the graph itself. Because the batch size B can be adjusted, the main memory consumption is from the feature array. For a P100 with 16 GB memory, if the feature length is 64, the maximum number of vertices it can handle before hitting OOM is about 60 million. The largest dataset tested so far is the `europe_osm` dataset with 50.9M vertices and 108M edges.

- **Data types** The vertex Ids and edge Ids are both presented as 32-bit unsigned integers. Input features, weights, output embeddings and intermedia results are represented as 32-bit floating-point numbers. A not so recent trend in machine learning research is to use less precision in neural networks. Half precision / 16-bit floating points are quite common,

and supported by recent GPUs. Using half precision cuts the computation time to about half, as compared to single precision, and also cuts the memory usage to store the features in half. It would be interesting to see what would happen if the data type is changed to half precision.

- **Graph types** The training process requires the graph to be undirected (enforced by `--undirected` in Gunrock's command line parameters). The behavior of sampling a zero-length neighbor list is undefined, and currently it will return the source vertex itself.

Comparison against existing implementations

Because computation on each vertex is independent from other vertices, GraphSAGE is an embarrassingly parallel problem when parallelized across vertices. Running a simple test with the `pokec` dataset, feature length as 64, num_children_per_source and num_leafs_per_child both at 10, the serial run (with omp-threads forced to 1) on the DGX-1 takes 366390.250 ms, as compared to 25242.941 ms using 32 threads; using 32 threads is about 14.5X faster than a single thread, which shows GraphSAGE scales pretty well on the CPU.

Comparing the running time of a 32-thread OpenMP and Gunrock's GPU implementation, the P100 is about 7.5X to 15X faster. Increasing the feature length from 64 to 128 roughly doubles the computation workload, and the speedup does not change very much for datasets with more than about 1M vertices. However, increasing the number of children per source and the number of leafs per child decreases the speedup. The OMP's running time increases slower than the number of neighbors selected, while the GPU's running time increases faster than the number of neighbors selected. This may be attributed to the cache effect: the parallelism on CPU is limited, so data reuse rate is high, even when the number of neighbors increases; however, the number of source or children processed on the GPU at the same time is much larger, with a much bigger working set, and this decreases the cache hit rate, so results in longer running time.

Also interesting is comparing the runtime on V100 and P100: V100 is about 3X faster than P100 when running GraphSAGE. This large performance difference is caused by the different limiting factors when running GraphSAGE on these two GPUs; details are in the the Performance limitations section. Compared to OpenMP, the V100 is about 20X to 30X faster.

Performance limitations

We profiled GraphSAGE with the `pokec` dataset on a Titan Xp GPU (profiling on P100 caused an internal error in the profiler itself; Titan Xp has roughly the same SM design as P100, but has only 30 SMs vs. 56 on the P100; P100 also has 16 GB HMB2 memory, and Titan Xp only has 12 GB GDDR5X; runtime on Titan Xp and P100 is similar). kernel2 takes up about 60% of the computation

of an batch, 10.64 ms out of 17.76 ms for `pokec` with 64 feature length, 10 neighbors, and batch size at 16384. Kernel1 takes 1.56 ms, or 8.8%, and Kernel3 takes 5.52 ms, or 31.1%.

Further detail on the profile of Kernel2 on the Titan Xp shows the utilization of the memory system:

Type	Transactions	Bandwidth	Utilization
Shared Loads	2129920	31.997 GB/s	
Shared Stores	1638400	24.613 GB/s	
Shared Total	3768320	56.611 GB/s	Idle to low
Local Loads	0	0 GB/s	
Local Stores	0	0 GB/s	
Global Loads	2685009922	1575.871 GB/s	
Global Stores	0	0 GB/s	
Texture Reads	671252480	2521.025 GB/s	
Unified Total	**3356262402**	**4096.897 GB/s**	**High**
L2 Reads	264170192	992.145 GB/s	
L2 Writes	10485773	39.381 GB/s	
L2 Total	274655965	1031.526 GB/s	Low to medium
Device Reads	2181833	8.194 GB/s	
Device Writes	543669	2.042 GB/s	
Device Total	2725502	10.236 GB/s	Idle to low

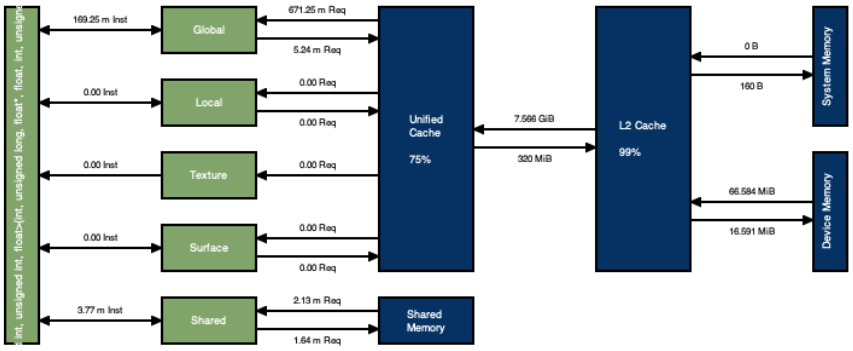

Figure 4.1: Sage_Pokec_TianXp

It's clear that the unified cache is almost fully utilized, at 4 TBps out of the 5 TBps theoretical upper bound, and is the bottleneck. This is because the `W` arrays and the intermediate arrays are highly reusable.

Running the same experiment on the V100 shows a different picture within the memory system:

Type	Transactions	Bandwidth	Utilization
Shared Loads	2138599	74.166 GB/s	
Shared Stores	1640842	56.904 GB/s	
Shared Total	3779441	131.070 GB/s	Idle to low
Local Loads	0	0 GB/s	
Local Stores	0	0 GB/s	
Global Loads	419594240	3637.862 GB/s	
Global Stores	0	0 GB/s	
Texture Reads	177448960	6153.897 GB/s	
Unified Total	597043200	9791.759 GB/s	Medium
L2 Reads	8209326	71.174 GB/s	
L2 Writes	5243176	45.458 GB/s	
L2 Total	274655965	116.633 GB/s	Idle to low
Device Reads	2402833	20.832 GB/s	
Device Writes	571925	4.959 GB/s	
Device Total	2974758	25.791 GB/s	Idle to low

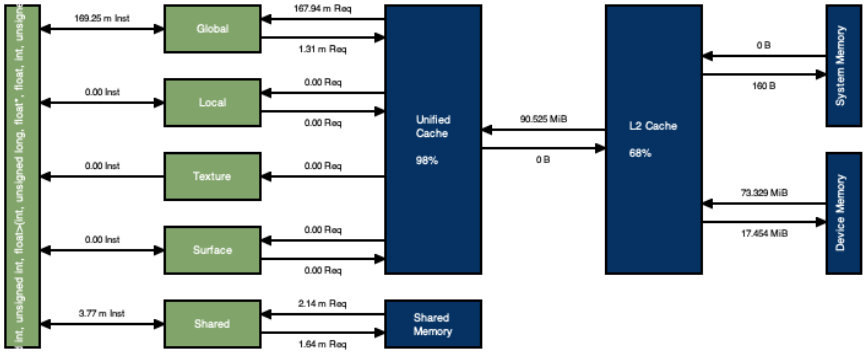

Figure 4.2: Sage_Pokec_V100

On the V100, kernel2 only takes 3.982 ms (about 60% of 6.67 ms per batch), and the unified-cache throughput increases to 9.8 TBps, more than double than on the Titan Xp. In fact, the theoretical upper bound of V100's L1 throughput is 28 TBps, resulted from doubling each SM's load throughput from 128 bytes per cycle to 256 bytes per cycle, and increasing the SM count to 80. This is the reason why the V100 can outperform P100 and Titan Xp by about 3X. The performance bottleneck is no longer the memory system, and switches to integer computations, which comes mainly from array index calculation. This particular kernel also takes up 32 registers per thread, which is the limit for full GPU occupancy. Storing intermediate index calculation results would help if the register usage is not so high.

Next Steps

Alternate approaches

Things we tried that didn't really work

An simple implementation that uses a thread to process the per-source or per-child computation is coded, but it runs about 10X slower than the current implementation that uses a block to process such units. One reason is the use of block-level parallel primitives, such as block reduce. Another reason is that by using a whole block, instead of a thread, to process the same computation, the working set is greatly reduced together with the parallelism, and the whole working set can fit into the cache system. When using higher parallelism, the working set is larger, and forced to be evicted into the global memory, and creates a bottleneck. Actually during the experiment, for the thread-level parallelism implementation, reducing the number of blocks of the kernel improves its running time, the opposite to normally what would be expected from running other kernels.

Gunrock implications

One thing that Gunrock does not provide, or intentionally hides, is block-level parallelism. However, it comes in handy when implementing the custom kernels for GraphSAGE: each block can process a one-dimension vector, with each thread holding one element, then use a block-level reduce to get the sum of those elements; this way is highly efficient, and actually reduces the parallelism and with it the size of the working set of data.

Notes on multi-GPU parallelization

The main memory usage is due to feature data, so it is critical to not duplicate features. The side effect is the computation needs to be divided into child-centric and source-centric parts, and exchange data in between. It should be scalable, and easy to implement.

Notes on dynamic graphs

GraphSAGE does not have a dynamic graph component, but it should able to work on a dynamic graph. Some of the data may be reusable if the graph has not been significantly changed, but the resulting memory requirement to store the intermediate data may make data reuse impossible.

Notes on larger datasets

If the dataset is so large that the graph and the per-vertex feature data are larger than the combined GPU memory, it's possible to accumulate the features of leafs and children on CPU, transfer the data on to GPU, and perform the computation.

Because of the cost of the transfer, runtime will increase significantly as compared to the cases when the full data can fit in the GPU memory, but whether that will cause an increase above the OpenMP implementation is still unknown.

Notes on other pieces of this workload

The main part of GraphSAGE workflow is actually the training process, which will be outside of Gunrock, provided by TensorFlow, PyTorch or other machine learning libraries. How to connect the training with the Gunrock GPU implementation is the main task for this workload going forward.

Research potential

The GPU implementation of the embedding part runs a lot faster than on the CPU, and hits a few GPU hardware limitations. It should have comparable runtime to other GPU implementations. But it's only useful as a part of the whole workload and achieves comparable prediction accuracy as conventional / reference implementations.

An interesting question raised from the GraphSAGE GPU implementation is whether it is useful to expose block-level parallelism to higher-level programming models/APIs, and if so, how to do that. It's clear that working at the block level provides benefits, such as the ability to use block-level primitives like scan and reduce. But it also comes with costs, most importantly, requiring the programmer to have knowledge about the GPU hardware. It also reduces the portability of the implementation, because two-level parallelism may not exist on other processors.

Chapter 5

GraphSearch

The graph search (GS) workflow is a walk-based method that searches a graph for nodes that score highly on some arbitrary indicator of interest.

The use case given by the HIVE government partner was sampling a graph: given some seed nodes, and some model that can score a node as "interesting", find lots of "interesting" nodes as quickly as possible. Their algorithm attempts to solve this problem by implementing several different strategies for walking the graph.

- `uniform`: given a node `u`, randomly move to one of `u`'s neighbors (ignoring scores)
- `greedy`: given a node `u`, walk to neighbor with maximum score
- `stochastic_greedy`: given a node `u`, choose neighbor to walk to with probability proportional to score

Use of these walk-based methods is motivated by the presence of homophily in many real world social networks: we expect interesting people to have relationships with interesting people.

Summary of Results

Graph search is a relatively minor modification to Gunrock's random walk application, and was straightforward to implement. Though random walks are a "worst case scenario" for GPU memory bandwidth, we still achieve 3–5x speedup over a modified version of the OpenMP reference implementation.

The original OpenMP reference implementation actually ran slower with more threads – we fixed the bugs, but the benchmarking experience highlights the need for performant and hardened CPU baselines.

Until recently, Gunrock did not support parallelism *within* the lambda functions run by the `advance` operator, so neighbor selection for a given step in the walk

is done sequentially. Methods for exposing more parallelism to the programmer are currently being developed via parallel neighbor reduce functions.

In an end-to-end graph search application, we'd need to implement the scoring function as well as the graph walk component. For performance, we'd likely want to implement the scoring function on the GPU as well, which makes this a good example of a "Gunrock+X" app, where we'd need to integrate the high-performance graph processing component with arbitrary user code.

Summary of Gunrock Implementation

The scoring model can be an arbitrary function (e.g., of node metadata). For example, if we were running GS on the Twitter friends/followers graph, the scoring model might be the output of a text classifier on each users' messages. Thus, we do not implement the scoring model in our Gunrock implementation – instead, we read scores from an input file and access them as necessary.

GS is a generalization of a random walk implementation, where there can be more variety in the transition function between nodes.

The GS `uniform` mode is exactly a uniform random walk, so we can use the pre-existing Gunrock application. Given a node, we compute the node to walk to as:

```
r = random.uniform(0, 1)
neighbors = graph.get_neighbors(node)
next_node = neighbors[floor(r * len(neighbors))]
```

Both the `GraphSearch` `greedy` and `stochastic_greedy` consist of small modifications to this transition function.

For `greedy`, we find the neighbor with maximum score:

```
neighbors = graph.get_neighbors(node)
next_node = neighbors[0]
next_node_score = scores[next_node]
for neighbor in neighbors:
    neighbor_score = scores[neighbor]
    if neighbor_score > next_node_score:
        next_node = neighbor
        next_node_score = neighbor_score
```

For `stochastic_greedy`, we sample neighbors proportional to their score – e.g.:

```
sum_neighbor_scores = 0
for neighbor in graph.neighbors(node):
```

```
   sum_neighbor_scores += scores[neighbor]

r *= sum_neighbor_scores

tmp = 0
for neighbor in graph.neighbors(node):
   tmp += scores[neighbor]
   if r < tmp:
       next_node = neighbor
       break
```

In Gunrock, we create a frontier containing all of the nodes we want to walk from. Then we map the transition function over the frontier using Gunrock's `ForEach` operator. Current nodes in the frontier are replaced with the chosen neighbor, and the walk is (optionally) recorded in an output array.

Because this is such a straightforward modification, we implement GS inside of the existing random walk `rw` Gunrock application. GS just requires adding a couple of extra flags and one extra array of size `|V|` to store the node values.

How To Run This Application on DARPA's DGX-1

Prereqs/input

```
git clone --recursive https://github.com/gunrock/gunrock -b dev-refactor
cd gunrock/tests/rw/
cp ../../gunrock/util/gitsha1.c.in ../../gunrock/util/gitsha1.c
make clean
make
```

Running the application

Application specific parameters

```
  --walk-mode
      0 = uniform
      1 = greedy
      2 = stochastic_greedy
  --node-value-path
      If --walk-mode != 0, this is the path to node scores
  --store-walks
      0 = just do the walk -- don't actually store it anywhere
      1 = store walks in memory
  --walk-length
      Length of each walk
  --walks-per-node
      Number of walks to do per seed node
```

```
  --seed
      Seed for random number generator
```

Example Command

```
# generate random features
python random-values.py 39 > chesapeake.values

# uniform random
./bin/test_rw_9.1_x86_64 --graph-type market --graph-file \
  ../../dataset/small/chesapeake.mtx --walk-mode 0 --seed 123

# greedy
./bin/test_rw_9.1_x86_64 --graph-type market --graph-file \
  ../../dataset/small/chesapeake.mtx --node-value-path chesapeake.values \
  --walk-mode 1

# stochastic greedy
./bin/test_rw_9.1_x86_64 --graph-type market --graph-file \
  ../../dataset/small/chesapeake.mtx --node-value-path chesapeake.values \
  --walk-mode 2 --seed 123
```

Example Output

```
# ----------------------------------------------
# uniform random

Loading Matrix-market coordinate-formatted graph ...
Reading from ../../dataset/small/chesapeake.mtx:
  Parsing MARKET COO format
 (39 nodes, 340 directed edges)...
Done parsing (0 s).
  Converting 39 vertices, 340 directed edges ( ordered tuples) to CSR format...
Done converting (0s).
--------------------------
--------------------------
 Elapsed: 0.001907
Using advance mode LB
Using filter mode CULL
num_nodes=39
--------------------------
0    0   0   queue3      oversize :  234 ->  682
0    0   0   queue3      oversize :  234 ->  682
0    1   0   queue3      oversize :  682 ->  1085
0    1   0   queue3      oversize :  682 ->  1085
0    5   0   queue3      oversize :  1085 ->     1166
```

```
0    5   0   queue3      oversize :  1085 ->     1166
-------------------------
Run 0 elapsed: 4.551888, #iterations = 10
[[0, 38, 8, 35, 11, 25, 13, 27, 37, 7, ],
[1, 34, 1, 38, 30, 38, 29, 37, 7, 37, ],
[2, 17, 2, 38, 4, 38, 10, 18, 14, 28, ],
...
[36, 33, 0, 22, 38, 27, 37, 18, 38, 8, ],
[37, 21, 31, 17, 25, 17, 18, 32, 37, 26, ],
[38, 7, 8, 34, 6, 5, 6, 5, 38, 19, ]]
-------- NO VALIDATION -----[rw] finished.
 avg. elapsed: 4.551888 ms
 iterations: 10
 min. elapsed: 4.551888 ms
 max. elapsed: 4.551888 ms
 load time: 60.925 ms
 preprocess time: 964.890000 ms
 postprocess time: 0.715017 ms
 total time: 970.350027 ms

# ------------------------------------------------
# greedy
# !! In this case, the output is formatted as `GPU_result:CPU_result`, for correctness chec

Loading Matrix-market coordinate-formatted graph ...
Reading from ../../dataset/small/chesapeake.mtx:
  Parsing MARKET COO format
 (39 nodes, 340 directed edges)...
Done parsing (0 s).
  Converting 39 vertices, 340 directed edges ( ordered tuples) to CSR format...
Done converting (0s).

--------------------------
--------------------------
 Elapsed: 0.085831
Using advance mode LB
Using filter mode CULL
num_nodes=39

--------------------------
0    0   0   queue3      oversize :  234 ->  682
0    0   0   queue3      oversize :  234 ->  682
0    1   0   queue3      oversize :  682 ->  770
0    1   0   queue3      oversize :  682 ->  770
--------------------------
Run 0 elapsed: 0.695944, #iterations = 10
[[0:0, 22:22, 32:32, 18:18, 11:11, 18:18, 11:11, 18:18, 11:11, 18:18, ],
[1:1, 22:22, 32:32, 18:18, 11:11, 18:18, 11:11, 18:18, 11:11, 18:18, ],
```

```
[2:2, 17:17, 2:2, 17:17, 2:2, 17:17, 2:2, 17:17, 2:2, 17:17, ],
...
[36:36, 33:33, 36:36, 33:33, 36:36, 33:33, 36:36, 33:33, 36:36, 33:33, ],
[37:37, 18:18, 11:11, 18:18, 11:11, 18:18, 11:11, 18:18, 11:11, 18:18, ],
[38:38, 2:2, 17:17, 2:2, 17:17, 2:2, 17:17, 2:2, 17:17, 2:2, ]]
0 errors occurred.
[rw] finished.
 avg. elapsed: 0.695944 ms
 iterations: 10
 min. elapsed: 0.695944 ms
 max. elapsed: 0.695944 ms
 load time: 44.2419 ms
 preprocess time: 974.721000 ms
 postprocess time: 0.731945 ms
 total time: 976.338863 ms

# ------------------------------------------------
# stochastic_greedy
# Output same format as `uniform` above.
# No correctness checking is implemented due to stochasticity.
```

Expected Output

When run in `--verbose` mode, the app outputs the walks. When run in `--quiet` mode, it outputs performance statistics (e.g., total number of steps taken). If running `greedy GraphSearch`, the app also outputs the results of a correctness check. Correctness checks for `uniform` and `stochastic_greedy` are omitted because of their inherent stochasticity.

Validation

The correctness of the implementation has been validated in outside experiments, by making sure that the output walks are valid and the distribution of transitions is as expected.

Performance and Analysis

Performance is measured by the runtime of the app, given

- an input graph `G=(U, E)`
- set of seed nodes (hardcoded to all nodes in `G`)
- number of walks per seed
- number of steps per walk
- a transition function (e.g., `uniform|greedy|stochastic_greedy`)

Implementation limitations

The output of the random walk is a dense array of size `(# seeds) * (steps per walk) * (walks per seed)`. When we have a large graph *or* long walks *or* multiple walks per seed, this array may exceed the size of GPU memory.

At the moment, we only support walks starting from *all* of the nodes in `G`. It would be straightforward to add a parameter that would allow the use to specify a smaller set of seed nodes.

This app can only be used for graphs that have scores associated w/ each node. In order to run benchmarks, if scores are not available we often assign uniformly random scores to nodes. The distribution of these scores may affect the runtime of the algorithm by changing data access patterns – we test on the provided Twitter dataset, but do not have a variety of other node attributed graphs to test on.

Comparison against existing implementations

We measure runtime on the HIVE graphsearch Twitter dataset. This graph has `|U|=9291392` nodes and `|E|=21741663` edges.

At a high level, the results show:

Variant	OpenMP w/ 64 threads	Gunrock GPU	Gunrock Speedup
Directed greedy	236ms	**64ms**	3.7x
Directed random	158ms	**34ms**	4.6x
Undirected random	3186ms	**630ms**	5.0x

The undirected random walks take ~ 10x longer because directed walks terminate when they encounter a node without any neighbors and thus have average length significantly shorter than the `--walk-length` parameter.

Details and raw data follow.

HIVE Python reference implementation

We run the HIVE Python reference implementation w/ the following settings:

- undirected graph
- uniform transition function
- 1000 random seeds
- 128 steps per walk

With the `uniform` transition function, the run took 41 seconds. Walks are done sequentially, so runtime will scale linearly with the number of seeds. This

implementation is *substantially* slower than even a single-threaded run of PNNLs OpenMP code. Thus, we omit further analysis.

PNNL OpenMP implementation

We run the PNNL OpenMP implementation on the Twitter graph w/ the following settings:

- commit: 69864383f0fc0e8aace52be34b329a2f8a58afb6
- 1,2,4,8,16,32 or 64 threads
- `greedy` or `uniform` transition function
- directed or undirected graph

We omit the `greedy` undirected case because the algorithm gets stuck jumping between a local maximum and its highest-scoring neighbor.

threads	method	directed?	nseeds	elapsed_sec	nsteps	steps_per_sec
1	greedy	yes	7199978	3.02876	16325873	5.39e+06
2	greedy	yes	7199978	2.83467	16325873	5.75e+06
4	greedy	yes	7199978	1.64405	16325873	9.93e+06
8	greedy	yes	7199978	0.870028	16325873	1.87e+07
16	greedy	yes	7199978	0.605769	16325873	2.69e+07
32	greedy	yes	7199978	0.43742	16325873	3.73e+07
64	greedy	yes	7199978	**0.236701**	16325873	6.89e+07
1	unif.	yes	7199978	**14.6291**	14510781	**991915**
2	unif.	yes	7199978	24.2175	14186833	585809
4	unif.	yes	7199978	25.1764	14487202	575427
8	unif.	yes	7199978	27.7312	13937449	502591
16	unif.	yes	7199978	30.5377	14062226	460488
32	unif.	yes	7199978	32.1057	13906144	433137
64	unif.	yes	7199978	31.2754	13876284	443680
1	unif.	no	100000	**12.3982**	12700000	**1.024+06**
2	unif.	no	100000	19.7925	12700000	641658
4	unif.	no	100000	22.5432	12700000	563362
8	unif.	no	100000	26.1053	12700000	486491
16	unif.	no	100000	28.275	12700000	449160
32	unif.	no	100000	28.334	12700000	448224
64	unif.	no	100000	28.7419	12700000	441864

Note that we use fewer seeds for the undirected uniform case due to slow runtime.

Observe that the `rand` modes have very bad scaling as a function of cores. After investigation, this was due to two issues. First, the neighbors were being

sampled incorrectly, which led to chaotic behavior. Second, the app was using a slow random number generator w/ an excessive number of seed resets. We created a PR to fix those issues here.

After these fixes, runtimes were as follows:

threads	method	directed?	nseeds	elapsed_sec	nsteps	steps_per_sec
1	greedy	yes	7199978	3.02876	16325873	5.39e+06
2	greedy	yes	7199978	2.83467	16325873	5.75e+06
4	greedy	yes	7199978	1.64405	16325873	9.93e+06
8	greedy	yes	7199978	0.870028	16325873	1.87e+07
16	greedy	yes	7199978	0.605769	16325873	2.69e+07
32	greedy	yes	7199978	0.43742	16325873	3.73e+07
64	greedy	yes	7199978	**0.236701**	16325873	**6.89e+07**
1	unif.	yes	7199978	1.49886	16529694	1.10e+07
2	unif.	yes	7199978	1.60176	16533004	1.03e+07
4	unif.	yes	7199978	0.974128	16538957	1.69e+07
8	unif.	yes	7199978	0.455227	16534756	3.63+07
16	unif.	yes	7199978	0.257524	16528617	6.42e+07
32	unif.	yes	7199978	**0.155722**	13906144	**1.06e+08**
64	unif.	yes	7199978	0.158828	16537488	1.04e+08
1	unif.	no	7199978	125.963	914397206	1.92e+08
2	unif.	no	7199978	78.927	914397206	1.80e+08
4	unif.	no	7199978	39.7097	914397206	2.96e+08
8	unif.	no	7199978	22.5195	914397206	6.35e+08
16	unif.	no	7199978	11.0047	914397206	1.12e+09
32	unif.	no	7199978	5.56317	914397206	**1.85e+09**
64	unif.	no	7199978	**3.18615**	914397206	1.82e+09

Note the improved runtimes and scaling. These experiments were run with this branch at commit 6c25a0687eecebfd4393e86fa4c7308d5594b73d.

All experiments are conducted on the HIVE DGX-1.

Gunrock GPU implementation

directed, greedy

```
./bin/test_rw_9.1_x86_64 --graph-type market --graph-file dir_gs_twitter.mtx \
    --node-value-path gs_twitter.values \
    --walk-mode 1 \
    --walk-length 32 \
    --undirected=0 \
    --store-walks 0 \
    --quick \
    --num-runs 10
```

```
Loading Matrix-market coordinate-formatted graph ...
Reading from dir_gs_twitter.mtx:
  Parsing MARKET COO format
 (7199978 nodes, 21741663 directed edges)...
Done parsing (7 s).
  Converting 7199978 vertices, 21741663 directed edges ( ordered tuples) to CSR format...
Done converting (0s).
============================================
 advance-mode=LB
Using advance mode LB
Using filter mode CULL
Run 0 elapsed: 65.273046, #iterations = 32
Run 1 elapsed: 64.157963, #iterations = 32
Run 2 elapsed: 64.009190, #iterations = 32
Run 3 elapsed: 64.055920, #iterations = 32
Run 4 elapsed: 64.069033, #iterations = 32
Run 5 elapsed: 64.002037, #iterations = 32
Run 6 elapsed: 64.031839, #iterations = 32
Run 7 elapsed: 64.036846, #iterations = 32
Run 8 elapsed: 64.065933, #iterations = 32
Run 9 elapsed: 64.047098, #iterations = 32
Validate_Results: total_neighbors_seen=298668024
Validate_Results: total_steps_taken=16325873
-------- NO VALIDATION --------
[rw] finished.
 avg. elapsed: 64.174891 ms
 iterations: 32
 min. elapsed: 64.002037 ms
 max. elapsed: 65.273046 ms
 load time: 7086.91 ms
 preprocess time: 1016.620000 ms
 postprocess time: 101.121902 ms
 total time: 2073.837996 ms
```

directed, uniform

```
./bin/test_rw_9.1_x86_64 --graph-type market --graph-file dir_gs_twitter.mtx \
    --node-value-path gs_twitter.values \
    --walk-mode 0 \
    --walk-length 128 \
    --undirected=0 \
    --store-walks 0 \
    --quick \
    --num-runs 10 \
    --seed 123
```

```
Loading Matrix-market coordinate-formatted graph ...
Reading from dir_gs_twitter.mtx:
  Parsing MARKET COO format
 (7199978 nodes, 21741663 directed edges)...
Done parsing (7 s).
  Converting 7199978 vertices, 21741663 directed edges ( ordered tuples) to CSR format...
Done converting (1s).
============================================
 advance-mode=LB
Using advance mode LB
Using filter mode CULL
------------------------
Run 0 elapsed: 38.613081, #iterations = 128
Run 1 elapsed: 34.458876, #iterations = 128
Run 2 elapsed: 34.530163, #iterations = 128
Run 3 elapsed: 33.849001, #iterations = 128
Run 4 elapsed: 33.759117, #iterations = 128
Run 5 elapsed: 33.967972, #iterations = 128
Run 6 elapsed: 33.873081, #iterations = 128
Run 7 elapsed: 33.970118, #iterations = 128
Run 8 elapsed: 33.756971, #iterations = 128
------------------------
Run 9 elapsed: 33.715963, #iterations = 128
Validate_Results: total_neighbors_seen=289124779
Validate_Results: total_steps_taken=16530404
-------- NO VALIDATION --------
[rw] finished.
 avg. elapsed: 34.449434 ms
 iterations: 128
 min. elapsed: 33.715963 ms
 max. elapsed: 38.613081 ms
 load time: 7176.17 ms
 preprocess time: 1016.720000 ms
 postprocess time: 101.902962 ms
 total time: 1781.071901 ms
```

undirected, uniform

```
./bin/test_rw_9.1_x86_64 --graph-type market --graph-file undir_gs_twitter.mtx \
    --node-value-path gs_twitter.values \
    --walk-mode 0 \
    --walk-length 128 \
    --store-walks 0 \
    --quick \
```

```
    --num-runs 10 \
    --seed 123

Loading Matrix-market coordinate-formatted graph ...
Reading from undir_gs_twitter.mtx:
  Parsing MARKET COO format
 (7199978 nodes, 43483326 directed edges)...
Done parsing (7 s).
  Converting 7199978 vertices, 43483326 directed edges ( ordered tuples) to CSR format...
Done converting (0s).
============================================
 advance-mode=LB
Using advance mode LB
Using filter mode CULL
Run 0 elapsed: 636.021852, #iterations = 128
Run 1 elapsed: 631.129026, #iterations = 128
Run 2 elapsed: 631.053925, #iterations = 128
Run 3 elapsed: 631.713152, #iterations = 128
Run 4 elapsed: 631.028175, #iterations = 128
Run 5 elapsed: 631.374836, #iterations = 128
Run 6 elapsed: 631.196976, #iterations = 128
Run 7 elapsed: 632.030964, #iterations = 128
Run 8 elapsed: 631.026983, #iterations = 128
Run 9 elapsed: 630.996943, #iterations = 128
Validate_Results: total_neighbors_seen=75443835041
Validate_Results: total_steps_taken=914397206
-------- NO VALIDATION --------
[rw] finished.
 avg. elapsed: 631.757283 ms
 iterations: 128
 min. elapsed: 630.996943 ms
 max. elapsed: 636.021852 ms
 load time: 7705.9 ms
 preprocess time: 1010.830000 ms
 postprocess time: 102.057934 ms
 total time: 7755.448818 ms
```

Performance limitations

- For the undirected uniform settings, profiling shows that 79% of compute time is spent in the `ForAll` operator and 20% is spent in the `curand` random number generator. Device memory bandwidth in the `ForAll` kernel is 193 GB/s.
- For the directed greedy settings, profiling shows that 99.5% of compute time is spent in the `ForAll` operator. Device memory bandwidth in the `ForAll` kernel is 136 GB/s.

When we do a large number of walks and/or the length of each walk is very long, there may not be enough GPU memory to store all of the walks in memory. For now, we expose the `--store-walks` parameter – when this is set to zero, the walk is discarded as it is computed and only the length of the walk is stored. A better solution that could be implemented in the future would be to move walks from GPU to CPU memory as they grow too large.

Optimization: In a directed walk, once we hit a node with no outgoing neighbors, we halt the walk. In the current Gunrock implementation, the enactor runs for a fixed number of iterations, regardless of whether any of the nodes are still active. It would be straightforward to add a check that terminates the app when no "living" nodes are left.

Next Steps

Alternate approaches

The size of the output array may become a significant bottleneck for large graphs. However, since all of the transition functions do not depend on anything besides the current node, we could reasonably move the results of the walk from GPU to CPU memory every N iterations. Properly executed, this should eliminate the largest bottleneck without unduely impacting performance.

Gunrock implications

For the `greedy` and `stochastic_greedy` transition function, we have to sequentially iterate over all of a node's neighbors. Simple wrappers for computing, e.g., the maximum of node scores across all of a node's neighbors could be helpful, both for ease of programming and performance. Gunrock has a newly added `NeighborReduce` kernel that supports associative reductions – it should be straightforward to implement (at least) the `greedy` transition function with this kernel. The `stochastic_greedy` transition function would require a more complex reduction function along the lines of reservoir sampling.

Notes on multi-GPU parallelization

If the graph is small enough to be duplicated on each GPU, the implementation is trivial: just do a subset of the walks on each GPU. The scalability will be perfect, as there is no communication involved at all.

When the graph is distributed across multiple GPUs, we expect to have very poor scalability, as the ratio of computation to communication is very low. A more detailed discussion is available here.

Notes on dynamic graphs

This workflow does not have an explicit dynamic component. However, because steps only depend on the current node, the underlying graph could change during the walks.

Notes on larger datasets

The random accesses inherent to graph search make it a particularly difficult workflow for larger-than-GPU memory datasets. The most straightforward solution would be to let Unified Virtual Memory (UVM) in CUDA automatically handle memory movement, but we should expect to see a substantial reduction in performance.

Notes on other pieces of this workload

In real use cases, the scoring function would be computed lazily – that is, we wouldn't have a precomputed array with scores for each of the nodes, and we would need to run the scoring function as the walk is running. Thus, it would be critical for us to be able to call the scoring function from within Gunrock quickly and without excessive programmer overhead.

Chapter 6

Community Detection (Louvain)

Community detection in graphs means grouping vertices together, so that those vertices that are closer (have more connections) to each other are placed in the same cluster. A commonly used algorithm for community detection is Louvain (https://arxiv.org/pdf/0803.0476.pdf).

Summary of Results

The Gunrock implementation uses sort and segmented reduce to implement the Louvain algorithm, different from the commonly used hash table mapping. The GPU implementation is about ~1.5X faster than the OpenMP implementation, and also faster than previous GPU works. It is still unknown whether the sort and segmented reduce formulation map the problem better than hash table on the GPU. The modularities resulting from the GPU implementation are within small differences as the serial implementation, and are better when the graph is larger. A custom hash table can potentially improve the running time. The GPU Louvain implementation should have moderate scalability across multiple GPUs in an DGX-1.

Summary of Gunrock Implementation

The commonly used approach to implement the Louvain algorithm uses a hash table. However, the memory access pattern that results from a hash table is almost totally random, and not GPU-friendly (more in the Alternative approaches section). Instead of using a hash table to accumulate the values associated with the same key, the Gunrock implementation on GPU tries another method: sort all key-value pairs, and use segmented reduce to accumulate the values in the continuous segments. Because Louvain always visits all edges in the graph, there is no need to use Gunrock frontiers, and the `advance` operator with the `ALL_EDGES` advance mode or a simple `ForAll` loop should be sufficient. The pseudocode is listed below:

```
m2 <- sum(edge_weights);
//Outer-loop
Do
    // Pass-initialization, assign each vertex to its own community
    For each vertex v in graph:
        current_communities[v] <- v;
        weights_v2any      [v] <- 0;
        weights_v2self     [v] <- 0;
    For each edge e<v, u> in graph: //an advance operator on all edges
        weights_v2any[v] += edge_weights[e];
        if (v == u)
            weights_v2self[v] += edge_weights[e];
    For each vertex v in graph:
        weights_community2any[v] <- weights_v2any[v];
    pass_gain <- 0;

    // Modularity optimizing iterations
    Do
        // Get weights between vertex and community
        For each edge e<v, u> in graph:
            edge_pairs  [e] <- <v, current_communities[u]>;
            pair_weights[e] <- edge_weights[e];
        Sort(edge_pairs, pair_weights)
            by edge_pair.first, then edge_pair.second if tie;
        segment_offsets <- offsets of continuous edge_pairs;
        segment_weights <- SegmentedReduce(pair_weights, segment_offsets, sum);

        // Compute base modularity gains
        // if moving vertices out of current communities
        For each vertex v in graph:
            comm <- current_communities[v];
            w_v2comm <- Find weights from v to comm in segment_weights;
            gain_bases[v] = weights_v2self[v] - w_v2comm
                - (weights_v2any[v] - weights_community2any[comm])
                    * weights_v2any[v] / m2;

        // Find the max gains if moving vertices into adjacent communities
        For each vertex v in graph:
            gains[v] <- 0;
            next_communities[v] <- current_communities[v];
        For each seg<v, comm> segment:
            if (comm == current_communities[v])
                continue;
            gain <- gain_bases[v] + segment_weights[seg]
                - weights_community2any[comm] * weights_v2any[v] / m2;
            atomicMax(max_gains + v, gain);
```

```
            seg_gains[seg] <- gain;
        For each seg<v, comm> segment:
            if (seg_gains[seg] != max_gains[v])
                continue;
            next_communities[v] <- comm;

        // Update communities
        For each vertex v in graph:
            curr_comm <- current_communities[v];
            next_comm <- next_communities[v];
            if (curr_comm == next_comm)
                continue;

            atomicAdd(weights_community2any[next_comm],  weights_v2any[v]);
            atomicAdd(weights_community2any[curr_comm], -weights_v2any[v]);
            current_communities[v] <- next_comm;

        iteration_gain <- Reduce(max_gains, sum);
        pass_gain += iteration_gain;
    While iterations stop condition not met
    // End of modularity optimizing iterations

    // Contract the graph
    // renumber occupied communities
    new_communities <- Renumber(current_communities);
    For each edge e<v, u> in graph: //an advance operator on all edges
        edge_pairs[e] <- <new_communities[current_communities[v]],
                          new_communities[current_communities[u]]>
    Sort(edge_pairs, edge_weights) by pair.x, then pair.y if tie;
    segment_offsets <- offsets of continuous edge_pairs;
    new_graph.Allocate(|new_communities|, |segments|);
    new_graph.edges <- first pair of each segments;
    new_graph.edge_values <- SegmentedReduce(edge_weights, segment_offsets, sum);

While pass stop condition not met
```

How To Run This Application on DARPA's DGX-1

Prereqs/input

CUDA should have been installed; `$PATH` and `$LD_LIBRARY_PATH` should have been set correctly to use CUDA. The current Gunrock configuration assumes boost (1.58.0 or 1.59.0) and Metis are installed; if not, changes need to be made in the Makefiles. DARPA's DGX-1 has both installed when the tests are performed.

```
git clone --recursive https://github.com/gunrock/gunrock/
cd gunrock
git checkout dev-refactor
git submodule init
git submodule update
mkdir build
cd build
cmake ..
cd ../tests/louvain
make
```

At this point, there should be an executable `louvain_main_<CUDA version>_x86_64` in `tests/louvain/bin`.

The datasets are assumed to have been placed in `/raid/data/hive`, and converted to proper matrix market format (.mtx). At the time of testing, `ca`, `amazon`, `akamai`, and `pokec` are available in that directory. `ca` and `amazon` are taken from PNNL's implementation, and originally use 0-based vertex indices; 1 is added to each vertex id to make them proper .mtx files.

The testing is done with Gunrock using the `dev-refactor` branch at commit `2699252` (Oct. 18, 2018), using CUDA 9.1 with NVIDIA driver 390.30.

Running the application

```
./bin/louvain_main_9.1_x86_64 --omp-threads=32 --iter-stats --pass-stats \
--advance-mode=ALL_EDGES --unify-segments=true --validation=each --num-runs=10 \
--graph-type=market --graph-file=/raid/data/hive/[DataSet]/[DataSet].mtx \
--jsondir=[LogDir] > [LogDir]/[DataSet].txt 2>&1
```

- Add `--undirected`, if the graph is indeed undirected.
- Remove `--iter-stats` or `--pass-stats`, if detailed timings are not required.
- Remove `--validation=each`, to only compute the modularity for the last run.

For example, when DataSet = `akamai`, and LogDir = `eval/DGX1-P100x1`, the command is

```
./bin/louvain_main_9.1_x86_64 --omp-threads=32 --iter-stats --pass-stats \
--advance-mode=ALL_EDGES --unify-segments=true --validation=each --num-runs=10 \
--graph-type=market --graph-file=/raid/data/hive/akamai/akamai.mtx \
--jsondir=eval/DGX1-P100x1 > eval/DGX1-P100x1/akamai.txt 2>&1
```

Output

The outputs are in the louvain directory. Look for the `.txt` files: running time is after `Run x elapsed:`, and the number of communities and the resulting modularity is in the line that starts with `Computed:`. There are 12 runs in each `.txt` file: 1 single thread CPU run for reference, 1 OpenMP multiple-thread (32 threads in the example, may not be optimal) run, and 10 GPU runs.

The output was compared against PNNL's results on the number of communities and modularity for the amazon and ca datasets. Note that PNNL's code does not count dangling vertices in communities. The results listed below use the number of communities minus dangling vertices; the dataset details are can be found in the next section.

The modularity of resulting communities:

DataSet	Gunrock GPU	OMP (32T)	Serial	PNNL (8T)	PNNL (serial)
amazon	0.908073	0.925721	0.926442	0.923728	0.925557
ca	0.711971	0.730217	0.731292	0.713885	0.727127

Note for these kind of small graphs, more parallelism could hurt the resulting modularity. Multi-thread CPU implementations from both Gunrock and PNNL yield modularities a little less than the serial versions, and the GPU implementation sees a ~0.02 drop. The reason could be concurrent updates to communities: vertex A moves to community C, thinking vertex B is in C; but B may have simultaneously moved to other communities.

However, when input graphs are larger in size, this issue seems to disappear, and modularities from the GPU implementation are sometimes even better than the serial implementation. (See detailed results below.)

The number of resulting communities:

DataSet	Gunrock GPU	OMP (32T)	Serial	PNNL (8T)	PNNL (serial)
amazon	7667	213	240	298	251
ca	1120	616	617	654	623

More parallelism also affects the number of resulting communities. On these two small datasets, the GPU implementation produces significantly more communities than all CPU implementations; on large datasets, the differences in the number of communities are much smaller. We believe the reason may also be concurrent community updates, especially when whole-community migration happens: all vertices in community A decide to move to community B, and all vertices in community B decide to move to community A. In the serial implementation, we may see these two communities combine into a single community,

but on the GPU, we instead see that community A and B just swap their labels and never become a single community.

Performance and Analysis

We measure Louvain performance with three metrics: the number of resulting communities (#Comm), the modularity of resulting communities (Q), and the running time (Time, in seconds). Higher Q and lower running time are better. * indicates the graph is given as undirected, and the number of edges is counted after edge doubling and removing of self loops or duplicate edges; otherwise, the graph is taken as directed, and self loops or duplicate edges are also removed. If edge weights are available in the input graph, they follow the input; otherwise, the initial edge weights are set to 1.

Details of the datasets:

DataSet	#V	#E	#dangling vertices
ca	108299	186878	85166
preferentialAttachment	100000	999970*	0
caidaRouterLevel	192244	1218132*	0
amazon	548551	1851744	213688
coAuthorsDBLP	299067	1955352*	0
webbase-1M	1000005	2105531	2453
citationCiteseer	268495	2313294*	0
cnr-2000	325557	3128710	0
as-Skitter	1696415	22190596*	0
coPapersDBLP	540486	30481458*	0
pokec	1632803	30622564	0
coPapersCiteseer	434102	32073440*	0
akamai	16956250	53300364	0
soc-LiveJournal1	4847571	68475391	962
channel-500x100x100-b050	4802000	85362744	0
europe_osm	50912018	108109320*	0
hollywood-2009	11399905	112751422*	32662
rgg_n_2_24_s0	16777216	265114400*	1
uk-2002	18520486	292243663	37300

Running time in seconds:

GPU	Dataset	Gunrock GPU	Speedup vs. OMP	OMP	Serial
P100	ca	0.108	0.24	**0.026**	0.065
V100	ca	0.089	0.33	**0.029**	0.067
V100	preferentialAttachment	**0.076**	1.26	0.096	0.235
V100	caidaRouterLevel	**0.063**	1.03	0.065	0.229

GPU	Dataset	Gunrock GPU	Speedup vs. OMP	OMP	Serial
P100	amazon	**0.160**	1.27	0.203	0.648
V100	amazon	**0.122**	1.62	0.198	0.631
V100	coAuthorsDBLP	**0.082**	1.62	0.133	0.414
V100	webbase-1M	**0.107**	1.57	0.168	0.318
V100	citationCiteseer	**0.074**	1.50	0.111	0.432
V100	cnr-2000	0.235	0.57	**0.133**	0.388
V100	as-Skitter	**0.376**	1.76	0.660	2.480
V100	coPapersDBLP	**0.358**	1.22	0.437	1.860
P100	pokec	**0.929**	1.34	1.244	6.521
V100	pokec	**0.624**	1.74	1.083	6.110
V100	coPapersCiteseer	**0.353**	1.11	0.391	1.592
P100	akamai	**1.278**	5.13	6.560	14.427
V100	akamai	**0.934**	6.79	6.343	13.266
V100	soc-LiveJournal1	**1.548**	2.59	4.016	16.311
V100	channel-500x100x100-b050	1.133	0.68	**0.768**	4.449
V100	europe_osm	**4.902**	7.11	34.875	101.320
V100	hollywood-2009	**1.230**	1.40	1.721	9.419
V100	rgg_n_2_24_s0	3.378	0.79	**2.664**	17.816
V100	uk-2002	**4.921**	1.15	5.682	31.006

Resulting modularity:

GPU	DataSet	Gunrock GPU	Gunrock - Serial	OMP	OMP - Serial	Serial
P100	ca	0.7112	-0.0193	0.7302	-0.0011	**0.7313**
V100	ca	0.7166	-0.0147	0.7290	-0.0025	**0.7313**
V100	preferentialAttachment	0.1758	-0.1095	0.2287	-0.0565	**0.2852**
V100	caidaRouterLevel	**0.8500**	+0.0065	0.8362	-0.0073	0.8436
P100	amazon	0.9081	-0.0184	0.9257	-0.0007	**0.9264**
V100	amazon	0.9089	-0.0175	0.9258	-0.0006	**0.9264**
V100	coAuthorsDBLP	0.8092	-0.0179	0.8136	-0.0135	**0.8271**
V100	webbase-1M	0.8945	-0.0613	0.9471	-0.0087	**0.9558**
V100	citationCiteseer	0.7888	-0.0137	0.7605	-0.0420	**0.8025**
V100	cnr-2000	0.8766	-0.0031	0.8784	-0.0013	**0.8797**
V100	as-Skitter	**0.8366**	+0.0234	0.8223	+0.0091	0.8132
V100	coPapersDBLP	**0.8494**	+0.0003	0.8440	-0.0051	0.8492
P100	pokec	0.6933	-0.0012	0.6914	-0.0032	**0.6945**
V100	pokec	0.6741	-0.0204	0.6763	-0.0183	**0.6945**
V100	coPapersCiteseer	0.9075	-0.0035	0.9059	-0.0051	**0.9110**
P100	akamai	**0.9334**	+0.0329	0.9072	+0.0067	0.9005
V100	akamai	**0.9333**	+0.0328	0.9074	+0.0070	0.9005
V100	soc-LiveJournal1	**0.7336**	+0.0097	0.5456	-0.1782	0.7239
V100	channel-500x100x100-b050	0.9004	+0.0498	**0.9512**	+0.1007	0.8505
V100	europe_osm	**0.9979**	+0.0142	0.9844	+0.0008	0.9836

GPU	DataSet	Gunrock GPU	Gunrock - Serial	OMP	OMP - Serial	Serial
V100	hollywood-2009	0.7432	-0.0079	0.7502	-0.0010	**0.7511**
V100	rgg_n_2_24_s0	**0.9921**	+0.0026	0.9920	+0.0024	0.9896
V100	uk-2002	0.9507	-0.0098	0.9604	+0.0000	**0.9604**

The number of resulting communities:

GPU	DataSet	Gunrock GPU	OMP	Serial
P100	ca	1120	616	617
V100	ca	1076	615	617
V100	preferentialAttachment	18	14	39
V100	caidaRouterLevel	410	467	745
P100	amazon	7667	213	240
V100	amazon	7671	233	240
V100	coAuthorsDBLP	95	138	273
V100	webbase-1M	4430	1469	1362
V100	citationCiteseer	67	48	141
V100	cnr-2000	65621	59219	59253
V100	as-Skitter	924	1945	2531
V100	coPapersDBLP	70	111	237
P100	pokec	154988	161709	166156
V100	pokec	155100	162464	166156
V100	coPapersCiteseer	108	110	358
P100	akamai	90285	130639	145785
V100	akamai	90245	127843	145785
V100	soc-LiveJournal1	506826	434272	447426
V100	channel-500x100x100-b050	24	54	12
V100	europe_osm	17320	784171	828662
V100	hollywood-2009	12218	12593	12741
V100	rgg_n_2_24_s0	344	359	311
V100	uk-2002	2402560	2245355	2245678

Implementation limitations

- **Memory usage** Each edge in the graph needs at least 88 bytes of GPU device memory: 32 bits for the destination vertex, 64 bits for edge weight, 64 bits x 2 x 4 for edge pairs and sorting, 32 bits for segment offsets and 64 bits for segment weights (assuming both vertex and edge ids are represented as 32-bit integers and edge weights are represented as 64-bit floating point numbers). So using a 32 GB GPU, the maximum graph the Louvain implementation can process is roughly 300 million edges. The largest graph successfully run so far is `uk-2002` with 292M edges and 18.5M vertices.

- **Data types** The edge weights and all computation around them are double-precision floating point values (64-bit `double` in C/C++); we tried single precision and found it resulted in very poor modularities. The `weight * weight / m2` part in the modularity calculation may be the reason for this limitation. Vertex ids should be 32-bit, as the implementation uses 64-bit integers to represent an edge pair for the sort function; if fast GPU sorting is available for 128-bit integers, 64-bit vertex ids might be used.

Comparison against existing implementations

We compare against serial CPU and OpenMP implementations; both are Gunrock's CPU reference routines. PNNL's results and previous published works are also referenced, to make sure the resulting modularities and running times are sane.

- **Modularity** The modularities have some variation from different implementations, mostly within +/- 0.05. On small graphs, the GPU implementation sees some modularity drops; on large graphs, the GPU implementation is more likely to yield modularity at least as good as the serial implementation. The larger the graph is, the better relative modularity is expected from Gunrock, as compared to the serial implementation. As mentioned in the output section, that variation could be caused by concurrent movement of vertices. Small graphs could suffer more than larger graphs, as movements to a community have a higher chance to happen concurrently.
- **Running time** Overall, the Gunrock implementation is 2x to 5x faster than previous work on GPU (Naim 2017, Cheong 2013). Our OMP implementation is a bit faster than PNNL's, and much faster than previous work using multiple CPU threads (Lu 2015, Naim 2016). The sequential CPU is an order of magnitude faster than previous sequential CPU work (Naim 2017, Naim 2016, Blondel 2008, Cheong 2013, Lu 2015). Comparing across different Gunrock implementations, the GPU is not always the fastest: on small graphs, GPU could actually be slower, caused by GPU kernel overheads and hardware underutilization; so for small graphs, the OpenMP implementation may be a better choice. Gunrock's GPU implementation in practice runs slower than OpenMP for mesh-like graphs, in which every vertex only has a very small neighbor list; the parallel formulation Gunrock uses does not work well on this kind of graph.

Published results (timing and modularity) from previous work are summarized in the louvain_results.xlsx file in the `louvain` directory.

Performance limitations

The GPU performance bottleneck is the sort function, especially in the first pass. It's true that sort on GPU is much faster than CPU; but the CPU implementations use hash tables, which may not be suitable for the GPU; the alternative approaches section has more details on this.

Using the `akamai` dataset to profile the GPU Louvain implementation on a V100, an iteration in the first pass takes 64.08 ms, and the sort takes 42.05 ms, which is two-thirds of the iteration time. The Louvain implementation uses CUB's radix-sort-pair function. CUB is considered to be one of the GPU primitive libraries that provide the best performance. Further profiling shows during the sort kernel, the device memory controller is ~75% utilized; in other words, the sort is memory bound. This is as expected, as in each iteration of radix sort, the whole `edge_pairs` and `pair_weights` arrays are shuffled, with cost on the order of `O(|E|)`, although the memory accesses are mostly coalesced. The memory system utilizations are as below (from NVIDIA profiler):

Type	Transactions	Bandwidth	Utilization
Shared Loads	2141139	1168.859 GB/s	
Shared Stores	2486946	1357.636 GB/s	
Shared Total	4628085	2526.495 GB/s	Low
L2 Reads	2533302	345.736 GB/s	
L2 Writes	2831732	386.464 GB/s	
L2 Total	5365034	732.200 GB/s	Low
Local Loads	588	80.248 MB/s	
Local Stores	588	80.248 MB/s	
Global Loads	2541637	346.873 GB/s	
Global Stores	2675820	365.186 GB/s	
Texture Reads	2515533	1373.242 GB/s	
Unified Cache Total	7734166	2085.462 GB/s	Idle to Low
Device Reads	2469290	336.999 GB/s	
Device Writes	2596403	354.347 GB/s	
Device Memory Total	**5065693**	**691.347 GB/s**	**High**
PCIe Reads	0	0 B/s	None
PCIe Writes	5	682.381 kB/s	Idle to Low

It's clear that the bottleneck is at the device memory: most data are read-once and write-once, with little possibility to reuse the data. The kernel achieved 691 GB/s bandwidth utilization, ~77% of the 32GB HBM2's 900 GB/s capability. This high-bandwidth utilization fits the memory access pattern: mostly regular and coalesced.

The particular issue here is not the kernel implementation itself, it's the usage of sorting: fully sorting the whole edge list is perhaps overkill. One possible improvement is to use a custom hash table on the GPU, to replace the sort +

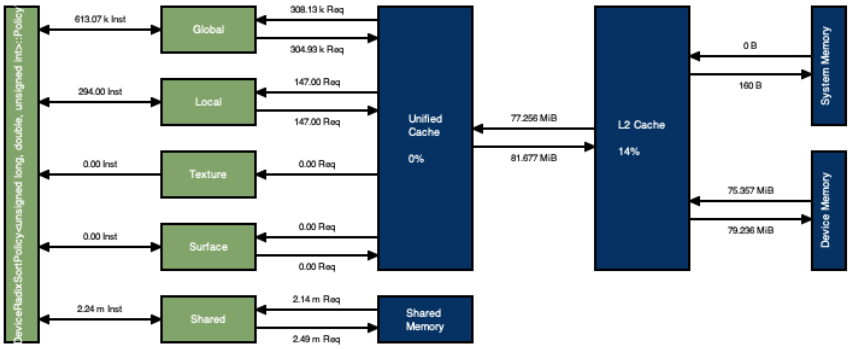

Figure 6.1: Louvain_akamai

segmented reduce part. The hash table could also cut the memory requirement by about 50%.

Next Steps

Alternate approaches

Things we tried that didn't work well

Segmented sort and CUB segmented reduce: the original idea for modularity optimization is to use CUB's segmented sort and segmented reduce within each vertex's neighborhood to get the vertex-community weights. However, CUB uses one block per each segment in these two routines, and that creates huge load imbalance, as the neighbor list length can have large differences. The solution is 1) use vertex-community pairs as keys, and CUB's unsegmented sort; 2) implement a load-balanced segmented-reduce kernel. This solution reduces the sort-reduce time by a few X, and can be enabled by the `--unify-segments` flag on the command line.

STL hash table on CPU: the `std::map` class has performance issues when used in a multi-threading environment, and yields poor scalability; it might be caused by using locks in the STL. The solution is to use a size |V| array per thread for the vertices that thread processes. Since within a thread, vertices are processed one by one, and the maximum number of communities is |V|, so instead of a hash table, a flat size |V| array can replace the hash table. This solution significantly reduces the running time, even using a single thread. The multi-thread scalability is also much better.

Vanilla hash table on GPU: this can't be used, as keys (vertex-community or community-community pair) and the values (edge weights) are both 64-bit, and there is currently no support of atomic-compare-and-exchange operations

for 128-bit data. Even if that's available, a vanilla table only provides insert and query operations, but not accumulation of values for the same key.

Custom hash table

Hash tables can be used to accumulate the vertex-to-community weights during modularity optimization iterations, and to get the community-to-community edge weights during the graph contraction part of the algorithm. Previous implementations use hash tables as a common practice. However, as mentioned above, vanilla hash tables that store key-value pairs are not a good choice for Louvain.

Louvain not only needs to store the key-value pairs, but also to accumulate values associated with the same key. That key may be the same vertex-community pair for modularity optimization, or the same community-community pair for graph contraction. Ideally, if the hash table provides the following functionality, it would be much more suitable for Louvain:

- Only insert the key (in the first phase of using the hash table).
- In the next phase, query the *positions* of the keys, and use atomics to accumulate the values belonging to the same key, in a separate array.
- There must be a barrier between the two phases; all insertions of the first phase need to be visible to the second phase.

This kind of hash table removes the strong restriction that the key-value pair needs to be able to support an atomic compare-and-exchange operation, which is imposed by vanilla hash table implementations. The custom hash table is also more value-accumulation-friendly. It replaces the sort-segmented reduce part, and can reduce the workload from about O(6|E|) to O(2|E|), and the memory requirement from 48|E| bytes to 24|E|. However, the memory access pattern now becomes irregular and uncoalesced, so it is still unknown whether it can actually yield a performance gain.

Iteration and pass stop conditions

The concurrent nature of the GPU implementation makes modularity gain calculation inaccurate. Community migrations are also observed. Because of these, the optimization iterations and the passes may run more than needed, and resulted in longer running times, especially in the first pass. Preliminary experiments to cap the number of iterations for the first pass can reduce the running time by about 40%, with the modularity value roughly unchanged. The actual cap is dataset-dependent, and more investigation is needed to get a better understanding of how to set the cap.

Gunrock implications

The core of the Louvain implementation mainly uses all-edges advance, sort, segmented reduce, and for loops. The sort-segmented reduce operation is actually a segmented keyed reduce; if that's a common operation that appears in more algorithms, it could be made into a new operator. The all-edges advance is used quite often in several applications, so wrapping it with a simpler operator interface could be helpful.

Notes on multi-GPU parallelization

When parallelizing across multiple GPUs, the community assignment of local vertices and their neighbors needs to available locally, either explicitly by moving them using communication functions, or implicitly by peer memory access or unified virtual memory. The communication volume is in the order of O(|V|) and the computation workload is at least in O(|E|), so the scalability should be manageable.

When the number of GPUs is small, 1D partitioning can be used to divide the edges, and replicate the vertices, so there is no need to do vertex id conversion across multiple GPUs. When the number of GPUs is large, the high-low degree vertex separation and partitioning scheme can be used: edges are still distributed across GPUs, high degree vertices are duplicated, and low degree vertices are owned by one GPU each. The boundary to use different partitioning scheme is still unclear, but it's likely that 8 GPUs within a DGX-1 can still be considered as a small number, and use the simple 1D partitioning.

Notes on dynamic graphs

Louvain is not directly related to dynamic graphs. But it should be able to run on a dynamic graph, provided the way to access all the edges is the same. Community assignment from the previous graph can be used as a good starting point, if the vertex ids are consistent and the graph is not dramatically changed.

Notes on larger datasets

The bottleneck of memory usage of the current implementation is in the edge pair-weight sort function: that makes up about half of the memory usage. Replacing sort-segmented reduce with a custom hash table could significantly lower the memory usage.

Louvain needs to go over the whole graph once in each modularity optimization iteration. If the graph is larger than the combined GPU memory space, which forces streaming of the graph in each modularity optimization iteration, the performance bottleneck will be CPU-GPU bandwidth. That can be an order of magnitude slower than when the graph can fully fit in GPU memory. Considering the OpenMP implementation is not that slow, using that may well be faster than moving the graph multiple times across the CPU-GPU bridge.

Notes on other pieces of this workload

All parts of Louvain are graph related, and fully implemented in Gunrock.

Research potential

Community detection on graphs is generally an interesting research topic, and others have targeted good GPU implementations for it. Our work is the first time Louvain is mapped to sort and segmented reduce, so more comparisons are needed to know whether it's better than the hash table mapping. The custom hash table implementation is worth trying out, and comparing with the current sort and segmented reduce implementation. Multi-GPU implementations, particularly the graph contraction part, can be a place for research investigation: it may be better to contract the graph onto a single GPU, or even the CPU, when the graph is small; but where is the threshold and how to do the multi-GPU to single-GPU or CPU switch?

Label propagation is another algorithm for community detection. It has a similar structure to Louvain, but has a simpler way to decide how to move the vertices. Comparing them side by side for both result quality (the modularity value) and computation speed (the running time) will be beneficial.

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Chapter 7

Local Graph Clustering (LGC)

From Andersen et al.:

> A local graph partitioning algorithm finds a cut near a specified starting vertex, with a running time that depends largely on the size of the small side of the cut, rather than the size of the input graph.

A common algorithm for local graph clustering is called PageRank-Nibble (PRNibble), which solves the L1 regularized PageRank problem. We implement a coordinate descent variant of this algorithm found in Fountoulakis et al., which uses the fast iterative shrinkage-thresholding algorithm (FISTA).

Summary of Results

This variant of local graph clustering (L1 regularized PageRank via FISTA) is a natural fit for Gunrock's frontier-based programming paradigm. We observe speedups of 2-3 orders of magnitude over the HIVE reference implementation.

The reference implementation of the algorithm was not explicitly written as `advance`/`filter`/`compute` operations, but we were able to quickly determine how to map the operations by using a lightweight Python implementation of the Gunrock programming API as a development environment. Thus, LGC was a good exercise in implementing a non-trivial end-to-end application in Gunrock from scratch.

Summary of Gunrock Implementation

We implement Algorithm 2 from Fountoulakis et al., which maps nicely to Gunrock. We present the pseudocode below along with the corresponding Gunrock operations:

```
A: adjacency matrix of graph
D: diagonal degree matrix of graph
Q: D^(-1/2) x (D - (1 - alpha)/2 x (D + A)) x D^(-1/2)
s: teleportation distribution, a distribution over nodes of graph
d_i: degree of node i
p_0: PageRank vector at iteration 0
q_0:  D^(-1/2) x p term that coordinate descent optimizes over
f(q): 1/2<q, Qq> - alpha x <s, D^(-1/2) x q>
grad_f_i(q_0): i'th term of the gradient of f(q_0) using q at iteration 0
rho: constant used to ensure convergence
alpha: teleportation constant in (0, 1)

Initialize: rho > 0
Initialize: q_0 = [0 ... 0]
Initialize: grad_f(q_0) = -alpha x D^(-1/2) x s

For k = 0, 1, ..., inf
    // Implemented using Gunrock ForAll operator
    Choose an i such that grad_f_i(q_k) < - alpha x rho x d_i^(1/2)
    q_k+1(i) = q_k(i) - grad_f_i(q_k)
    grad_f_i(q_k+1) = (1 - alpha)/2 x grad_f_i(q_k)

    // Implemented using Gunrock Advance and Filter operator
    For each j such that j ~ i
        Set grad_f_j(q_k+1) = grad_f_j(q_k) +
            (1 - alpha)/(2d_i^(1/2) x d_j^(1/2)) x A_ij x grad_f_i(q_k)

    For each j such that j !~ j
        Set grad_f_j(q_k+1) = grad_f_j(q_k)

    // Implemented using Gunrock ForEach operator
    // Note: ||y||_inf is the infinity norm
    if (||D^(-1/2) x grad_f(q_k)||_inf > rho x alpha)
            break
EndFor

return p_k = D^(1/2) x q_k
```

How To Run This Application on DARPA's DGX-1

Prereqs/input

```
# clone gunrock
git clone --recursive https://github.com/gunrock/gunrock.git \
        -b dev-refactor
```

```
cd gunrock/tests/pr_nibble
cp ../../gunrock/util/gitsha1.c.in ../../gunrock/util/gitsha1.c
make clean
make
```

Running the application

Example command

```
./bin/test_pr_nibble_9.1_x86_64 \
    --graph-type market \
    --graph-file ../../dataset/small/chesapeake.mtx \
    --src 0 \
    --max-iter 1
```

Example output

```
Loading Matrix-market coordinate-formatted graph ...
  Reading meta data from ../../dataset/small/chesapeake.mtx.meta
  Reading edge lists from ../../dataset/small/chesapeake.mtx.coo_edge_pairs
  Substracting 1 from node Ids...
  Edge doubleing: 170 -> 340 edges
  graph loaded as COO in 0.084587s.
Converting 39 vertices, 340 directed edges ( ordered tuples) to CSR format...Done (0s).
Degree Histogram (39 vertices, 340 edges):
    Degree 0: 0 (0.000000 %)
    Degree 2^0: 0 (0.000000 %)
    Degree 2^1: 1 (2.564103 %)
    Degree 2^2: 22 (56.410256 %)
    Degree 2^3: 13 (33.333333 %)
    Degree 2^4: 2 (5.128205 %)
    Degree 2^5: 1 (2.564103 %)


---------------------------
pr_nibble::CPU_Reference: reached max iterations. breaking at it=10
---------------------------
 Elapsed: 0.103951
============================================
 advance-mode=LB
Using advance mode LB
Using filter mode CULL
---------------------------
0    2   0   queue3      oversize :  234 ->  342
0    2   0   queue3      oversize :  234 ->  342
pr_nibble::Stop_Condition: reached max iterations. breaking at it=10
---------------------------
Run 0 elapsed: 1.738071, #iterations = 10
```

```
0 errors occurred.
[pr_nibble] finished.
 avg. elapsed: 1.738071 ms
 iterations: 140733299213840
 min. elapsed: 1.738071 ms
 max. elapsed: 1.738071 ms
 src: 0
 nodes_visited: 41513344
 edges_visited: 140733299212960
 nodes queued: 140733299212992
 edges queued: 5424992
 load time: 116.627 ms
 preprocess time: 963.004000 ms
 postprocess time: 0.080824 ms
 total time: 965.005875 ms
```

Expected Output

We do not print the actual output values of PRNibble, but we output the results of a correctness check of the GPU version against our CPU implementation. `0 errors occurred.` indicates that LGC has generated an output that exactly matches our CPU validation implementation.

Our implementations are validated against the HIVE reference implementation.

For ease of exposition, and to help in mapping the workflow to Gunrock primitives, we also implemented a version of PRNibble in pygunrock. This implementation is nearly identical to the actual Gunrock app, but in a way that more clearly exposes the logic of the app and eliminates a lot of Gunrock scaffolding/memory management/etc.

Performance and Analysis

Performance is measured by the runtime of the approximate PageRank solver, given

- a graph `G=(U, E)`
- a (set of) seed node(s) `S`
- some parameters controlling e.g., the target conductivity of the output cluster (`rho`, `alpha`, ...)

The reference implementation also includes a sweep-cut step, where a threshold is applied to the approximate PageRank values to produce hard cluster assignments. We do not implement this part of the workflow, as it is not fundamentally a graph operation.

Implementation limitations

PageRank runs on arbitrary graphs – it does not require any special conditions such as node attributes, etc.

- **Memory size**: The dataset is assumed to be an undirected graph (with no self-loops). We were able to run on graphs of up to 6.2 GB in size (7M vertices, 194M edges). The memory limitation should be the number of edges `2*|E| + 7*|U|`, which needs to be smaller than the GPU memory size (16 GB for a single P100 on DGX-1).
- **Data type**: We have only tested our implementations using an `int32` data type for node IDs. However, we could also support `int64` node IDs for graphs with more than 4B edges.

Comparison against existing implementations

We compare our Gunrock GPU implementation with two CPU reference implementations:

- HIVE reference implementation (Python wrapper around C++ library)
- Gunrock CPU reference implementation (C++)

We find the Gunrock implementation is 3 orders of magnitude faster than either reference CPU implementation. The minimum, geometric mean, and maximum speedups are 7.25x, 1297x, 32899x, respectively.

All runtimes are in milliseconds (ms):

Dataset	HIVE Ref. C++	Gunrock C++	Gunrock GPU	Speedup
delaunay_n13	21.52	16.33	2.86	8
ak2010	97.99	72.08	3.04	32
coAuthorsDBLP	1004	1399	4.86	207
belgium_osm	2270	1663	2.97	726
roadNet-CA	3403	2475	3.03	1123
delaunay_n21	5733	4084	2.98	1924
cit-Patents	40574	22148	16.41	2472
hollywood-2009	43024	30430	46.30	929
road_usa	48232	31617	3.01	16024
delaunay_n24	49299	34655	3.28	15030
soc-LiveJournal1	63151	37936	19.29	3274
europe_osm	97022	72973	2.95	32889
indochina-2004	101877	71902	11.05	9220
kron_g500-logn21	110309	89438	627.55	176
soc-orkut	111391	89752	18.05	6171

Performance limitations

We profiled the Gunrock GPU primitives on the `kron_g500-logn21` graph. The profiler adds approx. 100 ms of overhead (728.48 ms with profiler vs. 627.55 ms without profiler). The breakdown of runtime by kernel looks like:

Gunrock Kernel	Runtime (ms)	Percentage of Runtime
Advance (EdgeMap)	566.76	77.8%
Filter (VertexMap)	10.85	1.49%
ForAll (VertexMap)	2.90	0.40%
Other	147.89	20.3%

Note: "Other" includes HtoD and DtoH memcpy, smaller kernels such as scan, reduce, etc.

By profiling the LB Advance kernel, we find that the performance of `advance` is bottlenecked by random memory accesses. In the first part of the computation – getting row pointers and column indices – memory accesses can be coalesced and the profilers says we perform 4.9 memory transactions per access, which is close to the ideal of 4. However, once we start processing these neighbors, the memory access becomes random and we perform 31.2 memory transactions per access.

Next Steps

Alternate approaches

PRNibble can also be implemented in terms of matrix operations using our GPU GraphBLAS library – this implementation is currently in progress.

In theory, local graph clustering is appealing because you don't have to "touch" the entire graph. However, all LGC implementations that we are aware of first load the entire graph into CPU/GPU memory, which limits the size of the graph that can be analyzed. Implementations that load data from disk "lazily" as computation happens would be interesting and practically useful.

Ligra includes some high performance implementations of similar algorithms. In the future, it would be informative to benchmark our GPU implementation against those performance optimized multi-threaded CPU implementations.

Gunrock implications

Gunrock currently supports all of the operations needed for this application. In particular, the `ForAll` and `ForEach` operators were very useful for this application.

Additionally, `pygunrock` proved to be a useful tool for development – correctly mapping the original (serial) algorithm to the Gunrock operators required a lot of attention to detail, and having an environment for rapid expedited experimentation facilitated the algorithmic development.

Notes on multi-GPU parallelization

Since this problem maps well to Gunrock operations, we expect parallelization strategy would be similar to BFS and SSSP. The dataset can be effectively divided across multiple GPUs.

Notes on dynamic graphs

It is not obvious how this algorithm would be extended to handle dynamic graphs. At a high level, the algorithm iteratively spreads mass from the seed nodes to neighbors in the graph. As the connectivity structure of the graph changes, the dynamics of this mass spreading could change arbitrarily – imagine edges that form bridges between two previously distinct clusters. Thus, we suspect that adapting the app to work on dynamic graphs may require substantial development and study of the underlying algorithms.

Notes on larger datasets

If the data were too big to fit into the aggregate GPU memory of multiple GPUs on a single node, then we would need to look at multiple-node solutions. Getting the application to work on multiple nodes would not be challenging, because it is very similar to BFS. However, optimizing it to achieve good scalability may require asynchronous communication, an area where we have some experience (Pan et al.). Asynchronous communication may be necessary in order to reach better scalability in multi-node, because this application which can be formulated as sparse-matrix vector multiplication has limited computational intensity (low computation-to-communication).

Notes on other pieces of this workload

As mentioned previously, we do not implement the sweep-cut portion of the workflow where the PageRank values are discretized to produce hard cluster assignments. Though it's not fundamentally a graph problem, parallelization of this step is a research question addressed in Shun et al.

Potential future academic work

The coordinate descent implementation (developed by Ben Johnson) shows that Gunrock can be used as a coordinate descent solver. There has been more interest in coordinate descent recently, because coordinate descent can be used in ML as an alternative to stochastic gradient descent for SVM training.

References

Prof. Cho-Jui Hsieh from UC Davis is an expert in this field (see 1, 2, 3).

Chapter 8

Graph Projections

Given a (directed) graph `G`, graph projection outputs a graph `H` such that `H` contains edge `(u, v)` iff `G` contains edges `(w, u)` and `(w, v)` for some node `w`. That is, graph projection creates a new graph where nodes are connected iff they are neighbors of the same node in the original graph. Typically, the edge weights of `H` are computed via some (simple) function of the corresponding edge weights of `G`.

Graph projection is most commonly used when the input graph `G` is bipartitite with node sets `U1` and `U2` and directed edges `(u, v)`. In this case, the operation yields a unipartite projection onto one of the node sets. However, graph projection can also be applied to arbitrary (unipartite) graphs.

Summary of Results

Because it has a natural representation in terms of sparse matrix operations, graph projections gave us an opportunity to compare ease of implementation and performance between Gunrock and another UC-Davis project, GPU GraphBLAS.

Overall, we found that Gunrock was more flexible and more performant than GraphBLAS, likely due to better load balancing. However, in this case, the GraphBLAS application was substantially easier to program than Gunrock, and also allowed us to take advantage of some more sophisticated memory allocation methods available in the GraphBLAS cuSPARSE backend. These findings suggest that addition of certain commonly used API functions to Gunrock could be a fruitful direction for further work.

Summary of Gunrock Implementation

We implement two versions of graph projections: one using Gunrock and one using GraphBLAS.

Gunrock

First, we can compute graph projection in Gunrock via a single `advance` operation from all nodes w/ nonzero outgoing degree:

```
def _advance_op(self, G, H_edges, src, dest):
    for neib in G.neighbors(src):
        if dest != neib:
            H_edges[dest * G.num_nodes + neib] += 1
```

That is, for each edge in the graph, we fetch the neighbors of the source node in `G`, then increment the weight of the edge between `dest` and each of those neighbors in `H_edges`.

Note that we have only implemented the unweighted case and a single method for computing the edgeweights of `H`, but the extension to weighted graphs and different weighting functions would be straightforward.

We use a dense `|V|x|V|` array to store the edges of the output matrix `H`. This is simple and fast, but uses an unreasonably large amount of memory (a graph with 60k nodes requires 16 GB). In the worst-case scenario, `H` may actually have all `|V|x|V|` possible edges, but any typical real-world graph has *far* fewer edges in practice.

GraphBLAS

Second, we implement graph projection as a single sparse matrix-matrix multiply in our GraphBLAS GPU library, which wraps and extends cuSPARSE.

Graph projection admits a simple linear algebra formulation. Given the adjacency matrix `A` of graph `G`, the projection is just:

```
H = matmul(transpose(A), A)
```

which can be concisely implemented via cuSPARSE's `csr2csc` and `csrgemm` functions.

The `csrgemm` functions in cuSPARSE allocate memory more intelligently than we do above, on the order of the number of edges in the output. Thus, our GraphBLAS implementation can scale to substantially larger matrices than our Gunrock implementation. However, implementing graph projection via a single call to `csrgemm` requires both the input graph `G` and output graph `H` to fit in GPU memory (16 GB on the DGX-1). This limit can easily be hit, even for a moderately sized `G`, as the number of edges in `H` is often orders of magnitude larger than in `G`.

Thus, to scale to larger graphs, we implement graph projections via a chunked matrix multiply. Specifically, to compute `matmul(X, Y)` w/ `X.shape = (n,`

`m)` and `Y.shape = (m, k)`, we split `X` into `c` matrices `(X_1, ..., X_c)`, w/ `X_i.shape = (n / c, m)`. Then we compute `matmul(X_i, Y)` for each `X_i`, moving the output of each multiplication from GPU to CPU memory as we go. This implementation addresses the common case where we can fit both `X` and `Y` in GPU memory, but not `matmul(X, Y)`. Obviously, the chunked matrix multiply incurs a performance penalty, but allows us to run graph projections of much larger graphs on the GPU.

How To Run This Application on DARPA's DGX-1

Gunrock

Prereqs/input

```
git clone --recursive https://github.com/gunrock/gunrock -b dev-refactor
cd gunrock/tests/proj/
cp ../../gunrock/util/gitsha1.c.in ../../gunrock/util/gitsha1.c
make clean
make
```

Application specific parameters

None

Example Command

```
./bin/test_proj_9.1_x86_64 \
        --graph-type market \
        --graph-file ../../dataset/small/chesapeake.mtx
```

Example Output

```
Loading Matrix-market coordinate-formatted graph ...
Reading from ../../dataset/small/chesapeake.mtx:
  Parsing MARKET COO format edge-value-seed = 1539110067
 (39 nodes, 340 directed edges)...
Done parsing (0 s).
  Converting 39 vertices, 340 directed edges ( ordered tuples) to CSR format...
Done converting (0s).

--------------------------
--------------------------
 Elapsed: 0.026941
Using advance mode LB
Using filter mode CULL

--------------------------
0    0   0   queue3      oversize :  234 ->  342
0    0   0   queue3      oversize :  234 ->  342
```

```
--------------------------
Run 0 elapsed: 0.199080, #iterations = 1
edge_counter=1372
0->1 | GPU=9.000000 CPU=9.000000
0->2 | GPU=1.000000 CPU=1.000000
0->3 | GPU=2.000000 CPU=2.000000
...
38->35 | GPU=28.000000 CPU=28.000000
38->36 | GPU=2.000000 CPU=2.000000
38->37 | GPU=18.000000 CPU=18.000000
======= PASSED ======
[proj] finished.
 avg. elapsed: 0.199080 ms
 iterations: 38594739
 min. elapsed: 0.199080 ms
 max. elapsed: 0.199080 ms
 src: 0
 nodes_visited: 38578864
 edges_visited: 38578832
 nodes queued: 140734466796512
 edges queued: 140734466795232
 load time: 85.5711 ms
 preprocess time: 955.861000 ms
 postprocess time: 3.808022 ms
 total time: 960.005045 ms
```

Expected Output

When run in `verbose` mode, the app outputs the weighted edgelist of the graph projection `H`. When run in `quiet` mode, it only outputs performance statistics and the results of a correctness check.

GraphBLAS

Prereqs/input

```
git clone --recursive https://github.com/bkj/graphblas_proj
cd graphblas_proj
make clean
make
```

Application specific parameters

```
--unweighted
 1 = convert entries of adjacency matrix to 1
 0 = leave entries of adjacency matrix as-is
--proj-debug
```

```
 1 = print debug information
 0 = don't print debug information
--print-results
 1 = print the edges of the projected graph
 0 = don't print edges
--onto-cols
 1 = given adjacency matrix A w/ `A.shape = (m, n)`,
     compute projection `H = matmul(transpose(A), A)` w/ `H.shape = (n, n)`
 0 = given adjacency matrix A w/ `A.shape = (m, n)`,
     compute projection `H = matmul(A, transpose(A))` w/ `H.shape = (m, m)`
--num-chunks
 <= 1 = do matrix multiply in one step
  > 1 = break matrix multiply into multiple chunks (eg, so we can compute
        projections larger than GPU memory)
```

Example Command

```
# generate some random data `data/X.mtx`
python data/make-random.py --seed 111 \
        --num-rows 1000 --num-cols 1000 --density 0.1

# run graph projection
./proj --X data/X.mtx --unweighted 1 --proj-debug 1
```

Example Output

```
proj.cu: loading data/X.mtx
  done
proj.cu: computing transpose
  done
proj.cu: computing projection
mxm analyze successful!
mxm compute successful!
  done
proj_num_edges          = 999946  # number of edges in H, including self loops
dim_out                 = 1000    # dimension of projected graph
proj_num_edges (noloop) = 998946  # number of edges in H, excluding self loops
timer                   = 208.98  # elapsed time (no IO)
```

Expected Output

The app will print the number of edges in the projected graph. Additionally,

- When run w/ `--print-results=1`, the app prints the edges of the the graph projection `H`.
- When run w/ `--proj-debug=1`, the app prints a small number of progress messages.

Validation

We compared the results of the Gunrock implementation to the HIVE reference implementation and the PNNL implementation. These two implementations vary slightly in their output (e.g., handling of self loops). We validated the correctness of our results against the HIVE reference implementation.

Performance and Analysis

Performance is measured by the runtime of the app, given:

- an input graph `G` (possibly bipartite)
- whether to project onto the rows or columns of the graph.

Implementation limitations

Gunrock

The primary limitation of the current implementation is that it allocates a `|V|x|V|` array, where `|V|` is the number of nodes in the network. This means that the memory requirements of the app can easily exceed the memory available on a single GPU (16 GB on the DGX-1). The size of this array reflects the *worst case* memory requirements of the graph projection workflow; while some graphs can become exceptionally large and dense when projected, we should be able to run the app on larger graphs if we store the output in a different data structure and/or allocate memory more efficiently. Algorithms do exist for mitigating this issue: cuSPARSE's `csrgemm` method computes the row pointers in one pass, then allocates the exact amount of memory for `H`'s column and value arrays, then actually computes the matrix product. An interesting future direction would be to integrate this sort of algorithm into Gunrock.

It may be possible to improve performance by making assumptions about the topology of the graph. Graph projection is often used for bipartite graphs, but this app does not make any assumptions about the topology of the graph. This choice was made in order to remain consistent with the HIVE reference implementation.

There are various ways that the edges of the output graph `H` can be weighted. We only implement graph projections for unweighted graphs: the weight of the edge `(u, v)` in the output graph `H` is the count of (incoming) neighbors that `u` and `v` have in common in the original graph `G`. Implementation of other weight functions would be fairly straightforward.

GraphBLAS

Currently, for the chunked matrix multiply, the CPU memory allocation and GPU to CPU memory copies for `matmul(X_i, Y)` block the computation of

`matmul(X_[i+1], Y)`. We could implement this in a non-blocking way using CUDA streams, but this would require some redesign of the GraphBLAS APIs.

Certain weighting functions are easily implemented by applying a transformation to the values of the sparse adjacency matrix `A`, but others cannot. For instance, these weighting functions are easy to implement:

```
weight_out = 1                                (by setting both matrices entries to 1)
weight_out = weight_edge_1                    (by setting one matrix's entries to 1)
weight_out = weight_edge_1 / weight_edge_2 (by setting one matrix's entries to 1 / x)
...
```

while this function (from the HIVE reference implementation) is not easy to implement in the `cuSPARSE` plus/multiply semiring:

```
weight_out = weight_edge_1 / (weight_edge_1 + weight_edge_2)
```

Implementation of additional semirings in GraphBLAS is currently in progress, and will extend the family of weightings we could support.

Comparison against existing implementations

When the graph fits in its memory, the Gunrock implementation is approx. 5x faster than the GraphBLAS implementation and approx. 100x faster than PNNL's OpenMP CPU implemention w/ 64 threads. Somewhat surprisingly, PNNL's implementation is substantially slower than a single-threaded scipy sparse matrix multiplication.

When the graph does not fit in the Gunrock implementation's memory, our GPU GraphBLAS implementation is the fastest of the remaining implementations.

Existing implementations

PNNL

We compare our results against PNNL's OpenMP reference implementation. We make minor modifications to their code to handle unweighted graphs, in order to match the Gunrock and GraphBLAS implementations. That is, the weight of the edge in the output graph `H` is the number of shared neighbors in the original graph.

There is a `--simple` flag in PNNL's CLI, but examining the code reveals that it just changes the order of operations. Thus, all of our experiments are conducted with `--simple=1`, which is faster than `--simple=0` due to better data access patterns.

Scipy

A very simple baseline is sparse matrix-matrix multiplication as implemented in the popular `scipy` python package. This is a single-threaded C++ implementation with a Python wrapper. Note, this implementation comes with the same caveats about weighting functions as the Gunrock implementation.

Experiments

MovieLens

MovieLens is a bipartite graph `G=(U, V, E)` w/ `|U|=138493`, `|V|=26744` and `|E|=20000264`. We report results on the full graph, as well as several random subgraphs.

For PNNL's OpenMP implementation, we report results using {1, 2, 4, 8, 16, 32, 64} threads.

In all cases, we project onto the nodeset `|V|`, producing a `|V|x|V|` graph.

Note: Small differences in the number of nonzero entries in the output (nnz_out) are due to small book-keeping differences (specifically, keeping or dropping self-loops). These differences do not have any meaningful impact on runtimes.

1M edge subgraph (|U|=6743 |V|=13950 |E|=1M)

implementation	num_threads	nnz_out	elapsed_seconds
scipy	1	63104132	2.4912
PNNL OpenMP	1	63090182	61.4852
PNNL OpenMP	2	63090182	62.2842
PNNL OpenMP	4	63090182	60.1542
PNNL OpenMP	8	63090182	37.5853
PNNL OpenMP	16	63090182	22.0257
PNNL OpenMP	32	63090182	13.1482
PNNL OpenMP	64	63090182	9.055
Gunrock	1xP100 GPU	63090182	**0.060**
GraphBLAS	1xP100 GPU	63090182	0.366

5M edge subgraph (|U|=34395 |V|=20402 |E|=5M)

implementation	num_threads	nnz_out	elapsed_seconds
scipy	1	157071858	10.1052
PNNL OpenMP	1	157051456	357.511
PNNL OpenMP	2	157051456	309.723
PNNL OpenMP	4	157051456	218.519
PNNL OpenMP	8	157051456	113.987

implementation	num_threads	nnz_out	elapsed_seconds
PNNL OpenMP	16	157051456	57.4606
PNNL OpenMP	32	157051456	38.1186
PNNL OpenMP	64	157051456	29.0056
Gunrock	1xP100 GPU	157051456	**0.3349**
GraphBLAS	1xP100 GPU	157051456	1.221

MovieLens-20M graph (|U|=138493 |V|=26744 |E|=20M)

implementation	num_threads	nnz_out	elapsed_seconds
scipy	1	286857534	39.181
PNNL OpenMP	1	286830790	*I killed before finish*
PNNL OpenMP	2	286830790	1109.32
PNNL OpenMP	4	286830790	727.224
PNNL OpenMP	8	286830790	358.708
PNNL OpenMP	16	286830790	188.701
PNNL OpenMP	32	286830790	102.964
PNNL OpenMP	64	286830790	163.731
Gunrock	1xP100 GPU	286830790	*out-of-memory*
GraphBLAS	1xP100 GPU	286830790	**5.012**

Takeaway: When the graph is small enough, Gunrock graph projection is fastest, followed by GraphBLAS (approx. 5x slower). The PNNL OpenMP implementation is consistently substantially slower than the single threaded scipy implementation, even when using 32+ threads.

RMAT

Next we test on a scale 18 RMAT graph. This is *not* a bipartite graph, but the graph projection algorithm can still be applied.

This graph was chosen because it was used in benchmarks in PNNL's gitlab repo. However, their command line parameters appear to be incorrect, so our results here are substantially different than reported in their README.

RMAT-18 (|V|=174147 |E|=7600696)

implementation	num_threads	nnz_out	elapsed_seconds
scipy	1	2973926895	150.869
PNNL OpenMP	1	2973752748	*I killed before finish*
PNNL OpenMP	2	2973752748	*I killed before finish*
PNNL OpenMP	4	2973752748	812.453
PNNL OpenMP	8	2973752748	677.582

implementation	num_threads	nnz_out	elapsed_seconds
PNNL OpenMP	16	2973752748	419.468
PNNL OpenMP	32	2973752748	369.278
PNNL OpenMP	64	2973752748	602.69
Gunrock	1xP100 GPU	2973752748	*out-of-memory*
GraphBLAS	1xP100 GPU	2973752748	**26.478**

Takeaway: GraphBLAS is approx. 5.7x faster than scipy, the next fastest implementation. Again, the PNNL OpenMP implementation is substantially faster than the single-threaded scipy implementation.

When the dataset can fit into memory, Gunrock is ~ 4x faster than GraphBLAS. Since the two implementations use slightly different algorithms, it's hard to tell where the Gunrock speedup comes from. Our hunch is that Gunrock's superior load balancing gives better performance than GraphBLAS, but this is an interesting topic for further research.

Performance information

Gunrock

- Results of profiling indicate that the Gunrock implementation is bound by memory latency.
- The device memory bandwidth is 297 GB/s – within the expected range for Gunrock graph analytics.
- 92% of the runtime is spent in the advance operator (pseudocode in implementation summary)

GraphBLAS

- 99% of time is spent in cuSPARSE's `csrgemm` routines

Next Steps

Alternate approaches

As mentioned above, it would be worthwhile to implement a Gunrock version that does not require allocating the `|V|x|V|` array. It should be possible to achieve this by implementing the same kind of two-pass approach that cuSPARSE uses for `spgemm` – one pass computes the CSR offsets, then column and data values are inserted at the appropriate locations.

Gunrock implications

Gunrock does not natively support bipartite graphs, but it is straightforward for programmers to implement algorithms that expect bipartite graphs by

keeping track of the number of nodes in each node set. However, for multi-GPU implementations, the fact that a graph is bipartite may be useful for determining the optimal graph partitioning.

Notes on multi-GPU parallelization

Multiple GPU support for GraphBLAS is on the roadmap. Unlike the Seeded Graph Matching problem – which requires the `mxm`, `mxv` and `vxm` primitives, which in turn necessitates possible changes in data layout – this problem only requires the `mxm` primitive, so multiple GPU support for graph projections is easier than for SGM.

Even though extending matrix multiplication to multiple GPUs can be straightforward, doing so in a backend-agnostic fashion that abstracts away the placement (i.e. which part of matrix A goes on which GPU) may still be quite challenging.

Further discussion can be found here.

Notes on dynamic graphs

This workflow does not have an explicit dynamic component. The graph projection operation seems like it would be fairly straightforward to adapt to dynamic graphs – as nodes/edges are added to `G`, we create/increment the weight of the appropriate edges in `H`. However, this adds an additional layer of complexity to the memory allocation step, as we can't use the two-pass approach to allocate memory conservatively.

Notes on larger datasets

If the dataset were too big to fit into the aggregate GPU memory of multiple GPUs on a node, then two directions can be taken in order to be able to tackle these larger datasets:

- Out-of-memory: Compute using part of the dataset at a time on the GPU, and save the completed result to CPU memory. This method is slower than distributed, but cheaper and easier to implement.
- Distributed memory: If GPU memory of a single node is not enough, use multiple nodes. This method can be made to scale for infinitely large datasets provided the implementation is good enough (faster than out-of-memory, but more expensive and difficult).

Notes on other pieces of this workload

This workload does not involve any non-graph components.

Chapter 9

Seeded Graph Matching (SGM)

From Fishkind et al.:

> Given two graphs, the graph matching problem is to align the two vertex sets so as to minimize the number of adjacency disagreements between the two graphs. The seeded graph matching problem is the graph matching problem when we are first given a partial alignment that we are tasked with completing.

That is, given two graphs `A` and `B`, we seek to find the permutation matrix `P` that maximizes the number of adjacency agreements between `A` and `P * B * P.T`, where `*` represents matrix multiplication. The algorithm Fishkind et al. propose first relaxes the hard 0-1 constraints on `P` to the set of doubly stochastic matrices (each row and column sums to 1), then uses the Frank-Wolfe algorithm to minimize the objective function `sum((A - P * B * P.T) ** 2)`. Finally, the relaxed solution is projected back onto the set of permutation matrices to yield a feasible solution.

Summary of Results

SGM is a fruitful workflow to optimize, because the existing implementations were not written with performance in mind. By making minor modifications to the algorithm that allow use of sparse data structures, we enable scaling to larger datasets than previously possible.

The application involves solving a linear assignment problem (LSAP) as a subproblem. Solving these problems on the GPU is an active area of research – though papers have been written describing high-performance parallel LSAP solvers, reference implementations are not available. We implement a GPU LSAP solver via Bertsekas' auction algorithm, and make it available as a standalone library.

SGM is an approximate algorithm that minimizes graph adjacency disagreements via the Frank-Wolfe algorithm. Certain uses of the auction algorithm

can introduce additional approximation in the gradients of the Frank-Wolfe iterations. An interesting direction for future work would be a rigorous study of the effects of this kind of approximation on a variety of different graph tolopogies. Understanding of those dynamics could allow further scaling beyond what our current implementations can handle.

Summary of Gunrock Implementation

The SGM algorithm consists of:

- several matrix-matrix and matrix-vector multiplies
- solving a linear assignment problem at each iteration
- computing the trace of matrix products (e.g., `trace(A * B))`)

The formulation of SGM in the HIVE reference implementation does not take advantage of the sparsity of the problem. This is due to two algorithmic design choices:

1. In order to penalize adjacency disagreements, they convert the 0s in the input matrices `A` and `B` to -1s
2. They initialize the solution matrix `P` near the barycenter of the Birkhoff polytope of doubly-stochastic matrices, so almost all entries are nonzero.

In order to take advantage of sparsity and make SGM more suitable for HIVE analysis, we make two relatively small modifications to the SGM algorithm:

1. Rework the equations so we can express the objective function as a function of the sparse adjacency matrices plus some simple functions of node degree
2. Initialize `P` to a vertex of the Birkhoff polytope

A nice property of the Frank-Wolfe algorithm is that the number of nonzero entries in the intermediate solutions grows slowly – after the `n`th step, the solution is the convex combination of (at most) `n` vertices of the polytope (e.g., permutation matrices). Thus, starting from a sparse initialization point means that all of the Frank-Wolfe steps are fairly sparse.

The reference implementation uses the Jonker-Volgenant algorithm to solve the linear assignment subproblem. However, the JV algorithm (and the similar Hungarian algorithm) do not admit straightforward parallel implementations. Thus, we replace the JV algorithm with Bertsekas' auction algorithm, which is much more natural to parallelize.

Because SGM consists of linear algebra plus an LSAP solver, we implement it outside of the Gunrock framework, using a GPU GraphBLAS implementation from John Owens' lab, as well as the CUDA CUB library.

How To Run This Application on DARPA's DGX-1

Prereqs/input

```
git clone --recursive https://github.com/owensgroup/csgm.git
cd csgm

# build
make clean
make

# make data (A = random sparse matrix, B = permuted version of A,
# except first `num-seeds` vertices)
python data/make-random.py --num-seeds 100
wc -l data/{A,B}.mtx
```

Running the application

Command:

```
./csgm --A data/A.mtx --B data/B.mtx --num-seeds 100 --sgm-debug 1
```

Output:

```
===== iter=0 ================================
APB_num_entries=659238
counter=17
run_num=0 | h_numAssign=4096 | milliseconds=21.3737
APPB_trace = 196
APTB_trace = 7760
ATPB_trace = 7760
ATTB_trace = 109460
ps_grad_P  = 393620
ps_grad_T  = 16124208
ps_gradt_P = 407896
ps_gradt_T = 15879704
alpha      = -29.4213314
falpha     = 224003776
f1         = -15486084
num_diff   = 448756
------------
f1 < 0
iter_timer=74.0615005
...
===== iter=2 ================================
```

```
APB_num_entries=13464050
counter=1
run_num=0 | h_numAssign=4096 | milliseconds=5.71267223
APPB_trace = 333838
APTB_trace = 333838
ATPB_trace = 333838
ATTB_trace = 333838
ps_grad_P  = 16777216
ps_grad_T  = 16777216
ps_gradt_P = 16777216
ps_gradt_T = 16777216
alpha      = 0
falpha     = -1
f1         = 0
num_diff   = 0
------------
iter_timer=45.222271
total_timer=170.153473 | num_diff=0
```

Note: Here, the final `num_diff=0` indicates that the algorithm has found a perfect match between the input graphs.

Output

When run with `--sgm-debug 1`, we output information about the quality of the match in each iteration. The most important number is `num_diff`, which gives the number of disagreements between `A` and `P * B * P.T`. `num_diff=0` indicates that SGM has found a perfect matching between `A` and `B` (eg, there are no adjacency disagreements).

This implementation is validated against the HIVE reference implementation. Additionally, since the original reference implementation code was posted, Ben Johnson has worked with Johns Hopkins to produce other more performant implementations of SGM, found here.

Performance and Analysis

Given:

- two input graphs `A` and `B`
- a set of seeds `S`
- some parameters controlling convergence (`num_iters`, `tolerance`)

Performance is measured by runtime of the entire SGM procedure as well as the final number of adjacency disagreements between `A` and `P * B * P.T`.

Per-iteration runtime is not necessarily meaningful, because different iterations present dramatically more difficult LSAP instances than others. In particular, the LSAP solver in the first iteration tends to take 10-100x longer than in subsequent iterations.

Bertsekas' auction algorithm allows us to make a tradeoff between runtime and accuracy. With appropriate parameter settings, it produces the exact same answer as the JV or Hungarian algorithms. However, with different parameter settings, the auction algorithm may run substantially faster (>10x), at the cost of a lower quality assignment. Since SGM is already an approximate algorithm, *we do not currently know the SGM's sensitivity to this kind of approximation.* Experiments to explore these tradeoffs would be an interesting direction for future research. In general, we run our SGM implementation with some approximation, and thus we rarely produce the exactly optimal solution for the LSAP subproblems. However, we often produce *SGM solutions* of comparable quality to those SGM implementations that exactly solve the LSAP subproblems.

Implementation limitations

SGM is only appropriate for pairs of graphs w/ some kind of correspondence between the nodes. This could be an explicit correspondance (users on Twitter and users on Instagram, people in a cell phone network and people on an email network), or an implicit correspondence (two people play similar roles at similar companies).

Currently, our implementation of SGM only supports undirected graphs – an extension to directed graphs is mathematically straightforward, but requires a bit of code refactoring. We have only tested on unweighted graphs, though the code should also work on weighted graphs out-of-the-box.

We also currently assume that the number of nodes in `A` and `B` are identical. Fishkind et al. discuss various padding schemes to address the cases where `A` and `B` have a different number of nodes, but we assume all of these could be done in a preprocessing step before the graph is passed to our SGM implementation.

At the moment, the primary scaling bottleneck is that we allocate two `|V|x|V|` arrays as part of the LSAP auction algorithm. These could be replaced w/ 3 `|E|` arrays without much effort.

Currently, the auction algorithm does not take advantage of all available parallelism. Each CUDA thread gets a row of the cost matrix, and then does a serial reduction across the entries of the row. As the auction algorithm runs, the number of "active" rows rapidly decreases. This means that the majority of auction iterations have a small number of active rows, and thus use a small number of GPU threads. We could better utilize the GPU by using multiple threads per row. We have a preliminary implementation of this using the CUB library, but it has not been tested on various relevant edge cases.

Preliminary experiments suggest the CUB implementation may be 2–5x faster than our current implementation.

Comparison against existing implementations

Python SGM code

The original SGM implementation is a single-threaded R program. Preliminary tests on small graphs show that this implementation is not very performant. As part of other work, we've written a modular SGM package that allows the programmer to plug in different backends for the LSAP solver and the linear algebra operations. This package includes modes that transform the SGM problem to take advantage of sparsity to improve runtime. In particular, we benchmark our CUDA SGM implementation against the `scipy.sparse.jv` mode, which uses `scipy` for linear algebra and the gatagat/lap implementation of the JV algorithm for the LSAP solver.

Experiments

Connectome

The connectome graphs are generated from brain MRIs. Nodes represent a voxel in the MRI and edges indicate some kind of flow between voxels. By using voxels of different spatial resolutions, the researchers that collected the data produced pairs of graphs at a variety of sizes (smaller voxel = larger graph). Each graph in a pair represents one hemisphere of the brain. Thus, we know there is an actual approximate correspondence between nodes.

Note that these graphs are already partially aligned – the distance between the input graphs is far smaller than would be expected by chance. We attempt to use SGM to further improve this initial alignment, using all nodes as "soft seeds" (see Fishkind et al. for further discussion).

The size of the connectome graphs we consider are as follows:

name	num_nodes	num_edges
DS00833	00833	12497
DS01216	01216	19692
DS01876	01876	34780
DS03231	03231	64662
DS06481	06481	150012
DS16784	16784	445821
DS72784	72784	2418304

In the tables below, `orig_dist` indicates the number of adjacency disagreements between `A` and `B`, and `final_dist` indicates the number of adjacency disagreements between `A` and `P * B * P.T` w/ `P` found by SGM. We run CSGM

w/ two values of `eps`, which controls the precision of the auction algorithm (lower values = more precise but slower).

Python runtimes

name	orig_dist	final_dist	time_ms
DS00833	11650	11486	122.656
DS01216	20004	19264	278.739
DS01876	38228	36740	2275.141
DS03231	78058	73282	8900.371
DS06481	201084	183908	97658.378
DS16784	677754	593590	920436.387

CSGM runtimes

eps	name	orig_dist	final_dist	time_ms	speedup
1.0	DS00833	11650	11538	181.481	0.6
1.0	DS01216	20004	19360	324.908	0.8
1.0	DS01876	38228	36936	807.148	2.8
1.0	DS03231	78058	73746	3078.78	2.9
1.0	DS06481	201084	184832	9056.55	10.7
1.0	DS16784	677754	596370	42220.5	21.8
1.0	DS72784	—	—	OOM	—
0.5	DS00833	11650	11466	378.056	0.3 *
0.5	DS01216	20004	19288	965.915	0.3
0.5	DS01876	38228	36764	1258.65	1.8
0.5	DS03231	78058	73346	6257.87	1.4
0.5	DS06481	201084	183796	25931.2	3.7 *
0.5	DS16784	677754	592822	120799	7.6 *
0.5	DS72784	—	—	OOM	—

Takeaway: For small graphs (`|U| < ~2000`) the Python implementation is faster. However, as the size of the graph grows, CSGM becomes significantly faster – up to 20x faster in the low accuracy setting and up to 7.6x faster in the higher accuracy setting. Also, though in general the auction algorithm does not compute exact solutions to the LSAP, in several cases CSGM's accuracy outperforms the Python implementation, which uses an exact LSAP solver – these are denoted with a `*`.

Kasios

The Kasios call graph shows the communication pattern inside of a corporation – nodes represent a person and edges indicate that two people spoke on the phone.

The whole graph has 10M edges and 500K nodes, which is too large for any of our SGM implementations to handle. Thus, we sample subgraphs of size 2**10 - 2**15 by running a random walk until the desired number of nodes are observed, and then extracting the subgraph induced by those nodes. We generate pairs of graphs by random permutations (except for the first `num_seeds=100` nodes). Interestingly, with 100 seeds, SGM can almost always perfectly "reidentify" the permuted graph.

Python runtimes

num_nodes	orig_dist	final_dist	time_ms
1024	66636	0	242
2048	208144	0	1275
4096	580988	0	6530
8192	1449712	0	30763
16384	3235356	0	118072
32768	6587656	0	479181

CSGM runtimes (`eps=1`)

num_nodes	orig_dist	final_dist	time_ms	speedup
1024	66636	0	182.445	1.3
2048	208144	4	310.566	4.1
4096	580988	4	1026.07	6.4
8192	1449712	8	3108.9	9.9
16384	3235356	16	4926.85	24.0
32768	6587656	OOM!	—	—

Takeaway: Similar to in the connectome experiments, we see the advantage of CSGM increase as the graphs grow larger. In these examples, CSGM does not *quite* match the performance of the exact LSAP solver. However, this could be addressed by tuning and/or scheduling the `eps` parameter.

Performance limitations

- Results from profiling indicate that all of the SGM kernels are memory latency bound.
- 50% of time is spent in sparse-sparse matrix-multiply (SpMM)
- 39% of time is spent in the auction algorithm. Of this 39%:
  - 65% of time is spent in `run_bidding`
  - 26% of time is spent in `cudaMemset`
  - 9% of time is spent in `run_assignment`

Next Steps

Alternate approaches

It would be worthwhile to look into parallel versions of the Hungarian or JV algorithms, as even a single-threaded CPU version of those algorithms is somewhat competitive with Bertseka's auction algorithm implemented on the GPU. It's unclear whether it would be better to implement parallel JV/Hungarian as multi-threaded CPU programs or GPU programs. If the former, SGM would be a good example of an application that makes good use of both the CPU (for LSAP) and GPU (for SpMM) at different steps.

Gunrock implications

N/A

Notes on multi-GPU parallelization

GraphBLAS

Multiple GPU support for GraphBLAS is on the roadmap. This will involve dividing the dataset across multiple GPUs, which can be challenging, because the GraphBLAS primitives required by SGM (`mxm`, `mxv` and `vxm`) have optimal layouts that vary depending on data and each other. There will need to be a tri-lemma between inter-GPU communication, layout transformation, and compute time for optimal vs. sub-optimal layout.

Although extending matrix-multiplication to multiple GPUs can be straightforward, doing so in a backend-agnostic fashion that abstracts away the placement (i.e., which part of matrix `A` goes on which GPU) from the user may be quite challenging. This can be done in two ways:

1. Manually analyze the algorithm and specify the layout in a way that is application-specific to SGM (easier, but not as generalizable)
2. Write a sophisticated runtime that will automatically build a directed acyclic graph (DAG), analyze the optimal layouts, communication volume and required layout transformations, and schedule them to different GPUs (difficult and may require additional research, but generalizable)

Auction algorithm

The auction algorithm can be parallelized across GPUs in several ways:

1. Move data onto a single GPU and run the existing auction algorithm (simple, but not scalable).
2. Bulk-synchronous algorithm: Run auction kernel, communicate, then run next iteration of auction kernel (medium difficulty, scalable).

3. Asynchronous algorithm: Run auction kernel and communicate to other GPUs from within kernel (difficult, most scalable).

Notes on dynamic graphs

Real-world applications of SGM to eg. social media or communications networks often involve dynamic graphs. Application of SGM to streaming garphs could be a very interesting new research direction. To our knowledge, this problem has not been studied by the JHU group responsible for the algorithm. Given an initial view of two graphs, we could compute an initial match, and then update the match via a few iterations of SGM as new edges arrive.

Notes on larger datasets

If the dataset were too big to fit into the aggregate GPU memory of multiple GPUs on a node, then two directions can be taken in order to be able to tackle these larger datasets:

1. Out-of-memory: Compute using part of the dataset at a time on the GPU, and save the completed result to CPU memory. This method is slower than distributed, but cheaper and easier to implement.
2. Distributed memory: If the GPU memory on a single node is not enough, use multiple nodes. This method can be made to scale for arbitrarily large datasets provided the implementation is good enough (faster than out-of-memory, but more expensive and difficult).

Notes on other pieces of this workload

There are no non-graph pieces of the SGM workload.

How this work can lead to a paper publication

Ben and Carl think this work can lead to a nice paper, because there aren't a lot of highly optimized parallel Linear Assignment Problem (LAP) solvers. A lot of the research Ben could find from 20+ years ago tends to assume that the input matrices are uniformly random. However, our use case is on cost matrices formed by the dot product of sparse matrices (so the `(i, j)`th entry is the number of neighbors node `i` and `j` have in common), which has a totally different distribution (closer to a power law). There may be some optimizations we can find that target this distribution (similar to how direction-optimized BFS targets power law graphs).

There is potential research in tie-breaking for the auction algorithm. In one of the popular Python/C++ LAP solvers, they're clearly not handling ties smartly, and the runtime can be improved ~10x by adding random values in a specific way. For these types of data, we find a lot of people assuming there

aren't many ties. But with graphs, Ben notices many entries are ties, so some randomization is clearly beneficial.

Further development on the standalone auction algorithm will happen here. This will include porting the current implementation to CUDA CUB to take better advantage of available parallelism, as well as writing Python bindings for ease of use.

Chapter 10

Sparse Fused Lasso

Given a graph where each vertex on the graph has a weight, *sparse fused lasso (SFL)*, also named *sparse graph trend filter (GTF)*, tries to learn a new weight for each vertex that is (1) sparse (most vertices have weight 0), (2) close to the original weight in the l2 norm, and (3) close to its neighbors' weight(s) in the l1 norm. This algorithm is usually used in main trend filtering (denoising). For example, an image (grid graph) with noisy pixels can be filtered with this algorithm to get a new image without the noisy pixels, which are "smoothed out" by its neighbors. https://arxiv.org/abs/1410.7690

Summary of Results

The SFL problem is mainly divided into two parts, computing residual graphs from maxflow and renormalizing the weights of the vertices. Maxflow is parallelizable with the push-relabel algorithm, so we adopt this algorithm in Gunrock's implementation. Moreover, each vertex has its own work to compute which communities it belongs to, and normalize the weights with other vertices in the same community. This renormalization requires global synchronization. SFL iterates by calling maxflow and renormalization several times before it converges. We notice that the overall runtime is mostly spent in maxflow, and thus improving the maxflow implementation will bring substantial speedup in the SFL.

Because of the current state of our maxflow implementation, we notice a 30x slowdown of Gunrock's GPU SFL with respect to the benchmark implementation. This slowdown is mainly caused by the parallel push-relabel implementation taking too many iterations to converge, and making SFL kernel launching overhead-bound. We are looking into algorithmic optimizations to reduce the number of iterations maxflow takes, and also engineering optimizations to reduce the effects of kernel overheads in computation time.

Summary of Gunrock Implementation

The loss function is `0.5 * sum((y' - y)^2) + lambda1 * sum(abs(y_i' - y_j')) + lambda2 * sum(abs(yi'))`, where `y` is the input weight (observation) for each vertex and `y'` (fitted weight) is the new weight for each vertex. Lambda1 and Lambda2 are required parameters to process the graph in SFL.

The input graph is specified in two files. The first file contains the original vertices' weights and the second file contains the directed graph connectivity without weights (edge pairs only). These two files and a edge_regularization_strength (`lambda1`) of the directed graph edge weights are the input to preprocessing. Two extra vertices, source and sink, are added to the original graph as well. They serve as two "labels" of different segments on the graph. This results in a graph where edges that connect to the source or sink have edge-weights as in the `vertices' weights` file, and the other edges are assigned an edge weight of `lambda1`.

The Gunrock implementation of this application has two parts. The first part is the maxflow algorithm. We choose a push-relabel maxflow formulation, which is well-suited for parallelization on a GPU with Gunrock. Computing a valid maxflow also implies a solution to the mincut problem, which is a segmentation of a graph into two pieces where the division is across a set of edges with the minimum possible weights. The output of this maxflow algorithm is (1) a residual graph where each edge weight is computed as `capacity - edge_flow`, and (2) a Boolean array that marks which vertices are reachable from the source after the mincut.

The second part is a renormalization of the residual graph and clustering based on reachability of the vertex. The renormalization is a process where (1) averages of the new weights of vertices that are grouped together as communities are computed, and (2) the new weights then subtract their own community averages. After the renormalization is done, this renormalized residual graph is passed into the maxflow again. Several iterations of maxflow then renormalization are needed before the new weights of different communities converge because vertices can be reassigned to different communities. In each of the SFL iterations, two non-overlapped subgraphs will be generated by maxflow/mincut, and thus the big communities in the last SFL iteration will have split into small communities. The vertices in a specific community will have the same new weights assigned to them.

The outputs will be the normalized values assigned to each vertex.

Lastly, these values will be passed into a soft-threshold function with `lambda2` to achieve the sparse representation by dropping the small absolute values. More specifically, the new weight will be subtracted by `lambda2` if the new weight is positive and larger than `lambda2`, or added by `lambda2` if the new weight is negative and smaller than `-lambda2`. If the new weight is in between `-lambda2` to `lambda2`, then the new weights will be 0.

Pseudocode for the core SFL algorithm is as follows:

```
Load the graph and normalize edge weights

Repeat iteration till convergence:

    // First part: Maxflow
    // Push phase
    For each local vertex v:
        If (excess[v] <= 0) continue
        If (v == source || v == sink) continue
        For each edge e<v, u> of v:
            If (capacity[e] <= flow[e]) continue
            If (height[v] <= height[u]) continue
            move := min(capacity[e] - flow[e], excess[v])
            excess[v] -= move
            flow[e] += move
            excess[u] += move
            flow[reverse[e]] -= move

    // Relabel phase
    For each local vertex v:
        If (excess[v] <= 0) continue
        min_height := infinity
        For each e<v, u> of v:
            If (capacity[e] <= flow[e]) continue;
            If (min_height > height[u]) min_height := height[u]
        If (height[v] <= min_height)
           height[v] := min_height + 1

    // Min-cut
    Run a BFS to mark the accessibilities of vertices from the source vertex
    in the residue graph

    // Second part: renormalization
    // Reset available community
    For each community comm:
        community_weights[comm] := 0
        community_sizes  [comm] := 0
        next_communities [comm] := 0

    // Accumulate the weights and count the number of vertices belong to the communities
    For each vertex v:
        If v is accessible from the source
            comm := next_communities[curr_communities[v]];
            If (comm == 0) update comm
```

```
            community_sizes[comm]++
            community_weights[comm] += weight[source -> v]
        Else
            community_weights[comm] -= weight[v -> sink]
            community_sizes [comm] ++

    // Normalize community
    For each community comm:
        community_weights[comm] /= community_sizes[comm]
        community_accus [comm] += community_weights[comm]

    // Update the residual graph
    For each vertex v:
        comm = curr_communities[v]
        If (v is accessible from the source):
            weight[source->v] -= community_weights[comm]
            If (weight[source->v] < 0):
                Swap(-weight[source->v], weight[v->sink])
        Else
            weight[v->sink] += community_weights[comm]
            If (weight[v->sink] < 0):
                Swap(weight[source->v], -weight[v->sink])

    // End of Repeats

// Part 3 Sparsify community_accus by lambda2
For i in len(each community_accus):
    If (community_accus < 0):
        community_accus[i] := min(community_accus[i] + lambda2, 0)
    Else:
        community_accus[i] := max(community_accus[i] - lambda2, 0)

Return community_accus
```

How To Run This Application on DARPA's DGX-1

Prereqs/input

CUDA should have been installed; `$PATH` and `$LD_LIBRARY_PATH` should have been set correctly to use CUDA. The current Gunrock configuration assumes boost (1.58.0 or 1.59.0) and Metis are installed; if not, changes need to be made in the Makefiles. DARPA's DGX-1 has both installed when the tests are performed.

```
git clone --recursive https://github.com/gunrock/gunrock/
```

```
cd gunrock
git checkout dev-refactor
git submodule init
git submodule update
mkdir build
cd build
cmake ..
cd ../tests/gtf
make
```

At this point, there should be an executable `gtf_main_<CUDA version>_x86_64` in `tests/gtf/bin`.

The testing is done with https://github.com/wetliu/gunrock/tree/master using `dev-refactor` branch at commit `8f51a6369127204a87893b74a7b920ad3d3fdd58` (Oct. 31, 2018), using CUDA 9.1 with NVIDIA driver 390.30.

HIVE Data Preparation

Prepare the data; skip this step if you are just running the sample dataset.

Refer to `parse_args()` in `taxi_tsv_file_preprocessing.py` for dataset preprocessing options.

If you don't have the `e` or `n` files:

```
cd gunrock/tests/gtf/_data

export TOKEN= # get this Authentication TOKEN from https://api-token.hiveprogram.com/#!/use
mkdir -p _data
wget --header "Authorization:$TOKEN" \
  https://hiveprogram.com/data/_v0/sparse_fused_lasso/taxi/taxi-small.tar.gz
tar -xzvf taxi-small.tar.gz && rm -r taxi-small.tar.gz
mv taxi-small _data/

wget --header "Authorization:$TOKEN" \
  https://hiveprogram.com/data/_v0/sparse_fused_lasso/taxi/taxi-1M.tar.gz
tar -xzvf taxi-1M.tar.gz && rm -r taxi-1M.tar.gz
mv taxi-1M _data/

python taxi_tsv_file_preprocessing.py
```

Two files, `e` and `n`, are generated.

Set the `lambda1` (see equation above) in generate_graph.py. If you have the `e` and `n` files, generated by the above commands or copied from `/raid/data/hive/gtf/{small, medium, large}`, you can do the following (`/raid/data/hive/gtf/small/` as an example):

```
cd gunrock/tests/gtf/_data
cp /raid/data/hive/gtf/small/n .
cp /raid/data/hive/gtf/small/e .
python generate_graph.py
```

A file called `std_added.mtx` is generated for Gunrock input.

Running the application

```
--lambda2 is the sparsity regularization strength
```

Sample command line with argument.

```
./bin/test_gtf_10.0_x86_64 market ./_data/std_added.mtx --lambda2 3
```

Output

The code will output two files in the current directory. One is called `output_pr.txt` (for CPU reference) and the other is called `output_pr_GPU.txt` (for GPU SFL with push-relabel backend). Each vertex's new weight will be stored in each line of the two files. These outputs could be further processed into the resulting heatmap. The printout after running `gtf_main_<CUDA version>_x86_64` includes the timing of the application.

Sample `txt` output:

```
0
0
0
0
0
0
-11.375
-0.307292
0
```

Sample output on console:

```
______CPU reference algorithm______
offset is 58522 num edges 76366
!!!!!!!!!! avg is -0.876037
Iteration 0
Iteration 1
Iteration 2
Iteration 3
```

```
Iteration 4
Iteration 5
Iteration 6
Iteration 7
Iteration 8
Iteration 9
Iteration 10
Iteration 11
---------------------------------
Elapsed: 5500.730991 ms
in side that weird function1
offset in GPU preprocess is 58522 num edges 76366
avg in GPU preprocess is -0.876037
Using advance mode LB
Using filter mode CULL
Using advance mode LB
Using filter mode CULL
offset is 58522 num edges 76366
h_community_accus is -0.876037
______GPU SFL algorithm____
enact calling successfully!!!!!!!!!!!
---------------------------------
Run 0, elapsed: 3341.358185 ms, #iterations = 12
transfering to host!!!: 8924
[gtf] finished.
 avg. elapsed: 3341.358185 ms
 iterations: 0
 min. elapsed: 3341.358185 ms
 max. elapsed: 3341.358185 ms
 load time: 138.952 ms
 preprocess time: 342.184000 ms
 postprocess time: 0.258923 ms
 total time: 3845.412016 ms
```

Performance and Analysis

We measure the runtime and loss function `0.5 * sum((y' - y)^2) + lambda1 * sum(abs(y_i' - y_j')) + lambda2 * sum(abs(yi'))`, where `y` is the input weight (observation) for each vertex and `y'` (fitted weight) is the new weight for each vertex.

Implementation limitations

- **Memory usage** Each edge in the graph needs at least 20 bytes of GPU device memory: 64 bits for the capacity value, 64 bits for the flow value, 16 bits for the index of the reverse edge. Each node in the graph needs

at least 16 bytes of GPU device memory: 64 bits for the excess value, 16 bits for the height value and 16 bits for the index of the lowest neighbor.

- **Data type** For edges we have the following arrays: capacity, flow, reverse. For nodes we have the following arrays: height, excess, lowest_neighbor. Capacity, flow and excess arrays and all computation around them are double-precision floating point values (64-bit `double` in C/C++). We use an epsilon value of 1e-6 to compare floating-point numbers to zero. Reverse, height, and lowest_neighbor arrays and all computation around them are 32-bit integer values.

Comparison against existing implementations

Graphtv is an official implementation of the sparse fused lasso algorithm with a parametric maxflow backend. It is a CPU serial implementation https://www.cs.ucsb.edu/~yuxiangw/codes/gtf_code.zip. The Gunrock GPU runtime is measured between the application enactor and it is an output of the application.

DataSet	time starts	time ends	#E	#V	Graphtv runtime	Gunrock
NY Taxi-small	2011-06-26 12:00:00	2011-06-26 14:00:00	20349	8922	0.11s	3.23s*
NY Taxi-small	2011-06-26 00:00:00	2011-06-27 00:00:00	293259	107064	8.71s	
NY Taxi-1M	2011-06-19 00:00:00	2011-06-27 00:00:00	588211	213360	103.62s	

DataSet	time starts	time ends	#E	#V	Graphtv loss	Gunrock GP
NY Taxi-small	2011-06-26 12:00:00	2011-06-26 14:00:00	20349	8922	132789.32	132789.32*
NY Taxi-small	2011-06-26 00:00:00	2011-06-27 00:00:00	293259	107064		
NY Taxi-1M	2011-06-19 00:00:00	2011-06-27 00:00:00	588211	213360		

*: The GPU implementation of maxflow still has a bug that leads to different results per run. We only report the best result we can achieve with the current version of maxflow. Since this current version of maxflow is able to achieve the same loss as Graphtv, we presume that the results, both the runtime and loss, should be similar or even better with a bug-free maxflow.

Performance limitations

We observe a slowdown when we compare Graphtv and Gunrock's current SFL implementation on the `NY Taxi-small` dataset with time from `2011-06-26 12:00:00` to `2011-06-26 14:00:00` for the following reasons:

- Graphtv uses a serial argumenting path based max flow algorithm, and Gunrock uses a parallel implementation of the push relabel algorithm.

On this particular dataset, push relabel uses more than 20K iterations, and SFL runs about a hundred seconds on CPU.

- The large number of iterations is very harmful to the computation speed of our GPU implementation, because of the kernel launching overhead. In fact, profiling shows the computation kernels only takes about 20% of MF's computation time, and the rest (80%) is overhead. Since maxflow takes up about 95% of SFL's computation time, this makes SFL kernel launching overhead-bound. We are looking at optimizations to cut down the number of iterations, such as the one described by Bo Hong in "A Lock-free Multi-threaded Algorithm for the Maximum Flow Problem" http://people.cs.ksu.edu/~wls77/weston/projects/cis598/hong.pdf.
- This dataset with ~9k vertices and ~20k edges is too small to fill the GPU. It makes the kernel launching overhead issue much worse than it would with larger graphs.
- There are some engineering limitations in our current implementation:
  1. The relabeling heuristics in maxflow are performed on the CPU; although they only run once per 100 iterations, the data movement takes up time.
  2. The current min-cut finding and renormalization are serial on GPU (i.e. only use a single thread to perform the computation).

  We will improve on these issues when the number of iterations is reduced, which has a much larger impact on computation time.

Next Steps

Alternate approaches

For CPU, the parametric maxflow algorithm works well, but it is not parallelizable to GPU. The push-relabel algorithm is the best candidate for parallel implementation, but more optimizations are needed to get good running times on a GPU.

Gunrock implications

SFL is the first application in Gunrock that calls another application (maxflow). Some common data pre-processing on the CPU requires better designs of the APIs to facilitate this usage. For example, `gtf_enactor` needs to call `mf_problem.reset()`, but because the current maxflow code uses CPU to preprocess the graph, SFL has to transfer the data back and forth between CPU and GPU. Using GPU to preprocess the graph for maxflow would be preferable.

Notes on multi-GPU parallelization

To parallelize the push-relabel algorithm across multiple GPUs, all arrays related to the graph have to be stored on each GPU. Moreover, the GPUs have to update their adjacent neighbors' data. Because the push-relabel algorithm needs to store at least three arrays of size O(|E|) and three arrays of size O(|V|), communicating so much data efficiently between GPUs is challenging.

The SFL renormalization should be able to be easily parallelized across different GPUs, because it is array operations only. However, extra data transfer is necessary if the graph is not copied across multiple GPUs.

Notes on dynamic graphs

Push relabel is not directly related to dynamic graphs. But it should be able to run on a dynamic graph, provided the source and the sink are given at the beginning of the algorithm and the way to access all the nodes and the edges is the same. Capacities of edges from the previous graph can be used as a good starting point, if the edges and the node ids are consistent and the graph is not dramatically changed.

However, SFL would be a significant challenge with dynamic graphs (the topology of the graph would change). The residual graph includes a swapping edge value (see pseudocode above) and we need to know characteristics of the new graph in order to allocate enough memory space for the new edges and vertices.

Notes on larger datasets

SFL renormalization can be done without having its temporary arrays on the same GPU, but extra communication costs are needed, if these arrays are in different GPU memories. Gunrock needs no specific new support to support SFL renormalization on larger datasets.

Notes on other pieces of this workload

Currently there is no GPU library that addresses SFL renormalization.

Research opportunities

Prof. Sharpnack indicates that this implementation could be generalized to multi-graph fused lasso. The idea is to set multiple edge values for the edges connecting to source/sink, while keeping the graph topology and edge values (`lambda1`) for the edges in the original graph (excluding source and sink) the same.

Chapter 11

Vertex Nomination

The vertex nomination (VN) workflow is an implementation of the kind of algorithm discussed in Coppersmith and Priebe.

Often, we have an attributed graph where we know of some "interesting" nodes, and we want to rank the rest of the nodes by their likelihood of being interesting. Coppersmith and Priebe propose a general framework for using both node attributes ("content") and network features ("context") to rank nodes. The specific content, context, and fusion functions can be arbitrary, user-defined functions.

Summary of Results

The term "vertex nomination" covers a variety of different node ranking schemes that fuse "content" and "context" information. The HIVE reference code implements a "multiple-source shortest path" context scoring function, but uses a very suboptimal algorithm. By using a more efficient algorithm, our serial CPU implementation achieves 1-2 orders of magnitude speedup over the HIVE implementation and our GPU implementation achieves another 1-2 orders of magnitude on top of that. Implementation was straightforward, involving only a small modification to the existing Gunrock SSSP app.

Summary of Gunrock Implementation

Since HIVE is focused on graph analytics, the content scoring function is not relevant, and we only implement the context scoring function. Coppersmith and Priebe propose a number of possible network statistics that can be used for context scoring. The HIVE reference implementation ranks each node `u` in a graph `G = (U, E)` by the minimum distance from `u` to a node in a set of seed nodes `S`. This is the VN variant we have implemented in Gunrock.

This choice of context scoring function ends up being nearly identical to a single source shortest paths (SSSP) problem. The one difference is that we start from the set of seed nodes `S` instead of single node.

Because of this similarity to SSSP, the Gunrock VN implementation consists of making a minor modification to the Gunrock SSSP implementation, so that it can accept a list of source nodes instead of a single source node. Thus, the core of the VN algorithm is a Gunrock advance operator implementing a parallel version of the Bellman-Ford algorithm. Specifically, in `python`:

```
class IterationLoop(BaseIterationLoop):
    def _advance_op(self, src, dest, problem, enactor_stats):
        src_distance = problem.distances[src]
        edge_weight  = problem.edge_weights[(src, dest)]
        new_distance = src_distance + edge_weight

        old_distance = problem.distances[dest]
        problem.distances[dest] = min(old_distance, new_distance)

        return new_distance < old_distance

    def _filter_op(self, src, dest, problem, enactor_stats):
        if problem.labels[dest] == enactor_stats['iteration']:
            return False

        problem.labels[dest] = enactor_stats['iteration']
        return True
```

Note we could have used the Gunrock SSSP implementation directly by

1. adding a dummy node `d` to `G`
2. adding an edge `(d, s)` between `d` and each node `s` in `S` with `weight(d, s) = 0`
3. running SSSP from `d`

How To Run This Application on DARPA's DGX-1

Prereqs/input

```
git clone --recursive https://github.com/gunrock/gunrock -b dev-refactor
cd gunrock/tests/vn
cp ../../gunrock/util/gitsha1.c.in ../../gunrock/util/gitsha1.c
make clean
make
```

Application specific parameters

```
--src
  Comma separated list of seed nodes (eg, `0,1,2`) OR `random` (see below)
--srcs-per-run
  If `src=random`, number of randomly chosen source nodes per run
--num-runs
  Number of runs
```

Example command

```
./bin/test_vn_9.1_x86_64 \
    --graph-type market \
    --graph-file ../../dataset/small/chesapeake.mtx \
    --src random \
    --srcs-per-run 10 \
    --num-runs 2
```

Example output

```
Loading Matrix-market coordinate-formatted graph ...
  Reading meta data from ../../dataset/small/chesapeake.mtx.meta
  Reading edge lists from ../../dataset/small/chesapeake.mtx.coo_edge_pairs
  Assigning 1 to all 170 edges
  Substracting 1 from node Ids...
  Edge doubleing: 170 -> 340 edges
  graph loaded as COO in 0.090935s.
Converting 39 vertices, 340 directed edges ( ordered tuples) to CSR format...Done (0s).
Degree Histogram (39 vertices, 340 edges):
    Degree 0: 0 (0.000000 %)
    Degree 2^0: 0 (0.000000 %)
    Degree 2^1: 1 (2.564103 %)
    Degree 2^2: 22 (56.410256 %)
    Degree 2^3: 13 (33.333333 %)
    Degree 2^4: 2 (5.128205 %)
    Degree 2^5: 1 (2.564103 %)


------------------------
------------------------
Run 0 elapsed: 0.025034 ms, srcs = 21,19,3,28,20,25,23,26,13,38
------------------------
------------------------
Run 1 elapsed: 0.021935 ms, srcs = 21,15,5,23,3,29,22,26,33,4
============================================
 mark-pred=0 advance-mode=LB
Using advance mode LB
```

```
Using filter mode CULL

-------------------------
0  1   0   queue3    oversize :  234 ->  246
0  1   0   queue3    oversize :  234 ->  246
-------------------------
Run 0 elapsed: 0.442028 ms, srcs = 21,19,3,28,20,25,23,26,13,38, #iterations = 3
-------------------------
-------------------------
Run 1 elapsed: 0.329971 ms, srcs = 21,15,5,23,3,29,22,26,33,4, #iterations = 3
Distance Validity: PASS
First 40 distances of the GPU result:
[0:1 1:1 2:1 3:0 4:0 5:0 6:1 7:1 8:2 9:2 10:2 11:2 12:2 13:1 14:1 15:0 16:1 17:1 18:1 19:2
First 40 distances of the reference CPU result.
[0:1 1:1 2:1 3:0 4:0 5:0 6:1 7:1 8:2 9:2 10:2 11:2 12:2 13:1 14:1 15:0 16:1 17:1 18:1 19:2

[vn] finished.
 avg. elapsed: 0.386000 ms
 iterations: 3
 min. elapsed: 0.329971 ms
 max. elapsed: 0.442028 ms
 rate: 0.880830 MiEdges/s
 src: 3
 nodes_visited: 39
 edges_visited: 340
 load time: 113.31 ms
 preprocess time: 974.719000 ms
 postprocess time: 0.562906 ms
 total time: 976.519108 ms
```

Expected Output

Currently, the VN app does not write any output to disk. It prints runtime statistics and the results of a correctness check. A successful run will print `Distance Validity: PASS` in the output.

Validation

The Gunrock VN implementation was tested against the HIVE reference implementation to verify correctness. We also implemented a CPU reference implementation inside of the Gunrock VN app, with results that match the HIVE reference implementation.

Additionally, for ease of exposition, we implemented a pure Python version of the Gunrock algorithm that lets people new to Gunrock see the relevant logic without all of the complexity of C++/CUDA data structures, memory management, etc. In this case, we already knew how to implement VN using

Gunrock primitives. However, in other cases, where we're writing a Gunrock app from scratch, translation from some arbitrary serial implementation to `advance`/`filter`/`compute` can be complex and involve some trial and error to handle edge cases. In those cases, `pygunrock` has proven to be a useful tool for rapid prototyping and debugging.

Our implementation of VN is a deterministic algorithm, so all correct solutions have the same accuracy/quality.

Performance and Analysis

Performance is measured by the runtime of the app, given:

- an input graph `G=(U, E)`
- a set of seed nodes (or size/number of random seed sets)

Other implementations

Python reference implementation

The Python + SNAP reference implementation can be found here. This is a very naive implementation of the context function – rather than running the SSSP variant we describe above, it runs a separate BFS from each node `s` in the seed set `S` to each node `u` in `U`. Thus, its algorithmic complexity is approximately `|S|x|U|` times larger than the Gunrock implementation.

Performer OpenMP implementations

We were unable to locate any C/OpenMP implementation of VN from TA1/TA2 performers at the time of writing. (2018-10-20)

Gunrock CPU implementation

For correctness checking, we implement VN in single-threaded C++ within the Gunrock testing framework. This is a serial implementation of Djikstra's algorithm using a CSR graph representation and `std::priority_queue`. We expect this to be substantially faster than the HIVE Python+SNAP reference implementation due to superior algorithmic complexity.

Experiments

HIVE Enron dataset (|U|=15056, |E|=57075)

The Enron graph is a graph of email communications between employees of Enron.

The HIVE reference implementation implementation does 10 runs w/ 5 random seeds each on the Enron email dataset. Results are as follows:

implementation	elapsed_ms (avg of 10 runs)
Python+SNAP	4115.545
Gunrock CPU	7.305
Gunrock GPU	**0.921**

Takeaway: Due to improved algorithmic efficiency, the Gunrock CPU implementation is approximately 563x faster than the HIVE reference implementation. The Gunrock GPU implementation is approximately 7.9x faster than the Gunrock CPU implementation. However, this dataset may be too small for these numbers to be very precise.

Hollywood-2009 graph (|U|=1139905, |E|=57515616)

The Hollywood-2009 graph is a graph of Hollywood movie actors, where nodes are actors and edges indicate two actors appear in a movie together.

implementation	elapsed_ms (avg of 10 runs)
Python+SNAP	*> 10 minutes*
Gunrock CPU	2035.45
Gunrock GPU	**13.793**

Takeaway: Here, the Gunrock GPU implementation is approximately 150x faster than the Gunrock CPU implementation. The HIVE reference implementation did not finish in 10 minutes.

Indochina-2004 graph (|U|=7414866, |E|= 191606827)

The Indochina-2004 graph is an internet hyperlink graph, generated by a crawl of Asian country domains.

implementation	elapsed_ms (avg of 10 runs)
Python+SNAP	*> 10 minutes*
Gunrock CPU	9079.216
Gunrock GPU	**22.743**

Takeaway: Here, the Gunrock GPU implementation is approximately 400x faster than the Gunrock CPU implementation. The HIVE reference implementation did not finish in 10 minutes.

Implementation limitations

The size of the graph that can be processed will (usually) be limited by the number of edges `|E|` in the input graph. The VN algorithm only allocates an additional 1–3 arrays of size `|U|`, and thus does not require a large amount of storage for temporary data.

The Gunrock VN algorithm works on weighted/unweighted directed/undirected graphs. No particular graph topology or node/edge metadata is required. In general, VN would be run on graphs with node and/or edge attributes, but since our Gunrock app only implements context scoring, we are not subject to those restrictions.

Performance limitations

- Like SSSP, VN is bound by device memory latency.
- Profiling indicates that 64% of time is spent in the Gunrock `advance` operator and 20% of time is spent in in the `filter` operator (pseudocode above).
- The device memory bandwidth is 271 GB/s – within the expected range for Gunrock graph analytics. Random memory access means that we don't expect to get close to the reported maximum memory bandwidth.

Next Steps

Alternate approaches/further work

Because of its similarity to SSSP, this implementation of VN is fairly hardened. However, given more time, we could implement more variations on context similiarity as described in Coppersmith and Priebe's paper. Given the range of potential context similarity functions, this could involve implementing a wide variety of Gunrock operators.

Gunrock implications

This was a straightforward adapatation of an existing Gunrock app. SSSP is also one of the simpler apps – only one advance/filter operation without complex logic – so implementing VN was not very difficult. All of the core logic in VN is identical to SSSP.

Notes on multi-GPU parallelization

Discussion of multi-GPU scalability of VN can be found here.

Notes on dynamic graphs

The reference implementation does not cover a dynamic graph version of this workflow, though one could imagine having a static set of seed nodes and a streaming graph on which one would like to compute context scores in real time.

Notes on larger datasets

If the datasets are larger than a single or multi-GPU's aggregate memory, the straightforward solution would be to let Unified Virtual Memory (UVM) in CUDA automatically handle memory movement. Declaring the entire graph as managed memory for a single GPU implementation, will allow the users to simply oversubscribe for 1 GPU, and queue vertices and edges in from the host memory as needed (this will be very slow). Further optimizations can be done, where instead of utilizing host memory, we can leverage a multi-GPU implementation and move the entire graph over to device memory, using NVLink to move data between the devices' global memory. This can be further optimized by using MemAdvise hints such as pinning the memory to GPU's local memory where it is likely to be used, or create a direct map to all other GPUs to avoid page faulting on first touch.

Notes on other pieces of this workload

The context scoring component of vertex nomination is incredibly general, and could include versions ranging in complexity from simple Euclidean distance metrics to the output of complex deep learning pipelines. If we were to integrate these kinds of components more closely w/ Gunrock, we'd likely need to use other CUDA libraries (cuBLAS, cuDNN, etc.) as well as interface w/ higher-level machine learning libraries (TensorFlow, PyTorch, etc.).

Chapter 12

Scaling analysis for HIVE applications

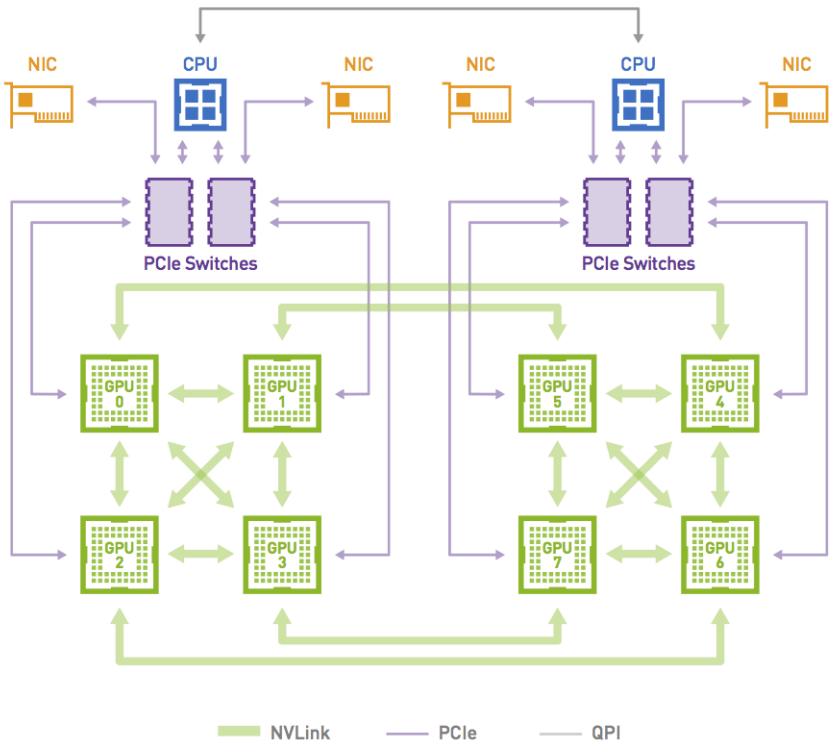
The purpose of this study is to understand how the HIVE v0 applications would scale out on multiple GPUs, with a focus on the DGX-1 platform. Before diving into per-application analysis, we give a brief summary of the potential hardware platforms, the communication methods and models, and graph partitioning schemes.

Hardware platforms

There are at least three kinds of potential multi-GPU platforms for HIVE apps. They have different GPU communication properties, and that may affect the choice of communication models and/or graph partitioning schemes, thus may have different scaling results.

DGX-1

The DGX-1 with P100 GPUs has 4 NVLink lanes per GPU, connected as follows.



Each of the NVLink links runs at 20 GBps per direction, higher than PCIe 3.0 x16 (16 GBps for the whole GPU). But the topology is not all-to-all, and GPUs may not be able to access every other GPU's memory. For example, GPU0 can't use peer access on GPUs 5, 6 and 7. This makes implementations using peer access more complex than a full all-to-all topology. DGX-1 with V100 GPUs increases the NVLink speed to 25 GBps per direction per lane, and increases the number of lanes per GPU to 6, but peer accessibility has not been changed. This issue is finally addressed in DGX-2 with the NVSwitch.

Using a benchmark program to test throughput and latency shows the following results. `Self` indicates local GPU accesses, `peer` indicates peer accesses, `host` indicates accesses to the CPU memory via UVM, and `all` indicates accesses to all peer-accessible GPUs. The `regular` operations access the memory in continous places by neighboring threads; in CUDA terms, these operations are coalesced memory accesses. The `random` operations access the memory space randomly, and neighboring threads may be touching memory that are far away from each other; in CUDA terms, these operations are non-coalesced memory accesses. The memory access patterns of graph workflows are a mix of both,

and one main target of kernel optimizations is to make the memory accesses as coalesced as possible. But at the end, depending on the algorithm, some random accesses may be unavoiable. Random accesses across GPUs are particularly slow.

Throughput in GBps:

Operation	Self	Peer	Host	All
Regular read	448.59	14.01	444.74	12.17
Regular write	442.98	16.21	16.18	12.17
Regular update	248.80	11.71	0.0028	6.00
Random read	6.78	1.43	2.39	4.04
Random write	6.63	1.14	3.47E-5	3.82
Random update	3.44	0.83	1.92E-5	2.08

Latency in microseconds (us):

Operation	Self	Peer	Host	All
Regular read	2.12	1.18	1.30	1.49
Regular write	1.74	1.00	13.83	1.01
Regular update	2.43	1.20	79.29	1.44
Random read	3.11	1.08	13.61	1.40
Random write	3.28	1.05	15.88	1.39
Random update	5.69	1.28	21.76	1.38

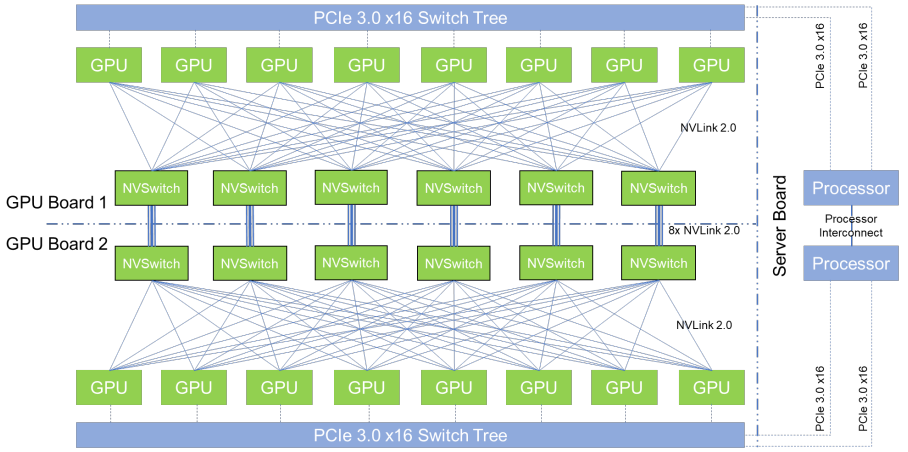
All the regular throughputs are at least 80% of their theoretical upper bounds. The latencies when accessing local GPUs seem odd, but other latencies look reasonable. It's clear that local regular accesses have much higher throughput than inter-GPU connections, about 20 to 30 times from this experiment. The ratio of random accesses are lower, but still at about 5 times. The implication on the scalabilities of graph applications is that for scalable behavior, the local-memory-access-to-communication ratio needs to be at least 10 to 1. Because most graph implementations are memory bound, the computation cost is counted by the number of elements accessed by the kernels; this means the computation to communication ratio should be at least 2.5 operations to 1 byte to exhibit scalable behavior.

Unified virtual memory (UVM) doesn't work as expected for most cases, instead only when the accesses are read only and the data can be duplicated on each GPU. Otherwise the throughputs are significantly lower, caused by memory migration and going over the PCIe interfaces. The less than 0.5 GBps throughputs from write and update operations via UVM could possibily caused by problems in the UVM support or the way how UVM is configured in the benchmark code. It must be noted that, at the time of testing, the DGX-1 has CUDA

9.1 and NVIDIA driver 390.30 installed, which are more than one year old. A newer CUDA version and NVIDIA driver could potentially improve the UVM performance. Testing using V100 GPUs with CUDA 10.0 and NVIDIA driver 410 shows considerablly better throughputs.

DGX-2

The DGX-2 system has a very different NVLink topology: the GPUs are connected by NVSwitches, and all to all peer accesses are available.



At the time of this report, the DGX-2 is hardly available, and not to us. What we have locally at UC Davis are two Quadro GV100 GPUs directly connected by 4 NVLink2 lanes. Although the setup is much smaller than the DGX-2, it still can provide some ideas on how the inter-GPU communication would perform on the DGX-2.

Throughput in GBps

Operation	Self	Peer	Host	All
Regular read	669.68	76.74	679.52	76.72
Regular write	590.01	85.00	170.113	76.28
Regular update	397.26	39.67	80.00	37.86
Random read	17.39	7.46	17.27	10.51
Random write	13.25	7.96	1.23	7.24
Random update	6.83	3.88	0.68	3.85

Latency in microsecond (us)

Operation	Self	Peer	Host	All
Regular read	0.37	0.47	0.37	0.41

Operation	Self	Peer	Host	All
Regular write	0.08	0.08	0.08	0.15
Regular update	0.37	0.47	0.43	0.41
Random read	0.11	0.10	0.10	0.16
Random write	0.13	0.08	0.08	0.15
Random update	0.15	0.09	0.09	0.17

On this machine configuration, the local-to-peer memory throughput ratios, about 8 for regular accesses and about 2 for random accesses, are much lower than the DGX-1. The decreases are mainly from using all the 4 lanes for communication, instead of 1 in the DGX-1 cases. If using only a single lane, the ratios would become 32 and 8, even higher than the DGX-1. The actual effect from the NVSwitch is still unclear, but DGX-2 is expected to have similar scalabilities as DGX-1 for graph applications.

GPU clusters

Going from multiple GPUs within the same node to multiple GPUs across different nodes significantly decreases the inter-GPU throughput. While NVLink runs at 80 GBps per direction per GPU for the DGX-1, the aggregated InfiniBand bandwidth is only 400 Gbps, which is only one twelfth of the aggregated inter-GPU bandwidth. This means the local access-to-communication-bandwidth ratio drops an order of magnitude, making scaling graph applications across nodes a corresponding order of magnitude harder. Using the same approximation method as the DGX-1, a graph implementation needs to have 30 operations / local memory operations for each byte going across the nodes. The implementation focus may need to switch to communication, rather than local computation, to achieve a scalable implementation on GPU clusters.

Communication methods / models

There are multiple ways to move data between GPUs: explicit movement, peer accesses, and unified virtual memory (UVM). They have different performance and implications in implementing graph workflows.

Explicit data movement

The most traditional way to communicate is to explicitly move the data: use `cudaMemcpyAsync` to copy a block of memory from one GPU to another. The source and destination GPUs are not required to be peer accessible. CUDA will automatically select the best route: if GPUs are peer-accessible, the traffic will go through the inter-GPU connection, be it NVLink or PCIe; if they are not peer-accessible, the data will be first copied to CPU memory, and then copied to the destination GPU.

One of the advantage of explicit data movement is throughput. `cudaMemcpyAsync` is highly optimized, and the data for communication are always dense. The throughput should be close to the hardware limit, if the size of data is not too small, say at least a few tens of MB. Explicit data movement also isolates local computation and communication. Because there is no need to consider the data layout or different access latencies from local or remote data, the implementation and optimization of computation kernels can be much simpler. It also enables connection to other communication libraries, such as MPI.

However, explicit memory copy requires that data for communication are packed in a continuous memory space. For most applications, this means additional computation to prepare the data. Since the computing power of GPUs is huge, and graph applications are mostly memory-bound, this extra computation should only have minimal impact on the running time.

Many graph algorithms are written using the bulk synchronous parallel (BSP) model: computations are carried out in iterations, and the results of computation are only guaranteed to be visible after the iteration boundary. The BSP model provides a natural communication point: at the iteration boundary. The current Gunrock multi-GPU framework follows the BSP model.

Depending on the algorithm, there are several communication models that can be used:

- *Peer to host GPU* This communication model is used when data of a vertex or edge on peer GPUs need to be accumulated / aggregated onto the host GPU of the vertex. When the vertex or edge is only adjacent to a few GPUs, it may be beneficial to use direct p2p communication; when the vertex is adjacent to most GPUs, a `Reduce` from all GPUs to the host GPU may be better.
- *Host GPU to peers* This is the opposite to the peer-to-host model. It propagates data of a vertex or edge from its host GPU to all GPUs adjacent to the vertex. Similarly, if the number of adjacent GPUs are small, point-to-point communication should do the work; otherwise, `broadcast` from the host GPU may be better.
- *All reduce* When updates on the same vertex or edge come from many GPUs, and the results are needed on many GPUs, `AllReduce` may be the best choice. It can be viewed as an `peers to host` followed by an `host to peers` communication. It can also be used without partitioning the graph: it works without knowing or assigning a host GPU to an vertex or edge.
- *Mix all reduce with peers to host GPU or host GPU to peers* This is a mix of `AllReduce` and peer-to-peer communications: for vertices or edges that touch a large number of GPUs, `AllReduce` is used; for other vertices or edges, direct peer-to-peer communications are used. This

communication model is coupled with the high / low degree partitioning scheme. The paper "Scalable Breadth-First Search on a GPU Cluster" https://arxiv.org/abs/1803.03922 has more details on this model.

Peer accesses

If a pair of GPUs is peer-accessible, they can directly dereference each other's memory pointers within CUDA kernels. This provides a more asynchronous way for inter-GPU communication: there is no need to wait for the iteration boundary. Atomic operations are also supported if the GPUs are connected by NVLink. The implementation can also be kept simple, since no data preparing and explicit movement is needed. The throughput is also acceptable, although not as good as explicit movement.

However, this essentially forces the kernel to work on a NUMA (non-uniform memory access) domain formed by local and remote GPU memory. Some kernels optimized under the assumption of a flat memory domain may not work well. Peer accesses also give up the opportunity to aggregate local updates on the same vertex or edge before communication, so the actual communication volume may be larger.

Unified virtual memory (UVM)

UVM is similar to peer accesses, as it also enables multiple GPUs to access the same memory space. However, the target memory space is allocated in the CPU memory. When needed on a GPU, a memory page will be moved to the GPU's memory via the page fault mechanism. Updates to the data are cached in GPU memory first, and will eventually be written to the CPU memory. UVM provides a transparent view of the CPU memory on GPU, and significantly reduces the coding complexity if running time is not a concern. It also enables the GPU to process datasets that can't fit in combined GPU memory without explicitly streaming the data from CPU to GPU.

But there are some caveats. The actual placement of a memory page/piece of data relies on hints given by `cudaMemAdvise`, otherwise it will need to be fetched from CPU to GPU when first used by any GPU, and bounces between GPUs when updated by multiple GPUs. The hints essentially come from partitioning the data, but sometimes there is no good way to partition, and data bouncing is unavoidable. In the worst cases, the data can be moved back to CPU, and any further access will need to go through the slow PCIe bridge again. The performance of UVM is not as good as explicit data movement or peer accesses; in the worst cases, it can be a few orders of magnitude slower. When data is larger than the GPU memory, UVM's throughput drops significantly; as a result, it's easier to code, but it will be slower than streaming the graph for datasets larger than GPU memory.

Graph partitioning scheme

Graphs may be cut into smaller pieces to put them onto multiple GPUs. Duplicating the graph on each may work for some problems, provided the graph is not too large; but duplication is not suitable for all problems, and does not scale in graph size. Graph partitioning is a long-lasting research topic, and we decided to use existing partitioners, such as Metis, instead of implementing some complicated ones of our own. A large number of graphs, especially those with high connectivities, are really difficult to partition; our results suggest that random partitioning works quite well in terms of time taken by the partitioner, load balancing, programming simplicity and still manageable communication cost. By default, Gunrock uses the random partitioner.

What makes a bigger difference is the partitioning scheme: whether the graph is partitioned in 1 dimension, 2 dimensions, or differently for low and high degree vertices.

1D partitioning

1D partitioning distributes the edges in a graph either by the source vertices or the destination vertices. It's simple to work with, and scales well when the number of GPUs are small. It should still work on the DGX-1 with 8 GPUs for a large number of graph applications. But that may approach 1D partitioning's scalability limit.

2D partitioning

2D partitioning distributes the edges by both the source and the destination vertices. When a graph is visualized in a dense matrix representation, 2D partitioning is like cutting the matrix by a 2D grid. 8 GPUs in the DGX-1 may be too small for 2D partitioning to be useful; it may worth trying out on DGX-2 with 16 GPUs. 2D partitioning of sparse graphs may create significant load imbalance between partitions.

High/low degree partitioning

The main idea of high/low degree partitioning is simple: for vertices with low out-degrees and their outgoing edges, distribute edges based on their source vertices; for vertices with high out-degrees and their outgoing edges, distribute edges based on the destination vertices; if both vertices have high out-degrees, distribute the edge based on the one with lower degree. The result is that low degree vertices are only adjacent to very few GPUs, while high degree vertices' edges are scattered among all GPUs. Graph applications scale very well when using the p2p communication model for low degree vertices, and the `AllReduce` model for high degree vertices.

Scaling of the HIVE applications

The target platform DGX-1 has 8 GPUs. Although that is more than we normally see for single scaling studies, the simple 1D graph partitioning scheme should (in general) still work. The marginal performance improvement by using more GPUs may be insignificant at this scale, and a small number of applications might even see performance decreases with some datasets. However, the 1D partitioning makes the scaling analysis simple and easily understandable. If other partitioning schemes could work better for a specific application, it would be noted.

How scaling is considered

The bandwidth of NVLink is much faster than PCIe 3.0: 20x3 and 25x6 GBps bidirectionally for each Tesla P100 and V100 GPUs respectively in an DGX-1. But compared to the several TFLOPs computing power and several hundred GBps device bandwidth, the inter-GPU bandwidth is still considerably less. For any application to have good scalability, the communication time should be able to be either: 1) hidden by overlap with computation, or 2) kept as a small portion of the computation. The computation-to-communication ratio is a good indicator to predict the scalability: a higher ratio means better scalability. Specific to the DGX-1 system with P100 GPUs, a ratio larger than about 10 to 1 is expected for an app to have at least marginal scalability. For GPUs newer than P100, the computation power and memory bandwidth improve faster than interconnect bandwidth, so the compute-to-communicate ratio needs to grow even more to start seeing positive scaling.

Community Detection (Louvain)

The main and most time-consuming part of the Louvain algorithm is the modularity optimization iterations. The aggregated edge weights between vertices and their respective adjacent communities, as well as the outgoing edge weights of each community, are needed for the modularity optimization. The vertex-community weights can be computed locally, if the community assignments of all neighbors of local vertices are available; to achieve this, a vertex needs to broadcast its new community when the assignment changes. The per-community outgoing edge weights can be computed by `AllReduce` across all GPUs. The modularity optimization with inter-GPU communication can be done as:

```
Do
    Local modularity optimization;
    Broadcast updated community assignments of local vertices;
    local_weights_community2any := sums(local edges from an community);
    weights_community2any := AllReduce(local_weights_community2any, sum);
While iterations stop condition not met
```

The local computation cost is on the order of O(|E| + |V|)/p, but with a large constant hidden by the O() notation. From experiments, the constant factor is about 10, considering the cost of sort or the random memory access penalty of hash table. The community assignment broadcast has a cost of |V| x 4 bytes, and the 'AllReduce' costs 2|V| x 8 bytes. These communication costs are the upper bound, assuming there are |V| communities, and all vertices update their community assignments. In practice, the communication cost can be much lower, depending on the dataset.

The graph contraction can be done as below on multiple GPUs:

```
temp_graph := Contract the local sub-graph based on community assignments;
Send edges <v, u, w> in temp_graph to host_GPU(v);
Merge received edges and form the new local sub-graph;
```

In the worst case, assuming the number of edges in the contracted graph is |E'|, the communication cost could be |E'| x 8 bytes, with the computation cost at about 5|E|/p + |E'|. For most datasets, the size reduction of graph from the contraction step is significant, so the memory needed to receive edges from the peer GPUs is manageable; however, if |E'| is large, it can be significant and may run out of GPU memory.

Summary of Louvain multi-GPU scaling

Because the modularity optimization runs multiple iterations before each graph contraction phase, the computation and communication of modularity optimization is dominant.

Parts	Comp cost	Comm cost	Comp/comm ratio	Scalability	Memory usage (B)
Modularity optim.	10(E + V) /p	20V bytes	E/p : 2V	Okay	88E/p + 12V
Graph contraction	5E / p + E'	8E' bytes	5E/p + E' : 8E'	Hard	16E'
Louvain	10(E + V) / p	20V bytes	E/p : 2V	Okay	88E/p + 12V + 16E'

Louvain could be hard to implement on multiple GPUs, especially for the graph contraction phase, as it forms a new graph and distributes it across the GPUs. But the scalability should be okay.

GraphSAGE

The main memory usage and computation of SAGE are related to the features of vertices. While directly accessing the feature data of neighbors via peer access is possible and memory-efficient, it will create a huge amount of inter-GPU traffic that makes SAGE unscalable in terms of running time. Using UVM to store the feature data is also possible, but that will move the traffic from inter-GPU to the GPU-CPU connection, which is even less desirable. Although

there is a risk of using up the GPU memory, especially on graphs that have high connectivity, a more scalable way is to duplicate the feature data of neighboring vertices. Depending on the graph size and the size of features, not all of the above data distribution schemes are applicable. The following analysis focuses on the feature duplication scheme, with other schemes' results in the summary table.

SAGE can be separated into three parts, depending on whether the computation and data access is source-centric or child-centric.

```
// Part1: Select the children
For each source in local batch:
    Select num_children_per_source children form source's neighbors;
    Send <source, child> pairs to host_GPU(child);

// Part2: Child-centric computation
For each received <source, child> pair:
    child_feature = feature[child];
    send child_feature to host_GPU(source);

    feature_sums := {0};
    For i from 1 to num_leaves_per_child:
        Select a leaf from child's neighbors;
        leaves_feature += feature[leaf];
    child_temp = L2_normalize( concatenate(
        feature[child] * Wf1, leaves_feature * Wa1));
    send child_temp to host_GPU(source);

// Part3: Source-centric computation
For each source in local batch:
    children_feature := sum(received child_feature);
    children_temp := sum(received child_temp);
    source_temp := L2_normalize( concatenate(
        feature[source] * Wf1, children_feature * Wa1));

    source_result := L2_normalize( concatenate(
        source_temp * Wf2, children_temp * Wa2));
```

Assume the size of local batch is B, the number of children per source is C, the number of leaves per child is L, and the feature length per vertex is F. Dimensions of 2D matrices are noted as (x, y). The computation and communication costs for each part are:

```
Part 1, computation  : B x C.
Part 1, communication: B x C x 8 bytes.
```

```
Part 2, computation  : B x C x F + B x C x (F + L x F + F x (Wf1.y + Wa1.y)).
Part 2, communication: B x C x (F + Wf1.y + Wa1.y) x 4 bytes.
Part 3, computation  : B x (C x (F + Wf1.y + Wa1.y) + F x (Wf1.y + Wa1.y) +
                       (Wf1.y + Wa1.y) x (Wf2.y + Wa2.y)).
Part 3, communication: 0.
```

For Part 2's communication, if C is larger than about 2p, using `AllReduce` to sum up `child_feature` and `child_temp` for each source will cost less, at B x (F + Wf1.y + Wa1.y) x 2p x 4 bytes.

Summary of Graph SAGE multi-GPU scaling

Parts	Comp. cost
Feature duplication	
Children selection	BC
Child-centric comp.	BCF x (2 + L + Wf1.y + Wa1.y)
Source-centric comp.	B x (CF + (Wf1.y + Wa1.y) x (C + F + Wf2.y + Wa2.y)
Graph SAGE	B x (C + 3CF + 3LCF + (Wf1.y + Wa1.y) x (CF + C + F + Wf2.y + Wa2.y))
Direct feature access	
Child-centric comp.	BCF x (2 + L + Wf1.y + Wa1.y)
Graph SAGE	B x (C + 3CF + 3LCF + (Wf1.y + Wa1.y) x (CF + C + F + Wf2.y + Wa2.y))
Feature in UVM	
Child-centric comp.	BCF x (2 + L + Wf1.y + Wa1.y)
Graph SAGE	B x (C + 3CF + 3LCF + (Wf1.y + Wa1.y) x (CF + C + F + Wf2.y + Wa2.y))

Parts	Comm. cost
Feature duplication	
Children selection	8BC bytes
Child-centric comp.	4B x (F + Wf1.y + Wa1.y) x min(C, 2p) bytes
Source-centric comp.	0 bytes
Graph SAGE	8BC + 4B x (F + Wf1.y + Wa1.y) x min(C, 2p) bytes
Direct feature access	
Child-centric comp.	4B x ((F + Wf1.y + Wa1.y) x min(C, 2p) + CLF) bytes
Graph SAGE	8BC + 4B x (F + Wf1.y + Wa1.y) x min(C, 2p) + 4BCFL bytes
Feature in UVM	
Child-centric comp.	4B x (F + Wf1.y + Wa1.y) x min(C, 2p) bytes over GPU-GPU + 4BCLF bytes over GPU-CPU
Graph SAGE	8BC + 4B x (F + Wf1.y + Wa1.y) x min(C, 2p) bytes over GPU-GPU + 4BCFL bytes over GPU-CPU

Parts	Comp/comm ratio	Scalability
Feature duplication		
Children selection	1 : 8	Poor
Child-centric comp.	~ CF : min(C, 2p) x 4	Good
Source-centric comp.	N.A.	N.A.
Graph SAGE	at least ~ CF : min(C, 2p) x 4	Good
Direct feature access		
Child-centric comp.	~ (2 + L + Wf1.y + Wa1.y) : 4L	poor
Graph SAGE	~ (2 + L + Wf1.y + Wa1.y) : 4L	poor
Feature in UVM		
Child-centric comp.	~ (2 + L + Wf1.y + Wa1.y) : 4L over GPU-CPU	very poor
Graph SAGE	~ (2 + L + Wf1.y + Wa1.y) : 4L over GPU-CPU	very poor

When the number of features is at least several tens, the computation workload will be much more than communication, and SAGE should have good scalability. Implementation should be easy, as only simple p2p or AllReduce communication models are used. If memory usage is an issue, falling back to peer-access or UVM will result in very poor scalability; problem segmentation (i.e,. only process portion of the graph at a time) may be necessary to have a scalable implementation for large graphs, but that will be quite complex.

Random walks and graph search

If the graph can be duplicated on each GPU, the random walk multi-GPU implementation is trivial: just do a subset of the walks on each GPU. The scalability will be perfect, as there is no communication involved at all.

A more interesting multi-GPU implementation would be when the graph is distributed across the GPUs. In this case, each step of a walk not only needs to send the `<walk#, step#, v>` information to `host_GPU(v)`, but also to the GPU that stores the result for such walk.

```
For each walk starting from local vertex v:
    Store v for <walk#, step 0>;
    Select a neighbor u of v;
    Store u for <walk#, step 1>;
    Send <walk#, 1, u> to host_GPU(u) for visit;

Repeat until all steps of walks finished:
    For each received <walk#, step#, v> for visit:
        Select a neighbor u of v;
        Send <walk#, step# + 1, u> to host_GPU(u) for visit;
        Send <walk#, step# + 1, u> to host_GPU_walk(walk#) for record;
```

```
For each received <walk#, step#, v> for record:
    Store v for <walk#, step#>;
```

Using W as the number of walks, for each step, we have

Parts	Comp. cost	Comm. cost	Comp/comm ratio	Scalability
Random walk	W/p	W/p x 24 bytes	1 : 24	very poor

Graph search is very similar to random walk, except that instead of randomly selecting any neighbor, it selects the neighbor with the highest score (when using the `greedy` strategy), or with probabilities proportional to the neighbors' scores (when using the `stochastic_greedy` strategy).

For the `greedy` strategy, a straightforward implementation, when reaching a vertex, goes through the whole neighbor list of thatsuch vertex and finds the one with maximum score. A more optimized implementation could perform a pre-visit to find the neighbor with maximum scored neighbor, with a cost of E/p; during the random walk process, the maximum scored neighbor will be known without going through the neighbor list.

For the `stochastic_greedy` strategy, the straightforward implementation would also go through all the neighbors, selecting one based on their scores and a random number. Preprocessing can also help: perform a scan on the scores of each vertex's neighbor list, with a cost of E/p; during the random walk, a binary search would be sufficient to select a neighbor, with weighted probabilities.

The cost analysis, depending on the walk strategy and optimization, results in:

Strategy	Comp. cost	Comm. cost	Comp/comm ratio	Scalability
Uniform	W/p	W/p x 24 bytes	1 : 24	Very poor
Greedy	Straightforward: dW/p	W/p x 24 bytes	d : 24	Poor
Greedy	Pre-visit: W/p	W/p x 24 bytes	1 : 24	Very poor
Stochastic Greedy	Straightforward: dW/p	W/p x 24 bytes	d : 24	Poor
Stochastic Greedy	Pre-visit: log(d)W/p	W/p x 24 bytes	log(d) : 24	Very poor

If the selection of a neighbor is weighted-random, instead of uniformly-random, it will increase the computation workload to Wd /p, where d is the average degree of vertices in the graph. As a result, the computation-to-communication ratio will increase to d:24; for most graphs, this is still not high enough to have good scalability.

Geolocation

In each iteration, Geolocation updates a vertex's location based on its neighbors. For multiple GPUs, neighboring vertices's location information needs to be available, either by direct access, UVM, or explicit data movement. The following shows how explicit data movement can be implemented.

```
Do
    Local geo location updates on local vertices;
    Broadcast local vertices' updates;
While no more update
```

The computation cost is on the order of O(|E|/p), if in each iteration all vertices are looking for possible location updates from neighbors. Because the spatial median function has a lot of mathematical computation inside, particularly a haversine() for each edge, the constant factor hidden by O() is large; for simplicity, 100 is used as the constant factor here. Assuming that we broadcast every vertex's location gives the upper bound of communication, but in reality, the communication should be much less, because 1) not every vertex updates its location every iteration and 2) vertices may not have neighbors on each GPU, so instead of broadcast, p2p communication may be used to reduce the communication cost, especially when the graph connectivity is low.

Comm. method	Comp. cost	Comm. cost	Comp/comm ratio	Scalability
Explicit movement	100E/p	2V x 8 bytes	25E/p : 4V	Okay
UVM or peer access	100E/p	E/p x 8 bytes	25 : 1	Good

Vertex Nomination

Vertex nomination is very similar to a single source shortest path (SSSP) problem, except it starts from a group of vertices, instead of a single source. One possible multi-GPU implementation is:

```
Set the starting vertex / vertices;
While has new distance updates
    For each local vertex v with distance update:
        For each edge <v, u, w> of vertex v:
            new_distance := distance[v] + w;
            if (distance[u] > new_distance)
                distance[u] = new_distance;

    For each u with distance update:
        Send <u, distance[u]> to host_GPU(u);
```

Assuming on average, each vertex has its distance updated `a` times, and the average degree of vertices is `d`, the computation and the communication costs are:

Parts	Comp. cost	Comm. cost	Comp/comm ratio	Scalability
Vertex nomination	aE/p	aV/p x min(d, p) x 8 bytes	E : 8V x min(d, p)	Okay

The min(d, p) part in the communication cost comes from update aggregation on each GPU: when a vertex has more than one distance update, only the smallest is sent out; a vertex that has a lot of neighbors and is connected to all GPUs has its communication cost capped by p x 8 bytes.

Scan Statistics

Scan statistics is essentially triangle counting (TC) for each vertex plus a simple post-processing step. The current Gunrock TC implementation is intersection-based: for an edge `<v, u>`, intersecting `neighbors[u]` and `neighbors[v]` gives the number of triangles including `edge <v, u>`. This neighborhood-intersection-based algorithm only works if the neighborhood of end points of all edges for which we need to count triangles can reside in the memory of a single GPU. For graphs with low connectivities, such as road networks and meshes, it is still possible to partition the graph; for graphs with high connectivity, such as social networks or some web graphs, it's almost impossible to partition the graph, and any sizable partition of the graph may touch a large portion of vertices of the graph. As a result, for general graphs, the intersection-based algorithm requires the graph can be duplicated on each GPU. Under this condition, the multi-GPU implementation is trivial: only count triangles for a subset of edges on each GPU, and no communication is involved.

A more distributed-friendly TC algorithm is wedge-checking-based (https://e-reports-ext.llnl.gov/pdf/890544.pdf). The main idea is this: for each triangle A-B-C, where `degree(A) >= degree(B) >= degree(C)`, both A and B are in C's neighborhood, and A is in B's neighborhood; when testing for possible triangle D-E-F, with `degree(D) >= degree(E) >= degree(F)`, the wedge (two edges that share the same end point) that needs to be checked is D-E, and the checking can be simply done by verifying whether D is in E's neighborhood. As this algorithm is designed for distributed systems, it should be well-suited for multi-GPU system. The ordering requirements are imposed to reduce the number of wedge checks and to balance the workload. The multi-GPU pseudo code is:

```
For each local edge < v, u >:
    If (degree(v) > degree(u)) continue;
    For each neighbor w of v:
        If (degree(v) > degree(w)) continue;
```

```
        If (degree(u) > degree(w)) continue;
        Send tuple <u, w, v> to host_GPU(u) for checking;

For each received tuple < u, w, v >:
    If (w in u's neighbor list):
        triangles[u] ++;
        triangles[w] ++;
        triangles[v] ++;

AllReduce(triangles, sum);

// For Scan statistics only
For each vertex v in the graph:
    scan_stat[v] := triangles[v] + degree(v);
    if (scan_stat[v] > max_scan_stat):
        max_scan_stat := scan_stat[v];
        max_ss_node := v;
```

Using T as the number of triangles in the graph, the number of wedge checks is normally a few times `T`, noted as `aT`. For the three graphs tested by the LLNL paper—Twitter, WDC 2012, and Rmat-Scale 34—`a` ranges from 1.5 to 5. The large number of wedges can use up the GPU memory, if they are stored and communicated all at once. The solution is to generate a batch of wedges and check them, then generate another batch and check them, loop until all wedges are checked.

Assuming the neighbor lists of every vertex are sorted, the membership checking can be done in log(#neighbors). As a result, using `d` as the average outdegree of vertices, the cost analysis is:

Parts	Comp. cost	Comm. cost (B)	Comp/comm ratio	Scalability
Wedge generation	dE/p			
Wedge communication	0	aE/p x 12		
Wedge checking	aE/p x log(d)			
AllReduce	2V	2V x 4		
Triangle Counting	(d + a x log(d))E/p + 2V	aE/p x 12 + 8V	~(d + a x log(d)) : 12a	Okay
Scan Statistics (with wedge checks)	(d + a x log(d))E/p + 2V + V/p	12aE/p + 8V	~(d + a x log(d)) : 12a	Okay
Scan Statistics (with intersection)	Vdd + V/p	8V	dd : 8	Perfect

Sparse Fused Lasso (GTF)

The sparse fused lasso iteration is mainly a max-flow (MF), plus some per-vertex calculation to update the capacities in the graph. The reference and

most non-parallel implementations of MF are augmenting-path-based; but finding the argumenting path and subsequent residual updates are both serial. The push-relabel algorithm is more parallelizable, and used by Gunrock's MF implementation. Each time the push operation updates the flow on an edge, it also needs to update the flow on the reverse edge; but the reverse edge may be hosted by another GPU, and that creates a large amount of inter-GPU traffic. The pseudocode for one iteration of MF with inter-GPU communication is:

```
// Push phase
For each local vertex v:
    If (excess[v] <= 0) continue;
    If (v == source || v == sink) continue;
    For each edge e<v, u> of v:
        If (capacity[e] <= flow[e]) continue;
        If (height[v] <= height[u]) continue;
        move := min(capacity[e] - flow[e], excess[v]);
        excess[v] -= move;
        flow[e] += move;
        Send <reverse[e], move> to host_GPU(u);
        If (excess[v] <= 0)
            break for each e loop;

For each received <e, move> pair:
    flow[e] -= move;
    excess[Dest(e)] += move;

// Relabel phase
For each local vertex v:
    If (excess[v] <= 0) continue;
    min_height := infinity;
    For each e<v, u> of v:
        If (capacity[e] <= flow[e]) continue;
        If (min_height > height[u])
            min_height = height[u];
    If (height[v] <= min_height)
        height[v] := min_height + 1;

Broadcast height[v] for all local vertex;
```

The cost analysis will not be on one single iteration, but on a full run of the push-relabel algorithm, as the bounds of the push and the relabel operations are known.

Parts	Comp. cost	Comm. cost (Bytes)	Comp/comm ratio	Scalability
Push	a(V + 1)VE/p	(V+1)VE/p x 8	a:8	Less than okay

Parts	Comp. cost	Comm. cost (Bytes)	Comp/comm ratio	Scalability
Relabel	VE/p	Vˆ2 x 8	d/p : 8	Okay
MF (Push-Relabel)	(aV + a + 1)VE/p	Vˆ2((V+1)d/p + 1) x 8	~ a:8	Less than okay

The GTF-specific parts are more complicated than MF in terms of communication: the implementation must keep some data, such as weights and sizes, for each community of vertices, and multiple GPUs could be updating such data simultaneously. It's almost impossible to do explicit data movement for this part, and the best option is to use direct access or UVM; each vertex may update its community once, so the communication cost is still manageable. One iteration of GTF is:

```
MF;
BFS to find the min-cut;
Vertex-Community updates;
Updates source-vertex and vertex-destination capacities;
```

with scaling characteristics:

Parts	Comp. cost	Comm. cost (Bytes)	Comp/comm ratio	Scalability
MF (Push-Relabel)	(aV + a + 1)VE/p	Vˆ2((V+1)d/p + 1) x 8	~ a:8	Less than okay
BFS	E/p	2V x 4	d/p : 8	Okay
V-C updates	E/p	V/p x 8	d : 8	Okay
Capacity updates	V/p	V/p x 4	1 : 4	Less than okay
GTF	(aV + a + 1)VE/p + 2E/p + V/p	Vˆ2((V+1)d/p + 1) x 8 + 2V x 4 + V/p x 4	~ a:8	Less than okay

It's unsurprising that GTF may not scale: the compute- and communicate-heavy part of GTF is the MF, and in MF, each push needs communication to update its reverse edge. A more distributed-friendly MF algorithm is needed to overcome this problem.

Graph Projection

Graph projection is very similar to triangle counting by wedge checking; but instead of counting the triangles, it actually records the wedges. The problem here is not computation or communication, but rather the memory requirement of the result: projecting all vertices may create a very dense graph, which may be much larger than the original graph. One possible solution is to process the results in batches:

```
vertex_start := 0;
```

```
While (vertex_start < num_vertices)
    markers := {0};
    current_range := [vertex_start, vertex_start + batch_size);
    For each local edge e<v, u> with u in current_range:
        For each neighbor t of v:
            If (u == t) continue;
            markers[(u - vertex_start) * ceil(num_vertices / 32) + t / 32] |=
                1 << (t % 32);

    For each vertex u in current_range:
        Form the neighbor list of u in the new graph by markers;

    For each local edge e<v, u> with u in current_range:
        For each neighbor t of v:
            If (u == t) continue;
            e' := edge_id of <u, t> in the new graph,
                by searching u's neighbor list;
            edge_values[e'] += 1;

    For each edge e'<u, t, w> in the new graph:
        send <u, t, w> to host_GPU(u);

    Merge all received <u, t, w> to form projection
        for local vertices u in current_range;
    Move the result from GPU to CPU;

    vertex_start += batch_size;
```

Using `E'` to denote the number of edges in the projected graph, and `d` to denote the average degree of vertices, the costs are:

Parts	Comp. cost	Comm. cost	Comp/comm ratio	Scalability
Marking	dE/p	0 byte		
Forming edge lists	E'	0 byte		
Counting	dE/p	0 byte		
Merging	E'	E' x 12 bytes		
Graph Projection	2dE/p + 2E'	12E' bytes	dE/p + E' : 6E'	Okay

If the graph can be duplicated on each GPU, instead of processing distributed edges, each GPU can process only `u` vertices that are hosted on that GPU. This eliminates the merging step; as a result, there is no communication needed, and the computation cost reduces to 2dE/p + E'.

Local Graph Clustering

The Gunrock implementation of Local Graph Clustering (LGC) uses PageRank-Nibble, a variant of the PageRank algorithm. PR-Nibble's communication pattern is the same as standard PR: accumulate changes for each vertex to its host GPU. As a result, PR-Nibble should be scalable, just as standard PR. PR-Nibble with communication can be done as:

```
// Per-vertex updates
For each active local vertex v:
    If (iteration == 0 && v == src\_neighbor) continue;
    If (iteration > 0 && v == src)
        gradient[v] -= alpha / #reference_vertices / sqrt(degree(v));
    z[v] := y[v] - gradient[v];
    If (z[v] == 0) continue;

    q_old := q[v];
    threshold := rho * alpha * sqrt(degree(v));
    If (z[v] >= threshold)
        q[v] := z[v] - threshold;
    Else if (z[v] <= -threshold)
        q[v] := z[v] + threshold;
    Else
        q[v] := 0;

    If (iteration == 0)
        y[v] := q[v];
    Else
        y[v] := q[v] + (1 - sqrt(alpha)) / (1 + sqrt(alpha)) * (q[v] - old_q);

    gradient[v] := y[v] * (1 + alpha) / 2;

// Ranking propagation
For each edge e<v, u> of active local vertex v:
    change := y[v] * (1 - alpha) / 2 / sqrt(degree(v)) / sqrt(degree(u));
    gradient_update[u] -= change;

For each u that has gradient updates:
    send < u, gradient_update[u]> to host_GPU(u);

For each received gradient update < u, gradient_update>:
    gradient[u] += gradient_update;

// Gradient updates
For each local vertex u with gradient updated:
    If (gradient[u] == 0) continue;
```

```
Set u as active for next iteration;

val := gradient[u];
If (u == src)
    val -= (alpha / #reference_vertices) / sqrt(degree(u));
val := abs(val / sqrt(degree(u)));
if (gradient_scale_value < val)
    gradient_scale_value = val;
if (val > gradient_threshold)
    gradient_scale := 1;
```

The cost analysis is:

Parts	Comp. cost	Comm. cost	Comp/comm ratio	Scalability
Per-vertex updates	~10 V/p	0 bytes		
Ranking propagation	2E/p	V * 8 bytes	d/p : 4	
Gradient updates	V/p	0 bytes		
Local graph clustering	(12V + 2E)/p	8V bytes	(6 + d)/p : 4	good

Seeded Graph Matching and Application Classification

The implementations of these two applications are linear-algebra-based, as opposed to other applications where we used Gunrock and its native graph (vertex-edge) data structures. The linear-algebra-based (BLAS-based) formulations, especially the ones that require matrix-matrix multiplications, may impose a large communication requirement. Advance matrix-matrix and vector-matrix multiplication kernels use optimizations that build on top of a specific layout of the data, which may be not distribution-friendly. A different method of analyzing the computation and the communication costs—the computation vs. communication ratio—is needed for these applications.

Summary of Results

Application	Computation to communication ratio	Scalability	Implementation diff.
Louvain	E/p : 2V	Okay	Hard
Graph SAGE	~ CF : min(C, 2p)x4	Good	Easy
Random walk	Duplicated graph: infinity	Perfect	Trivial
Random walk	Distrib. graph: 1 : 24	Very poor	Easy
Graph search: Uniform	1 : 24	Very poor	Easy
Graph search: Greedy	Straightforward: d : 24	Poor	Easy
Graph search: Greedy	Pre-visit: 1:24	Very poor	Easy
G.S.: Stochastic greedy	Straightforward: d : 24	Poor	Easy
G.S.: Stochastic greedy	Pre-visit: log(d) : 24	Very poor	Easy

Application	Computation to communication ratio	Scalability	Implementation diff.
Geolocation	Explicit movement: 25E/p : 4V	Okay	Easy
Geolocation	UVM or peer access: 25 : 1	Good	Easy
Vertex nomination	E : 8V x min(d, p)	Okay	Easy
Scan statistics	Duplicated graph: infinity	Perfect	Trivial
Scan statistics	Distrib. graph: ~ (d + a * log(d)) : 12	Okay	Easy
Sparse fused lasso	~ a:8	Less than okay	Hard
Graph projection	Duplicated graph : infinity	Perfect	Easy
Graph projection	Distrib. graph : dE/p + E' : 6E'	Okay	Easy
Local graph clustering	(6 + d)/p : 4	Good	Easy

Seeded graph matching and application classification are matrix-operation-based and not covered in this table.

From the scaling analysis, we can see these workflows can be roughly grouped into three categories, by their scalabilities:

Good scalability GraphSAGE, geolocation using UVM or peer accesses, and local graph clustering belong to this group. They share some algorithmic signatures: the whole graph needs to be visited at least once in every iteration, and visiting each edge involves nontrivial computation. The communication costs are roughly at the level of V. As a result, the computation vs. communication ratio is larger than E : V. PageRank is a standard graph algorithm that falls in this group.

Moderate scalability This group includes Louvain, geolocation using explicit movement, vertex nomination, scan statistics, and graph projection. They either only visit part of the graph in an iteration, have only trivial computation during an edge visit, or communicate a little more data than V. The computation vs. communication is less than E : V, but still larger than 1 (or 1 operation : 4 bytes). They are still scalable on the DGX-1 system, but not as well as the previous group. Single source shortest path (SSSP) is an typical example for this group.

Poor scalability Random walk, graph search, and sparse fused lasso belong to this group. They need to send out some data for each vertex or edge visit. As a result, the computation vs communication ratio is less than 1 (or 1 operation : 4 bytes). They are very hard to scale across multiple GPUs. Random walk is an typical example.

End of report