Gunrock: A Fast and Programmable Multi-GPU Graph Processing Library

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Why use GPUs for Graph Processing?

Graphs

- Found everywhere
  - Road & social networks, web, etc.
- Require fast processing
  - Memory bandwidth, computing power and GOOD software
- Becoming very large
  - Billions of edges
- Irregular data access pattern and control flow
  - Limits performance and scalability

GPUs

- Found everywhere
  - Data center, desktops, mobiles, etc.
- Very powerful
  - High memory bandwidth (288 GBps) and computing power (4.3 Tflops)
- Limited memory size
  - 12 GB per NVIDIA K40
- Hard to program
  - Harder to optimize

Scalability

Performance

Programmability

What we want to achieve with Gunrock?

Performance

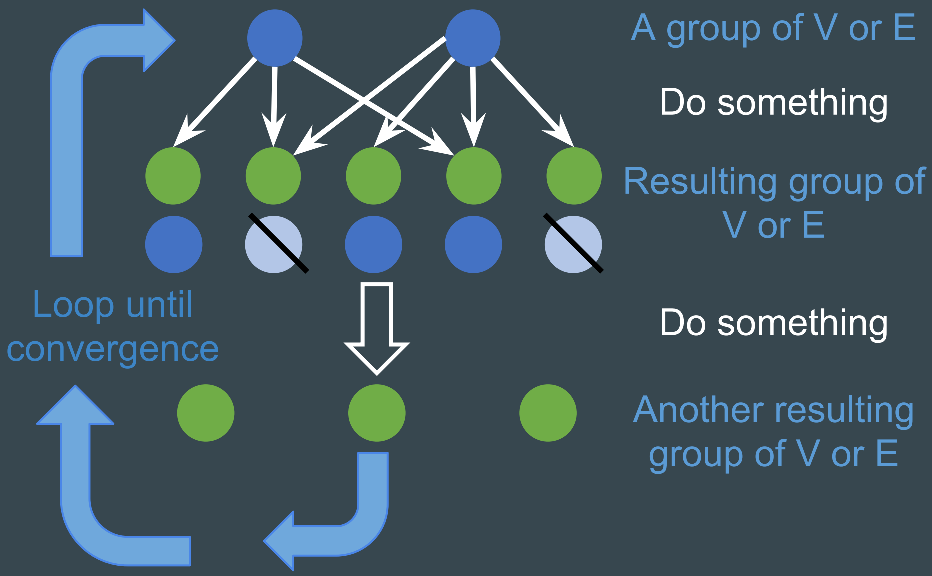
- High performance GPU computing primitives
- High performance framework
- Optimizations
- Multi-GPU capability

Programmability

- A data-centric abstraction designed specifically for the GPU
- Simple and flexible interface to allow user-defined operations
- Framework and optimization details hidden from users, but automatically applied when suitable

Idea: Data-Centric Abstraction & Bulk-Synchronous Programming

A generic graph algorithm:



Data-centric abstraction

- Operations are defined on
  a group of vertices or edges $\stackrel{\text{def}}{=}$ a frontier

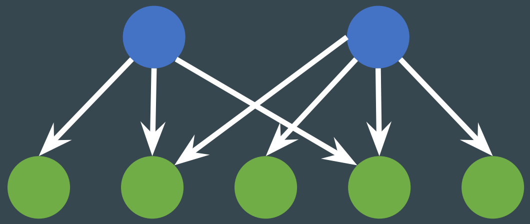
=> Operations = manipulations of frontiers

Bulk-synchronous programming

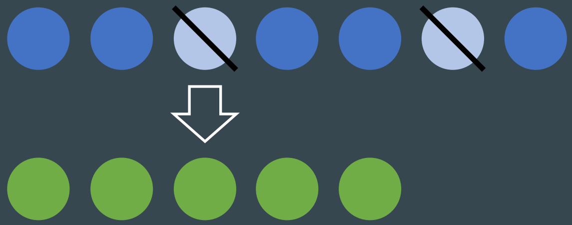
- Operations are done one by one, in order
- Within a single operation, computing on multiple elements can be done in parallel, without order

Gunrock's Operations on Frontiers

Generation

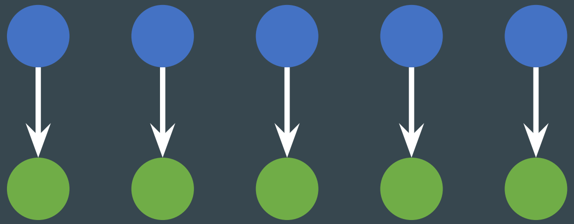


Advance: visit neighbor lists



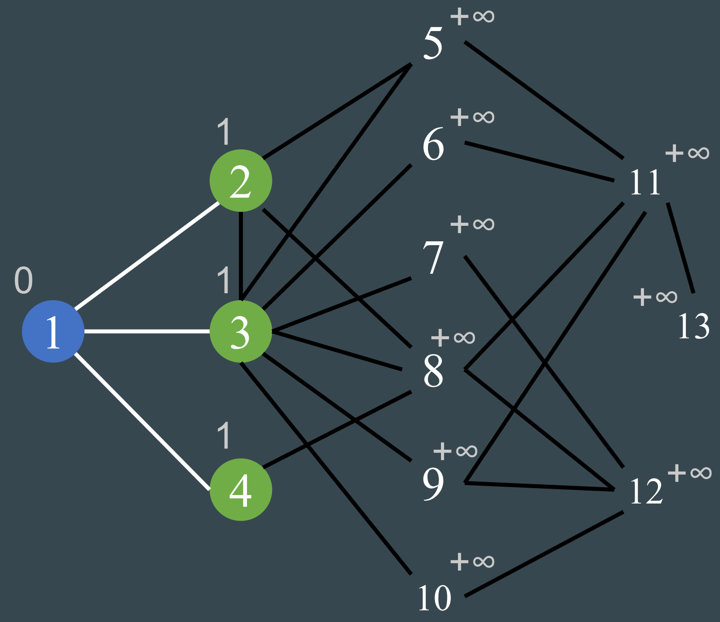
Filter: select and reorganize

Computation



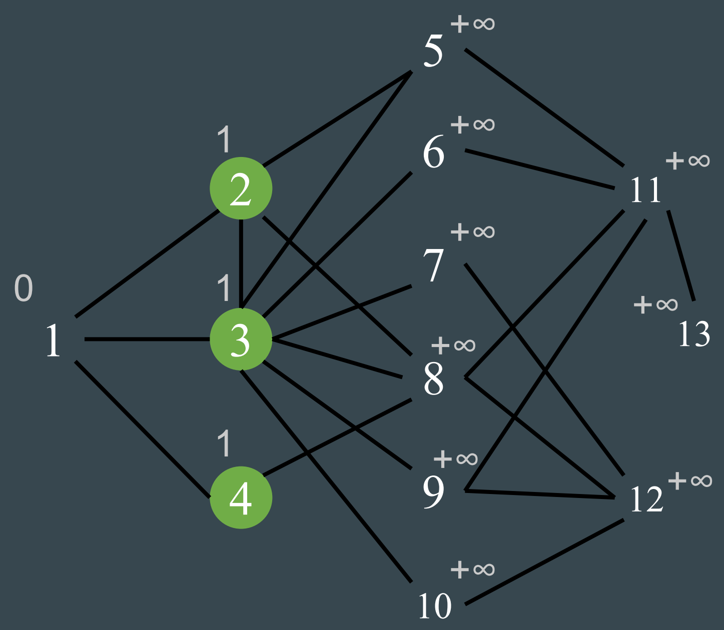
Compute: per-element computation, in parallel
can be combined with advance or filter

Example: BFS with Gunrock



Advance + Compute (+1, AtomicCAS)

Example: BFS with Gunrock



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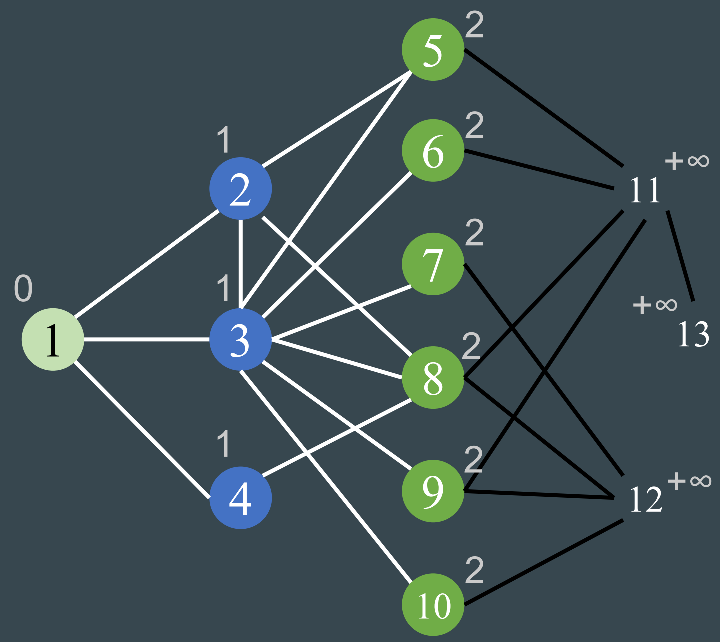
Advance + Compute (+1, AtomicCAS)

Filter

Example: BFS with Gunrock



1

Advance + Compute (+1, AtomicCAS)

3 4 2

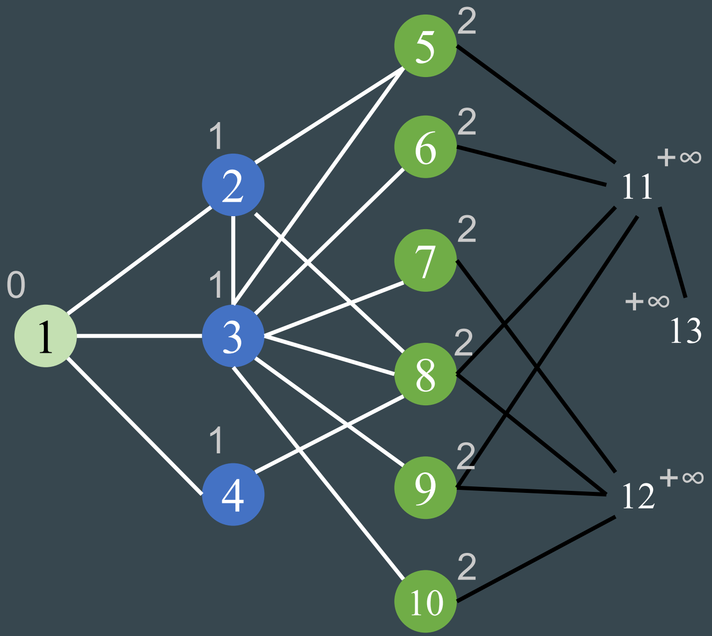
Filter

3 4 2

Advance + Compute (+1, AtomicCAS)

1 2 5 6 7 8 9 10 | 1 8 | 1 3 5 8

Example: BFS with Gunrock



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Advance + Compute

3 4 2

Filter

3 4 2

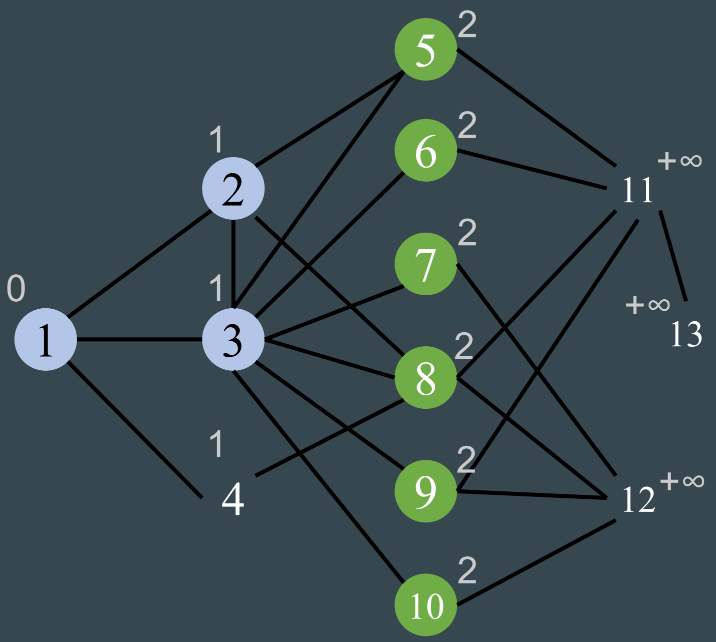
Advance + Compute (+1, AtomicCAS)

1 2 5 6 7 8 9 10 | 1 8 | 1 3 5 8

P: uneven neighbor list lengths (v4 vs. v3)

P: Concurrent discovery conflict (v5,8)

Example: BFS with Gunrock



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Advance + Compute

3 4 2

Filter

3 4 2

Advance + Compute (+1, AtomicCAS)

1 2 5 6 7 8 9 10 | 1 8 | 1 3 5 8

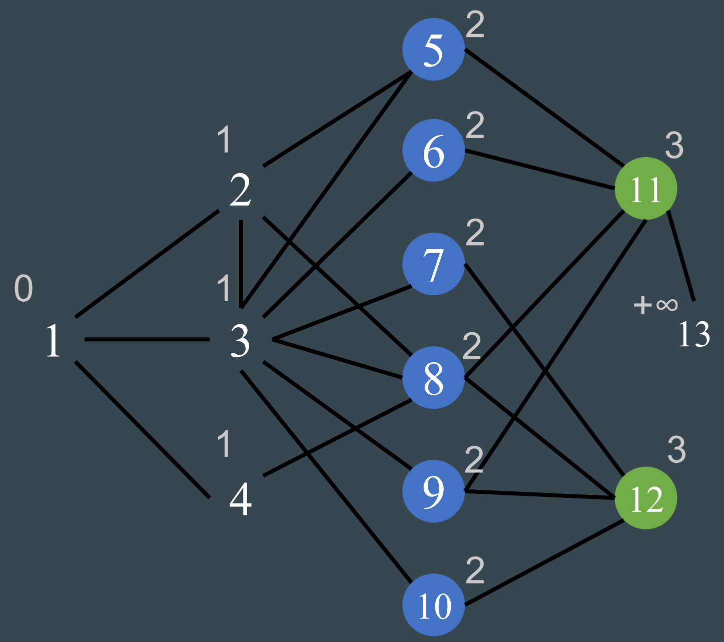
Filter

6 7 9 10 8 5

P: uneven neighbor list lengths (v4 vs. v3)

P: Concurrent discovery conflict (v5,8)

Example: BFS with Gunrock



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Advance + Compute

3 4 2

Filter

3 4 2

Advance + Compute (+1, AtomicCAS)

1 2 5 6 7 8 9 10 ¦ 1 8 ¦ 1 3 5 8

Filter

6 7 9 10 8 5

Advance + Compute, Filter

11 12

P: uneven neighbor list lengths (v4 vs. v3)

P: Concurrent discovery conflict (v5,8)

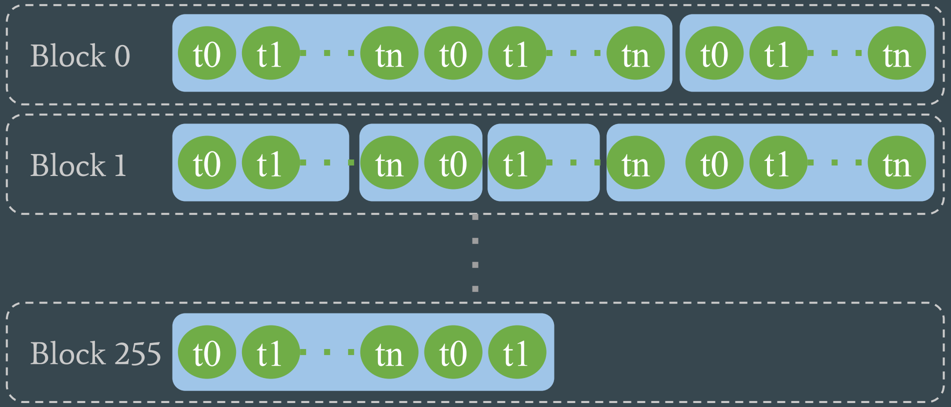
P: From many to very few (v5,6,7,8,9,10 -> v11, 12)

Optimizations: Workload mapping and load-balancing

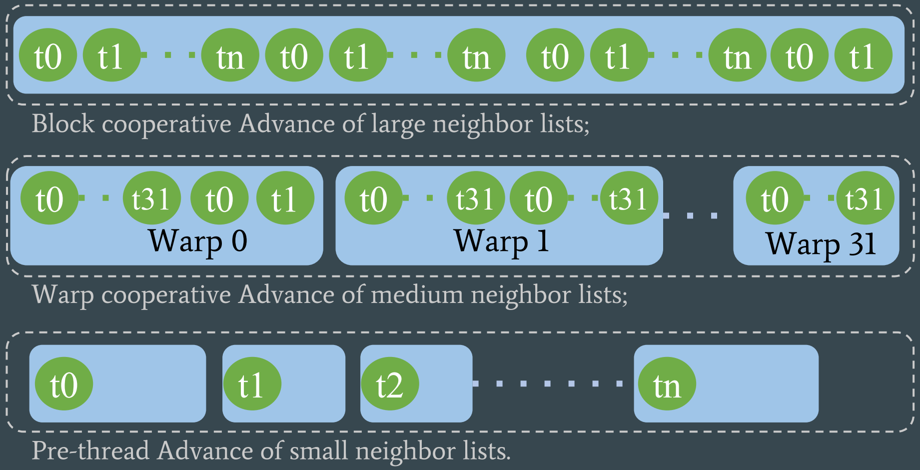
P: uneven neighbor list lengths

S: trade-off between extra processing and load balancing

First appeared in various BFS implementations, now available for all advance operations



Load-Balanced Partitioning [3]



Per-thread fine-grained, Per-warp and per-CTA coarse-grained [4]

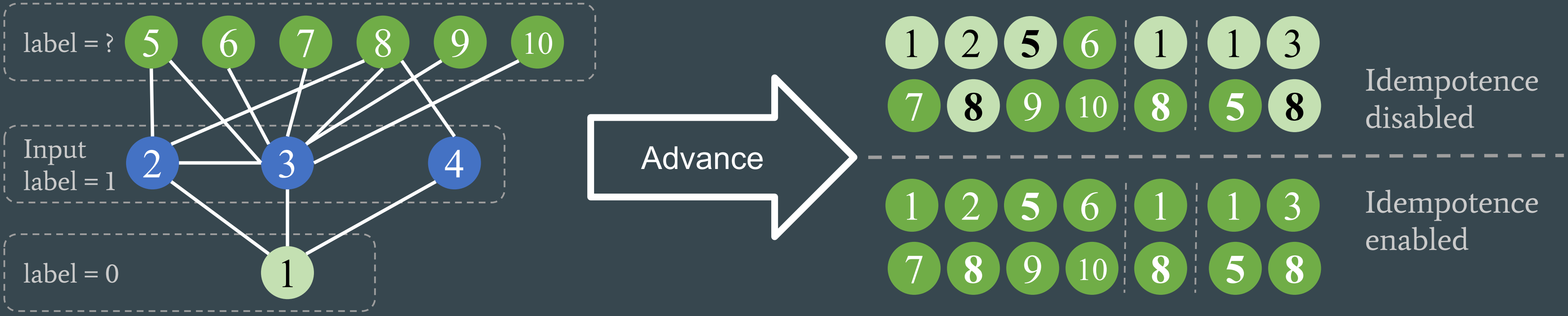
Optimizations: Idempotence

P: Concurrent discovery conflict (v5,8)

S: Idempotent operations (frontier reorganization)

- Allow multiple concurrent discoveries on the same output element
- Avoid atomic operations

First appeared in BFS [4], now available to other primitives



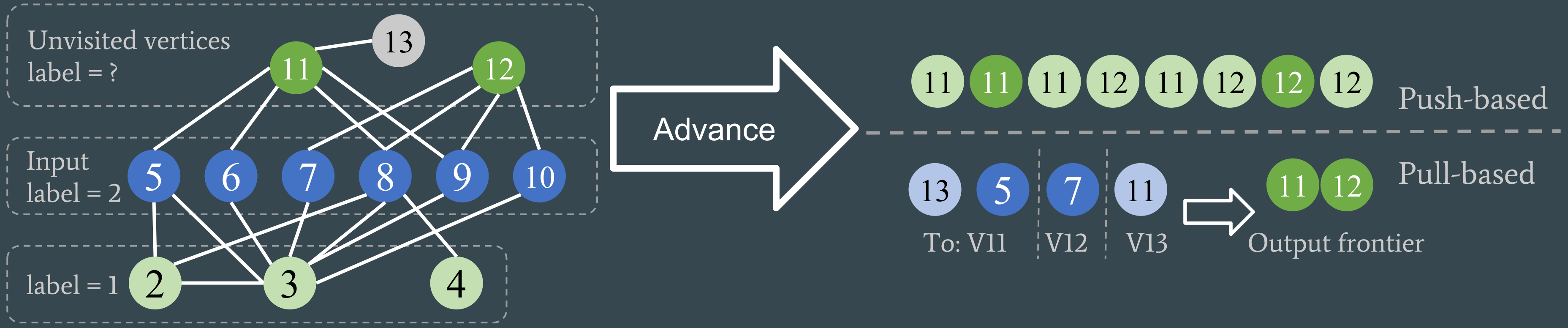
Optimizations: Pull vs. push traversal

P: From many to very few (v5,6,7,8,9,10 -> v11, 12)

S: Pull vs. push operations (frontier generation)

- Automatic selection of advance direction based on ratio of undiscovered vertices

First appeared in DO-BFS [5], now available to other primitives



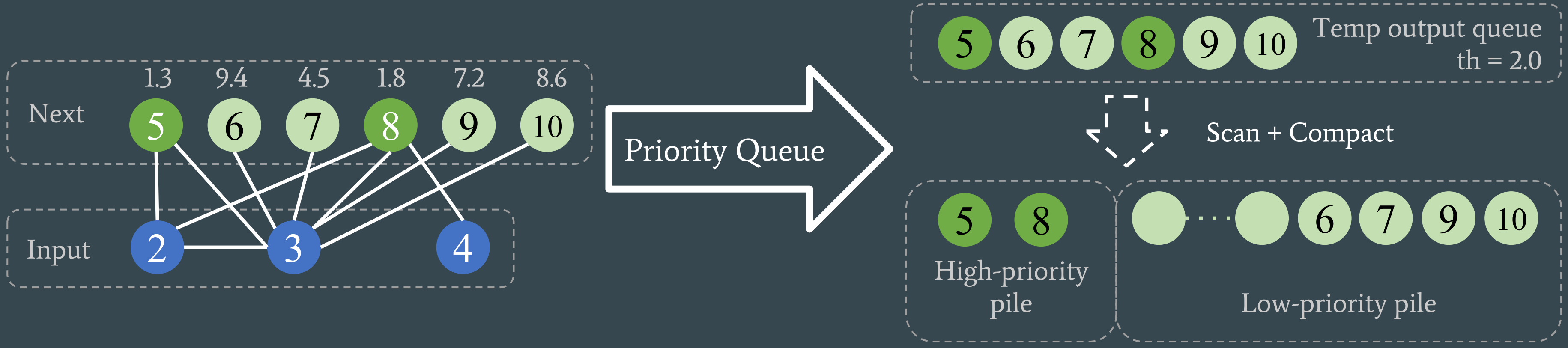
Optimizations: Priority queue

P: A lot of redundant work in SSSP-like primitives

S: Priority queue (frontier reorganization)

- Expand high-priority vertices first

First appeared in SSSP[3], now available to other primitives



Idea: Multiple GPUs

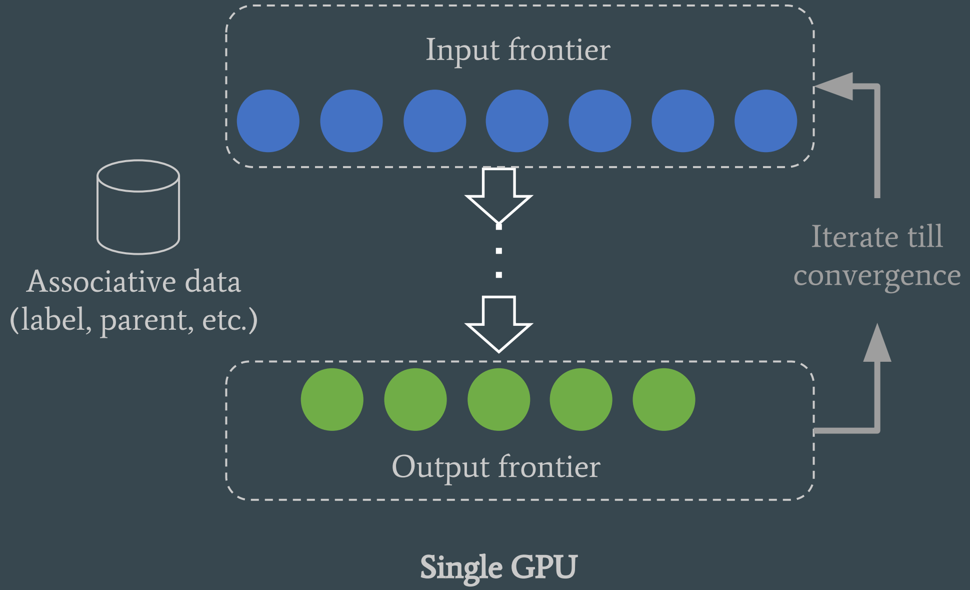
P: Single GPU is not big and fast enough
S: use multiple GPUs
-> larger combined memory space and computing power

P: Multi-GPU program is very difficult to develop and optimize
S: Make algorithm-independent parts into a multi-GPU framework
-> Hide implementation details, and save user's valuable time

P: Single GPU primitives can’t run on multi-GPU
S: Partition the graph, renumber the vertices in individual sub-graphs and do data exchange between super steps
-> Primitives can run on multi-GPUs as it is on single GPU

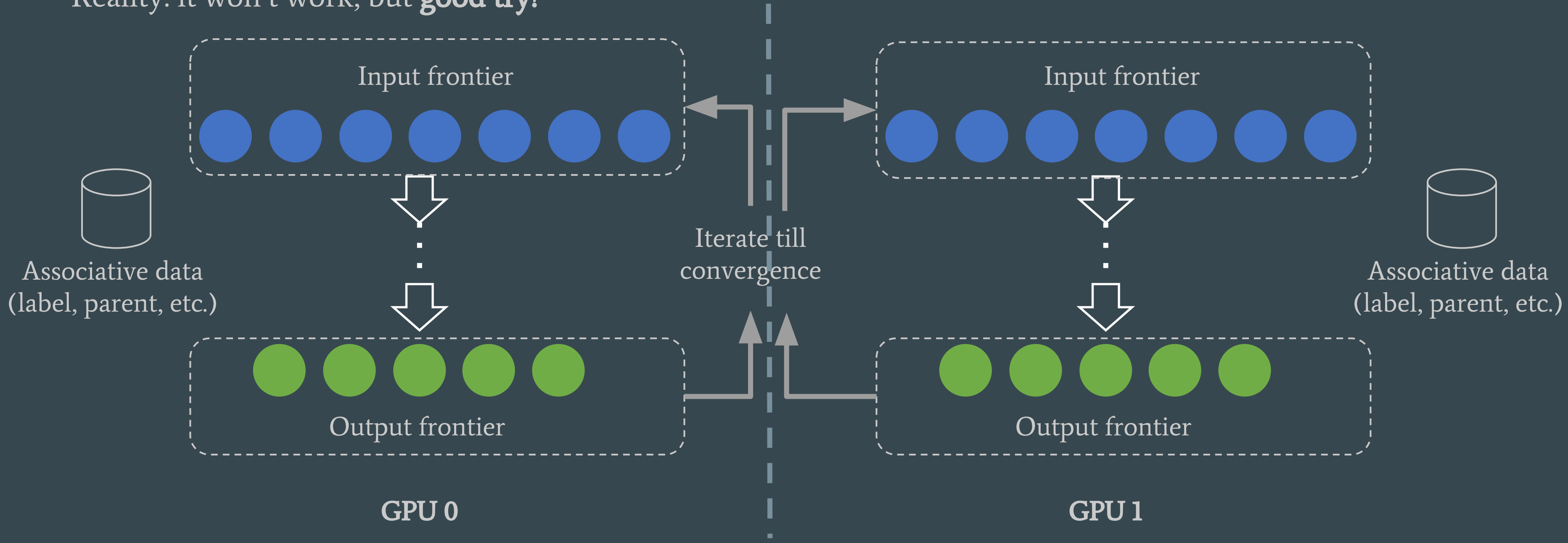
Multi-GPU Framework (for programmers)

Recap: Gunrock on single GPU



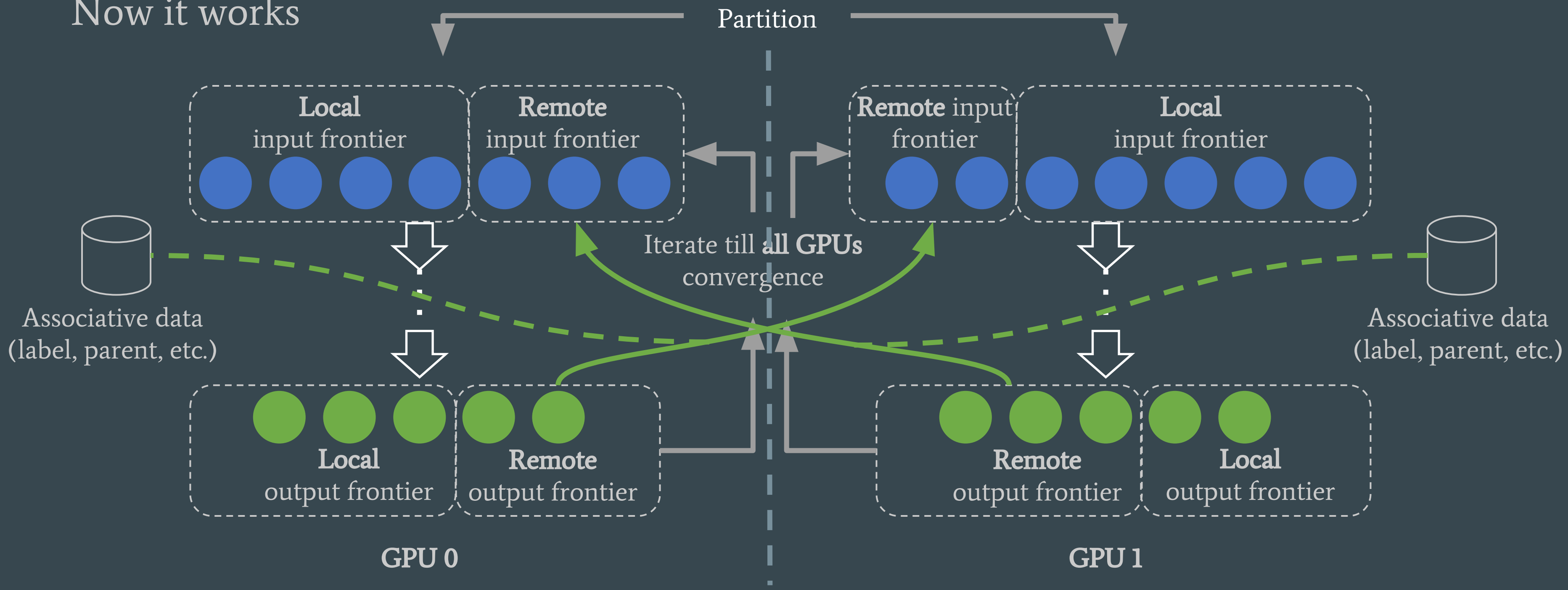
Multi-GPU Framework (for programmers)

Dream: just duplicate the single GPU implementation
Reality: it won't work, but **good try!**

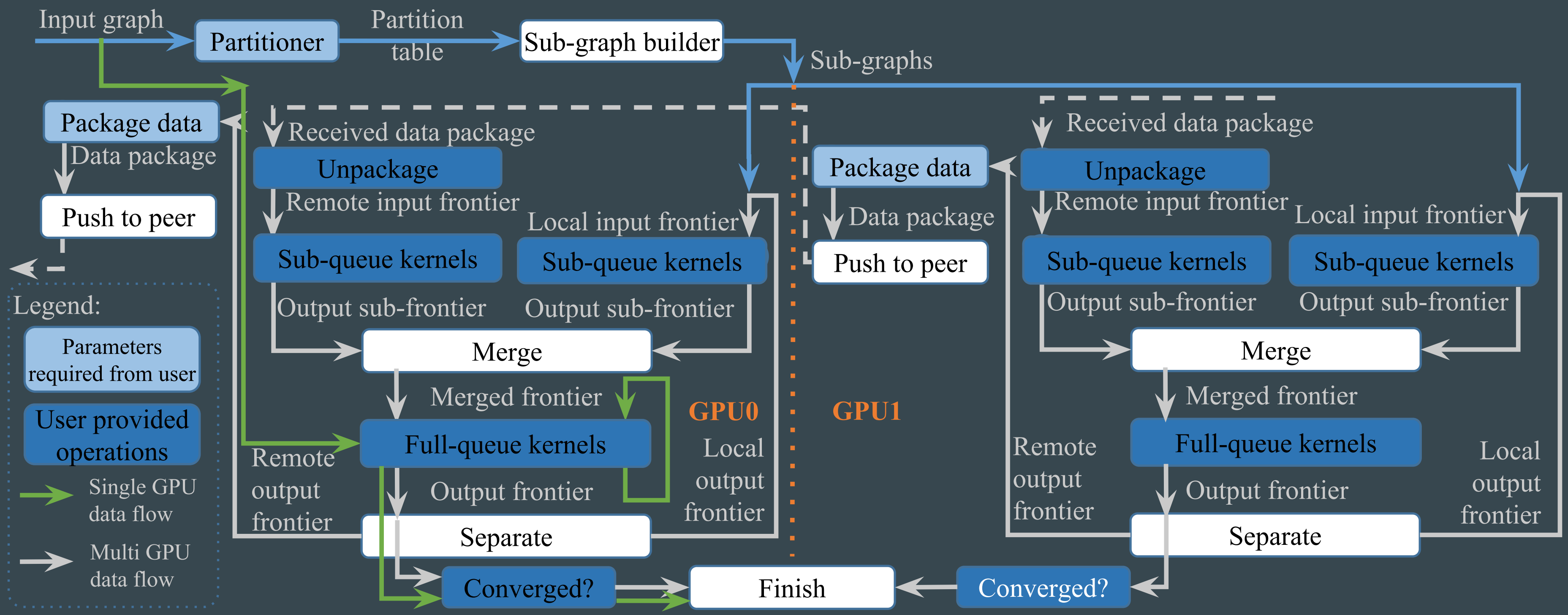


Multi-GPU Framework (for programmers)

Now it works



Multi-GPU Framework (for programmers)



Multi-GPU Framework (for end users)

```
gunrock_executable input_graph --device=0,1,2,3 other_parameters
```

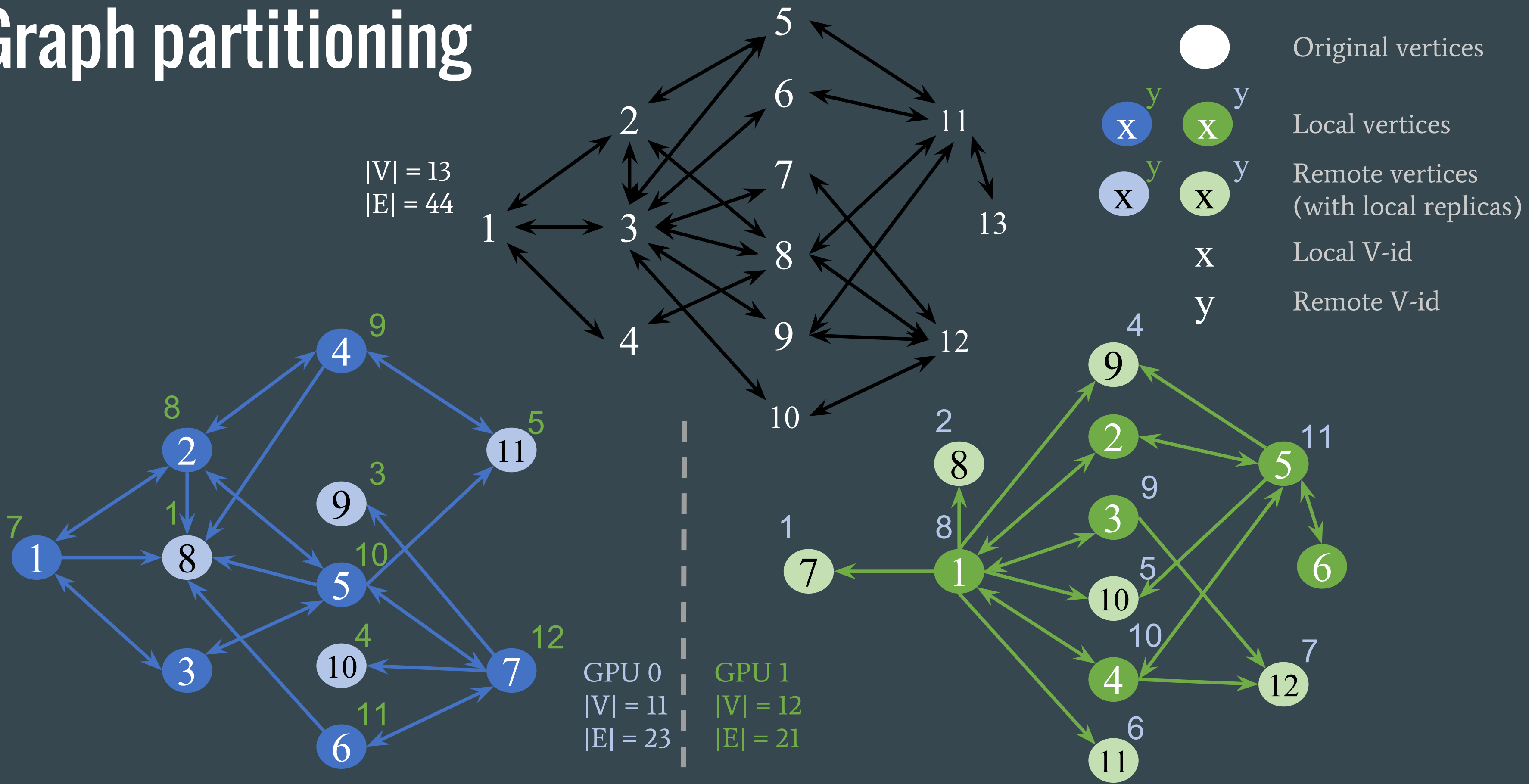
Graph partitioning

- Distribute the vertices
- Host edges on their sources' host GPU
- Duplicate remote adjacent vertices locally
- Renumber vertices on each GPU

-> Primitives no need to know peer GPUs
-> Local and remote vertices are separated
-> Partitioning algorithm not fixed

P: Still looking for good partitioning algorithm /scheme

Graph partitioning



Optimizations: Multi-GPU Support & Memory Allocation

P: Serialized GPU operation dispatch and execution

S: Multi CPU threads and multiple GPU streams

≥1 CPU threads with multiple GPU streams to control each individual GPUs

-> overlap computation and transmission

-> avoid false dependency

P: Memory requirement only known after advance / filter

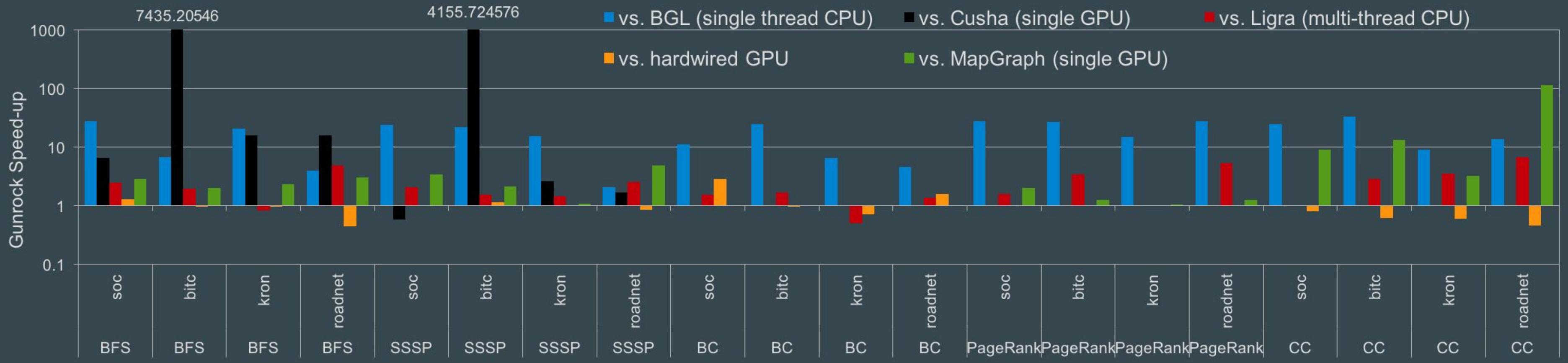
S: Just-enough memory allocation

check space requirement before every possible overflow

-> minimize memory usage

-> can be turned off for performance, if requirements are known (e.g. from previous runs on similar graphs)

Results: Single GPU Gunrock vs. Others



* 17x (avg.) vs. BGL [6], a single thread CPU graph library;
* 2.4x (avg.) vs. Ligra [8], a multi-thread CPU graph library;
* beats Cusha [7] with bitcoin dataset;
* comparable with hardwired GPU implementations,
  some speed-up from applying optimizations across primitives;
* 10x (avg.) vs. MapGraph [9], especially for CC

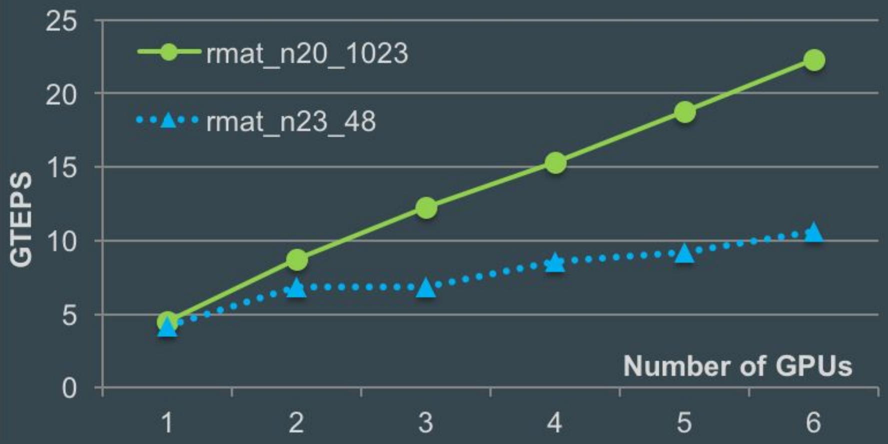
Results: Multi-GPU Gunrock vs. Others (BFS)

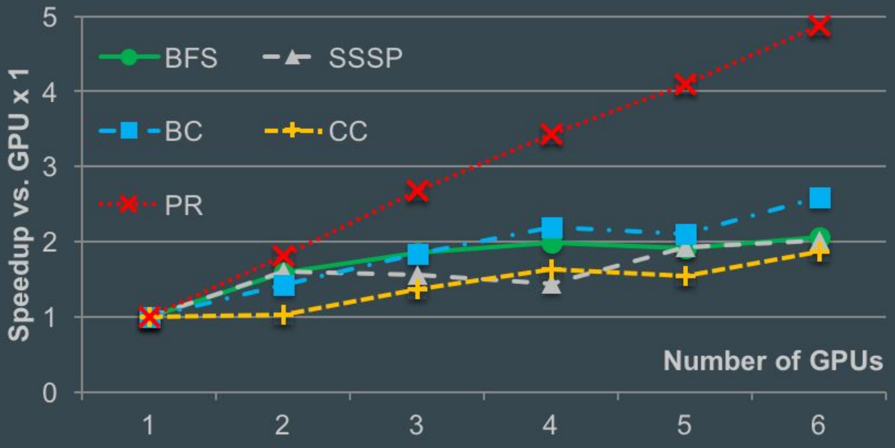
	Ref.	Ref. hardware	Ref. performance	Our hardware	Our performance
rmat_n20_128	Merrill et al. [4]	4x Tesla C2050	8.3 GTEPS	4x Tesla K40	11.2 GTEPS
rmat_n20_16	Zhong et al. [10]	4x Tesla C2050	15.4 ms	4x Tesla K40	9.29 ms
peak performance	Fu et al. [9]	16x Tesla K20	15 GTEPS	6x Tesla K40	22.3 GTEPS
peak performance	Fu et al. [11]	16x Tesla K20	29.1 GTEPS	6x Tesla K40	22.3 GTEPS

* ~ 35% faster than Merrill et al.'s results. Their results on > 3-year-old hardware are impressive, though only customized to BFS.
* > 50% faster than Medusa (Zhong et al.), another programmable graph framework.
* 6 GPU peak performance comparable to MapGraph (Fu et al.) using 16 GPU cluster

Results: Multi-GPU Scaling

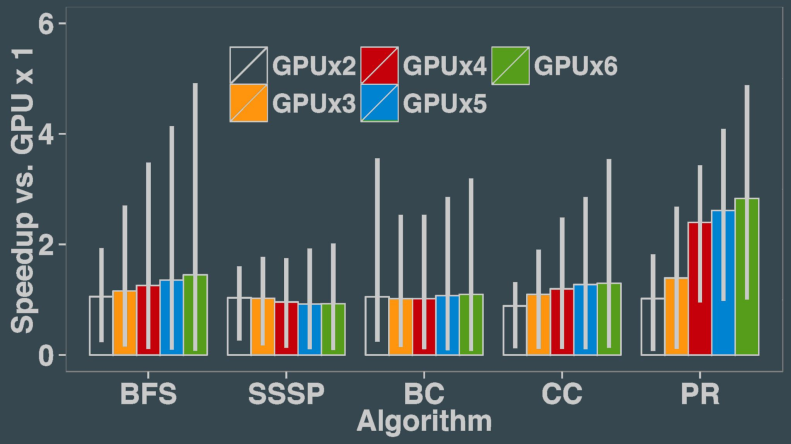
* Traversed edges per sec (TEPS) for BFS→
* Strong scaling on rmat_n22_48 ↓
* Weak scaling on R-MAT graphs (scale 48, each GPU hosting ~180M edges) ↘



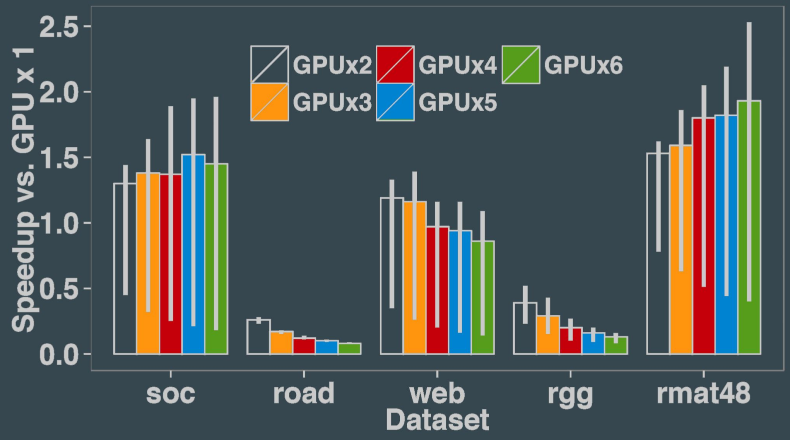


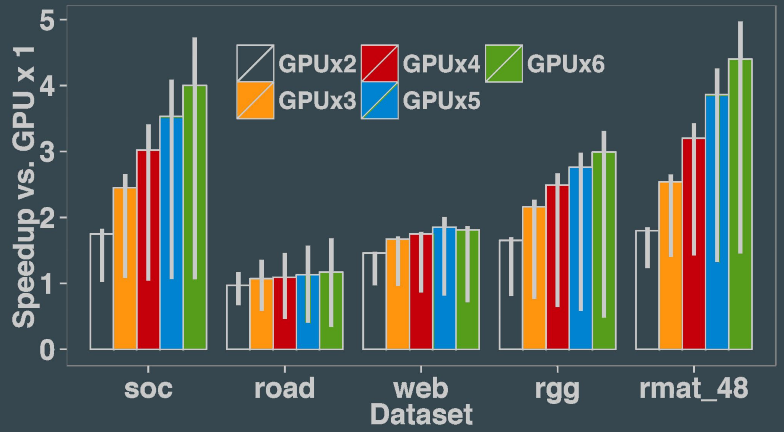
Things that we can improve on

* Partitioning
* Inter-iteration overhead
* Long tail / small frontier issue



Speedup of 5 algorithms (→), BFS (↙) and PR (↘)





Current Status

Open source, available @ http://gunrock.github.io/

It has over 10 graph primitives
* traversal-based, node-ranking, global (CC, MST)
* LOC ≤ 10 to use a primitive
* LOC ≤ 300 to program a new primitive
* Good balance between performance and programmability

Multi-GPU framework under major revision
* use circular-queue for better scheduling and smaller overhead
* extendable onto multi-node usage

More graph primitives are coming
* graph coloring, maximum independent set, community detection, subgraph matching

Future Work

* Multi-node support with NVLink
* Performance analysis and optimization
* Graph BLAS
* Asynchronized graph algorithms
* Fixed partitioning / 2D partitioning
* Global, neighborhood, and sampling operations
* More graph primitives
* Dynamic graphs
* Kernel fusion
* ...

Acknowledgment

The Gunrock team

Onu Technology and Royal Caliber team

Erich Elsen, Vishal Vaidyananthan, Oded Green and others

For their discussion on library development and dataset generating code

All code contributors to the Gunrock library

NVIDIA

For hardware support, GPU cluster access, and all other supports and discussions

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* DARPA STTR award D14PC00023

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Questions?

Q: How can I find Gunrock?
A: http://gunrock.github.io/

Q: Is it free and open?
A: Absolutely (under Apache License v2.0)

Q: Papers, slides, etc.?
A: https://github.com/gunrock/gunrock#publications

Q: Requirements?
A: CUDA ≥ 5.5, GPU compute capability ≥ 3.0, Linux || Mac OS

Q: Language?
A: C/C++, with a simple wrapper connects to Python

Q: ... (continue)

Example python interface - breadth-first search

```
from ctypes import *
### load gunrock shared library - libgunrock
gunrock = cdll.LoadLibrary('../../build/lib/libgunrock.so')

### read in input CSR arrays from files
row_list = [int(x.strip()) for x in open('toy_graph/row.txt')]
col_list = [int(x.strip()) for x in open('toy_graph/col.txt')]

### convert CSR graph inputs for gunrock input
row = pointer((c_int * len(row_list))(*row_list))
col = pointer((c_int * len(col_list))(*col_list))
nodes = len(row_list) - 1
edges = len(col_list)

### output array
labels = pointer((c_int * nodes)())

### call gunrock function on device
gunrock.bfs(labels, nodes, edges, row, col, 0)

### sample results
print ' bfs labels (depth):',
for idx in range(nodes): print labels[0][idx],
```