Extreme-scale Graph Analysis on Blue Waters

2016 Blue Waters Symposium

George M. Slota[1,2],
Siva Rajamanickam[1], Kamesh Madduri[2], Karen Devine[1]

[1]Sandia National Laboratories[a]
[2]The Pennsylvania State University
www.gmslota.com gslota@psu.edu

13 June 2016

[a]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

About Me

Past:

- PhD in Computer Science & Engineering from Penn State in 2016
- Supported by *Blue Waters Fellowship* in 2014-2015
- Intern at Sandia National Labs from 2013-2016

Present:

- Staff at Sandia National Labs

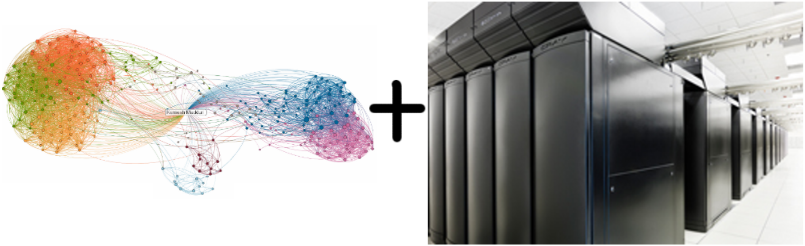
Future:

- Assistant Professor at Rensselaer Polytechnic Institute

Hi

What?

Graph Analytics and HPC



Or, given modern extreme-scale graph-structured datasets (web crawls, brain graphs, human interaction networks) and modern high performance computing systems (Blue Waters), how can we develop a generalized approach to efficiently study such datasets on such systems?

Why?

Why do want to study these large graphs?

Human Interaction Graphs:

- Finding hidden communities, individuals, malicious actors
- Observe how information and knowledge propagates

Brain Graphs:

- Study the topological properties of neural connections
- Finding latent computational substructures, similarities to other information processing systems

Web Crawls:

- Identifying trustworthy/important sites
- Spam networks, untrustworthy sites

Prior Approaches

Can we use them to analyze large graphs on HPC?

- Some limited by shared-memory and/or specialized hardware
- Some run in distributed memory but graph scale is still limited
- Others, graph scale isn't limiting factor but performance can be

Graph analytics on HPC

So why do we want to run graph analytics on HPC?

- Scalability for analytic performance and graph size
  - Efficient implementations should be limited only by distributed memory capacity
  - Graph500.org - demonstration of performance achievable for irregular computations through breadth-first search (BFS)
- Relative availability of access in academic/research communities
  - Private clusters of various scales, shared supercomputers
  - Access for domain experts, those using analytics on real-world graphs

Can we create an approach that is as simple to use as the aforementioned frameworks but runs on common cluster hardware and gives state-of-the-art performance?

Challenges

Scale

- This work considers "extreme-scale" graphs – billion+ vertices and up to trillion+ edges
- Processing these graphs requires at least hundreds to thousands of compute nodes or tens of thousands of cores
- Graph analytic algorithms are generally memory-bound instead of compute-bound; in the distributed space, this results in a ratio of communication versus computation that increases with core/node count

Complexity

- Real-world extreme-scale graphs have similar characteristics: small-world nature with skewed degree distributions
- Small-world graphs are difficult to partition for distributed computation or to optimize in terms of cache due to "too much locality"
- Skewed degree distributions make efficient parallelization and load balance difficult to achieve
- Multiple levels of cache/memory and increasing reliance on wide parallelism for modern HPC systems compounds the above challenges

Approach

Identifying Communication Patterns

Observation: many iterative graph algorithms have similar communication patterns

- (Vanilla) *BFS-like*: frontier expansion, information *pushed* from vertices to adjacencies, volume of data exchanged is **variable** or fixed across iterations
- (Vanilla) *PageRank-like*: information *pulled* from incoming arcs, either **fixed** or variable communication pattern in every iteration

We develop optimized skeleton code for these two (or four) patterns, and can use it to fill in analytic-specific details

Analytics Fitting these Patterns

Some examples

BFS-like:

- **SCC**: Strongly connected components
- **WCC**: Weakly connected components
- **K-Core**: Iterative approach to find approximate vertex coreness
- **Harmonic Centrality**: Routine for calculating harmonic centrality value of any given vertex

PageRank-like:

- **PageRank**: Well-known centrality algorithm
- **Label Propagation**: Community detection algorithm
- **Color Propagation**: Connectivity algorithm for CC, WCC, SCC

Implementation Considerations

Choices, choices, choices ...

Tradeoffs (ease of implementation vs. scalability):

- **1D** (vertex-based) vs. 2D (edge-based) partitioning and graph layout
- **Bulk-synchronous** vs. asynchronous communication
- Programming language and parallel programming model
  - High-level language (e.g., Scala) vs. **C/C++**
  - High-level model (e.g., Spark) vs. MPI-only vs. **MPI+OpenMP**

Other considerations:

- In-memory graph representation
  - **Vanilla CRS-like** vs. compressed (e.g., with RLE) adjacencies
- Partitioning strategy (with 1D layout)
  - **Vertex-balanced, Edge-balanced, Random** vs. Explicit partitioning

Performance Results

Experimental Setup

Test systems, Graphs

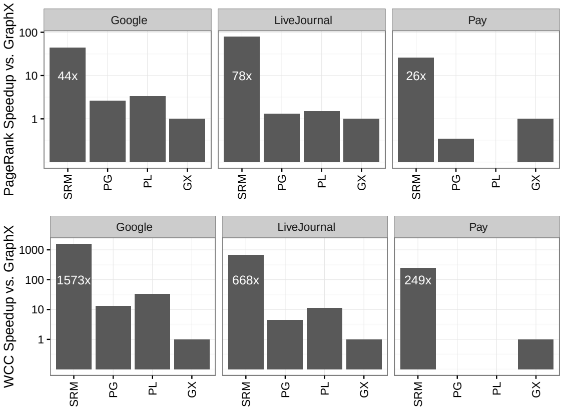
- *Blue Waters*: dual-socket AMD Interlagos 6276, 16 cores, 64 GB memory
- *Compton* cluster: dual-socket Intel Xeon E5-2670, 16 cores, 64 GB memory

Graph	n	m	D_{avg}	Source
Web Crawl (WC)	3.6 B	129 B	36	[?]
R-MAT	3.6 B	129 B	36	[?]
Rand-ER	3.6 B	129 B	36	Erdös-Rényi
R-MAT	2^{25}-2^{36}	2^{29}-2^{40}	16-64	[?]
Rand-ER	2^{25}-2^{36}	2^{29}-2^{40}	16-64	Erdös-Rényi
Pay	39 M	623 M	16	[?]
LiveJournal	4.8 M	69 M	14	[?]
Google	875 K	5.1M	5.8	[?]

Comparison to Distributed Graph Frameworks

Our approach vs. GraphX, PowerGraph, PowerLyra

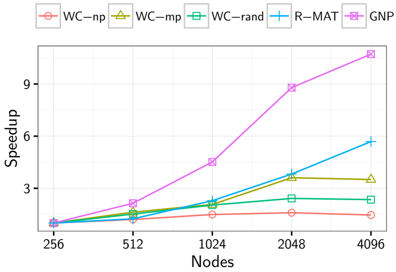
- Compared GraphX (GX), PowerGraph (PG), and PowerLyra (PL) on 16 nodes of *Compton* to our code (SRM)
- About 38× faster on average for PageRank (top), 201× faster for WCC (bottom) against distributed memory frameworks

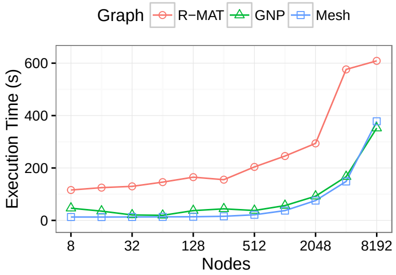


Weak and Strong Scaling

Label propagation-based analytics

- Strong scaling on *Blue Waters* for label propagation community detection with WC and random graphs
- Weak scaling on *Blue Waters* for label propagation-based algorithm on random graphs and meshes





Performance on WC with 256 node of Blue Waters

How can we improve?

- Perf. units are similar to GTEPS (Giga Traversed Edges Per Second): $\frac{m * n_{\text{iter}}}{t \times 10^9}$

Analytic	Time (s)	Perf.	Our evaluation
PageRank	87	29.6	🙂
Label Propagation	367	3.5	😐
WCC	63	2.0	🙁
Harmonic Centrality	46	2.8	🙁
K-core	363	9.6	😐
Largest SCC	108	2.4	🙁
Overall	1034	7.6	😐
Graph500 (estimate)		119.2	🙂

Possible Future Extensions

- Processing **quadrillion-edge** (petascale) graphs?
- **10x** performance improvement by next year? Direction optimization, asynchronous communication, graph compression, other partitioning strategies
- Identify and implement additional analytics that fit push/pull/fixed/variable communication patterns
- Open-source code
  - Contact gslota@psu.edu for current version

Acknowledgments

- **Sandia and FASTMATH**
  - This research is supported by NSF grants CCF-1439057 and the DOE Office of Science through the FASTMath SciDAC Institute. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energys National Nuclear Security Administration under contract DE-AC04-94AL85000.
- **Blue Waters Fellowship**
  - This research is part of the Blue Waters sustained petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070, ACI-1238993, and ACI-1444747) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana Champaign and its National Center for Supercomputing Applications.
- **Kamesh Madduri's CAREER Award**
  - This research was also supported by NSF grant ACI-1253881.

Conclusions and Thanks!

- Graphs are ubiquitous, massive, and complex: scalability and efficiency are important considerations for real-world analytics
- We identified and optimized several distinct communication patterns that fit large classes of graph algorithms
- Implemented several algorithms fitting these patterns and demonstrated scalability up to 131k cores of *Blue Waters*
- Demonstrated 26-1573× speedup vs. GraphX on 256 cores of *Compton*

Thank you! Questions? gslota@psu.edu, www.gmslota.com

Bibliography I