Irregular Graph Algorithms on Modern Multicore, Manycore, and Distributed Processing Systems

Doctoral Defense

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Defense Overview

- Motivation
- Summaries of Research
- Manycore graph processing
- Distributed graph processing
- Conclusions

Motivation

- Graph analysis is key for the study of biological, chemical, social, and other networks
- Real-world graphs are big, irregular, complex
  - Graph analytics is one of DARPA's 23 toughest mathematical challenges
  - Facebook graph: 1.6B people, 500B friendships
  - Brain graph: 100B neurons, 1,000T synaptic connections
  - Skewed degree distributions, small-world nature make parallelization difficult
- Modern computational systems are also big and complex
  - Multiple levels of parallelism, memory hierarchy, configurations
  - Heterogeneous – host, GPU, coprocessors (Xeon Phi)
  - Optimization – account for socket-level, node-level, and distributed

Motivation
Goals of Research

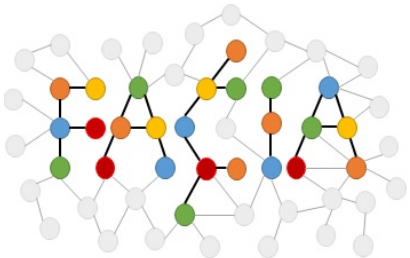
- How do we design parallel graph algorithms for computational efficiency under all of the aforementioned difficulties?
- What algorithmic traits are common to various irregular graph algorithms that we can optimize for?
- How do we store/organize and access graphs and associated data efficiently in shared and distributed memory?

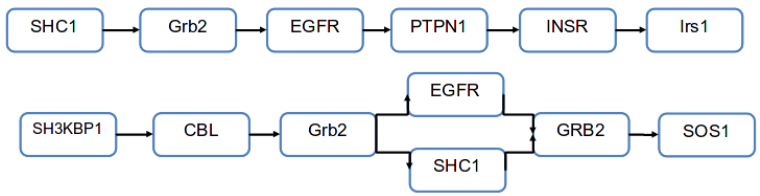
Research Summaries

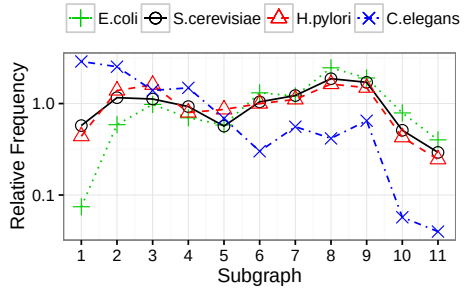
Summaries of Research: Color-coding, Connectivity, Partitioning, In-memory Layout

Topic 1: Summary of Color-coding

FASCIA subgraph enumeration and FASTPATH min-weight path finding







Overview:

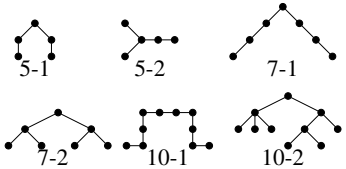
- Subgraph Counting: Find and count the number of occurrences of some input template in a larger graph (∼NP-complete)
- Minimum Weight Path Finding: In an edge-weighted network, find the k length simple path with the least sum of weights (NP-hard)
- Applications: Motif/anti-motif finding, network classification/clustering, network alignment, signaling pathways detection

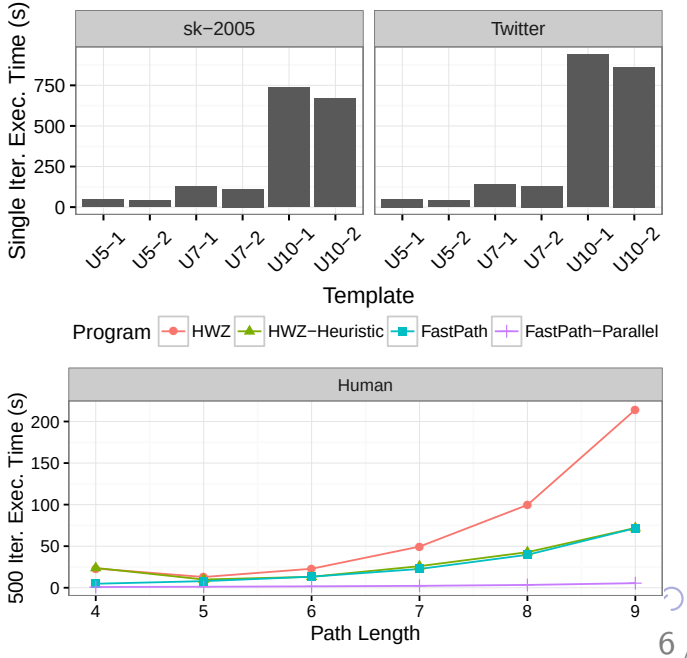
Contributions:

- Highly optimized implementation of the color-coding technique [Alon et al., 2008] for tree-structured subgraph counting; up to five orders-of-magnitude faster than prior work
- Extended baseline code for minimum weight path finding

Software:

- **Fascia**: Fast Approximate Subgraph Counting
- **FastPath**: Fast Minimum Weight Path Finding





Topic 2: Summary of Graph Connectivity Research

Multistep and BiCC Algorithms

Overview:

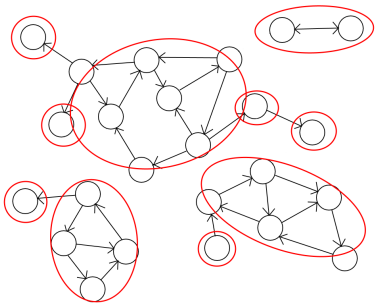
- Connectivity and Weak Connectivity: Find maximal components of a graph where a path exists between all vertices (ignore directivity of edges for weak)
- Strong Connectivity: Find maximal components of a directed graph where each vertex in a component has a path to every other vertex in the component
- Biconnectivity: Find maximal components of an undirected graph where the removal of any single vertex would not disconnect the component
- Applications: Social network analysis, scientific computing, network resilience analysis

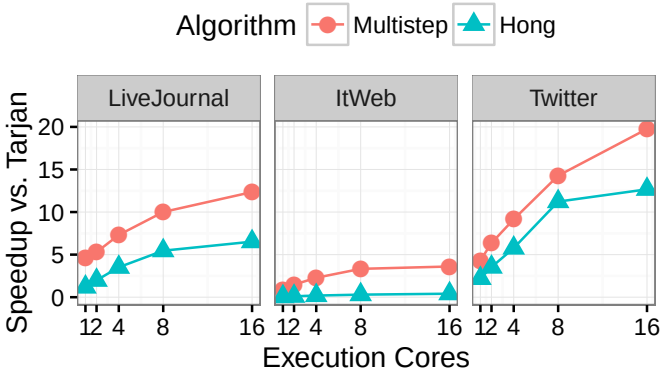
Contributions:

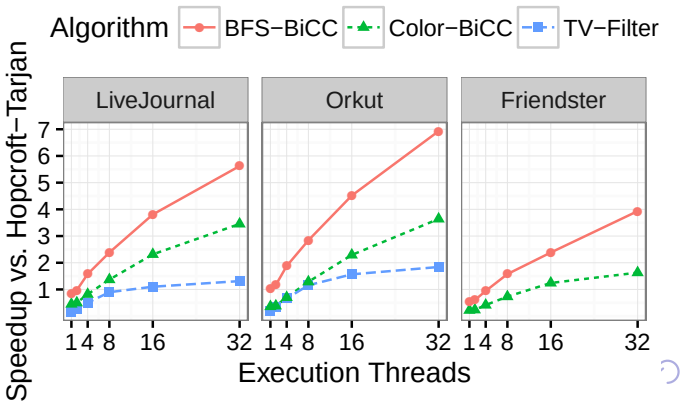
- New parallel algorithms for connected (CC), weakly connected (WCC), strongly connected (SCC), and biconnected components (BiCC)
- Identified several shared-memory optimizations (multi-level queues, minimize synchronizations, efficient algorithm design)
- Demonstrated over **2-7x average speedup** to state-of-the-art

Software:

- **Multistep**: Parallel methods for CC, WCC, and SCC
- **BiCC**: Open-source implementations available

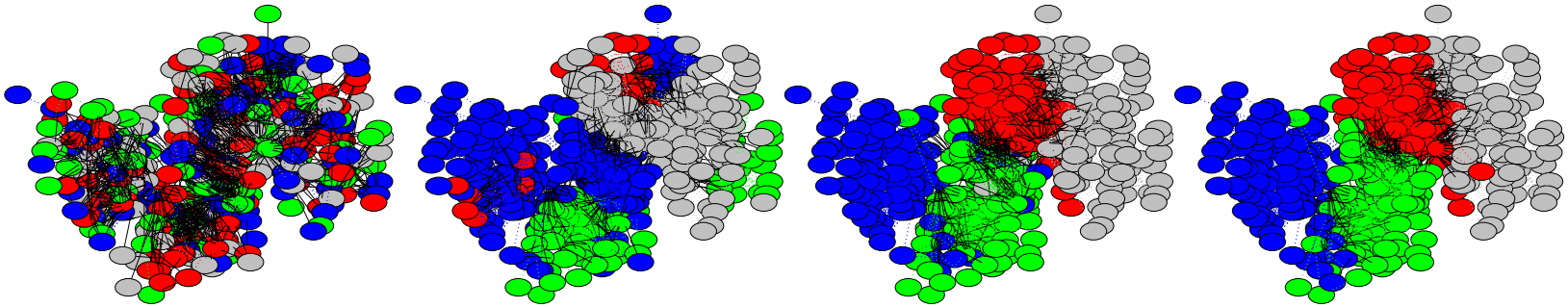






Topic 3: Summary of Graph Partitioning Research

PuLP: Partitioning Using Label Propagation



Overview:

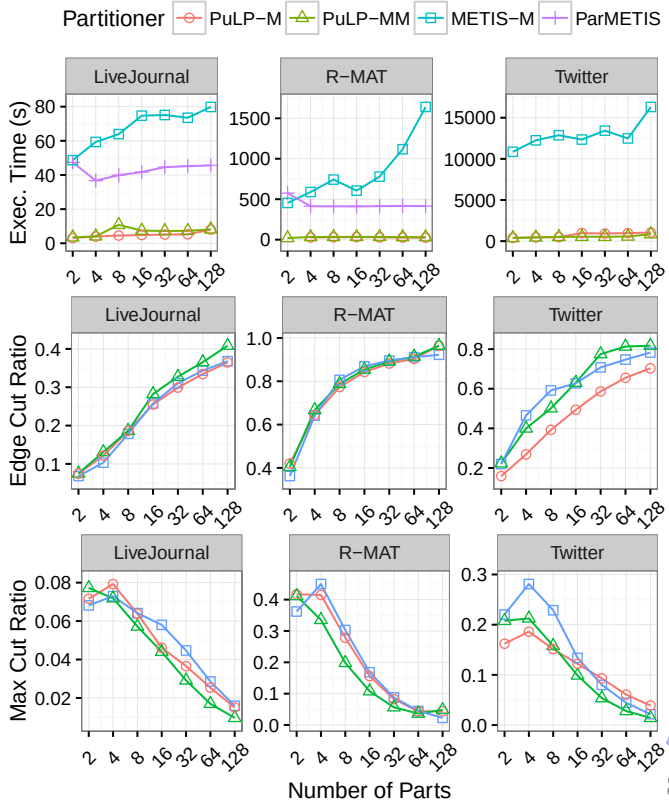
- Graph Partitioning: Separate a graph into k balanced *parts* with minimal inter-part edges (edge cut) for distributed computations (NP-complete problem)
- Label Propagation: Efficient (linear work) and scalable (naïvelyparallel) community detection and clustering algorithm [Raghavan et al., 2007]

Contributions:

- Parallel (OpenMP and soon MPI) multi-constraint multi-objective graph partitioning method for small-world networks that exploits Label Propagation community detection algorithm
- On suite of test graphs, **14.5× faster** and **38× less memory** on average relative to (Par)METIS with comparable or better cut quality
- Distributed version scales to **hundred billion edge networks**

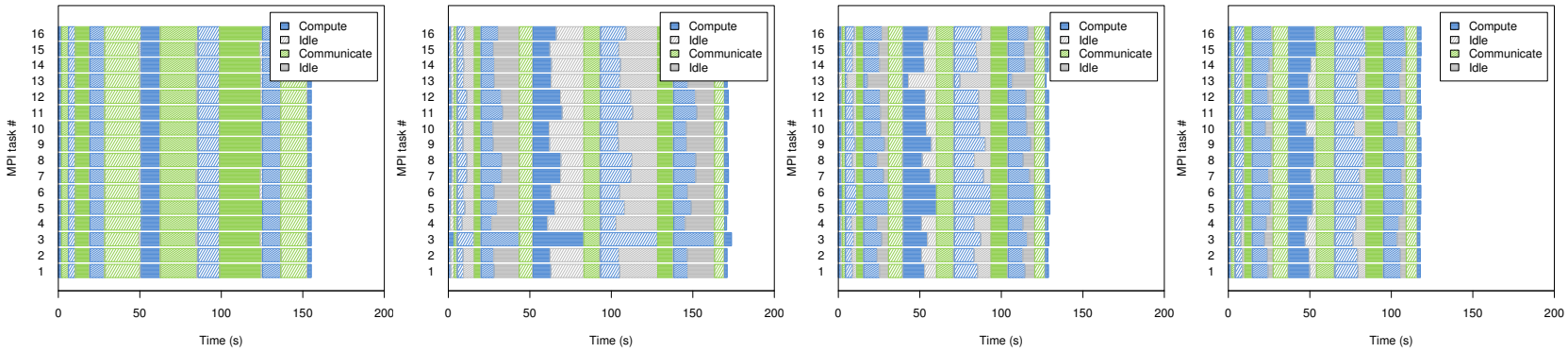
Software:

- **PuLP**: Interface now available in **Zoltan2** package of **Trilinos**



Topic 4: Summary of Distributed Layout Research

DGL: Distributed Graph Layout



Overview:

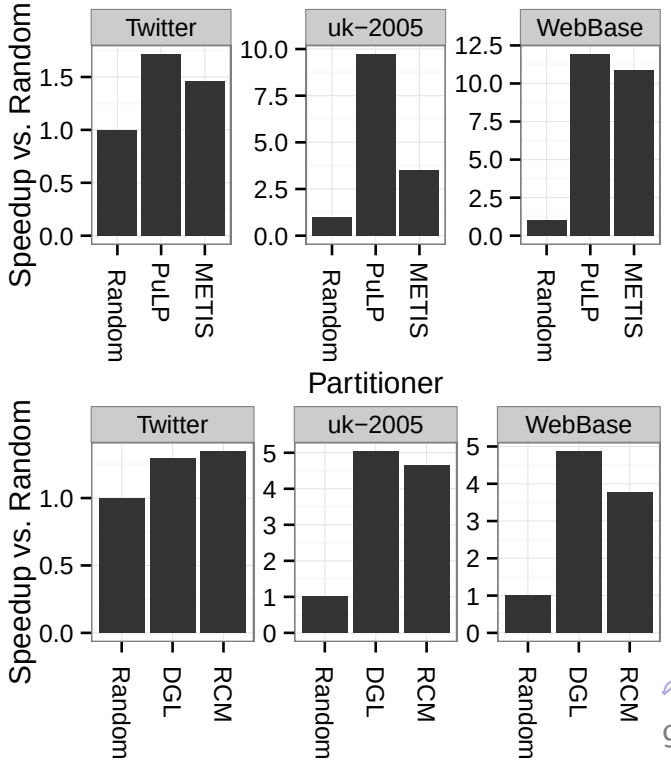
- Graph Layout: How to store a graph in distributed memory in terms of graph partitioning and intra-node vertex ordering

Contributions:

- Methodology for distributed in-memory layout for graphs
- Uses PuLP for partitioning and novel BFS-based ordering scheme
- Speedups for distributed computation (**up to 4x**) and communication (**up to 12x**) relative to naive methods for running PageRank with PuLP and DGL ordering
- Both PuLP and DGL ordering are faster to compute than other methods

Software:

- **DGL**: Distributed Graph Layout with PuLP and DGL ordering



Graph Algorithms for Manycore

Part 1: **Manycore graph algorithms** – abstraction for wide parallelism

Motivating questions for this work

- **Q**: What are some **common abstractions** that we can use to develop parallel graph algorithms for manycores?
- **Q**: What **key optimization strategies** can we identify to design new parallel graph algorithms for manycores?
- **Q**: Is it possible to develop **performance-portable implementations** of graph algorithms using advanced **libraries and frameworks** using the above optimizations and abstractions?

Contributions

- **Q**: **Common abstractions** for manycores?
  - We use array-based data structures, express computation in the form of nested loops.
- **Q**: **Key optimization strategies**
  - We improve load balance by manual loop collapse, coalesce memory access, and use collective operations when possible.
- **Q**: **Performance-portable implementations** of graph algorithms using advanced **libraries and frameworks**?
  - We use Kokkos [Carter Edwards et al., 2014].
- We compare high-level implementations using new framework to hand-optimized code + vary graph computations + vary graph inputs + vary manycore platform.

Background
GPU and Xeon Phi microarchitecture

- **GPU**
  - Multiprocessors (up to about 15/GPU)
  - Multiple groups of stream processors per MP (12×16)
  - *Warps* of threads all execute SIMT on single group of stream processors (32 threads/warp, two cycles per instruction)
  - Irregular computation (high degree verts, if/else, etc.) can result in most threads in warp doing NOOPs
- **Xeon Phi (MIC)**
  - Many simple (Pentium 4) cores, 57-61
  - 4 threads per core, need at least 2 threads/core for OPs on each cycle
  - Highly vectorized (512 bit width) - difficult for irregular computations to exploit

Background
Kokkos and GPU microarchitecture

- Kokkos
  - Developed as back-end for portable scientific computing
  - Polymorphic multi-dimensional arrays for varying access patterns
  - Thread parallel execution for fine-grained parallelism
- Kokkos model - performance portable programming to multi/manycores
  - Thread team - multiple warps on same multiprocessor, but all still SIMT for GPU
  - Thread league - multiple thread teams, over all teams all work is performed
  - Work statically partitioned to teams before parallel code is called

- **Observation**: many (synchronous) graph algorithms follow a tri-nested loop structure
  - Optimize for this general algorithmic template
  - Transform structure for more parallelism

```
1:  Initialize temp/result arrays A_t[1..n], 1 ≤ t ≤ l.        ▷ l = O(1)
2:  Initialize S_1[1..n].
3:  for i = 1 to niter do                                      ▷ niter = O(log n)
4:      Initialize S_{i+1}[1..n].                              ▷ Σ_i |S_i| = O(m)
5:      for j = 1 to |S_i| do                                  ▷ |S_i| = O(n)
6:          u ← S_i[j]
7:          Read/update A_t[u], 1 ≤ t ≤ l.
8:          for k = 1 to |E[u]| do                             ▷ |E[u]| = O(n)
9:              v ← E[u][k]
10:             Read/update A_t[v].
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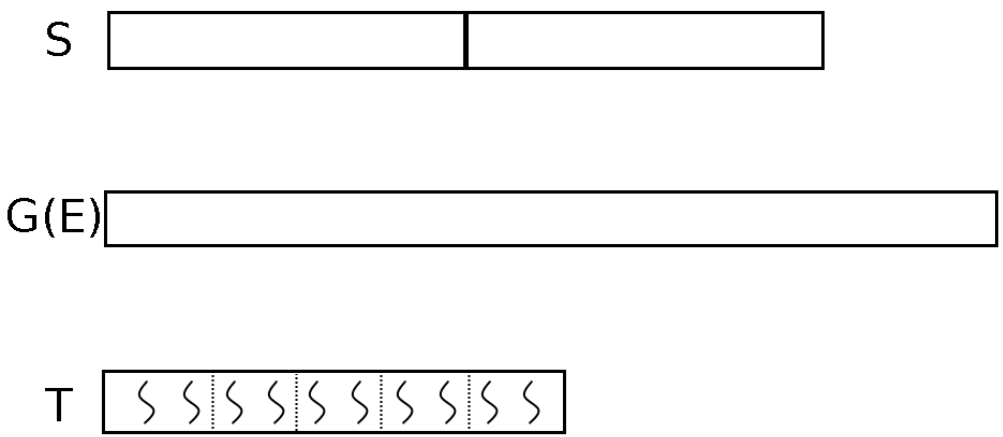
Graph Algorithms for Manycore
Parallelization strategies

- Baseline parallelization



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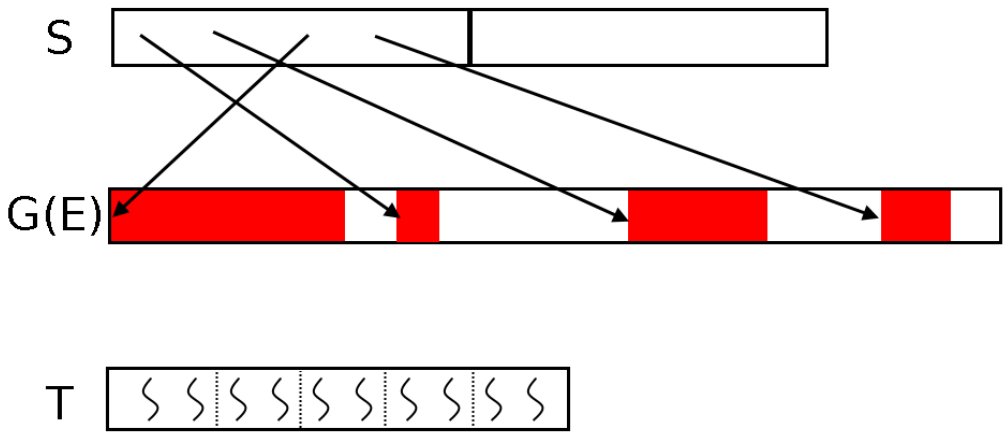

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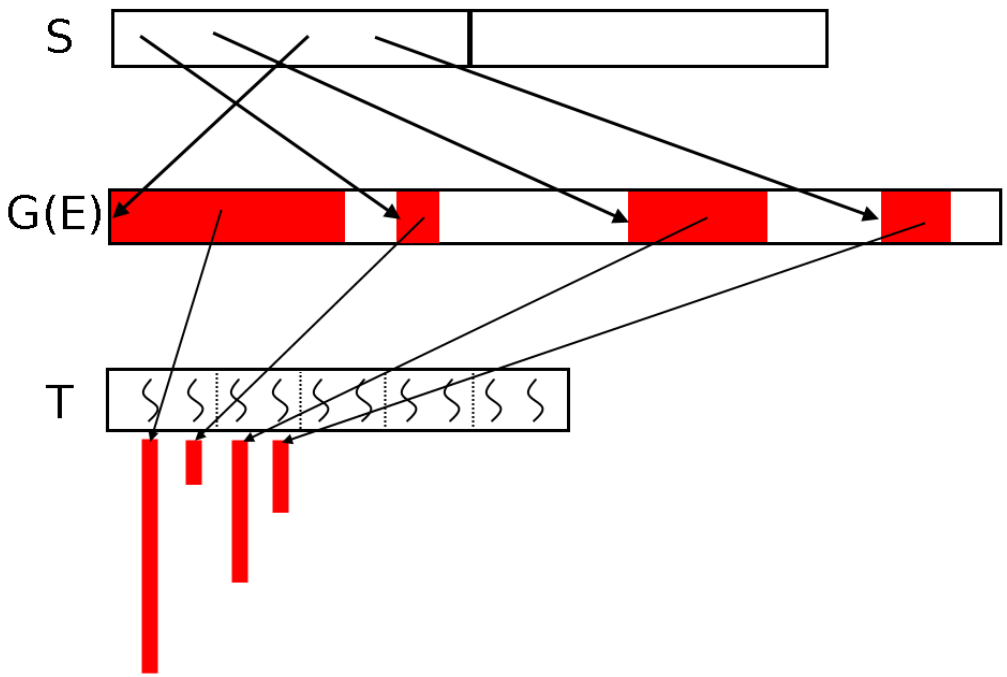

Graph Algorithms for Manycore
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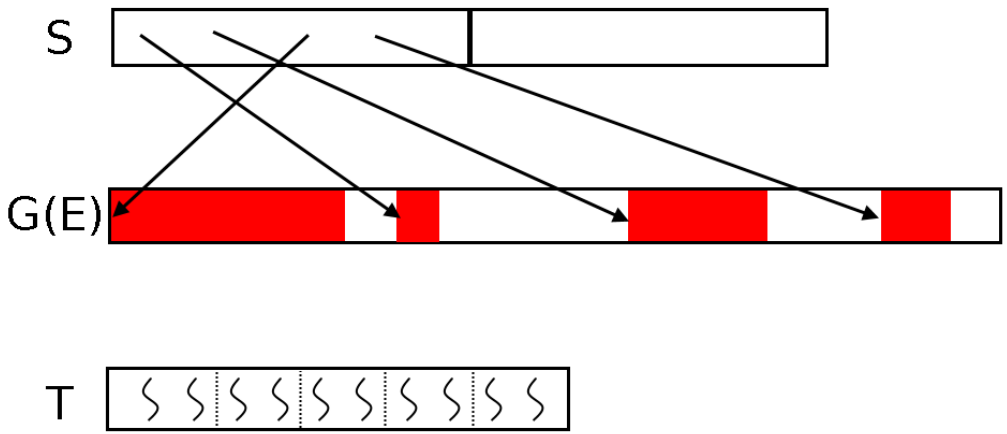
- Baseline parallelization
- Hierarchical expansion (e.g. [Hong et al., 2011])



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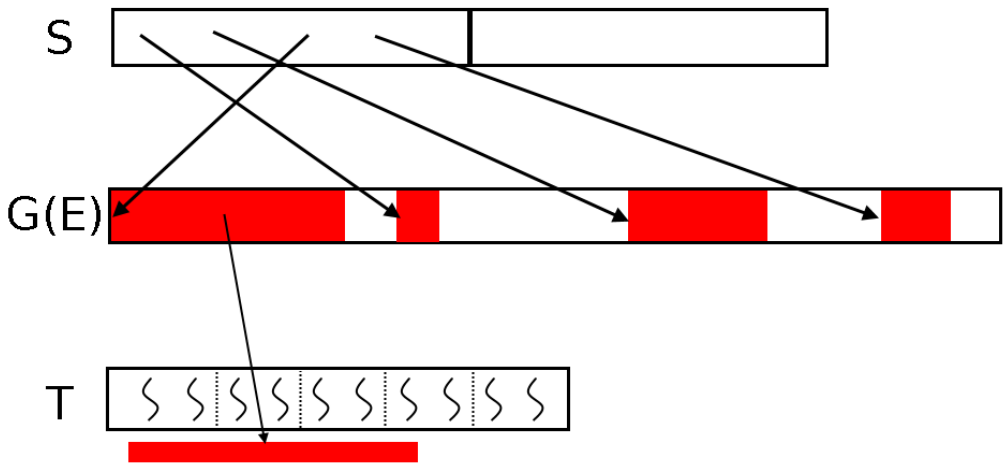

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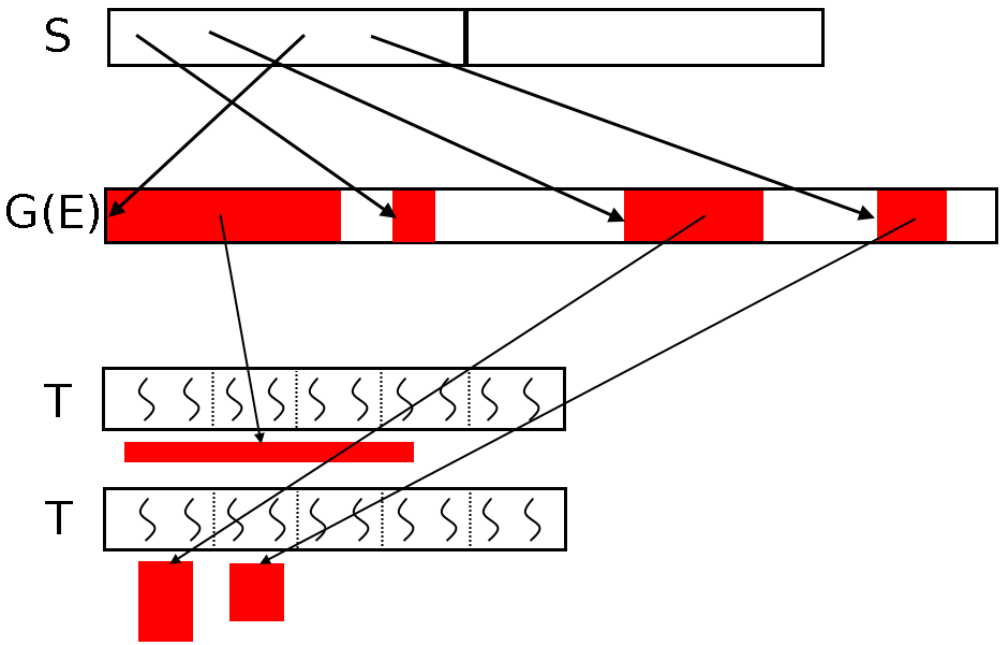

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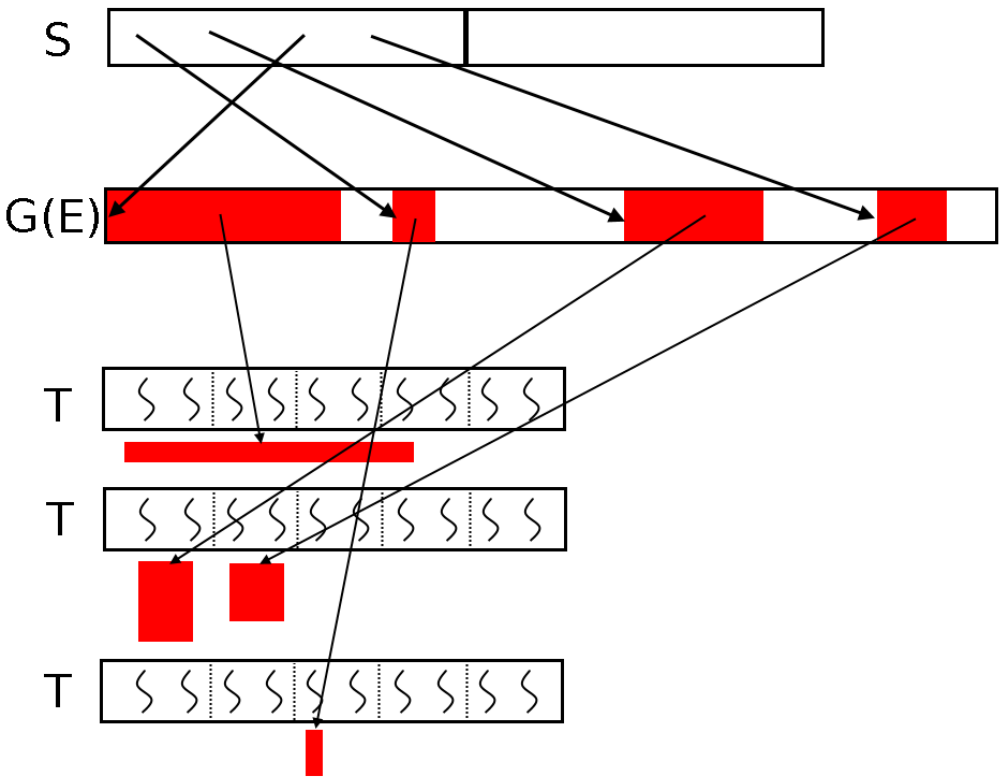

Graph Algorithms for Manycore
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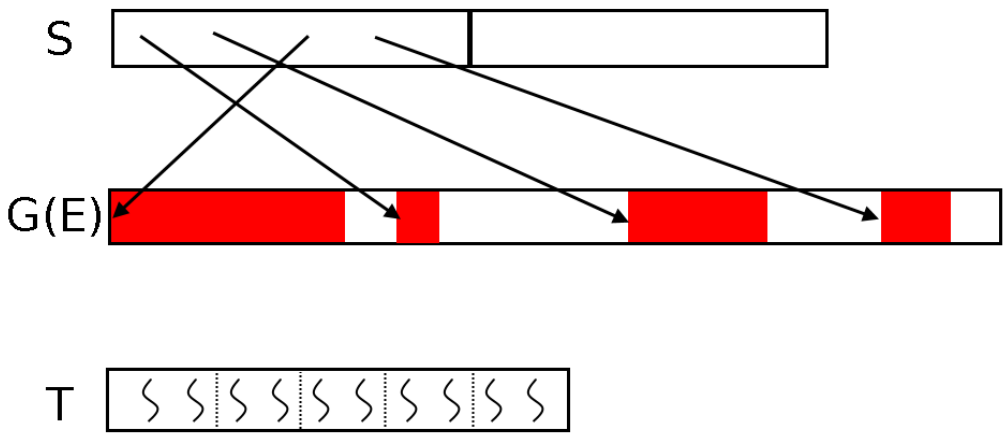
- 'Manhattan collapse - local' (e.g. [Merrill et al., 2012])



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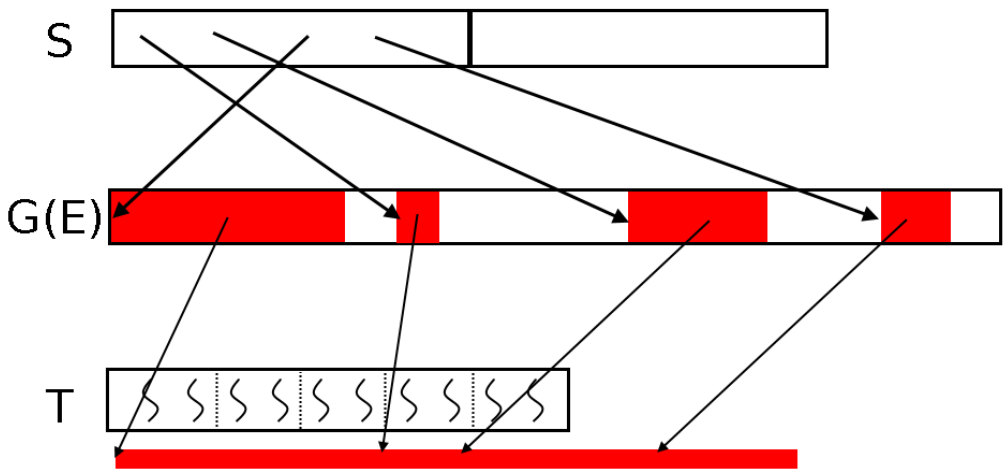

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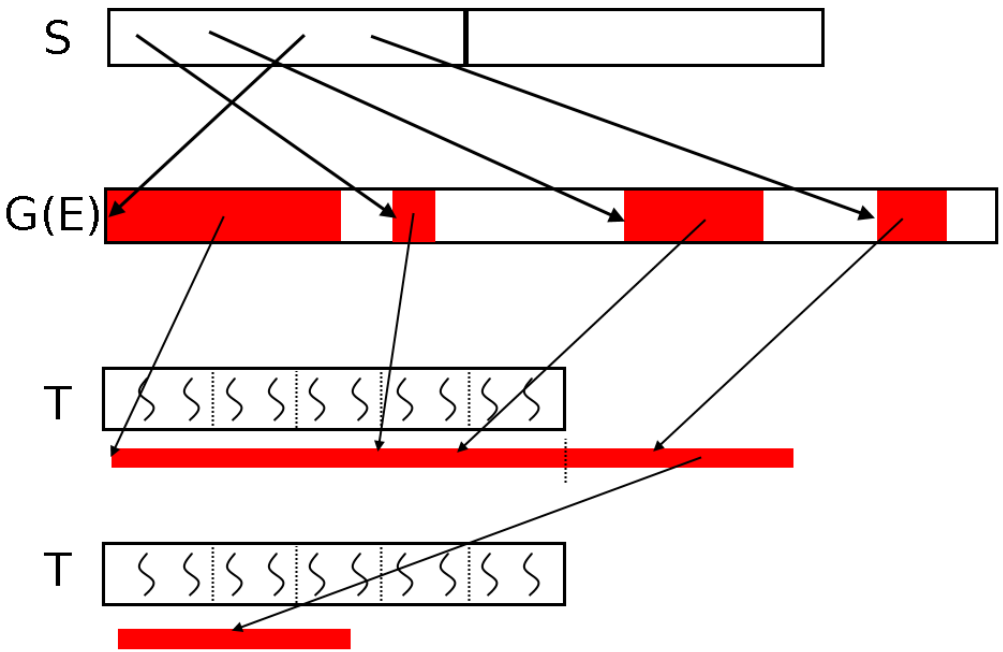

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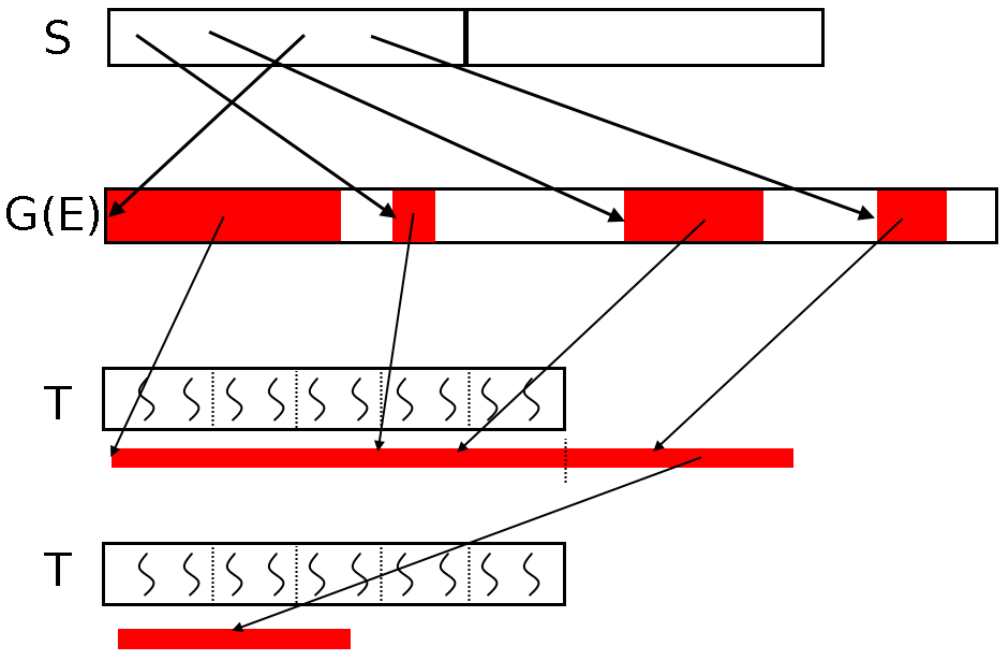
- 'Manhattan collapse - global' (e.g. [Davidson et al., 2014])



- Implementation
  - Develop with Kokkos for cross-platform compatibility
  - Implement MULTISTEP SCC algorithm for testing
- Memory access optimizations
  - Explicit shared memory utilization on GPU
  - Coalescing memory access (locality)
  - Minimize access to global/higher-level memory
- Collective operation optimizations
  - Warp and team-based operations (team scan, team reduce)
  - Minimize global atomics (team-based atomics)

Graph computations
Implemented algorithms

- Breadth-first search
- Color propagation
- Trimming
- The MULTISTEP algorithm [Slota et al., 2014] for Strongly Connected Components (SCC) decomposition

Graph computations
Breadth-first search

- Useful subroutine in other graph computations

```
1:  A_1[1..n] ← −1
2:  S_1[1] ← root
3:  level ← 0
4:  while |S_i| ≠ ∅ do
5:      Initialize S_{i+1}
6:      for j = 1 to |S_i| do
7:          u ← S_i[j]
8:          for k = 1 to |E[u]| do
9:              v ← E[u][k]
10:             if A_1[v] < 0 then
11:                 A_1[v] ← level
12:                 S_{i+1} ← v
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Graph computations
Breadth-first search

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Graph computations
Color propagation

- Basic algorithm for connectivity
- General approach applies to other algorithms (e.g., label propagation)

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```

Graph computations
Trimming

- Routine for accelerating connectivity decomposition
- Iteratively trim 0-degree vertices

```
1:  A_1[1..n] ← 1
2:  S_1[1..n] ← [1..n]
3:  while |S_i| ≠ ∅ do
4:      Initialize S_{i+1}
5:      for j = 1 to |S_i| do
6:          u ← S_i[j]
7:          trim ← true
8:          for k = 1 to |E[u]| do
9:              v ← E[u][k]
10:             if A_1[v] = 1 then
11:                 trim ← false
12:         if trim = true then
13:             A_1[u] ← 0
14:             S_{i+1} ← E[u]
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Graph computations
Trimming

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Graph computations

Multistep SCC decomposition [Slota et al., 2014]

- Combination of trimming, BFS, and color propagation

1: $T \leftarrow \text{Trim}(G)$
2: $V \leftarrow V \setminus T$
3: Select $v \in V$ for which $d_{in}(v) * d_{out}(v)$ is maximal
4: $D \leftarrow \text{BFS}(G(V, E(V)), v)$
5: $S \leftarrow D \cap \text{BFS}(G(D, E'(D)), v)$
6: $V \leftarrow V \setminus S$
7: **while** $\text{NumVerts}(V) > 0$ **do**
8: $\quad C \leftarrow \text{ColorProp}(G(V, E(V)))$
9: $\quad V \leftarrow V \setminus C$

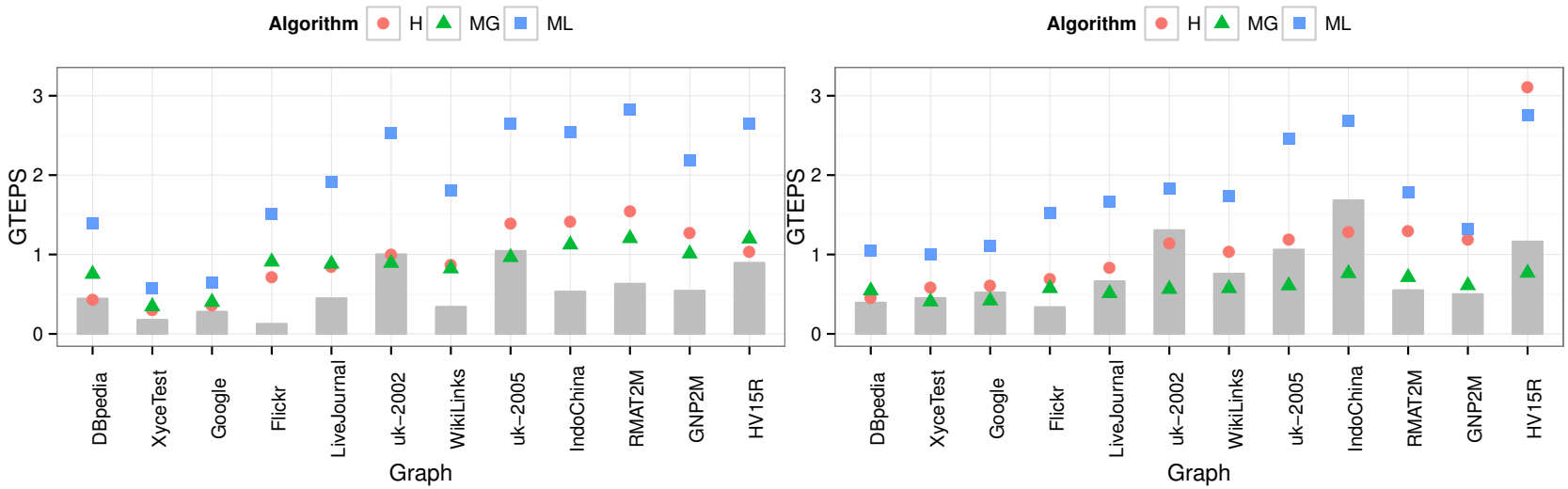
Performance Results

Experimental Setup

- Test systems: One node of *Shannon* and *Compton* at Sandia and *Blue Waters* at the NCSA
  - Intel Xeon E5-2670 (Sandy Bridge), dual-socket, 16 cores, 64-128 GB memory
  - NVIDIA Tesla K40M GPU, 2880 cores, 12 GB memory
  - NVIDIA Tesla K20X GPU, 2688 cores, 6 GB memory
  - Intel Xeon Phi (KNC, ∼3120A), 228 cores, 6 GB memory
- Test graphs:
  - Various real and synthetic small-world graphs, 5.1 M to 936 M edges
  - Social networks, circuit, mesh, RDF graph, web crawls, R-MAT and $G(n, p)$ random graphs, Wikipedia article links

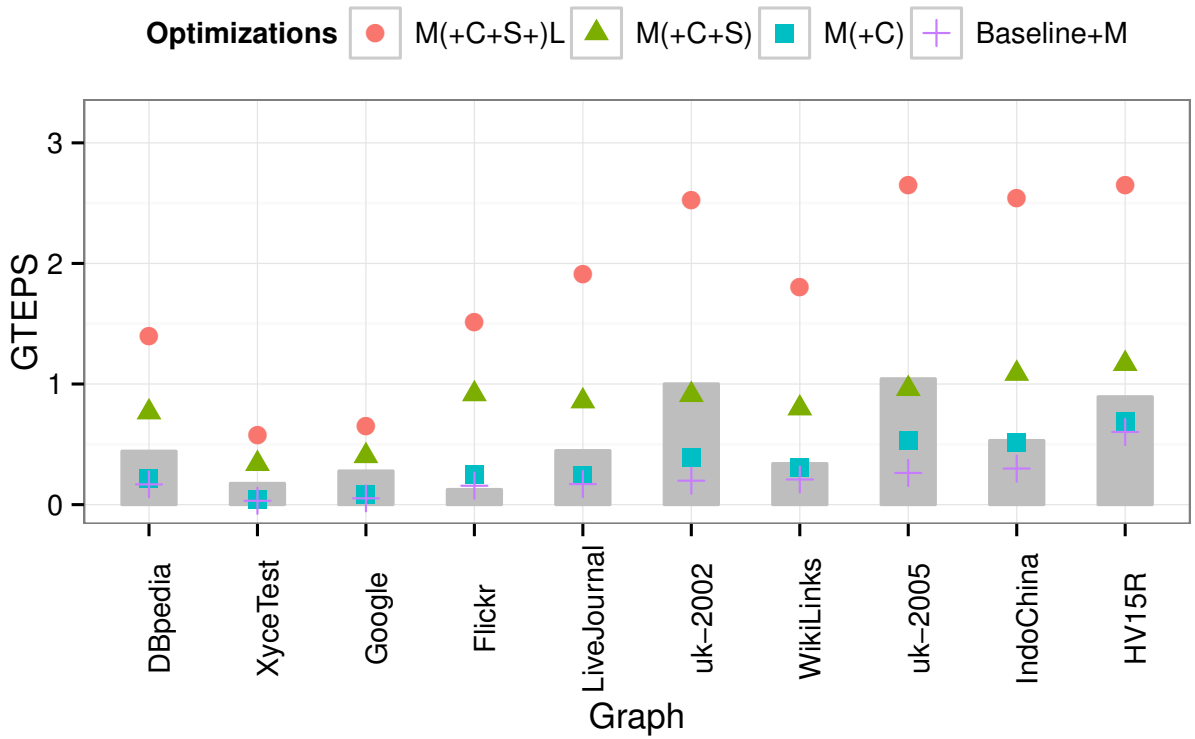
BFS and Coloring versus Loop Strategies
Tesla K40M

- Performance in GTEPS (10^9 trav. edges per second) for BFS (left) and color propagation (right) on Tesla K40M.
- Graphs ordered by increasing density from left to right
- Gray Bar: Baseline, H: Hierarchical, ML: Local collapse, MG: Global collapse,



BFS - Cumulative Impact of Optimizations
Tesla K40M

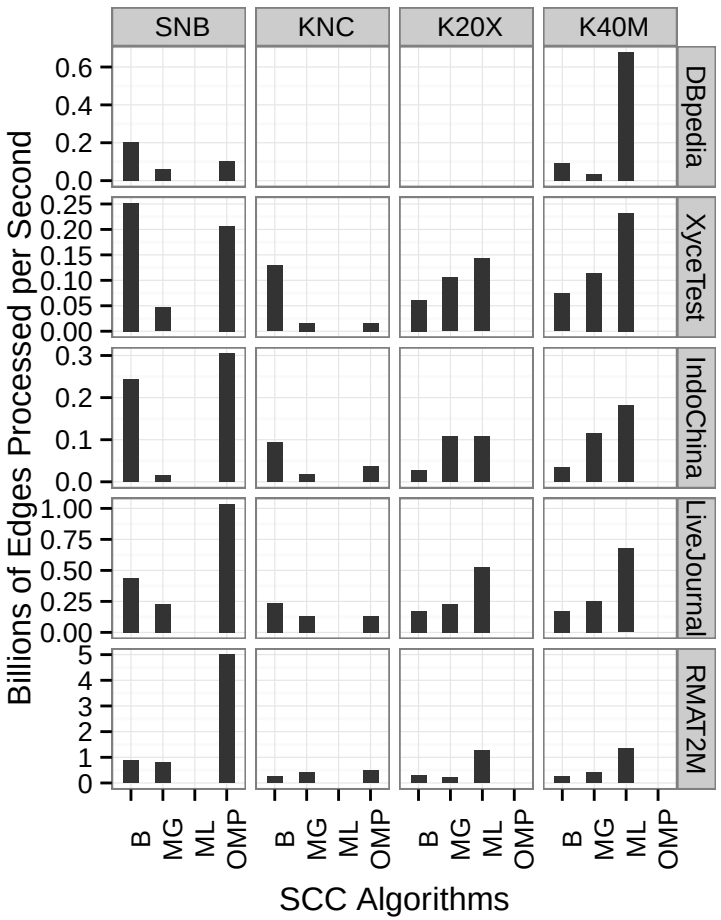
- Gray Bar: baseline, M: local collapse, C: coalescing memory access, S: shared memory use, L: local team-based primitives



SCC Cross-platform Performance Comparison

Sandy bridge (SB), MIC Knight's Corner (KNC), K40M, K20M

- B: Baseline, MG: Manhattan Global, ML: Manhattan Local, OMP: Optimized OpenMP code



Conclusions

- We express several graph computations in the **Kokkos** programming model using an **algorithm design abstraction** that allows portability across both multicore platforms and **accelerators**.
- The **SCC** code on GPUs (using the **Local Manhattan Collapse** strategy) demonstrates up to a 3.25× speedup relative to a state-of-the-art parallel CPU implementation running on a dual-socket compute node.
- Future work: Expressing other computations using this framework; Heterogeneous CPU-GPU processing; Newer architectures.

Large Graph Analysis – Full-scale Optimization

Part 2: **Large Graph Analysis** – Techniques for multi-billion vertex scale graph analysis

Large Graph Analysis – Full-scale Optimization

Current state-of-the-art:

- Many frameworks exist for large graph analysis
- Single-node parallel frameworks demonstrate good performance, but are limited by shared-memory (Ligra, Green-Marl, etc.)
- Disk-based frameworks are slow at all scales (MapReduce-like)
- Most distributed-memory frameworks often run slower than serial C code without massive parallelism, also fail for large graphs (GraphX, GraphLab and its variants, most others)
- Some can scale to large graphs, but only give reasonable relative performance at that scale (Giraph)
- Some are performant, but require specialized hardware (FlashGraph)

Motivating questions for this work

- **Q**: What is needed to analyze the **largest publicly-available graph instances** on modern distributed **HPC** systems ?
- **Q**: What **optimizations strategies and abstractions** can we identify to simplify implementation efforts ?
- **Q**: Is it possible to be both **highly performant** while keeping the implementation effort as **simple** as possible ?

Contributions

- **Q**: **Needed to analyze large graphs on HPC** ?
  - We develop optimized MPI+OpenMP code that uses 256 nodes of the Blue Waters supercomputer to analyze the 3.5B page and 130B link 2012 Web Data Commons web crawl.
- **Q**: **Optimizations strategies and abstractions** ?
  - We recognize three classes of communication patterns common to many graph algorithms and develop optimizations for them.
- **Q**: **Highly performant and simple** ?
  - Yes. Each algorithm can be implemented in only a couple hundred lines of C++ code while outperforming state-of-the-art frameworks by orders-of-magnitude.

Research Goals

Goals of this research:

- Develop methodology for analyzing the **largest publicly available graph instances** on **HPC systems**
- Identify **optimization strategies and abstractions** that can simplify implementation efforts
- Strive for **ease of implementation** while retaining **high performance**, identify and evaluate potential performance and scalability tradeoffs
- Use these implementations to gain novel insight into graph structure

Design Tradeoffs and Considerations

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 vs. **C/C++**
  - High-level model vs. MPI only vs. **MPI+OpenMP**

Other considerations:

- In-memory graph representation
  - Compressed vs. **uncompressed**, efficiency in accessing structural information
- Partitioning strategy (with 1D layout)
  - Vertex block vs. Edge block vs. Random
- Generalizability for many graph algorithms

Communication in Distributed Graph Algorithms

Observation: many iterative graph algorithms have similar communication patterns

- *BFS-like*: build and exchange global queue of vertices on each iteration
- *PageRank-like*: exchange all per-vertex values on each iteration
- *ColorProp-like*: exchange subset of per-vertex values on each iteration

Takeaway: develop optimized outlines for each of these patterns, fill in algorithm-specific details

BFS-like Algorithms

- Build and exchange global queue (Q) of vertices on each iteration

1: $Q \leftarrow v_{root}$
2: $Data[V_{local} \cup V_{ghost}] \leftarrow$ InitData()
3: **while** $Q \neq \varnothing$ **do**
4: **for all** $v \in Q$ **do**
5: $Data[v] \leftarrow$ PerformWork($v, Data$)
6: **for all** $\langle v, u \rangle \in E$ **do**
7: $Data[u] \leftarrow$ PerformWork($u, Data$)
8: **if** CriteraSatisfied() **then**
9: $Q_n \leftarrow u$
10: $Q \leftarrow$ Exchange(Q_n)

PageRank-like Algorithms

- Exchange all per-vertex *Data* with neighbors on each iteration

1: $Data[V_{local} \cup V_{ghost}] \leftarrow \text{InitData}()$
2: **for** $iter = 1 \cdots NumIter$ **do**
3: **for all** $v \in V_{local}$ **do**
4: $Data[v] \leftarrow \text{PerformWork}(v, Data)$
5: **for all** $\langle v, u \rangle \in E$ **do**
6: $Data[v] \leftarrow \text{PerformWork}(u, Data)$
7: $Q_{Data} \leftarrow Data[v]$
8: $Data[V_{ghost}] \leftarrow \text{Exchange}(Q_{Data})$

ColorProp-like Algorithms

- Exchange subset of per-vertex *Data* on each iteration

1: $Q \leftarrow V_{local}$
2: $Data[V_{local} \cup V_{ghost}] \leftarrow \text{InitData}()$
3: **for** $iter = 1 \cdots NumIter$ **or** $Q \neq \varnothing$ **do**
4: **for all** $v \in Q$ **do**
5: $Data[v] \leftarrow \text{PerformWork}(v, Data)$
6: **for all** $\langle v, u \rangle \in E$ **do**
7: $Data[v] \leftarrow \text{PerformWork}(u, Data)$
8: **if** CriteraSatisfied() **then**
9: $Q_n \leftarrow v$
10: $Q_{Data} \leftarrow Data[v]$
11: $Q \leftarrow \text{Exchange}(Q_n)$
12: $Data[V_{ghost}] \leftarrow \text{Exchange}(Q_{Data})$

Distributed Graph Processing

Large-scale graph analysis on HPC systems

- Optimized parallel graph I/O and pre-processing
- Fully parallel – almost no serial work (tasks & threads)
- Implemented algorithms:
  - *BFS-like*: MULTISTEP SCC (1st stage), MULTISTEP WCC (1st stage), K-core, Harmonic Centrality
  - *PageRank-like*: PageRank, Label Propagation (this implementation)
  - *ColorProp-like*: MULTISTEP WCC (2nd stage), PULP
- Compact and efficient: ~2,000 total lines of code

Performance Results

Experimental Setup

Test systems and test networks

- Test systems: and *Compton* at Sandia and *Blue Waters* at NCSA
  - Intel Xeon E5-2670, dual-socket, 16 cores, 64 GB memory
  - AMD Interlagos 6276, dual-socket, 16 cores, 64 GB memory

Graph	n	m	D_{avg}	Source
Web Crawl	3.5 B	129 B	36	Meusel et al. [2015]
R-MAT	3.5 B	129 B	36	Chakrabarti et al. [2004]
$G(n,p)$	3.5 B	129 B	36	
R-MAT	2^{25}-2^{32}	2^{29}-2^{36}	16	Chakrabarti et al. [2004]
$G(n,p)$	2^{25}-2^{32}	2^{29}-2^{36}	16	
Host	89 M	2.0 B	22	Meusel et al. [2015]
Pay	39 M	623 M	16	Meusel et al. [2015]
Twitter	53 M	2.0 B	38	Cha et al. [2010]
LiveJournal	4.8 M	69 M	14	Leskovec et al. [2009]
Google	875 K	5.1M	5.8	Leskovec et al. [2009]

End-to-end Analysis

256 nodes of Blue Waters

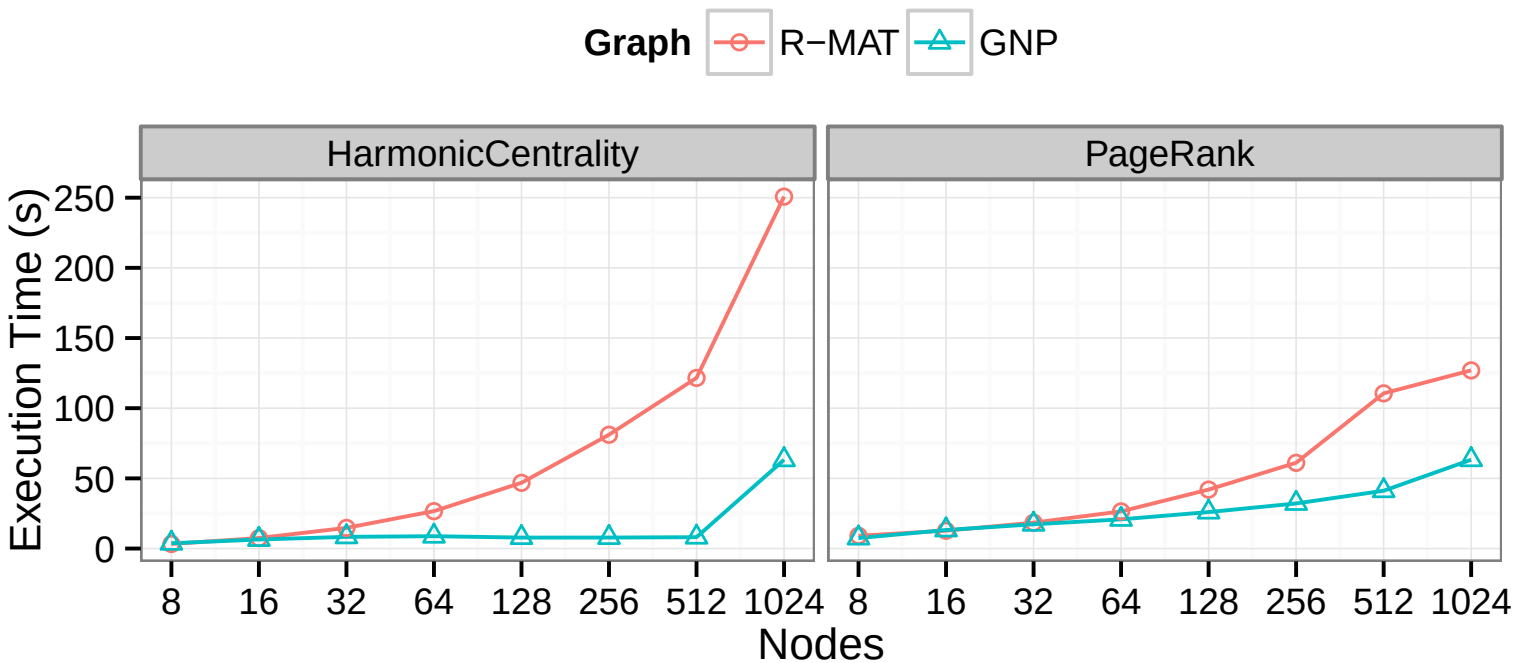
- Ran all six analytics on the web crawl (with three partitioning strategies) and the $G(n, p)$ and R-MAT graphs
- With $\frac{n}{p}$ partitioning strategy, end-to-end times are about 20 minutes (3 minutes for I/O+PP), expect up to 50% further reduction possible with PuLP

Analytic	WC-np	WC-mp	WC-rand	R-MAT	$G(n, p)$
PageRank	87	111	227	125	121
Label Propagation	400	435	367	993	992
WCC	88	63	112	68	77
Harmonic Centrality	54	46	101	252	84
K-core	445	363	583	579	481
SCC	184	108	184	89	83

Weak Scaling

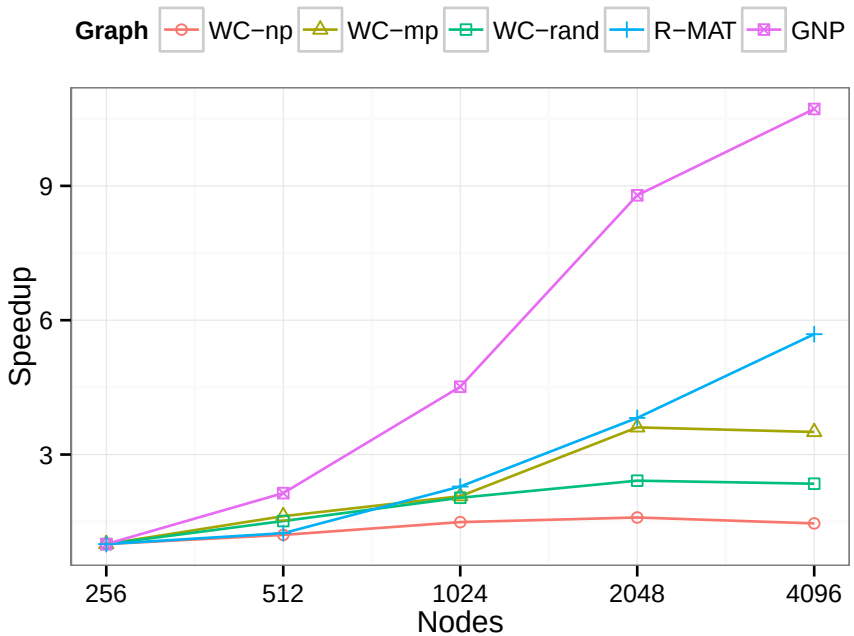
Blue Waters from 8 to 1024 nodes

- Harmonic Centrality and PageRank on R-MAT and $G(n, p)$ graphs with vertex block partitioning
- 2^{22} vertices per node and 2^{26} edges per node



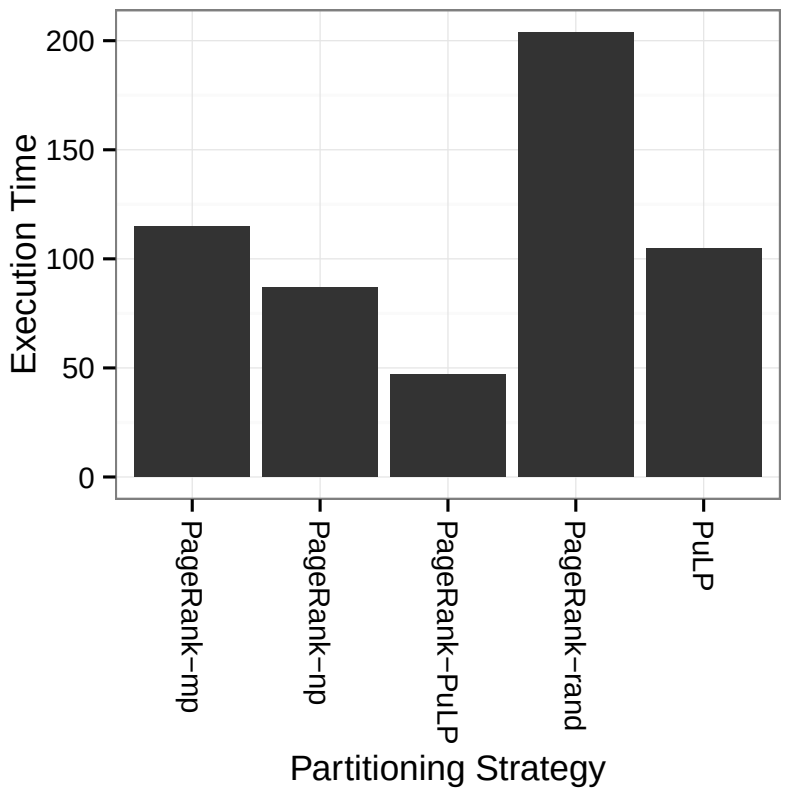
Strong Scaling
Blue Waters from 256 to 4096 nodes

- Label propagation – shows strong scaling from 256 to 4096 nodes
- PageRank-like and ColorProp-like strong scale nicely; BFS-like more dependent on graph structure (high number of synchronizations and low computation per iteration)



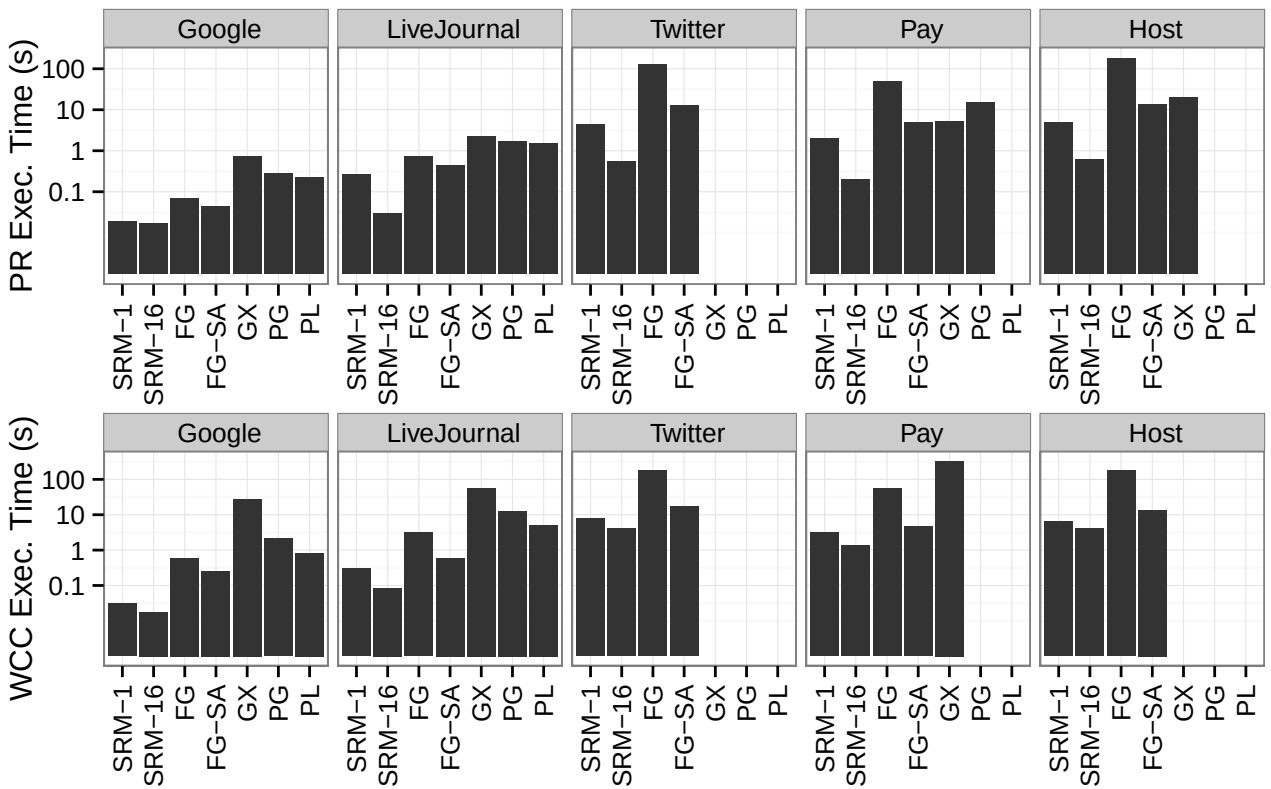
Ongoing work: PuLP in distributed memory

- Tentative distributed version of PuLP
- 20 iterations of PageRank on the web crawl with various partitioning strategies ($\frac{n}{p}$, $\frac{m}{p}$, random, PuLP)
- Using PuLP cuts best-case execution time in half



Comparison to popular frameworks

- Compared SRM-16 (Slota-Rajamanickam-Madduri) to GraphX (GX), PowerGraph (PG), and PowerLyra (PL) on 16 nodes of *Compton*; compared SRM-1 to FlashGraph (FG) and FlashGraph standalone (FG-SA) on a single node
- About 38× faster on average for PageRank (top), 201× faster for WCC (bottom) against distributed memory frameworks
- About 2.4× and 2.6× faster in shared-memory than FlashGraph

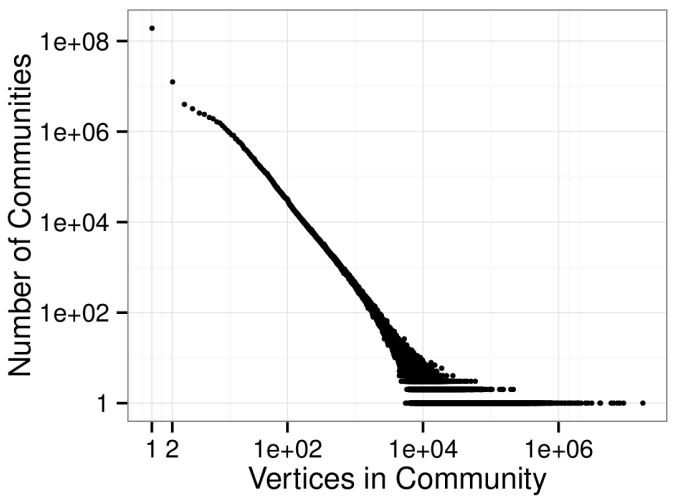


Community Detection in Web Crawl

- Used label propagation to study community structure of the web crawl
- Largest communities discovered after 30 iterations in table below
- Community frequencies from label propagation appear to follow a heavy-tailed power law

Largest Communities (numbers in millions)

Pages	In-Links	Out-Links	Rep. Page
112	2126	32	YouTube
18	548	277	Tumblr
9	516	84	Creative Commons
8	186	85	WordPress
7	57	83	Amazon
6	41	21	Flickr



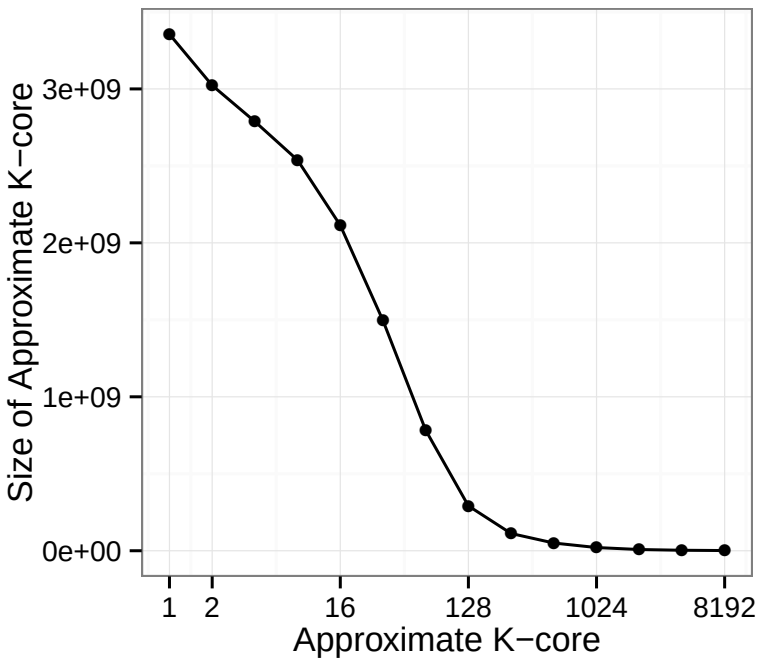
Centrality Measurements of Web Crawl

- Determined the top 10 web pages according to different centrality indices
- Similar to results found in prior work using smaller host-level graph [Meusel et al., 2014]
- Note that out-degree demonstrates very little importance as a centrality index

Out-degree	In-degree	PageRank	Harmonic Centrality
photoshare.ru/..	youtube.com	youtube.com	wordpress.org
dvderotik.com/..	wordpress.org	youtube.com/t/..	twitter.com
zoover.be/..	youtube.com/t/..	youtube.com/testtube	twitter.com/privacy
cran.r-project.org/..	youtube.com/..	youtube.com/t/..	twitter.com/about
cran.rakanu.com/..	youtube.com/t/..	youtube.com/t/..	twitter.com/tos
linkagogo.com/..	youtube.com/..	tumblr.com	twitter.com/account/..
cran.r-project.org/..	youtube.com/t/..	google.com/intl/en/..	twitter.com/account/..
fussballdaten.de/..	gmpg.org/xfn/11	wordpress.org	twitter.com/about/resources
fussballdaten.de/..	google.com	google.com/intl/..	twitter.com/login
fussballdaten.de/..	google.com/intl/..	google.com	twitter.com/about/contact

K-core Decomposition of Web Crawl

- Performed k-core decomposition using our approximation algorithm (gives upper-bound power-of-two)
- Plotted below is number of total pages in k-core versus k-core values
- K-cores appear quite large; ~300M pages in 128 k-core and ~20M pages in 1024 k-core



Future work

- Complete implementation of PuLP and DGL for communication and computation acceleration
- Continue to develop general purpose engine for many more graph analytics
- Use techniques to perform more in-depth studies of large and complex networks

Conclusions
Overall lessons learned

- Parallel algorithm design
  - Minimizing synchronization costs
  - Keeping memory accesses local
  - Even work distribution among threads and tasks
- Identifying algorithmic traits across graph algorithms
  - Many graph algorithms follow an iterative nested-loop structure
  - Many graph algorithms use common subroutines such as BFS, etc.
- Storing and organizing graphs efficiently in memory
  - Optimizing layout for specific graph types and applications
  - Balance cost tradeoffs for both communication and computation
  - Need for parameter tuning and experimental evaluation

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Thank you! Questions?

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