Parallel Breadth First Search on GPU Clusters

http://mapgraph.io

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This work was (partially) funded by the DARPA XDATA program under AFRL Contract #FA8750-13-C-0002. This material is based upon work supported by the Defense Advanced Research Projects Agency (DARPA) under Contract No. D14PC00029. The authors would like to thank Dr. White, NVIDIA, and the MVAPICH group at Ohio State University for their support of this work.

Many-Core is Your Future
Graphs are everywhere and need for graph analytics is growing rapidly.

- **Facebook has ~ 1 trillion edges in their graph.**
- **Over 30 minutes per iteration using 200 machines.**
- **All computations require multiple iterations (6-50).**
- **We could do it in seconds on a cluster of GPUs.**
Graph Database
- High performance, Scalable
  - 50B edges/node
  - High level query language
  - Efficient Graph Traversal
  - High 9s solution
- Open Source
  - Subscriptions

GPU Analytics
- Extreme Performance
  - 100s of times faster than CPUs
  - 10,000x faster than graph databases
  - 30,000,000,000 edges/sec on 64 GPUs
- DARPA funding
- Disruptive technology
  - Early adopters
  - Huge ROIs
SYSTAP is focused on building software that enable graphs at speed and scale.

- **Blazegraph™** for Property and RDF Graphs
  - High Availability (HA) Architecture with Horizontal Scaling

  *Blazegraph™ Comparison*

- **Mapgraph™** GPU-accelerated data parallel graph analytics
  - Vertex-Centric API.
  - Single or multi-GPU.
  - 10,000X faster than Accumulo, Neo4J, Titan, etc.
  - 3x faster then Cray XMT-2 at 1/3rd the price.
GPU Hardware Trends

- K40 GPU (today)
  - 12G RAM/GPU
  - 288 GB/s bandwidth
  - PCIe Gen 3
- Pascal GPU (Q1 2016)
  - 32G RAM/GPU
  - 1 TB/s bandwidth
  - Unified memory across CPU, GPUs
- NVLINK
  - High bandwidth access to host memory
MapGraph: Extreme performance

- GTEPS is Billions ($10^9$) of Traversed Edges per Second.
  - This is the basic measure of performance for graph traversal.

<table>
<thead>
<tr>
<th>Configuration</th>
<th>Cost</th>
<th>GTEPS</th>
<th>$/GTEPS</th>
</tr>
</thead>
<tbody>
<tr>
<td>4-Core CPU</td>
<td>$4,000</td>
<td>0.2</td>
<td>$5,333</td>
</tr>
<tr>
<td>4-Core CPU + K20 GPU</td>
<td>$7,000</td>
<td>3.0</td>
<td>$2,333</td>
</tr>
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<td>XMT-2 (rumored price)</td>
<td>$1,800,000</td>
<td>10.0</td>
<td>$188,000</td>
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<tr>
<td>64 GPUs (32 nodes with 2x K20 GPUs per node and InfiniBand DDRx4 – today)</td>
<td>$500,000</td>
<td>30.0</td>
<td>$16,666</td>
</tr>
<tr>
<td>16 GPUs (2 nodes with 8x Pascal GPUs per node and InfiniBand DDRx4 – Q1, 2016)</td>
<td>$125,000</td>
<td>&gt;30.0</td>
<td>&lt;$4,166</td>
</tr>
</tbody>
</table>
SYSTAP’s MapGraph APIs Roadmap

- Vertex Centric API
  - Same performance as CUDA.
- Schema-flexible data-model
  - Property Graph / RDF
  - Reduce import hassles
  - Operations over merged graphs
- Graph pattern matching language
- DSL/Scala => CUDA code generation
Breadth First Search

- Fundamental building block for graph algorithms
  - Including SPARQL (JOINs)
- In level synchronous steps
  - Label visited vertices
- For this graph
  - Iteration 0
  - Iteration 1
  - Iteration 2
- Hard problem!
  - Basis for Graph 500 benchmark
GPUs – A Game Changer for Graph Analytics

- Graphs are a hard problem
  - Non-locality
  - Data dependent parallelism
  - Memory bus and communication bottlenecks
- GPUs deliver effective parallelism
  - 10x+ memory bandwidth
  - Dynamic parallelism

BFS Results: MapGraph vs GraphLab

- CPU vs GPU
- GPU 15x-300x faster
- More CPU cores does not help

MapGraph Speedup vs GraphLab (BFS)
PageRank: MapGraph vs GraphLab

- CPU vs GPU
- GPU 5x-90x faster
- CPU slows down with more cores!
2D Partitioning (aka Vertex Cuts)

- p x p compute grid
  - Edges in rows/cols
  - Minimize messages
    - \( \log(p) \) (versus \( p^2 \))
  - One partition per GPU

- Batch parallel operation
  - Grid row: out-edges
  - Grid column: in-edges

- Representative frontiers

- Parallelism – work must be distributed and balanced.
- Memory bandwidth – memory, not disk, is the bottleneck
Scale 25 Traversal

- Work spans multiple orders of magnitude.
Distributed BFS Algorithm

1: procedure BFS(Root, Predecessor)  
2:     \[ I_{i,j}^{0} \leftarrow \text{LocalVertex}(Root) \]  \hspace{1cm} \text{Starting vertex}
3:     \text{for } t \leftarrow 0 \text{ do}
4:         \text{Expand}(I_{i,j}^{t}, O_{i,j}^{t}) \hspace{1cm} \text{Data parallel 1-hop expand on all GPUs}
5:         \text{LocalFrontier}_{t} \leftarrow \text{Count}(O_{i,j}^{t}) \hspace{1cm} \text{Local frontier size}
6:         \text{GlobalFrontier}_{t} \leftarrow \text{Reduce}(\text{LocalFrontier}_{t}) \hspace{1cm} \text{Global frontier size}
7:         \text{if } \text{GlobalFrontier}_{t} > 0 \text{ then}
8:             \text{Contract}(O_{i,j}^{t}, O_{i,j}^{t}, I_{i,j}^{t+1}, \text{Assign}_{i,j}) \hspace{1cm} \text{Global Frontier contraction ("wave")}
9:             \text{UpdateLevels}(O_{i,j}^{t}, t, \text{level}) \hspace{1cm} \text{Record level of vertices in the In / Out frontier}
10:         \text{else}
11:             \text{UpdatePreds}(\text{Assign}_{i,j}, \text{Preds}_{i,j}, \text{level}) \hspace{1cm} \text{Compute predecessors from local In / Out levels (no communication)}
12:         \text{break} \hspace{1cm} \text{Done}
13:     \text{end if}
14:     t++ \hspace{1cm} \text{Next iteration}
15: \text{end for}
16: end procedure
Distributed BFS Algorithm

1: procedure BFS(Root, Predecessor)
2: \[In_{ij}^{0} \leftarrow \text{LocalVertex}(Root)\] \(\rightarrow\) Starting vertex
3: for \(t \leftarrow 0\) do
4: \[\text{Expand}(In_{i}^{t}, Out_{ij}^{t})\] \(\rightarrow\) Data parallel 1-hop expand on all GPUs
5: \[\text{LocalFrontier}_{t} \leftarrow \text{Count}(Out_{ij}^{t})\] \(\rightarrow\) Local frontier size
6: \[\text{GlobalFrontier}_{t} \leftarrow \text{Reduce}(\text{LocalFrontier}_{t})\] \(\rightarrow\) Global frontier size
7: if \(\text{GlobalFrontier}_{t} > 0\) then
8: \[\text{Contract}(Out_{ij}^{t}, Out_{ij}^{t}, In_{i}^{t+1}, \text{Assign}_{ij})\] \(\rightarrow\) Global Frontier contraction (“wave”)
9: \[\text{UpdateLevels}(Out_{ij}^{t}, t, \text{level})\] \(\rightarrow\) Record level of vertices in the In / Out frontier
10: else
11: \[\text{UpdatePreds}(\text{Assign}_{ij}, \text{Preds}_{ij}, \text{level})\] \(\rightarrow\) Compute predecessors from local In / Out levels (no communication)
12: break \(\rightarrow\) Done
13: end if
14: \(t++\) \(\rightarrow\) Next iteration
15: end for
16: end procedure

- Key differences
  - \(\log(p)\) parallel scan (vs sequential wave)
  - GPU-local computation of predecessors
  - 1 partition per GPU
  - GPUDirect (vs RDMA)
Expand

1: procedure EXPAND($In_i^t$, $Out_{ij}^t$)
2:         $L_{in} \leftarrow \text{convert}(In_i^t)$
3:         $L_{out} \leftarrow \emptyset$
4:     for all $v \in L_{in}$ in parallel do
5:          for $i \leftarrow \text{RowOff}[v], \text{RowOff}[v+1]$ do
6:              $c \leftarrow \text{ColIdx}[i]$
7:              $L_{out} \leftarrow c$
8:     end for
9:     end for
10:     $Out_{ij}^t \leftarrow \text{convert}(L_{out})$
11: end procedure

- The GPU implementation uses multiple strategies to handle data-dependent parallelism. See our SIGMOD 2014 paper for details.
Global Frontier Contraction and Communication

1: \textbf{procedure} \textsc{contract}(Out}_{i,j}^t, Out}_{j}^t, In}_{i}^{t+1}, \text{Assign}_{i,j} \) \\
2: \quad \text{Prefix}_{i,j}^t \leftarrow \text{ExclusiveScan}_j(Out}_{i,j}^t) \\
3: \quad \text{Assigned}_{i,j} \leftarrow \text{Assigned}_{i,j} \cup (Out}_{i,j}^t - \text{Prefix}_{i,j}^t) \\
4: \quad \textbf{if} \ i = p \ \textbf{then} \\
5: \quad \quad \text{Out}_{j}^t \leftarrow \text{Out}_{i,j}^t \cup \text{Prefix}_{i,j}^t \\
6: \quad \textbf{end if} \\
7: \quad \text{Broadcast}(\text{Out}_{j}^t, p, ROW) \\
8: \quad \textbf{if} \ i = j \ \textbf{then} \\
9: \quad \quad \text{In}_{i}^{t+1} \leftarrow \text{Out}_{j}^t \\
10: \quad \textbf{end if} \\
11: \quad \text{Broadcast}(\text{In}_{i}^{t+1}, i, COL) \\
12: \textbf{end procedure}
Global Frontier Contraction and Communication

1: procedure CONTRACT(Out\^t_{ij}, Out\^t_j, In\^t_{i+1}, Assign\_{ij})
2: Prefix_{ij} ExclusiveScan_j (Out\^t_{ij})
8: if i = j then
9: In\^t_{i+1}\rightarrow Out\^t_j
10: end if
11: Broadcast( In\^t_{i+1}, i, COL )
12: end procedure

« Distributed prefix sum. Prefix is vertices discovered by your left neighbors (log p)
« Vertices first discovered by this GPU.

« Right most column has global frontier for the row
« Broadcast frontier over row.

« Broadcast frontier over column.
Global Frontier Contraction and Communication

1: procedure CONTRACT\( (Out^t_{ij}, Out^t_j, In^{t+1}_i, Assign_{ij}) \)
2: Prefix\( t_{ij} \) \( \text{ExclusiveScan}_{j}(Out^t_{ij}) \)
3: \( \text{Assign}_{ij} \) \( \text{Assign}_{ij}[\text{Prefix}_t_{ij}] \)
4: if \( i = p \) then
5: \( \text{Out}_j \) \( \text{Out}_{ij}[\text{Prefix}_t_{ij}] \)
6: end if
7: Broadcast\( (\text{Out}^{t+1}_i, p, \text{ROW}) \)
8: if \( i = j \) then
9: \( \text{In}^{t+1}_i \) \( \text{Out}_j \)
10: end if
11: Broadcast\( (\text{In}^{t+1}_i, i, \text{COL}) \)
12: end procedure

- We use a parallel scan that minimizes communication steps (vs work).
- This improves the overall scaling efficiency by 30%.

\( \Rightarrow \) Distributed prefix sum. Prefix is vertices discovered by your left neighbors \((\log p)\)
\( \Rightarrow \) Vertices first discovered by this GPU.

\( \Rightarrow \) Right most column has global frontier for the row
\( \Rightarrow \) Broadcast frontier over row.

\( \Rightarrow \) Broadcast frontier over column.
Global Frontier Contraction and Communication

1: procedure CONTRACT(Out^t_{ij}, Out^t_j, In^{t+1}_i, Assign_{ij})
2: Prefix^t_{ij} ExclusiveScan j (Out^t_{ij})
3: Assigned_{ij} = Assigned_{ij}[Prefix^t_{ij}]
4: if i = p then
5: Out^t_j = Out^t_{ij}[Prefix^t_{ij}]
6: end if
7: Broadcast(Out^{t+1}_i, p, ROW)
8: if i = j then
9: In^{t+1}_i = Out^t_j
10: end if
11: Broadcast(In^{t+1}_i, i, COL)
12: end procedure

• We use a parallel scan that minimizes communication steps (vs work).
• This improves the overall scaling efficiency by 30%.

↓ Distributed prefix sum. Prefix is vertices discovered by your left neighbors (log p)
↓ Vertices first discovered by this GPU.

↓ Right most column has global frontier for the row
↓ Broadcast frontier over row.

↓ Broadcast frontier over column.
Global Frontier Contraction and Communication

1: procedure CONTRACT(\(Out^t_{ij}, \ Out^t_{j}, \ In^{t+1}_i, \ Assign_{ij}\))
2: Prefix\(t\)ij ExclusiveScan\(j\) (\(Out^t_{ij}\))
3: Assigned\(ij\) Assigned\(ij\) [\(Prefix\(t\)ij\)]
4: if \(i = p\) then
5: \(Out^t_{j}\) \(Out^t_{ij}\) [\(Prefix\(t\)ij\)]
6: end if
7: Broadcast(\(In^{t+1}_i, \ i, \ COL\))
8: if \(i = j\) then
9: \(In^t_i\) \(Out^t_{j}\)
10: end if
11: Broadcast(\(In^{t+1}_i, \ i, \ COL\))
12: end procedure

We use a parallel scan that minimizes communication steps (vs work).
This improves the overall scaling efficiency by 30%.
Global Frontier Contraction and Communication

1: procedure CONTRACT(Out$_t$$_i$, Out$_t$$_j$, In$_{i+1}^t$, Assign$_{ij}$)
2:  Prefix$_{ij}$ ExclusiveScan$_j$(Out$_t$$_i$$_j$)
3:  Assigned$_{ij}$ Assigned$_{ij}$[Prefix$_{ij}$]
4:  if $i = p$ then
5:    Out$_j$ Out$_t$$_i$$_j$[Prefix$_{ij}$]
6:  end if
7:  Broadcast(Out$_t$$_j$, p, ROW)
8:  if $i = j$ then
9:    In$_{i+1}^t$ Out$_t$$_j$
10:  end if
11:  Broadcast(In$_{i+1}^t$, i, COL)
12: end procedure

- Distributed prefix sum. Prefix is vertices discovered by your left neighbors ($\log p$)
- Vertices first discovered by this GPU.
- Right most column has global frontier for the row
- Broadcast frontier over row.
- Broadcast frontier over column.
Global Frontier Contraction and Communication

1: procedure CONTRACT(Out$^t_j$, Out$^t_i$, In$^{t+1}_i$, Assign$_{ij}$)
2: Prefix - ExclusivScan(Out$^t_{ij}$)
3: Assigned$^t_{ij}$
4: if $i = p$ then
5: Out$_j$ Out$^t_{ij}$
6: end if
7: Broadcast(Out$^t_j$, $p$, ROW)
8: if $i = j$ then
9: In$^{t+1}_i$ Out$_j$
10: end if
11: Broadcast(In$^{t+1}_i$, $i$, COL)
12: end procedure

- Distributed prefix sum. Prefix is vertices discovered by your left neighbors (log p)
- Vertices first discovered by this GPU.
- Right most column has global frontier for the row
- Broadcast frontier over row.
- Broadcast frontier over column.

- All GPUs now have the new frontier.
Update Levels

1: procedure UPDATELEVELS($Out^t_j$, t, level)
2:   for all $v \in Out^t_j$ in parallel do
3:     level[$v$] $\leftarrow$ t
4:   end for
5: end procedure

- We store both the In and Out levels.
- This allows us to compute the predecessors in a GPU local manner.
Predecessor Computation

1: **procedure** UPDATEPREDs(Assigned\(_{ij}\), Preds\(_{ij}\), level)
2:   **for all** \( v \in \text{Assigned}_{ij} \) **in parallel** **do**
3:     \( \text{Pred}[v] \leftarrow -1 \)
4:     **for** \( i \leftarrow \text{ColOff}[v], \text{ColOff}[v + 1] \) **do**
5:       **if** \( \text{level}[v] = \text{level}[	ext{RowIdx}[i]] + 1 \) **then**
6:         \( \text{Pred}[v] \leftarrow \text{RowIdx}[i] \)
7:       **end if**
8:     **end for**
9: **end for**
10: **end procedure**

- Predecessors are computed after the traversal is complete using node-local In/Out levels.
- No inter-node communication is required.
Weak Scaling

• Scaling the problem size with more GPUs
  – Fixed problem size per GPU.

• Maximum scale 27 (4.3B edges)
  – 64 K20 GPUs => .147s => 29 GTEPS
  – 64 K40 GPUs => .135s => 32 GTEPS

  • K40 has faster memory bus.

<table>
<thead>
<tr>
<th>GPUs</th>
<th>Scale</th>
<th>Vertices</th>
<th>Edges</th>
<th>Time (s)</th>
<th>GTEPS</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>21</td>
<td>2,097,152</td>
<td>67,108,864</td>
<td>0.0254</td>
<td>2.5</td>
</tr>
<tr>
<td>4</td>
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<td>8,388,608</td>
<td>268,435,456</td>
<td>0.0429</td>
<td>6.3</td>
</tr>
<tr>
<td>16</td>
<td>25</td>
<td>33,554,432</td>
<td>1,073,741,824</td>
<td>0.0715</td>
<td>15.0</td>
</tr>
<tr>
<td>64</td>
<td>27</td>
<td>134,217,728</td>
<td>4,294,967,296</td>
<td>0.1478</td>
<td>29.1</td>
</tr>
</tbody>
</table>
Central Iteration Costs (Weak Scaling)

- Communication costs are not constant.
- 2D design implies cost grows as $2 \log(2p)/\log(p)$
- How to scale?
  - Overlapping
  - Compression
    - Graph
    - Message
  - Hybrid partitioning
  - Heterogeneous computing
• Chart shows the different costs for each GPU in each iteration (64 GPUs).
• Wave time is essentially constant, as expected.
• Compute time peaks during the central iterations.
• Costs are reasonably well balanced across all GPUs after the 2nd iteration.
Strong Scaling

- Speedup on a constant problem size with more GPUs
- Problem scale 25
  - $2^{25}$ vertices (33,554,432)
  - $2^{26}$ directed edges (1,073,741,824)
- Strong scaling efficiency of 48%
  - Versus 44% for BG/Q

<table>
<thead>
<tr>
<th>GPUs</th>
<th>GTEPS</th>
<th>Time (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>16</td>
<td>15.2</td>
<td>0.071</td>
</tr>
<tr>
<td>25</td>
<td>18.2</td>
<td>0.059</td>
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<tr>
<td>36</td>
<td>20.5</td>
<td>0.053</td>
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<tr>
<td>49</td>
<td>21.8</td>
<td>0.049</td>
</tr>
<tr>
<td>64</td>
<td>22.7</td>
<td>0.047</td>
</tr>
</tbody>
</table>
Directions to Improve Scaling

• Overlap computation with communication
  – Multiple partitions per GPU
  – Frontier compression

• Hybrid partitioning
  – Degree aware data layout + bottom up search optimization
    • This also requires asynchronous communications and per-target node buffers.
  – Graph aware partitioning plus 2D data layout

• Uintah style data warehouse
  – Hand off tasks to workers (Uintah)
  – Hybrid CPU/GPU computation strategies (TOTEM)
Concept: Accelerate Key Value Stores

**ACCUMULO CLOUD**

- Entity Link Graph

1. Graph data in Accumulo

**MAP/REDUCE CLOUD**

- Compute 2D partitioning

2. Parallel reduce writes 2D edge partitioning

**GPU CLUSTER**

3. Parallel read of 2D data GPU DRAM

4. Extreme speed for graph analytics.

5. Parallel reduction writes output to HDFS or other target.

Paralle File System (HDFS)

1 BFS step @ 270 MTEPS => 2 Hours

- Accumulo + MR
- 1200 nodes
- 1T edges

Assuming 10000x Speedup => .72s/step
MapGraph Timings (single GPU)

- Orkut social network 2.3M vertices, 92M edges. Most time is *load* on CPU.
- Next step eliminates overhead: 62500ms => 63ms (1000x faster)

Once on the GPU, it is very cheap to run other algorithms, different starting vertices, etc.
Current and Future Code Streams

Implemented

Multi-MapGraph
32 GTEPS on 64 GPUs, 4.3 Billion edge graph

Implemented

MapGraph + Java
Single GPU
JNI Interface
Schema Flexible Data Model (PG/RDF)

Current Activity

Multiple Partitions per GPU

Next Steps

• Updates pushed to GPU in background.
  • No ETL latency impact
  • Full GPU Acceleration

Overlap computation with communication for better scaling.

• Horizontal Scaling
  • Extreme Performance

http://BlazeGraph.com
http://MapGraph.io

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3/10/15
MapGraph Beta Customer?

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