Tree contraction, connected components, minimum spanning trees: a GPU path to vertex fitting

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September 9, 2014
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PBBS and Graph500

- PBBS: The Problem Base Benchmark Suite
  - Benchmark designed to compare
    - parallel algorithmic approaches;
    - parallel programming languages;
    - machine architectures;

- Graph500
  - a benchmark to use graph problems to compare computer architectures and compiler design.

- CMS (LHC experiment)
  - Minimum Spanning Tress computations are reported as part of ZVMVST in vertex finding.
Connected components and Minimal spanning tree computations can be demanding.

- Lower bound on work for computation of a Minimum Spanning Tree over an \( m \) edges graph is \( O(m) \).
- Lower bound on space also \( O(m) \).
- Euclidean Graph with \( 2^{21} \) vertices might demand 16 TB of RAM just to represent the edges.
Connected components and Minimal spanning tree computations can be demanding.

- Lower bound on work for computation of a Minimum Spanning Tree over an $m$ edges graph is $O(m)$.
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- Euclidean Graph with $2^{21}$ vertices might demand $16\ TB$ of RAM just to represent the edges.

Challenging as a Computer Science problem.
Theoretical limit

- Connected components and Minimal spanning tree computations can be demanding.
  - Lower bound on work for computation of a Minimum Spanning Tree over an $m$ edges graph is $O(m)$.
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- Challenging as a Computer Science problem.

- Could it have applications in CMS or any other LHC project or even HEP in general? Do they work with large dense graphs?
Kruskal plus lock-free transactions

- Parallel algorithm based on Kruskal MST algorithm with:
  - Lock-free transactions for edge selection based on database style distributed reserve and commit of vertices.
  - Parallel tree contraction as form of disjoint find-union set implementation.
Parallel approximation algorithm based on fair split that will lead to *Well Separated Pair Decomposition*.

- Parallel tree implementation for vertices indexing that doesn’t demand explicit edge representation.
- Approximation algorithm that can lead to MST computation with $O(n \lg n)$ work, given $n$ vertices.
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8. **Disclaimer**
A graph $G$ is a pair $(V, E)$ where
- $V$ is a set of $n$ vertices.
- $E \subseteq \{\{v_i, v_j\} : v_i, v_j \in V\}$ is a set of $m$ edges.
- a map $w$ assigns weight to edges.
Some sort of metric defines the weight of edges.

Graph can possibly be Euclidean.
  - $w$ is the Euclidean distance between the respective vertices.
  - graph is possibly complete: an edge between each pair of vertices.
Spanning tree of a graph $G$

a subgraph $G$ that:
- connects all vertices of $G$;
- contains exactly one path connecting each pair of vertices.
Minimal spanning tree

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  - A spanning tree whose sum edge weights is minimal when compared to all spanning trees of $G$. 
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  A union of minimum spanning trees of each component of $G$. 
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The challenge

- Benchmarks and all that
  - No parallel algorithm for \texttt{mst} computation in PBBS
  - 1 Parallel algorithm approximates \texttt{mst} through \texttt{msf}.
  - Efficiency of parallel \texttt{msf} algorithm is less than 30%.
  - No GPU algorithm for parallel \texttt{mst} or \texttt{msf} computation, even if a few algorithms for connected components can be found.

Lower bounds do matter $\omega(m)$: General \texttt{mst} in 3 or more dimensions cannot be computed in less than $m$ comparisons, possibly close to $n^2$.

$\omega(m)$ again: 1 to 4 TB for a dense graph with 1 million vertices.

Why bother? Kruskal algorithm can build an \texttt{mst} for a dense graph with 1K vertices in less than a second. 2 days when number vertices gets to 1M.
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A Lemma and 700 algorithms

Lemma: Let $X$ be any subset of vertices of $G$, and let $e$ be lightest edge connecting $X$ to $G - X$. Then $e$ is part of the mst of $G$. 
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- Prim-Dijkstra: start with a one vertex tree and add the lightest edge connecting the tree to a vertex not in it.
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- Kruskal: add lightest edge first.
- Prim-Dijkstra: start with a one vertex tree and add the lightest edge connecting the tree to a vertex not in it.
- Borůvka: start with $n$ trees and join pairs with lightest edges. *(Extremely parallel, but...)*
- Separated blobs: subgraphs can be seen as blobs, worked on separately and in parallel and...
A graph

Edges in increasing order of weight:

(4, 1)
(2, 1)
(10, 5)
(10, 6)
(2, 5)
(1, 10)
Kruskal order

- Kruskal: loop invariant based on \textbf{mst} Lemma.
  
  \textit{start with empty} \( t \)
  
  \textit{for each edge} \( e \) \textit{in increasing order of weight}
  
  \textit{if vertices of} \( e \) \textit{are disconnected in} \( t \)
  
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  \item add \textit{e} to \textit{t}
  \end{itemize}

- The tree
  \begin{itemize}
  \item 4 \quad 1
  \item 2
  \item 5
  \item 6
  \item 10
  \end{itemize}
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```
4  —  1
  |
  2
```

```
10
5
6
```
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  5

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  \[
  \begin{array}{c}
  4 \quad 1 \\
  \hline
  2 \\
  5 \quad 6
  \end{array}
  \]
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Sequence of parallel bunch adds

- Process edges in order, but in parallel 2 steps a time if you have 2 processors.
  - add (4, 1) and (2, 1) concurrently;
  - (10, 5) and (10, 6) concurrently;
  - (2, 5) and (1, 10) concurrently, but watch out!
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- The tree

  4 — 1
    |
  2 — 10
    |
  5 — 6

- red edges created a cycle.
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The tree:

```
   4 — 1
   |   |
  2   5
  |   |
  6
```

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- The tree

```
  4 — 1 — [red] — 10
     |                    |
    2 — [red] — 5 — 6
```

- red edges created a cycle.
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```
    4 — 1 —— 10
      |       |
      2 ----- 5
          |
          6
```
- red edges created a cycle.
Non interference demanded

- Blue lines delimit supervertices

Sequential execution helps the lazy programmer.

Concurrent steps should not interfere with each other.
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```
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\\
2
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- Concurrent steps should not interfere with each other.
Linearization to avoid interference

- The two red edges interfere with each other.
- Their addition must be *linearized*. 
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- Elipse on the left and circle on the right represent two different trees.
- Options:
  - Mutual exclusion through atomic execution.
    Concurrent access to one tree is disallowed by explicit use of atomic transactions. For example, through semaphores.
Linearization to avoid interference

- The two red edges interfere with each other.
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- Ellipse on the left and circle on the right represent two different trees.
- Options:
  - Mutual exclusion through atomic execution.
    Concurrent access to one tree is disallowed by explicit use of atomic transactions. For example, through semaphores.
  - Linearization without atomic instructions
    Each concurrent step request the right to change a tree.
    Requests are prioritized.
    First request that does not create a circle is committed.
    Other requests are rejected and must be resubmitted.
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Limitations of parallel Kruskal

- Dense graphs always an obstacle.
  - All edges have to scanned: a dense graph with a million vertices might demand many terabytes of RAM memory.
  - Linearization of concurrent steps may lead to inefficient sequential processing of too many edges.

- Mitigation: Prune 30% heaviest edges of dense graphs.
  However...

Red edges are in 30% heaviest.
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2

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Vertex-centric processing

- Kruskal’s limitations are edge scanning limitations
  - Scanning all edges in graph can be quadratic in space and work on the number of vertices.
Vertex-centric processing

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  - Updating the mst in constructions and the super-vertices will always lead to slow sequential execution of parallel algorithms due to linearization of concurrent executions.
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  - Problem is intrinsic to Kruskal, Prim-Dijkstra and Borůvka algorithms.

- Divide-and-conquer might be the path to success.
Vertex-centric processing

- Kruskal’s limitations are edge scanning limitations
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  - Updating the **mst** in construction and the super-vertices will always lead to slow sequential execution of parallel algorithms due to linearization of concurrent executions.
  - Problem is intrinsic to Kruskal, Prim-Dijkstra and Borůvka algorithms.
- The **mst** construction will be more efficient if vertex centered.
- Divide-and-conquer might be the path to success.

\[
\begin{align*}
4 & \quad 1 \\
2 & \\
\end{align*}
\quad \quad \quad \\
\begin{align*}
10 & \\
5 & \quad 6
\end{align*}
\]
A graph $G = (V, E)$ with $n$ vertices and Euclidean distances is assumed.

- A k-d Tree or Ball Tree can be constructed with parallel work $O(n \lg n)$.
- A well separated decomposition of vertices $W = (A_1, B_1), \ldots, (A_w, B_w)$ can be constructed in $O(n \lg n)$ work, see CHEP 2013.
- In $O(n \lg n)$ work a subset $E' \subseteq E$ can be built where each $(a_i, b_i) \in E'$ is the Bichromatic Closest Pair of $(A_i, B_i)$. 
The idea of decomposing the vertices in *balls* originates in a 1977 paper and theorem by Yao:

- decompose given vertices to balls of up to 16 vertices, followed by computation \texttt{mst} of each ball, \texttt{mst} of super-vertices.
- Time reduction obtained to $O((n \lg n)^{1.8}$ down from $O((n \lg n)^2)$

Idea of decomposition to well separated balls originated in 1989 work by Vaidya, directed at sequential computations.

$O(n \lg n)$ work bounds obtained with uniform distributions.

For non-uniform distributions good bounded approximations for spanning trees weight can be guaranteed.
Experimental comparisons

- Euclidean graphs with uniform distributions of 3-d. Time in seconds.
- GPU: Tesla 2070.
- CPU: Intel Xeon E5620, 2.40GHz.
- \textbf{spmst}: Separated pair decomposition \textbf{mst} on 1 thread.
- \textbf{4-spmst}: Separated pair decomposition \textbf{mst} on 4 thread.
- \textbf{8-spmst}: Separated pair decomposition \textbf{mst} on 8 thread.
- \textbf{gpu-spms}\textbf{t}: Separated pair decomposition \textbf{mst} on GPU.
- \textbf{Kruskal}: standard sequential Kruskal.

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GPU computation of Spanning Trees
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Much to do yet

- This VERY much work in development.
- Work needed in:
  - Testing of parallel Kruskal and the filtering policy based on J Bentley D Johnson’s work.
  - Intensive test for both Kruskal and decomposition algorithms needed.
  - Transactional memory and delayed reservation should be tested with a parallel Borůvka algorithm.
  - No test has been performed so far with non-uniform distributions.
  - Intensive comparison of behaviours in presence of dense and sparse graphs has not been performed.

- This works is not part of the CMS development and we do not even know if CMS has a demand for the sort of algorithm here presented.