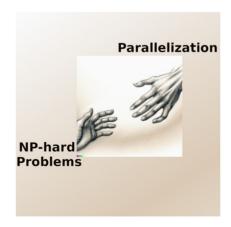
NP-Hard Problems Meet Parallelization





23-Apr-2024



Outline



- Motivation
 - Philosophy
 - Landscape
- Steiner Tree
 - Algorithm
 - Halt-Optimization
 - GPU-Optimization
 - Two-level parallelism
- Vehicle Routing
 - Local-search algorithm
- Summary
- Future Directions



Our Philosophy



... take a **fresh look** at some of the classic graph algorithms and devise **faster** and more parallel GPU and CPU implementations.

+

- Fallin et al.

NP-hard

=

Our Philosophy

A High-Performance MST Implementation for GPUs

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lines. In this example, the cheapest distribution grid that allows everyone to deliver or receive electricity is the MST shown.

B 2 C B 2 C 2 A 1 D

SC'23

ABSTRACT

Finding a minimum spanning tree (MST) is a fundamental graph algorithm with applications in many fields. This paper presents ECL-MST, a fast MST implementation designed specifically for GPUs. ECL-MST is based on a parallelization approach that unifies Kruskal's and Borůvka's algorithm and incorporates new and existing optimizations from the literature, including implicit path compression and edge-centric operation. On two test systems, it outperforms leading GPU and CPU codes from the literature on all of our 17 input graphs from various domains. On a Titan V GPU,

Current status



Irregular Mem. access

Poly-time Problems

- Parallelization is easier
- Algorithms are simpler
- Run few seconds on million/billion-scale
- Solution search space is small
- Exact solution

Examples

- Minimum Spanning Tree
- Single Source Shortest Path

Goal: Solve largest benchmark instances from DIMACS/PACE Challenges

NP-Hard Problems

- Comparitively difficult
- Complicated algorithms
- Few hours for thousand-sized instances
- Solution search space is large
- Tradeoff: Solution vs Time

- Steiner Tree Problem
- Travelling Salesman Problem
- Vehicle Routing Problem
- More practical applications

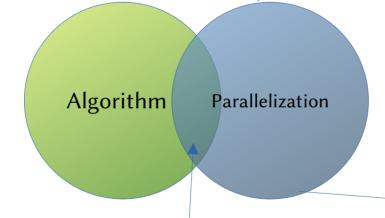
Algorithms and Optimizations



- Parallel Implementations chosen from
 - Efficient serial algorithm
 - Proven algorithm amenable for parallelization

Design parallelism-friendly algorithms

Optimizations



Peak performance

Data-driven versus Topology-driven Irregular Computations on GPUs

Rupesh Nasre The University of Texas Austin, Texas, USA Email: nagrafflices uteras adu

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Compiling Graph Applications for GPUs with GraphIt

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Abstract-The performance of graph programs depends highly on the algorithm, the size and structure of the input graphs, as well as the features of the underlying hardware. No single set of optimizations or one hardware platform works well across all settings. To achieve high performance, the programmer must carefully select which set of optimizations and hardware platforms to use. The GraphIt programming language make easy for the programmer to write the algorithm once and optimize it for different inputs using a scheduling language However, GraphIt currently has no support for generating high performance code for GPUs, Programmers must resort to re implementing the entire algorithm from scratch in a low-level language with an entirely different set of abstractions and optimizations in order to achieve high performance on GPUs.

We propose G2, an extension to the GraphIt compiler framework, that achieves high performance on both CPUs and GPUs using the same algorithm specification. G2 significantly expands the optimization space of GPU graph processing frameworks with a novel GPU scheduling language and compiler that enables combining load balancing, edge traversal direction, active vertexset creation, active vertexset processing ordering, and kernel fusion rations. G2 also introduces two performance optimization Edge-based Thread Warps CTAs load balancing (ETWC) and EdgeBlocking, to expand the optimization space for GPUs. ETWC improves load balancing by dynamically partitioning the edges of each vertex into blocks that are assigned to threads, warps, and CTAs for execution. EdgeBlocking improves the locality of the program by reordering the edges and restricting random memory accesses to fit within the L2 cache. We evaluate G2 on 5 algorithms and 9 input graphs on both Pascal and Volta generation NVIDIA GPUs, and show that it achieves up to 5.11× eedup over state-of-the-art GPU graph processing frameworks, and is the fastest on 66 out of the 90 experiments.

Index Terms—Compiler Optimizations, Graph Processing, [13], [14], [15], researchers have also used different hard-GPUs, Domain-Specific Languages

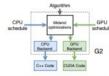


Fig. 1. G2 adds a new GPU backend to Graphlt that produces CUDA from the same Graphit algorithm language and a scheduling language tai

In prior work, we built the GraphIt DSL compiler [7] to generate high-performance CPU code from a h level algorithm language. GraphIt achieves state-of-the performance on CPUs across different algorithms and gr inputs by introducing a scheduling language to tune opting tions. The algorithm language has primitives for topol driven algorithms, data-driven algorithms, and priority-by algorithms. This algorithm and schedule representation m it easy for the programmer to write an algorithm once generate different highly-optimized implementations by sir changing the schedule. We will discuss in detail the Gra algorithm and scheduling languages in Section IV.

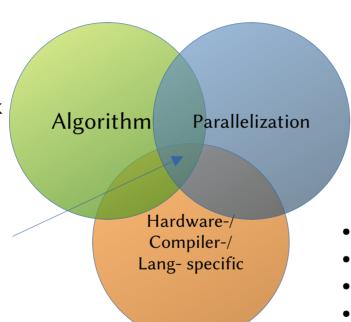
Apart from a large body of work for optimizing algorit on different inputs on CPUs [6], [8], [9], [10], [11], platforms for high-performance graph processing, inclu-GPUs [16], [17], [18], [19], [20], [21], [22], [23], [24],

Optimizing for peak performance



- Input Charateristics
 - Diameter
 - Max degree
 - Road/social network
- Properties of substeps

Peak performance



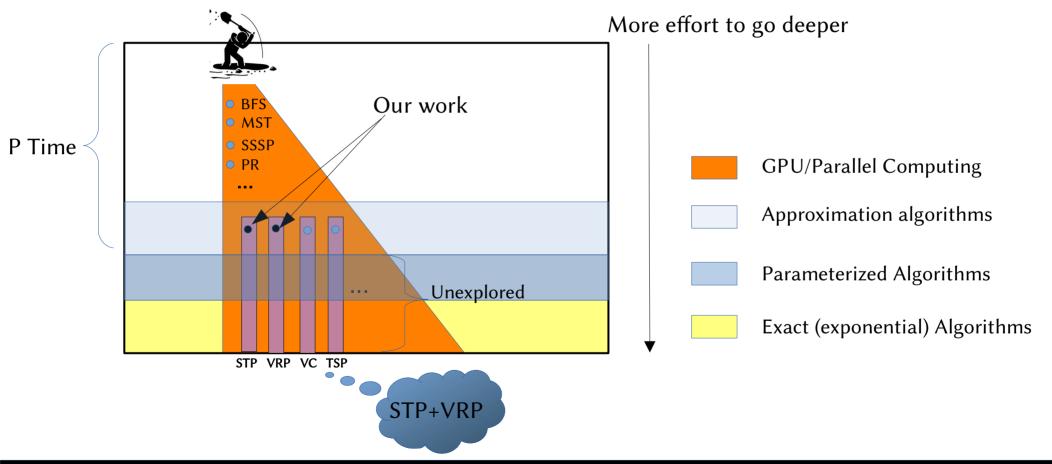
- Vertex-/Edge- centric
- Data-/Topology-driven
- Push-/Pull-based
- Load-balancing

...

- Architecture-specific
- Shared memory
- Warp-Intrincics
- Data accesses within reg/caches
- Vectorization loads/adds
- Language-specific 128b CAS CC9+
- Use profilers and https://godbolt.org

Landscape of Parallelization



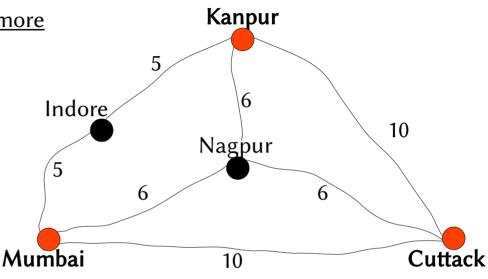


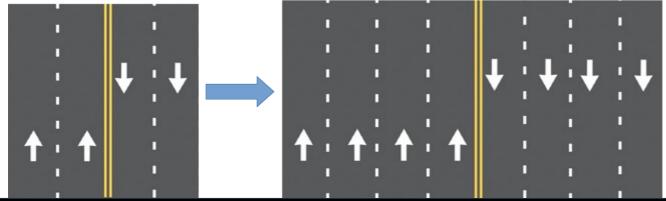
Steiner Tree - Example



 Let's say Highway Department wants to <u>add more</u> <u>lanes</u> to connect K, M and C

- Say K, M & C are important.
- Overall budget should be minimum
- Budget ∝ Distance





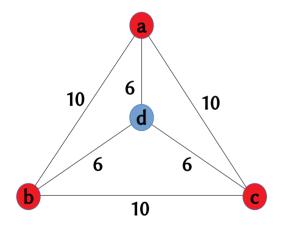
Steiner Tree Problem (STP) - Example



<u>Input</u>: Graph G(V, E, W) W:E → Z^+ and L⊆V terminals.

Output: A tree T'(V'⊇L, E'⊆E) of G such that minimize W(E').

// Minimum weighted tree with all terminals.



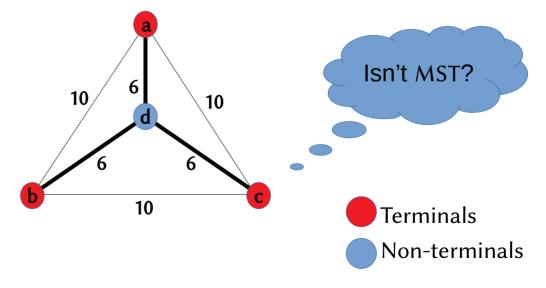


Fig 1 (a)

Fig 1 (b)

Steiner Tree Problem (STP) - Example



Input : Graph G(V, E, W) W: $E \rightarrow Z^+$ and L $\subseteq V$ terminals

Output: Minimum weighted tree with all terminals

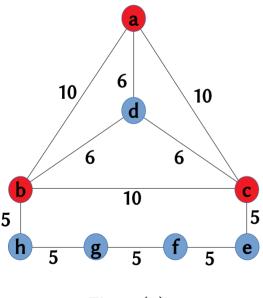


Fig 2 (a)

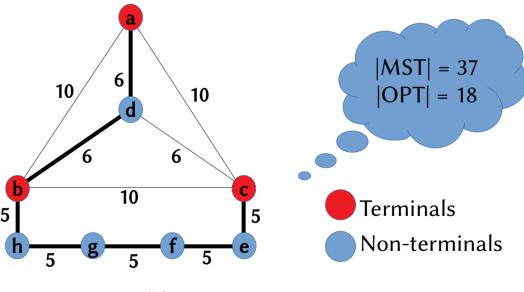


Fig 2 (b)

Steiner Tree Problem (STP) - Hardness



Input : Graph G(V, E, W) W: $E \rightarrow Z^+$ and $L \subseteq V$ terminals

Output: Minimum weighted tree with all terminals

Take away

MST solution is a valid feasible Steiner Tree solution

However, solution can be arbitrarily bad w.r.t OPT.

Special cases

•
$$L = \{u,v\}$$
 or $k = 2$ STP=ShortestPath_In_G(u,v)

• L = V or k = n STP=MST(G)

In general

STP is NP-Hard



In P Time

n

How to deal with NP-Hardness



What could be naive solutions? Enumerate all Spanning trees.

Approximation algorithm

- Runs in Polynomial time.
- Outputs an approximate solution with some guarantee.
 - e.g 2 or some constant, log n, etc.
- There are several algorithms
 - Kou, Markowsky and Berman[KMB81]
 - Mehlhorn [M88]
 - Robins and Zelikovsky [RZ2000]



L. Kou, G. Markowsky, and L. Berman. A fast algorithm for Steiner trees. Acta Informatica, 1981.

KMB Algorithm G(V,E,W,L)



Phase 1

// Input G

Computes the shortest distance between every pair of terminals

Phase 2

// Construct G'= K_L

Build a graph G' over terminals, having edge-weights corresponding to the shortest distances computed in Phase 1

// Every edge in G' corresponds
to a path in G

MST (G')

Phase 3

// Construct G''

For every edge in MST(G') substitute the edges with the corresponding shortest path in G

// Collect all the edges & vertices of the corresponding path to construct G"

MST(G")

Takeaway: One more invocation for SSSP/MST algorithm. $G \rightarrow G' \rightarrow G''$

KMB Algorithm - Running example



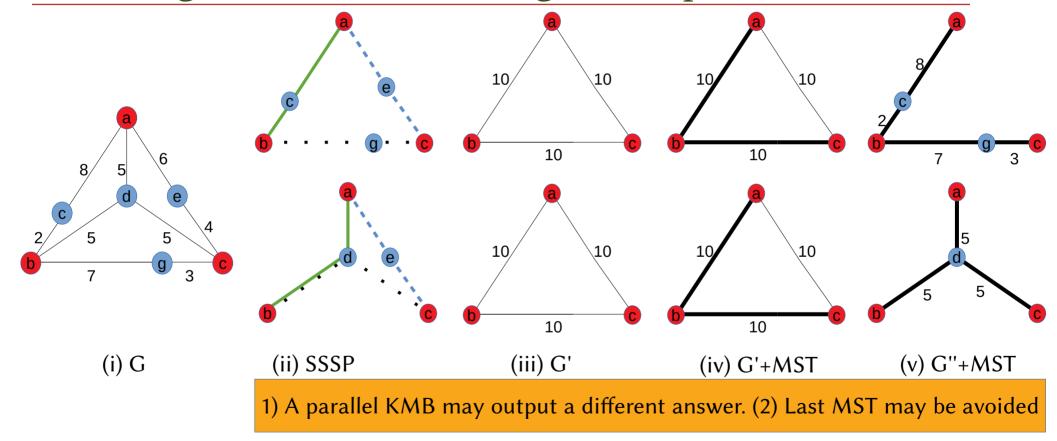


Fig. 3 Execution steps of KMB algorithm, where • are terminals and • are non-terminals.

KMB Algorithm G (V,E,W,L)



Phases 1 & 2 Observe: Two For-loops. For u in L { Naive? For v in L { $P_{uv} = ShortestPath(u,v)$ $W'(u,v) = |P_{uv}|$ T' = MST(G', W')

```
Phase 3

For (u,v) in edges of T' {

G'' = G'' \cup P_{uv}

//Add vertices & edges of P_{uv}
}

T'' = MST (G'', W)
```

KMB Algorithm G (V,E,W,L)



```
Input: Graph G(V, E, W, L)
Output: 2-approx Steiner Tree T (V_{\tau}, E_{\tau}) V_{\tau} \supseteq L
                                                Single For-loop
For u \in L {
                                               but runs SSSP to
  SSSP (G, W, L, u) with Halt
                                                  Completion
  Compute W' incrementally
T' = MST(G', W')
Compute G" and its vertices, adjList using T'
T'' = MST(G'', W)
return T"
```

CPU Implementation - Optimization



SSSP-halt optimization

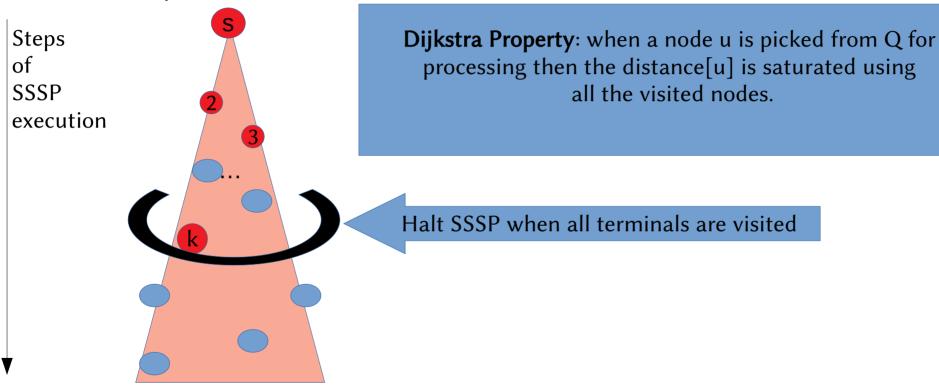


Fig. 4 SSSP-halt visualization

KMB Algorithm G (V,E,W,L)



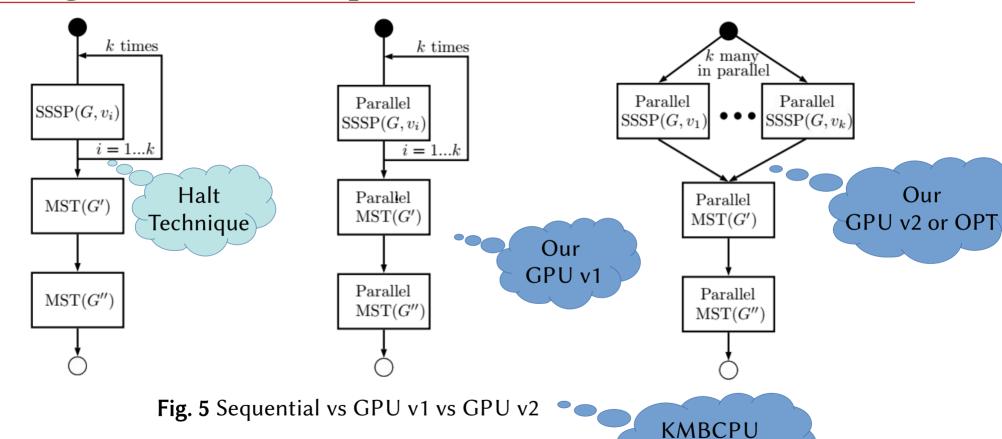
```
Input: Graph G(V, E, W, L)
Output: 2-approx Steiner Tree T (V_{\tau}, E_{\tau}) V_{\tau} \supseteq L
For u \in L
  parallel SSSP(G, W, L, u);
  Compute W' incrementally;
T' = parallel MST(G', W');
Compute G" and its vertices, adjList;
T'' = parallel MST(G'', W);
return T"
```

A novel aspect of our work is to run multiple parallel-SSSPs in parallel.

Subroutines?
Gunrock

Design choice for parallelization

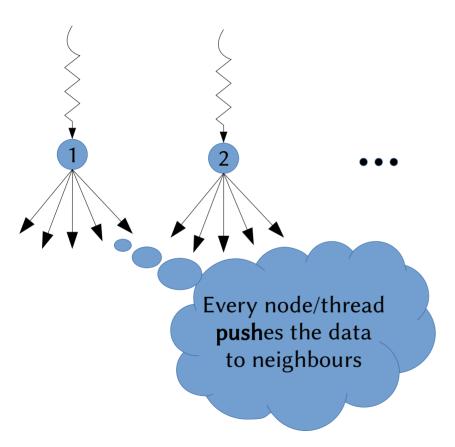


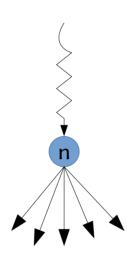


KMBGPU

GPU Implementation - SSSP







- n-threads
- One thread for each node
- Performs RELAX in parallel
- RELAXes its neighbours
- Till there is no change

Fig. 6 push-SSSP

KMB Algorithm G(V,E,W,L)



```
MAIN
For s in L {
 ThdsPerBlk = 512; // or 1024
 Blks = [n/ThdsPer Blk];
 do {
   INIT-KERNEL<Blks,ThdsPerBlk>(s, d, p, n);
   RELAX-KERNEL<Blks,ThdsPerBlk>(.., s, d, p, changed, n);
                       //= = = = =
   CopyTo(DArray, d<sub>s</sub>);
   CopyTo(PArray, p<sub>s</sub>);
                       // From Device to Host
   } while (hChanged);
```

 We need the p[] for knowing the intermediate vertices in the shortest path

KMB Algorithm G(V,E,W,L)



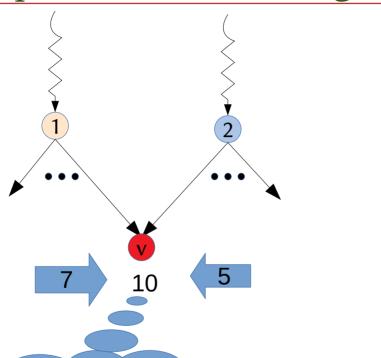
```
RELAX-KERNEL(..,s, d, p, changed, n) {
                                                                   Note:
u = tid // compute tid;
If tid < n {
  For v \in adjacent[u] \{ // Using CSR arrays \}
     // Relax Operation (u, v, W(u,v))
     newCost = d_s[u] + W(u, v);
     old = d_s[v];
      If newCost < old
         Atomic-MIN(d<sub>s</sub>[v], newCost);
                                                     Is it enough?
     // Updates Parent array
     If Atomic-MIN is success {
        p_{s}[v] = u;
         changed = true;
```

NP-Hard Problems meet Parallelization

 Parent of v should be updated if the Atomic-MIN is success.

Parent update - Challenge





Two threads want to update distance of their common neighbour v

```
<snip>
newCost = d_s[u] + W(u, v);
old = d_s[v];
If newCost < old
     Atomic-MIN(d<sub>s</sub>[v], newCost);
// Updates Parent array
If Atomic-MIN is success {
    p_{s}[v] = u;
     changed = true;
</snip>
```

Fig. 7 Challenges in parent update

Even **Gunrock** has a challenges in updating p array consistently. Listed as known issues https://github.com/gunrock/gunrock/releases/tag/v1.0

Parent update - Challenge





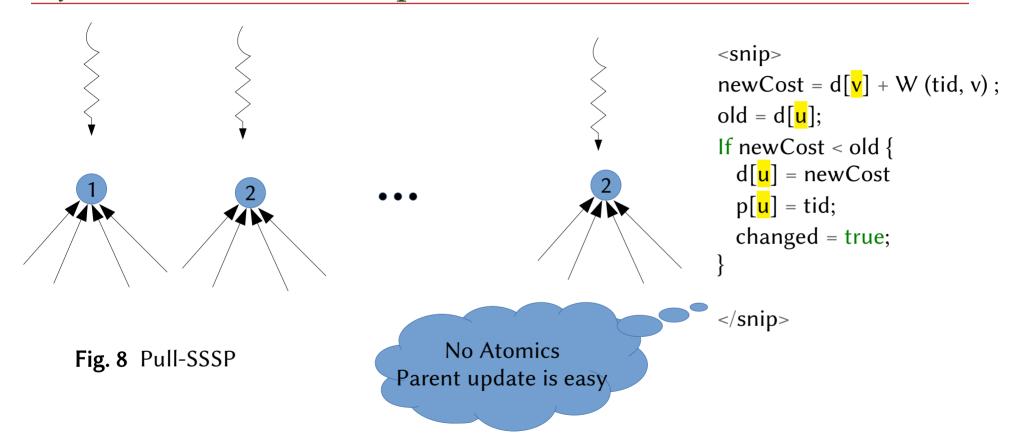
Thread 1	<u> </u>	Thread 2		
	1 2		<snip></snip>	
newCost=7	Time	newCost=5	newCost = d[u] + W(u, v);	
old=10	7 5	old=10	old = d[v];	
			If newCost < old	
d[v]=7 //oldA=10			oldA=Atomic-MIN(d[v], newCost);	
		d[v]=5 //oldA=7		
			// Update's Parent array	
			If Atomic-MIN is success {	
		p[v]=2		
		P['] ~	p[v] = u;	
			changed = true;	
p[v] = 1			}	
	It is a challen	It is a challenge to find which "thread" updated d[v] to the minimum		

How to update both distance and parent at the same time?

Wrong!

Synchronization optimization • Pull





Because, one thread is writing to an index

GPU Optimizations



- Synchronization
 - Push
 - Pull
- Computation
 - Data-driven
 - Edge-based
 - Controlled Computation unrolling
 - ∆²
 - 2Δ
 - t∆
- Memory
 - Shared memory

 Δ – max degree of the graph

GPU Optimizations



- Synchronization
 - Push
 - Pull
- Computation
 - Data-driven
 - Edge-based
 - Controlled Computation unrolling
 - Δ²
 - 2Δ
 - <u>t∆</u>
- Memory
 - Shared memory



 Δ – max degree of the graph

Compute optimization



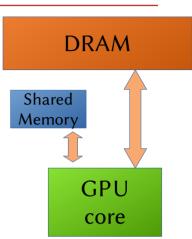
- Computation Unrolling
 - Instead of one thread doing Δ work, perform more work per thread
 - Update also neighbours of neighbours (Δ^2)
 - Repeat the work; Say 2 times or t times $(2\Delta \text{ or } t\Delta)$; e.g. we do pull 3 times in the kernel 3-pull
- Data-driven
 - Needs Worklist (WL)
 - Active/Change nodes are inserted into WL
- Edge-based optimization
 - m-threads are launched
 - RELAXes one edge or a group of edges



Memory optimization



- Programmable shared memory can be useful
- When there are multiple reads to DRAM
- We can move data to shared memory
- For e.g. In 3-pull, we moved CSR AdjList to shared
- As the neighbours AdjList is accessed 3 times
- Of the total 48K per block
- when using 512 threadPerBlock we have 24 words to store per thread
- Hence, if degree(node) < 25 we use shared, we move CSR AdjList[node] to Shared
- With shared memory we achieve 25% of improvement in 3-pull



Double-barrel approach



- SSSP happens in parallel
- To run two SSSP, we have to run one after the other
- Instead we use Double-barrel approach
- This can be generalized (p-SSSP)



In our Double-barrel approach, we run two individually parallel SSSPs also in parallel.

Image source: https://stock.adobe.com/

Double-barrel approach



```
Result Array: d[n]
Initialize(d=INTMAX)
d[src] = 0
FixedPoint{
     doRELAX(G, d, changed ...);
Result Array: d[2n]
Initialize(d=INTMAX)
d[src1] = 0; d[n+src2] = 0
FixedPoint{
    doRELAX(G, dist, changed, ...);
```

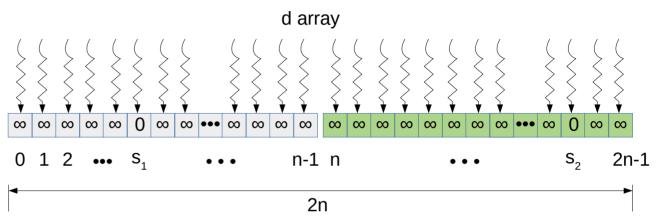


Fig. 9 Double-barrel approach.



Key takeaways so far



- Solving Steiner Tree Problem is NP-hard
- KMB Algorithm, a 2-approximation algorithm
- CPU implementation has SSSP-halt optimization
- SSSP with parent array update <u>was</u> challenging
- Pull-based SSSP is great for KMBGPU even without SSSP-halt
- Parallel-SSSPs in parallel (p-SSSP)

Experimental setup & Graphsuite



CPU

- Intel(R) Xeon(R) E5-2640 v4 @ 2.40GHz
- 64GB RAM

GPU

- Tesla P100 @ 1.33 GHz
- 12GB global memory
- •
- GCC 7.3.1 with O3
- CUDA 10.2

Graphsuite

- Total 14 Graphs
 - 11 from PACE Challenge [PACE2018]
 - 2 from SteinLib
 - 1 from SNAP

Baselines

- PACE'18 Winner CIMAT [PACE2018]
- ODGF's KMB/JEA [BC19]

- CIMAT Team https://github.com/HeathcliffAC/SteinerTreeProblem
- S. Beyer and M. Chimani, Strong Steiner Tree Approximations in Practice, JEA 2019.

Experiments: Speed-up



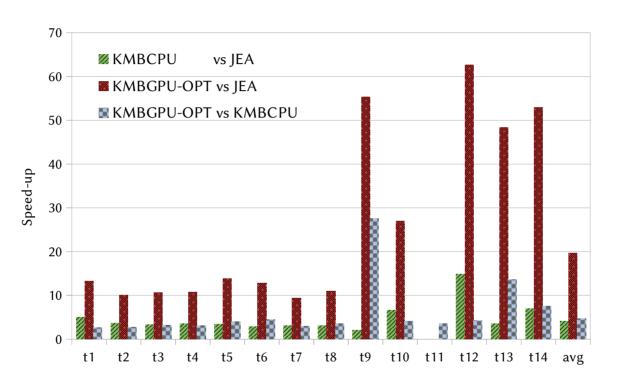


Fig. 10 Speed-up comparisons of the implementations (higher is better). JEA timed-out on t11

Takeaway: KMBCPU and KMBGPUOPT is better than JEA

Comparison of GPU time with Shared mem.



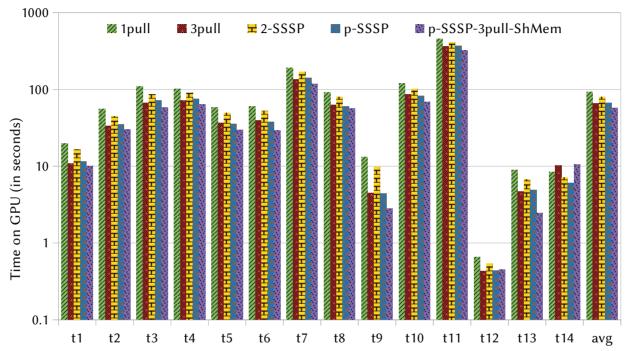


Fig. 11 Comparison of 1-Pull, 3-Pull, Double-barrel & KMBGPU-OPT

Takeaway: Combining GPU optimizations p-SSSP, 3-Pull & Shared memory performs best.

Comparison of p-SSSP



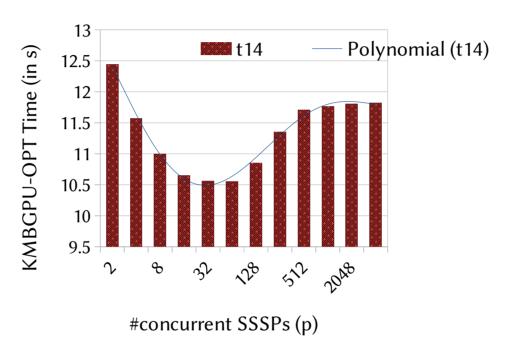


Fig. 12 KMBGPU with varying p-SSSP for the same graphs t14 (Smaller is better).

Takeaway: As we increase the #parallel SSSPs it reaches a point and then increases.

Experiments - Scalability of GPU and CPU



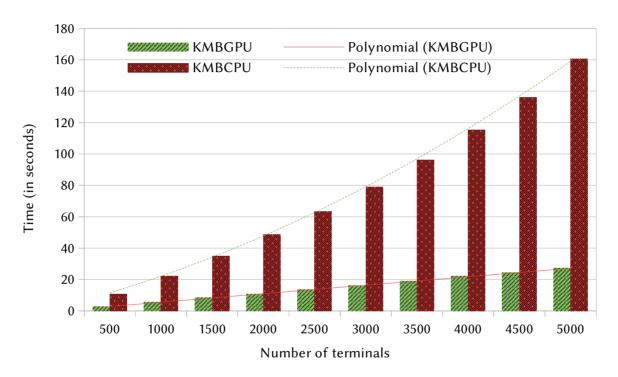


Fig. 13 Scalability plot on **t14** with increasing terminal size (lower is better)

Takeaway: KMBGPU-OPT scales better than KMBCPU

Summary - STP



- Optimized CPU implementation for KMB algorithm
 - Novel SSSP-halt technique
 - Speed-up of 4x (average) over JEA/OGDF's KMB[BC19]
- Optimized GPU implementation for KMB algorithm
 - Novel p-SSSP technique (multiple parallel-SSSP in parallel)
 - Speed-up of 20x (average) over sequential JEA[BC19]



S. Beyer and M. Chimani, Strong Steiner Tree Approximations in Practice, JEA 2019.

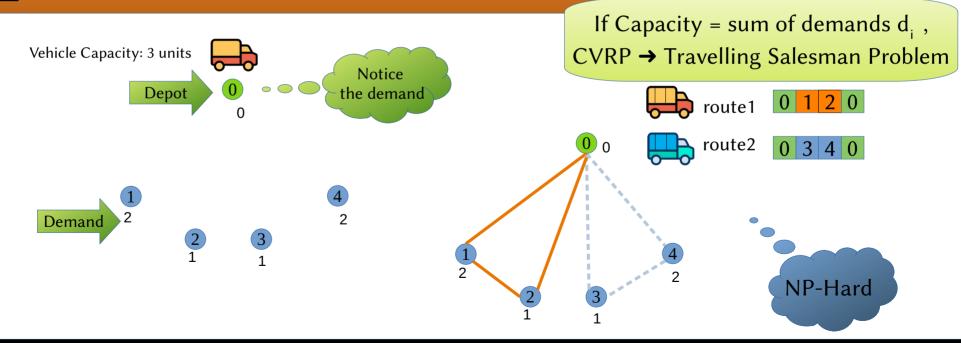
Capacitated Vehicle Routing Problem (CVRP)



Input : Given n nodes (single Depot and customers) with their coordinates (x_i, y_i) and demands $d_i > 0$ for $i \in n$, Vehicle capacity C. Node 0 is Depot and has zero demand.

Output: Set of routes serving all the customers respecting the vehicle capacity from/to Depot.

Goal : Minimize total distance travelled.



CVRP Limitations



Current state-of-the-art

- work only on smaller instances
- has a large solution Gap
- takes a lot of time

Instance	Number of	Time (s)	
	customers	Base2	Base1
Flanders2	30,000	8,355	2,534
Flanders1	20,000	7,768	2,031
Brussels1	15,000	7,164	871

Table 4: State-of-the-art GPU methods are time-consuming.



RQ1. Can we invent a simpler algorithm? RQ2. Can we reduce Gap on large instances?



RQ3. Design Parallelization friendly algorithms?

Our ParMDS

- Serial and **Parallel** implementation
- Combining MST and DFS
- Uses Local-search approach
- Uses Randomization approach

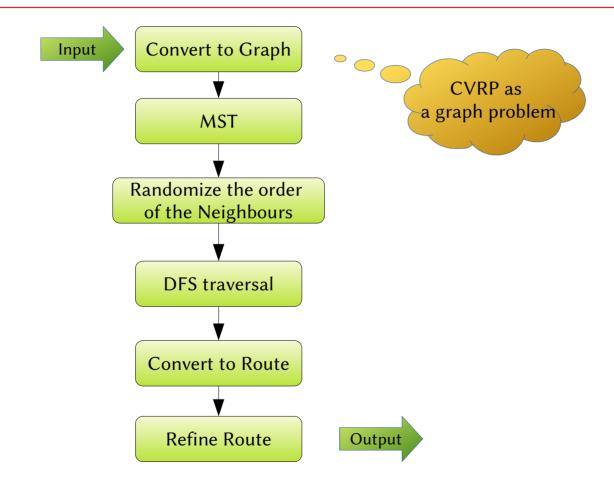
$$Gap = \frac{Z_S - Z_{BKS}}{Z_{BKS}} \times 100$$

Baseline 1: P. Yelmewad and B. Talawar. Parallel Version of Local Search Heuristic Algorithm to Solve Capacitated Vehicle Routing Problem, Cluster Computing, 2021.

M. Abdelatti and M. Sodhi. An improved GPU-accelerated heuristic technique applied to the Capacitated Vehicle Routing Problem, GECCO, 2020.

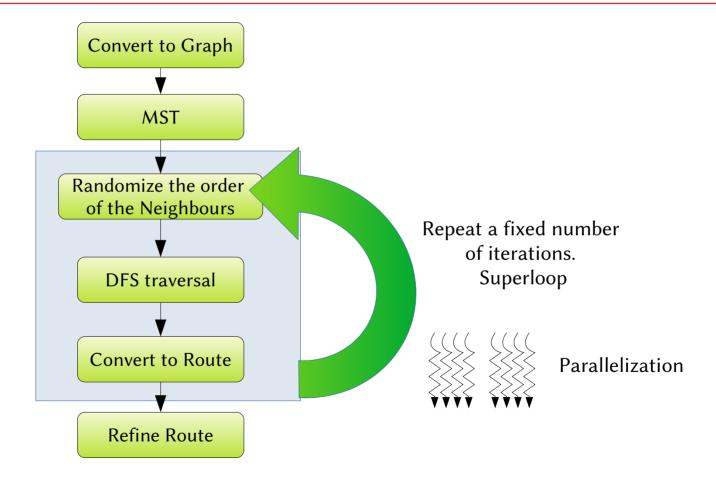
Overview - ParMDS





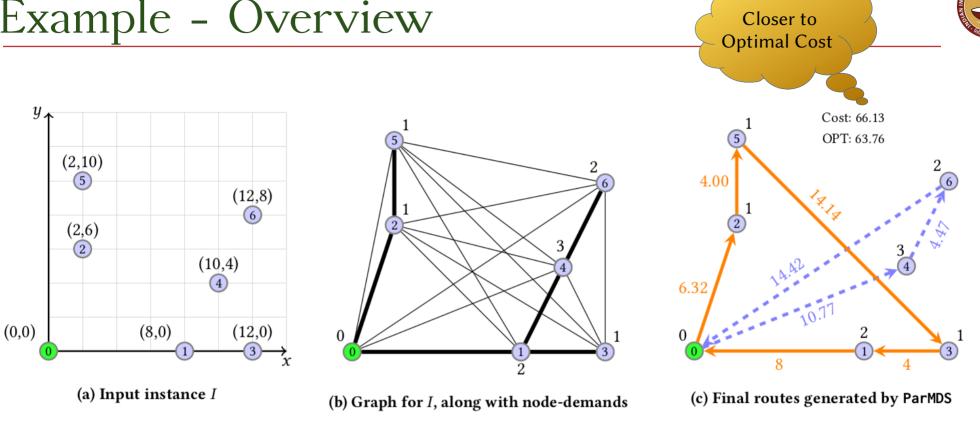
Overview - ParMDS





Example - Overview

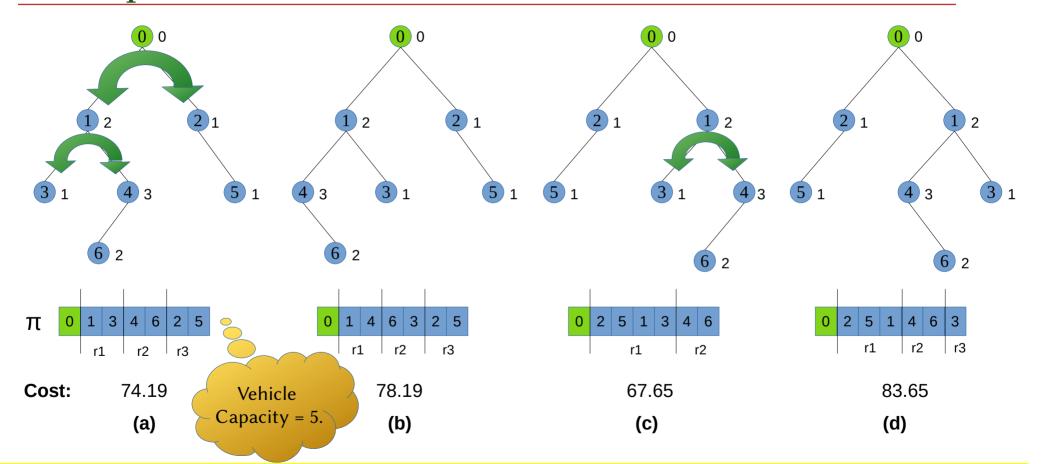
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ParMDS on an example input instance with n = 7 and Vehicle Capacity = 5.

Example - DFS and Randomization

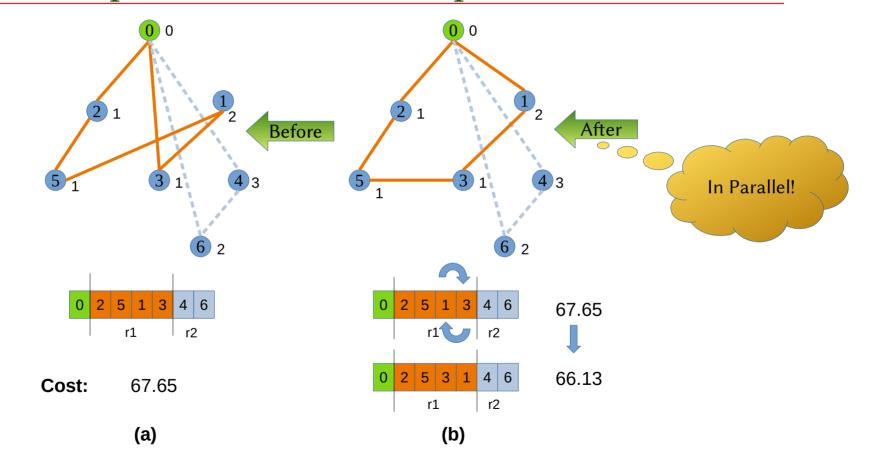




Takeaway: Randomizing neighbours of MST may yield a different DFS ordering. Hence, a different route!

Intra-route optimization - 20pt





ParMDS Algorithm

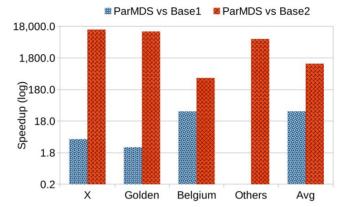


```
Input: G = (V, E), Demands D := \bigcup_{i=1}^n d_i, Capacity Q
   Output: R, a collection of routes as a valid CVRP solution
            C_R, the cost of R
1 T \leftarrow PRIMS MST(G)
                                                    /* Step 1 */
_2 C_R \leftarrow \infty
for i \leftarrow 1 to \rho do /* Superloop */ /* Parallel */
                                                                                       /* Standard: stride = 1;
                                                                        Zoom-in
       T_i \leftarrow \text{Randomize}(T) / * \text{Shuffle Adjacency List } * /
                                                                                       /* Strided : stride = #CPU cores
       \pi_i \leftarrow \text{DFS\_Visit}(T_i, \text{Depot})
                                         /* Step 2 */
                                                                                       /* Parallel for loop: Standard/Strided
                                                                                                                                                        */
       R_i \leftarrow \text{Convert To Routes}(\pi_i, Q, D) /* Step 3 */
                                                                                     1 for i \leftarrow 1; i \leq \rho; i = i + stride do
      C_{R_i} \leftarrow \text{CALCULATE\_COST}(R_i) /* Parallel */
                                                                                           for v \in V do
      if C_{R_i} < C_R then
                                                                                               /* seed ← constant or i or rand()
                                                                                                                                                       */
          C_R \leftarrow C_{R_i} /* Current Min Cost */
R' \leftarrow R_i /* Current Min Cost Route */
                                                                                               Shuffle-neighbors(AdjList(v), seed);
                                                                                           end
       end
12 end
                                                                                     6 end
13 R \leftarrow \text{Refine}_{\text{ROUTES}}(R')
                                                     /* Step 4 */
                                                                                     7 ...
14 return R, C_R
```

Experiments

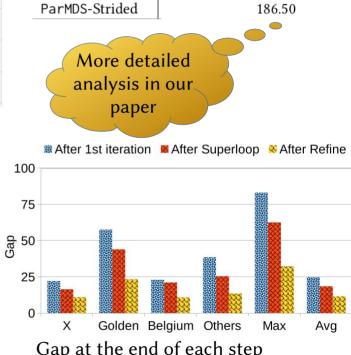


- 130 Instances of CVRPLIB
- Intel Xeon CPU F5-2640 v4
- Baselines on GPU
 - NVIDIA's Tesla P100
 - **CUDA 11.5**



Speedup of ParMDS vs. baselines

- Our Code uses
 - SeqMDS: GCC 9.3.1
 - ParMDS: nvc++ compiler NVIDIA's HPC SDK 22.11



Execution Time (s)

using Random

1,722.44

1,522.26

Gap at the end of each step

Method

SeaMDS

ParMDS-Standard

Summary



- Fresh perspective to <u>design</u> parallelism-friendly algorithms
- Performance: Algorithmic-, Parallelism- & Platform- specific Optimizations
- Our techniques are applicable
 - Two-level parallelism (p-SSSP) technique
 - Strided parallel Local-search
- Promising future directions in our area (next 3-10 years)
 - Paradigm specific parallelization: Greedy, Dynamic Programming
 - Most STL algorithms would run parallel // My Prediction
 - Single source code for muti-core GPU and GPU

Thank you!

Questions?

