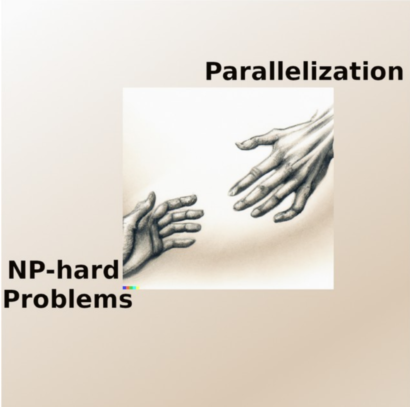
NP-Hard Problems Meet Parallelization

https://bit.ly/rajesh-viva



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Outline

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

PhD journey

Our Philosophy

... take a **fresh look** at some of the classic graph algorithms and devise **<u>faster</u>** 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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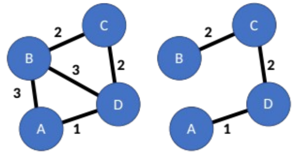
SC’23

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,

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



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

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

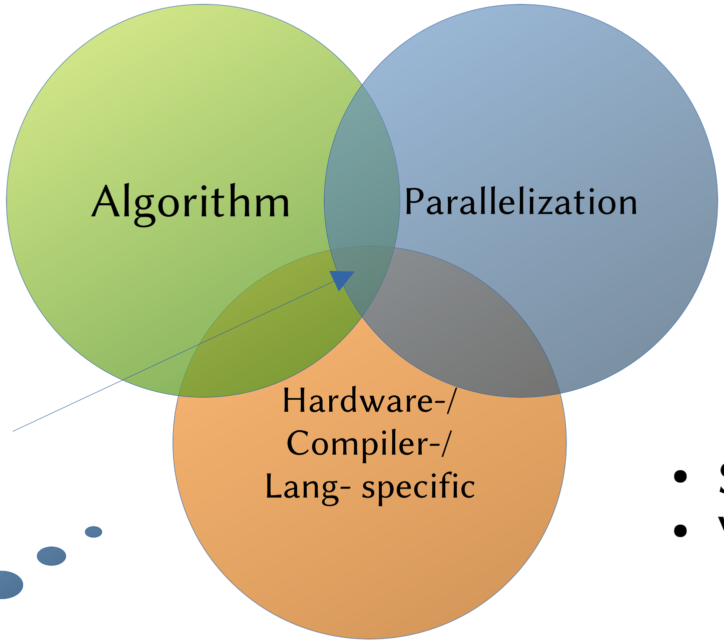
Goal: Solve largest benchmark instances from DIMACS/PACE Challenges

Optimizing for peak performance

- Input Charateristics
- Properties of substeps

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

  …

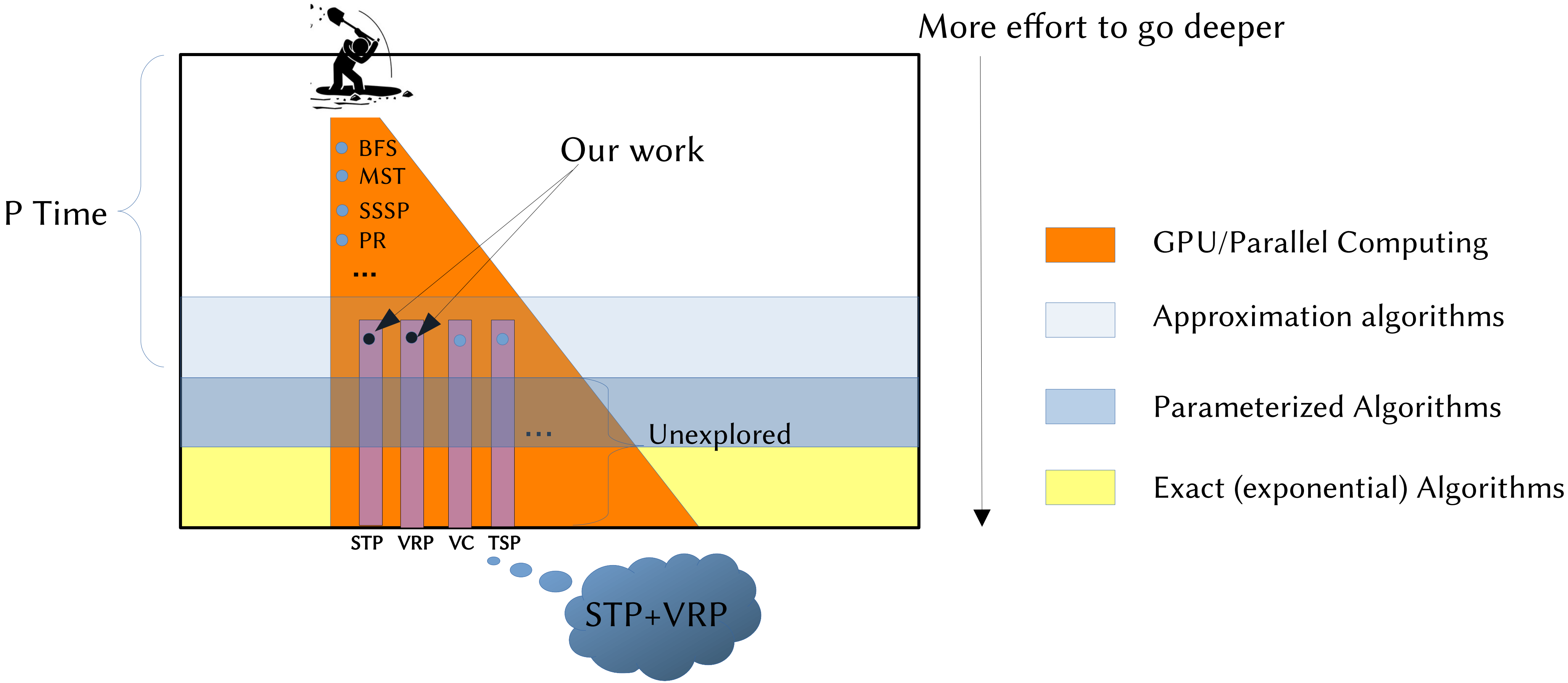


Peak performance

- Shared memory
- Warp-Intrincics

Is that all?

Landscape of Parallelization



Steiner Tree Problem (STP) – Example

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

Output: A tree $T'(V' \supseteq L, E' \subseteq E)$ of G such that minimize $W(E')$.

// Minimum weighted tree with all terminals.

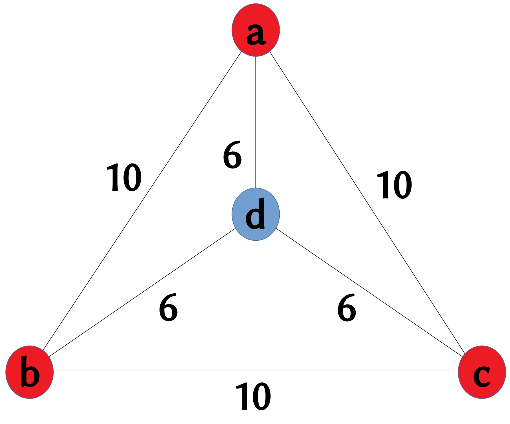


Fig 1 (a)

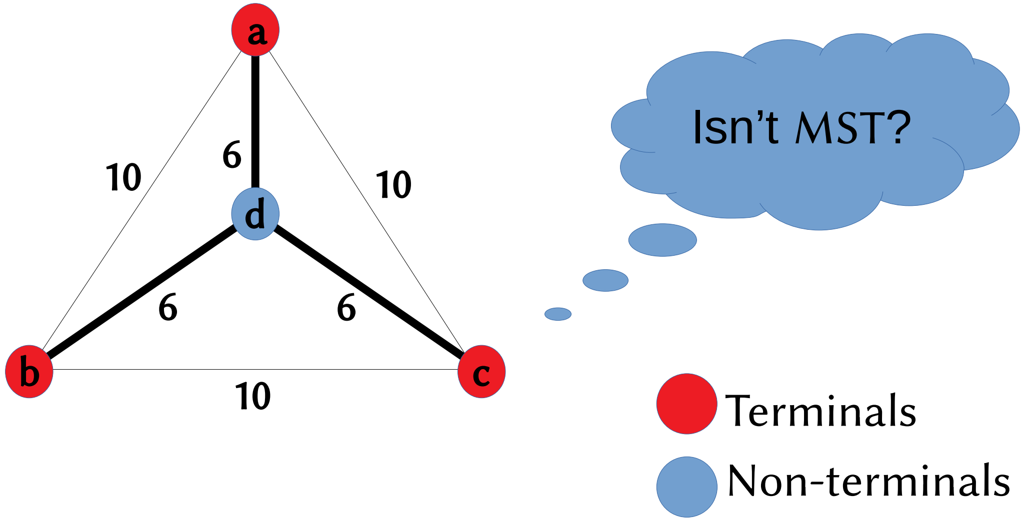


Fig 1 (b)

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

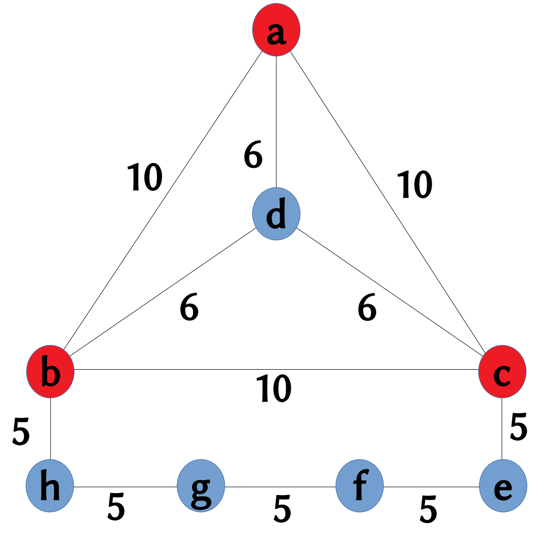


Fig 2 (a)

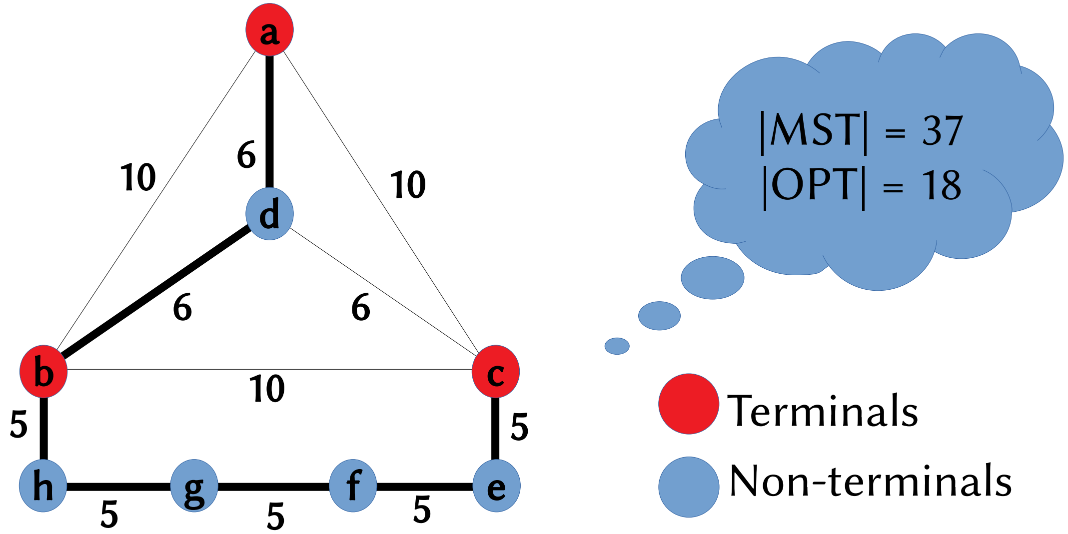


Fig 2 (b)

Steiner Tree Problem (STP) - Hardness

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

<u>Output</u> : Minimum weighted tree with all terminals

2 n

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 P Time

- In general STP is NP-Hard

Approximation algorithms

How to deal with NP-Hardness

- What could be naive solutions? Enumerate all Spanning trees.

<u>Approximation algorithm</u>

- 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]

KMB

$|ALG| <= 2 \, |OPT|$

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→G'→G''

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

Phases 1 & 2

Observe:
Two For-loops.
Naive?

```
For u in L {
  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'' ∪ 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_T , E_T) $V_T \supseteq L$

For u ∈ L {

SSSP (G, W , L, u) with Halt

Compute W' incrementally

}

T' = MST(G' ,W')

Compute G'' and its vertices, adjList using T'

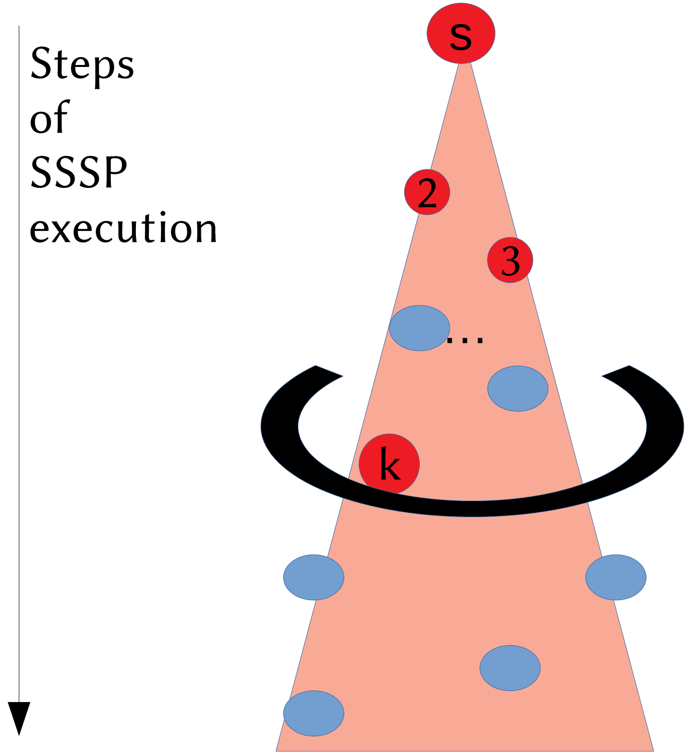
T'' = MST(G'' ,W)

return T''

Single For-loop but runs SSSP to Completion

CPU Implementation - Optimization

- SSSP-halt optimization



Dijkstra Property: when a node u is picked from Q for processing then the distance[u] is saturated using all the visited nodes.

Halt SSSP when all terminals are visited

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_T , E_T) $V_T \supseteq L$

For u ∈ 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

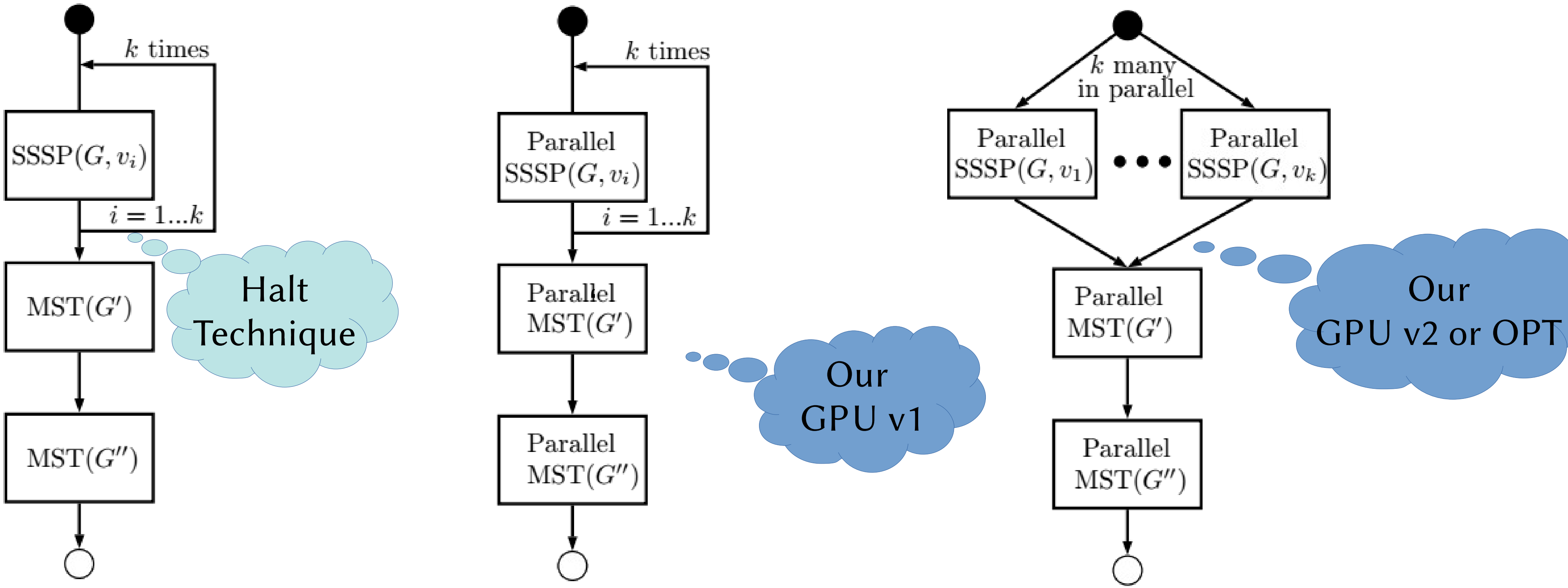


Fig. 5 Sequential vs GPU v1 vs GPU v2

KMBCPU
KMBGPU

GPU Implementation - SSSP

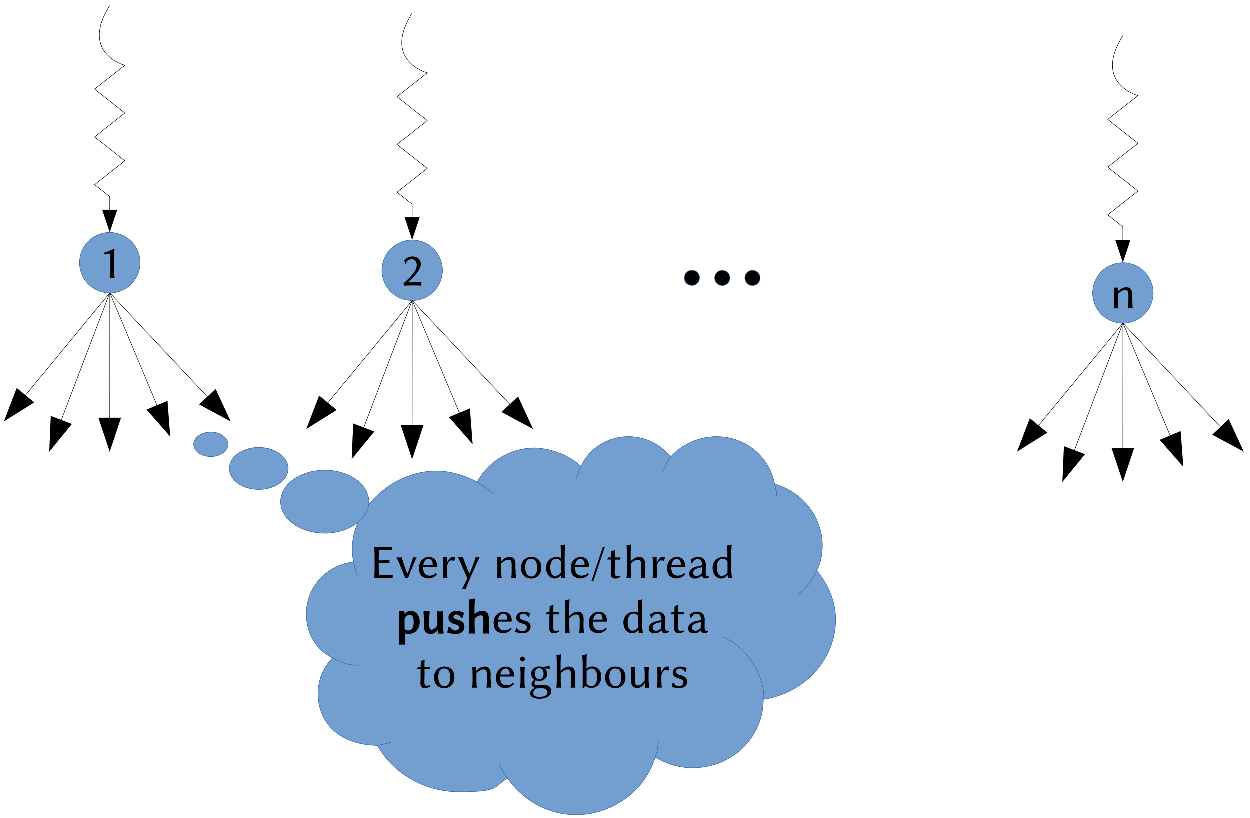


Fig. 6 push-SSSP

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

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_s , p_s , n);
    RELAX-KERNEL<Blks,ThdsPerBlk>(.., s, d_s , p_s , changed, n);
    CopyTo(DArray, d_s );            //= = = = =
    CopyTo(PArray, p_s );            // From Device to Host
    CopyTo(hChanged, changed); // = = = = =
  } while (hChanged);
}
```

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

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

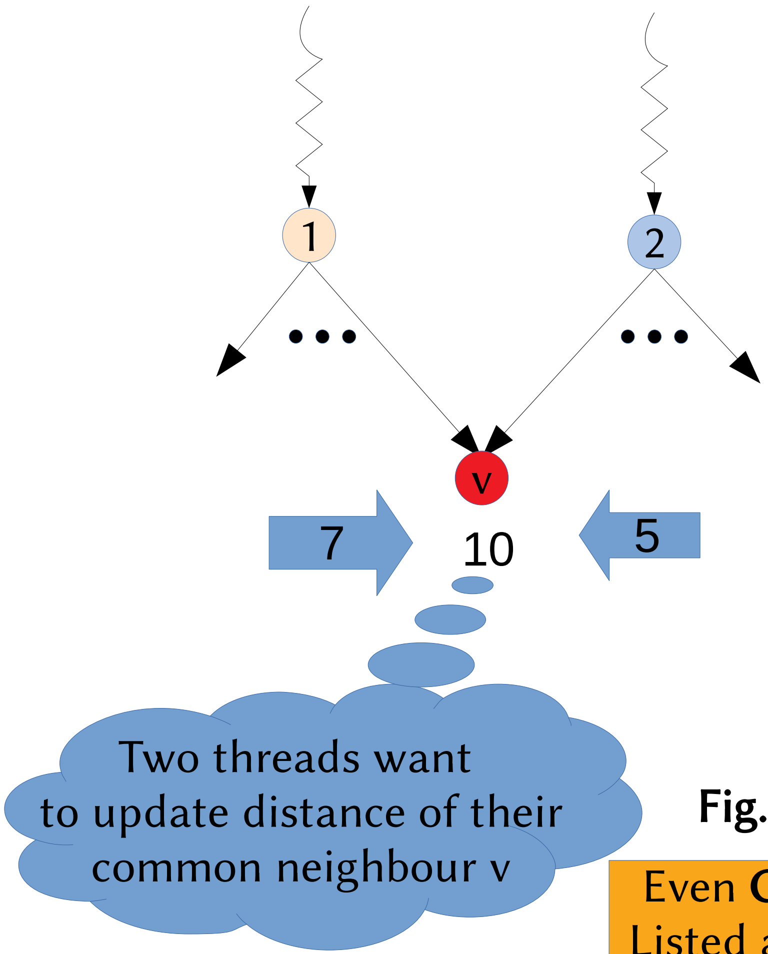
```
RELAX-KERNEL(..,s, d_s , p_s , changed, n) {
u = tid  // compute tid;
If tid < n  {
   For v ∈ adjacent[u] { // Using CSR arrays
      // Relax Operation (u, v, W(u,v))
      newCost = d_s[u] + W(u, v) ;
      old = d_s[v];
      If newCost < old
           Atomic-MIN(d_s[v], newCost);
      // Updates Parent array
     If Atomic-MIN is success {
         p_s[v] = u;
         changed = true;
     }
}}
```

Is it enough?

Note :

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

Parent update - Challenge



<snip>

..

newCost = d_s[u] + W(u, v) ;

old = d_s[v];

If newCost < old

    Atomic-MIN(d_s[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

Synchronization optimization • Pull

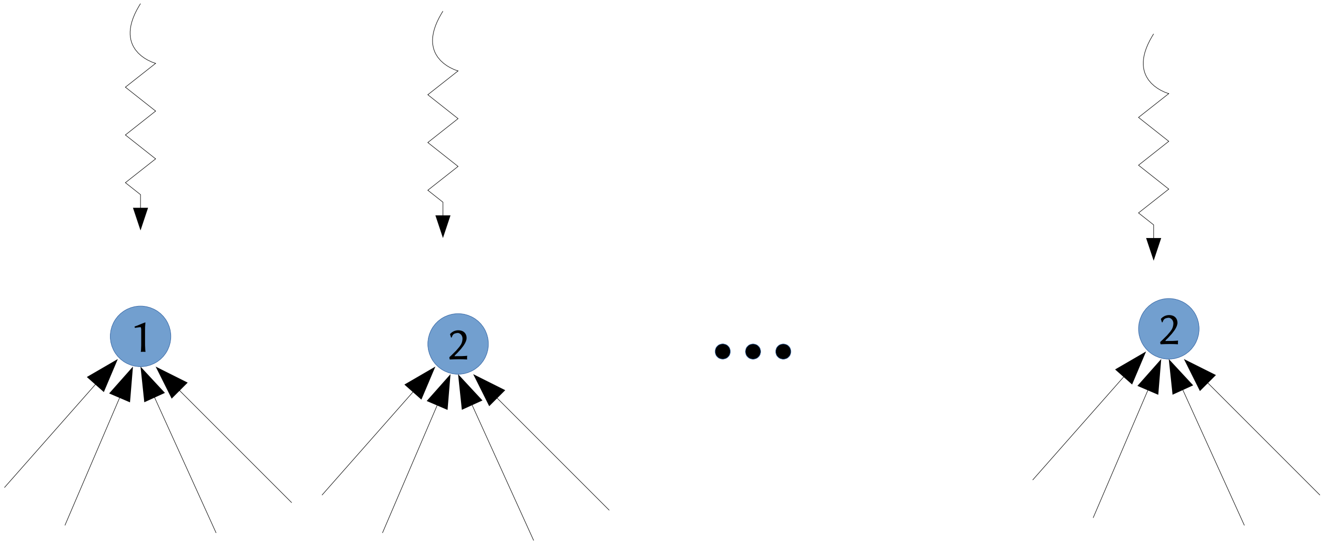


Fig. 8 Pull-SSSP

```
<snip>
newCost = d[v] + W (tid, v) ;
old = d[u];
If newCost < old {
   d[u] = newCost
   p[u] = tid;
   changed = true;
}

</snip>
```

No Atomics
Parent update is easy

Because, one thread is writing to an index

GPU Optimizations

- Synchronization
  - Push
  - Pull
- Computation
  - Data-driven
  - Edge-based
  - Controlled Computation unrolling
    - Δ^2
    - 2Δ
    - $t\Delta$
- Memory
  - Shared memory

Δ – max degree of the graph

GPU Optimizations

- Synchronization
  - Push
  - **Pull**
- Computation
  - Data-driven
  - Edge-based
  - **Controlled Computation unrolling**
    - Δ^2
    - 2Δ
    - **$t\Delta$**
- Memory
  - **Shared memory**

These worked best for us!

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 (2Δ or tΔ); 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

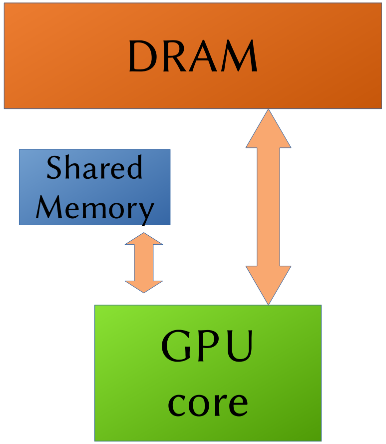
Give more work
or repeat the work?

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, …);
}

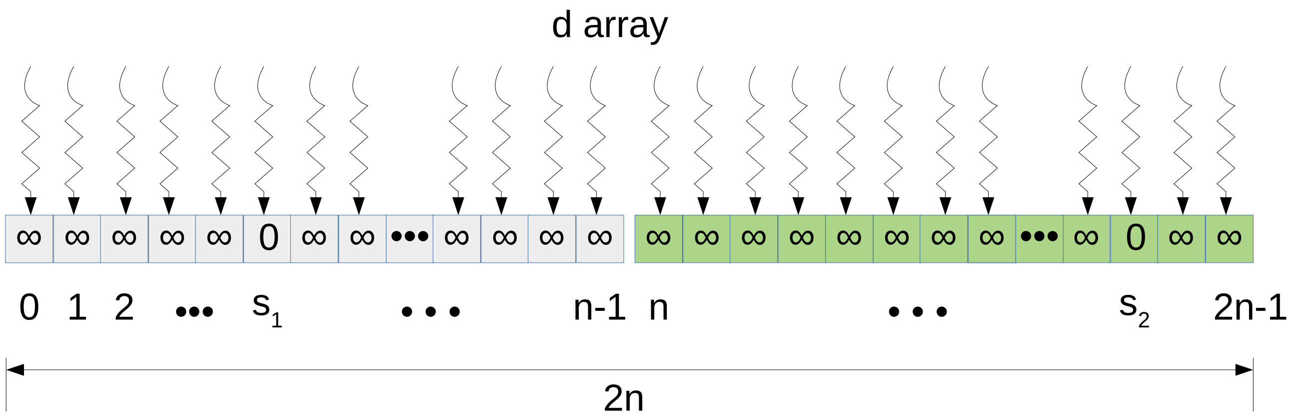
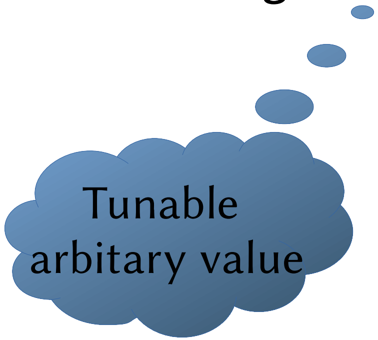


Fig. 9 Double-barrel approach.



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

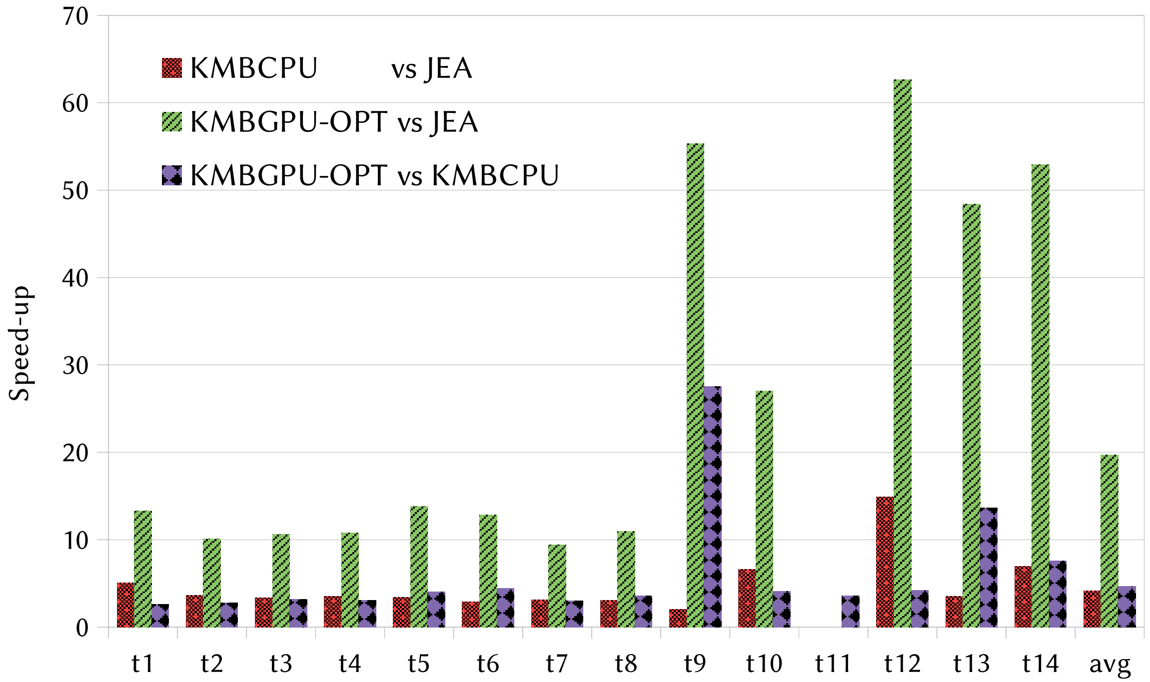


Fig. 10 Speed-up comparisons of the implementations (higher is better). JEA timed-out on t11

Takeaway: KMBCPU and KMBGPUOPT is better than JEA

Comparison of p-SSSP

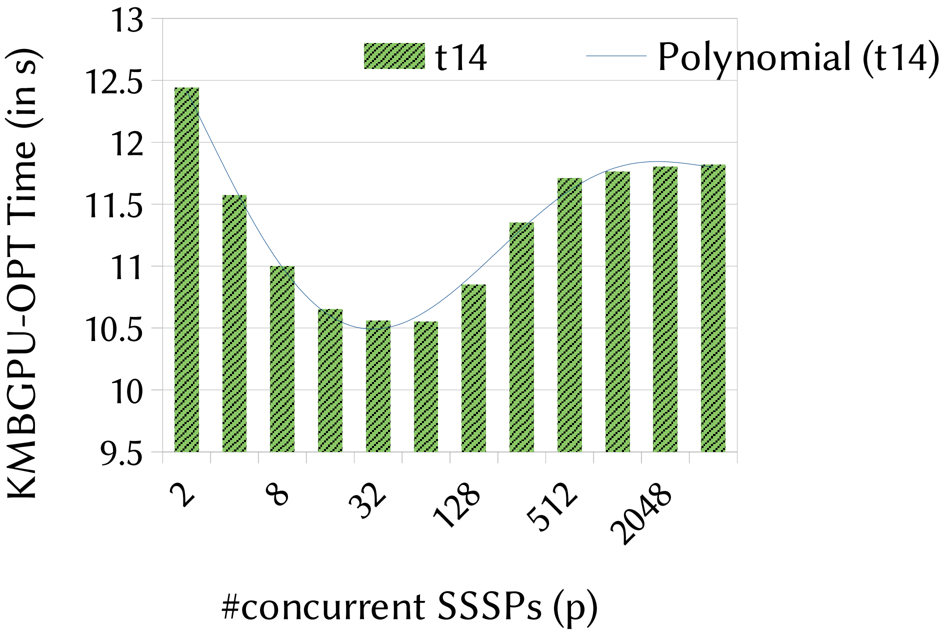


Fig. 12 KMBGPU with varying p-SSSP for the same graphs t14 (Smaller is better).

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

Experiments – Scalability of GPU and CPU

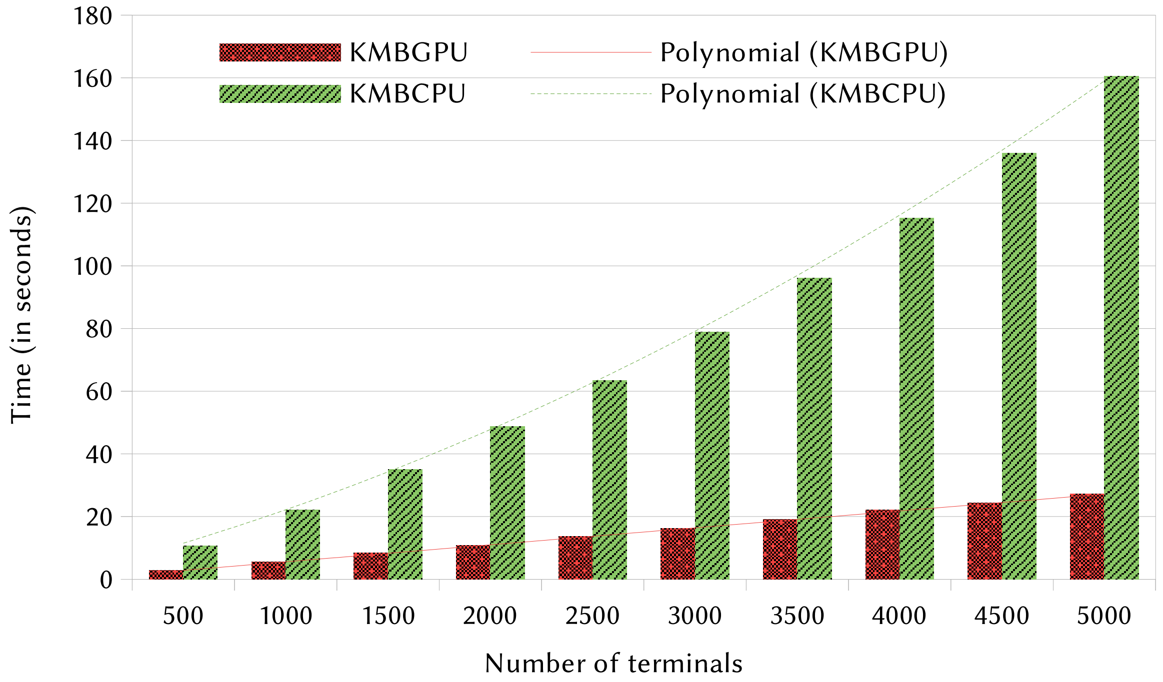


Fig. 13 Scalability plot on **t14** with increasing terminal size (lower is better)

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]

</work>

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

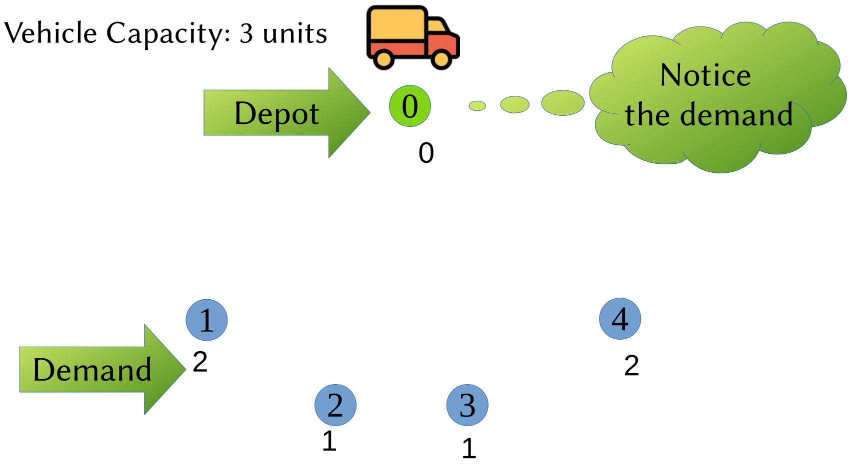
Capacitated Vehicle Routing Problem (CVRP)

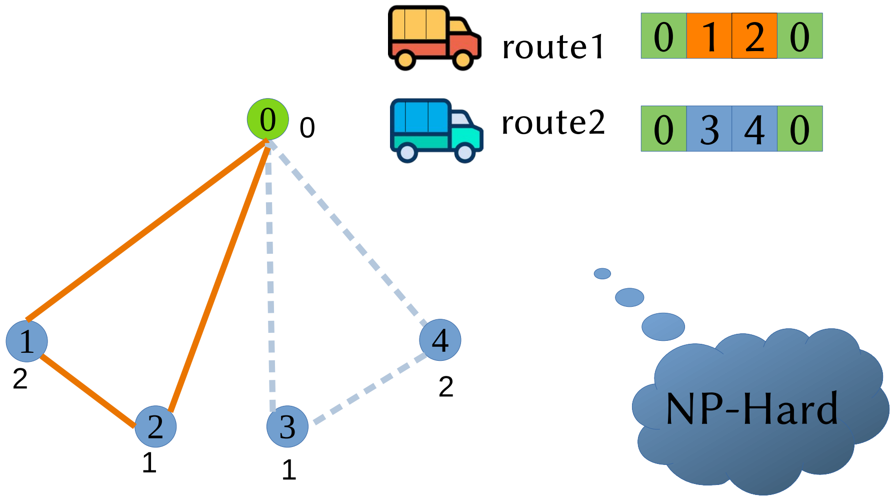
Input : Given *n* nodes (single Depot and customers) with their coordinates (x_i, y_i) and demands $d_i > 0$ for $i \in n$, Vehicle capacity C. Node 0 is Depot and has zero demand.

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

Goal : Minimize total distance travelled.

If Capacity = sum of demands d_i ,
CVRP ➜ Travelling Salesman Problem





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 customers	Time (s)	
		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**

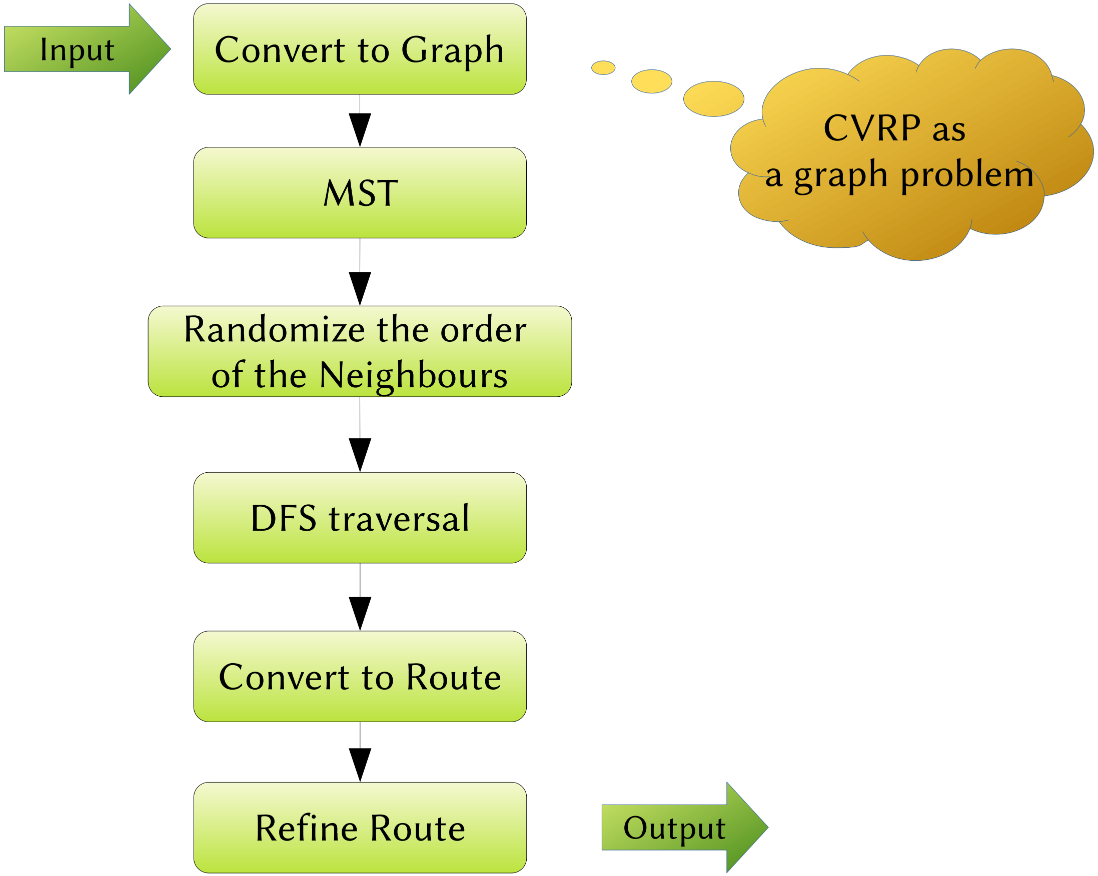
- Serial and Parallel implementation
- Combining MST and DFS
- Uses Local-search approach
- Uses Randomization approach

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

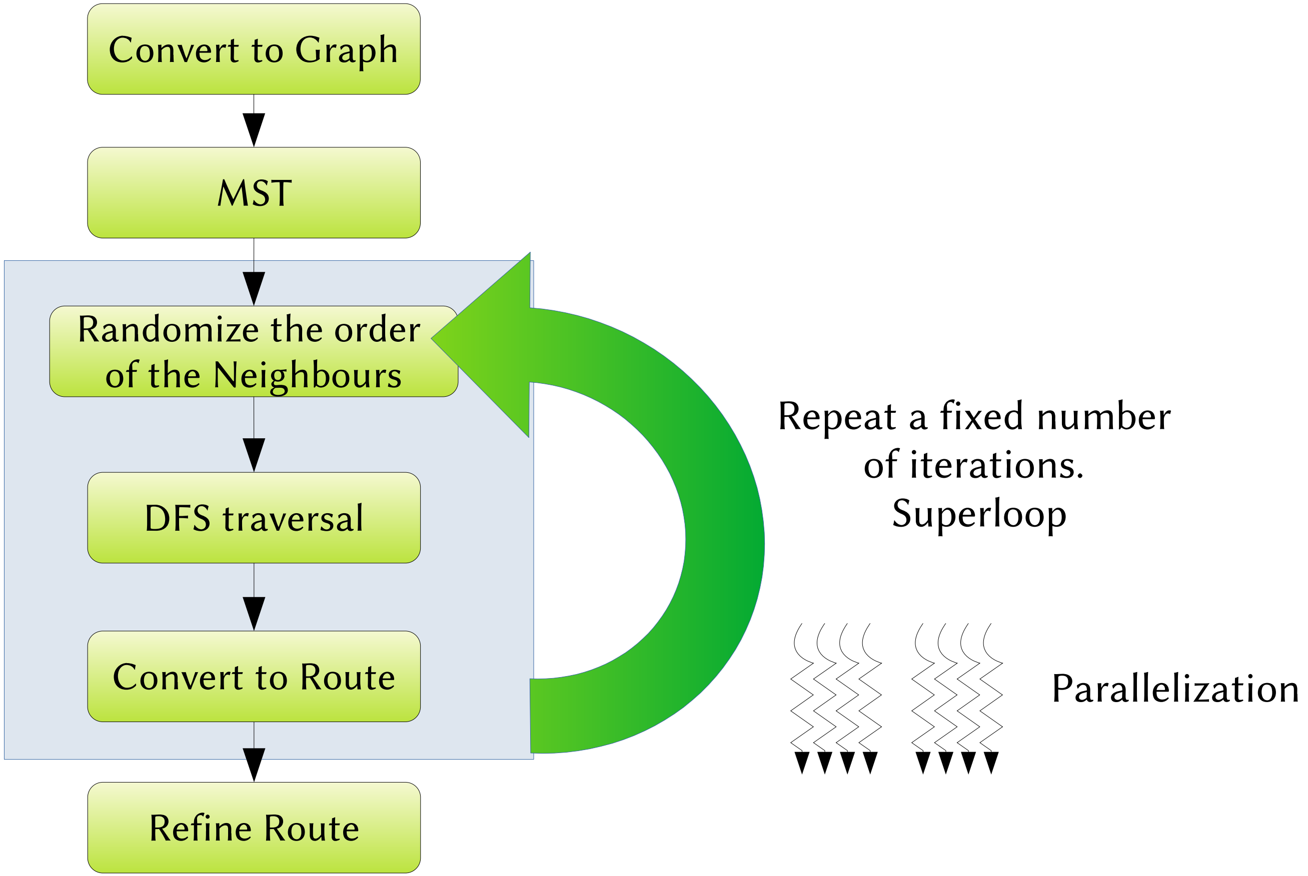
Baseline1: P. Yelmewad and B. Talawar. Parallel Version of Local Search Heuristic Algorithm to Solve Capacitated Vehicle Routing Problem, Cluster Computing, 2021.

Baseline2: M. Abdelatti and M. Sodhi. An improved GPU-accelerated heuristic technique applied to the Capacitated Vehicle Routing Problem, GECCO, 2020.

Overview - ParMDS

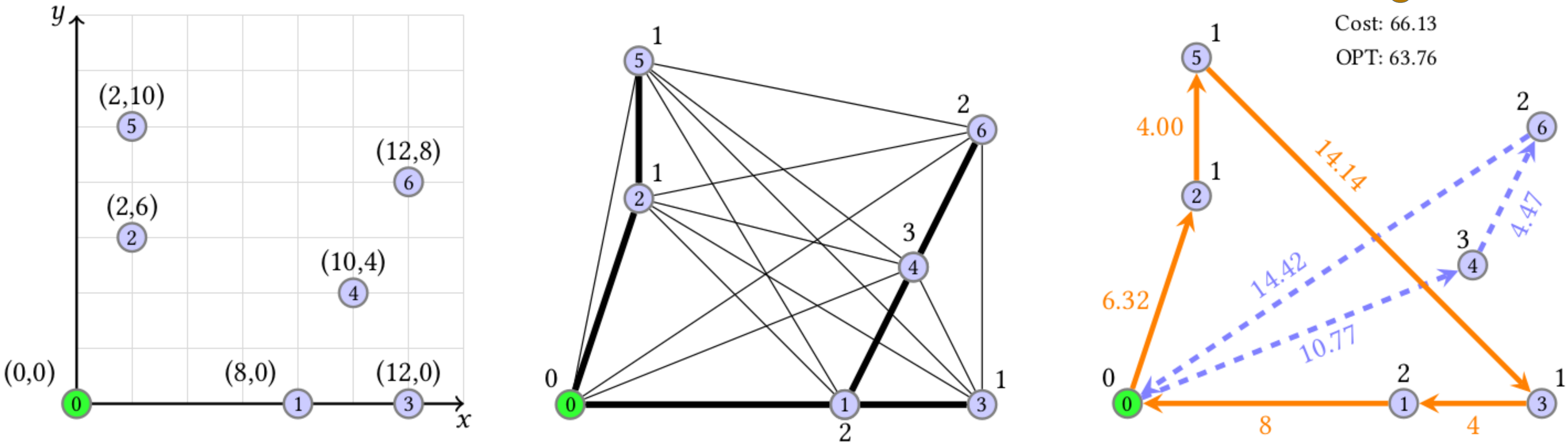


Overview - ParMDS



Example - Overview

Closer to Optimal Cost



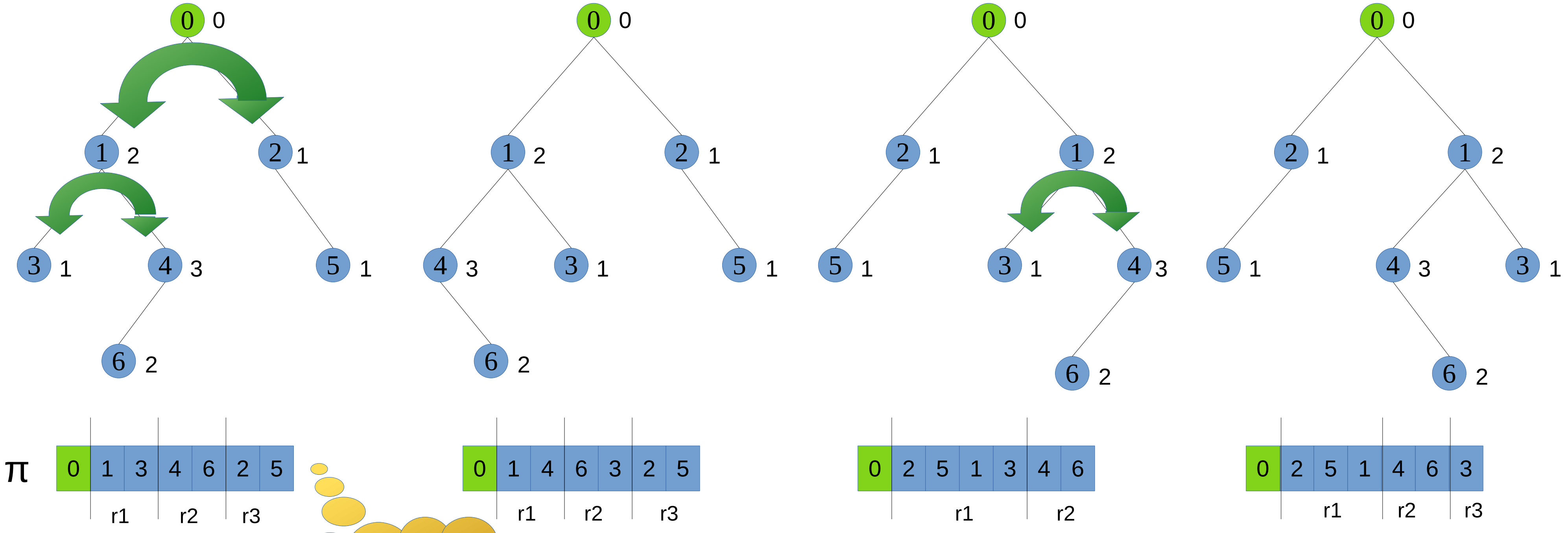
(a) Input instance I

(b) Graph for I, along with node-demands

(c) Final routes generated by ParMDS

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

Example – DFS and Randomization

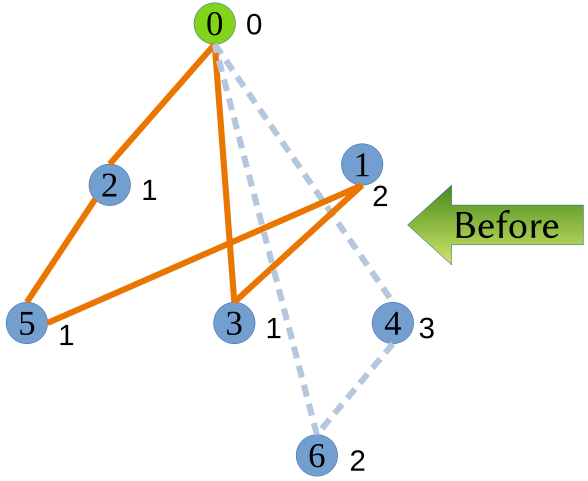


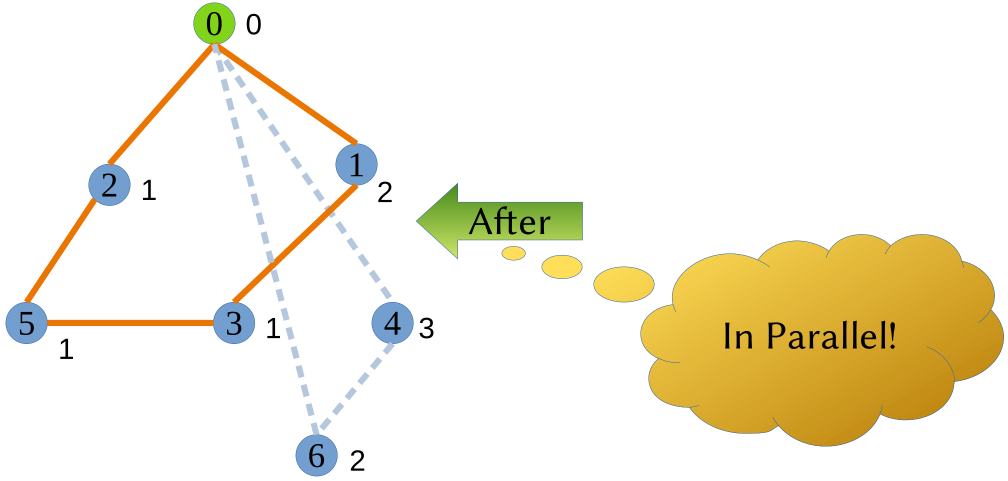
Vehicle Capacity = 5.

Cost:	74.19	78.19	67.65	83.65
	(a)	**(b)**	**(c)**	**(d)**

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

Intra-route optimization - 2Opt





0	2	5	1	3	4	6
	r1				r2	

Cost: 67.65

(a)

0	2	5	1	3	4	6
	r1				r2	

67.65

0	2	5	3	1	4	6
	r1				r2	

66.13

(b)

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

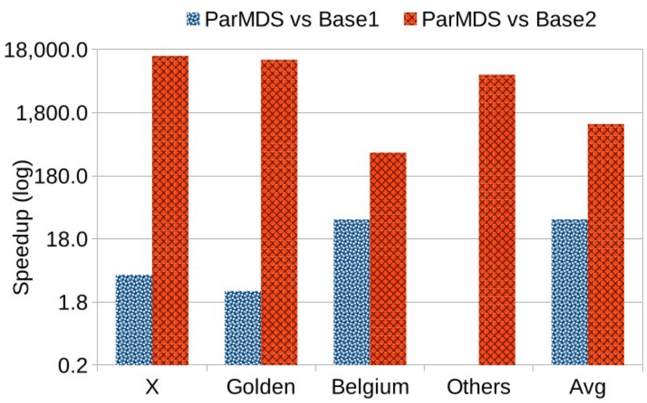
```
T ← PRIMS_MST (G)                                  /* Step 1 */
C_R ← ∞
for i ← 1 to ρ do            /* Superloop */ /* Parallel */
    T_i ← RANDOMIZE (T) /* Shuffle Adjacency List */
    π_i ← DFS_VISIT (T_i, Depot)                   /* Step 2 */
    R_i ← CONVERT_TO_ROUTES (π_i, Q, D)            /* Step 3 */
    C_{R_i} ← CALCULATE_COST (R_i)                 /* Parallel */
    if C_{R_i} < C_R then
        C_R ← C_{R_i}                              /* Current Min Cost */
        R' ← R_i                                   /* Current Min Cost Route */
    end
end
R ← REFINE_ROUTES (R')                             /* Step 4 */
return R, C_R
```

Zoom-in

```
/* Standard: stride = 1;                            */
/* Strided : stride = #CPU cores                    */
/* Parallel for loop: Standard/Strided              */
for i ← 1; i ≤ ρ; i = i + stride do
    for v ∈ V do
        /* seed ← constant or i or rand()           */
        SHUFFLE-NEIGHBORS(AdjList(v), seed);
    end
    ...
end
...
```

Experiments

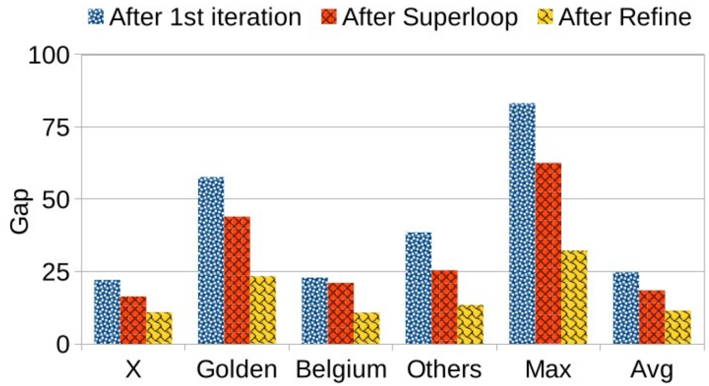
- 130 Instances of CVRPLIB
- Intel Xeon CPU E5-2640 v4
- Baselines on GPU
  - NVIDIA's Tesla P100
  - CUDA 11.5
- Our Code uses
  - **SeqMDS:** GCC 9.3.1
  - **ParMDS:** nvc++ compiler NVIDIA's HPC SDK 22.11



Speedup of ParMDS vs. baselines

Method	Execution Time (s) using Random
SeqMDS	1,722.44
ParMDS-Standard	1,522.26
ParMDS-Strided	186.50

More detailed analysis in our paper



Gap at the end of each step

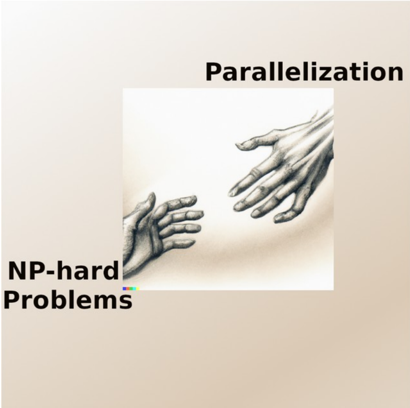
Summary

- Fresh perspective to <u>design</u> parallelism-friendly algorithms
- Performance: Algorithmic- and Parallelism- specific Optimizations

- Our techniques are applicable in general
  - Two-level parallelism (p-SSSP) technique
  - Strided parallel Local-search

- Immediate future directions
  - Substituting our SSSP with faster SSSP
  - Extending DD-based pSSSP
  - Supporting parMDS on GPU

Thank you!
Questions?



https://bit.ly/rajesh-viva