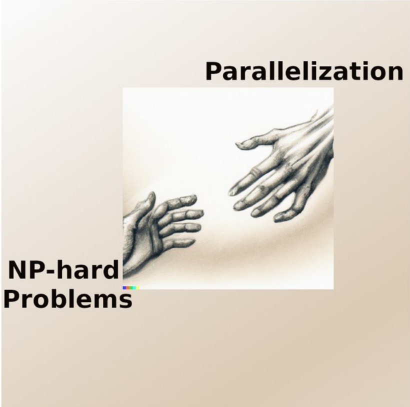
NP-Hard Problems Meet Parallelization

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 **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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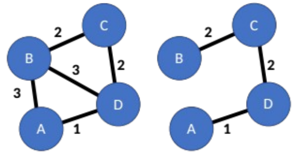
ABSTRACT

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 Memory access pattern

Polynomial-time Problems

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

- **Examples**
  - Minimum Spanning Tree
  - Single Source Shortest Path

NP-Hard Problems

- Comparatively difficult
- Complicated algorithms
- Few hours for thousand-sized instances
- Solution search space is large
- Trade-off: Solution quality vs Time

  - Steiner Tree Problem
  - Travelling Salesman Problem
  - Vehicle Routing Problem

- More practical applications

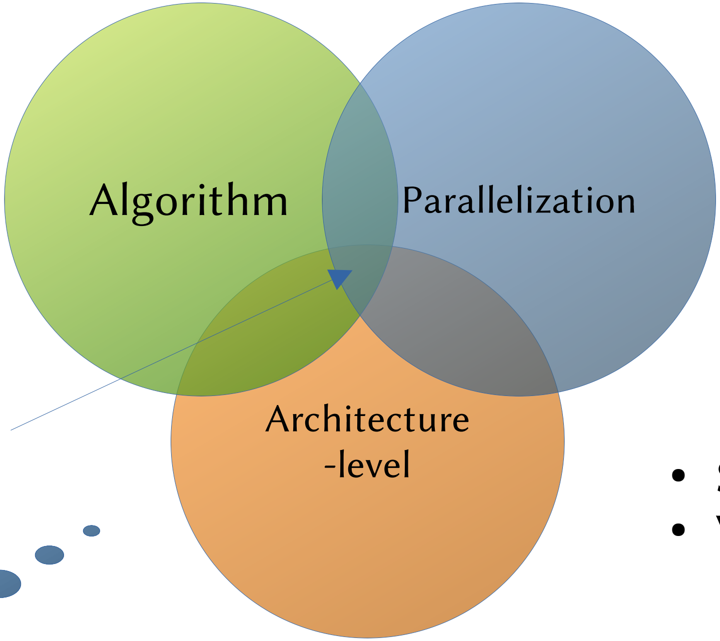
Goal: Solve on largest benchmark instances from DIMACS/PACE Challenges

Optimizing for peak performance

- Input Characteristics
- Properties of substeps

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

…



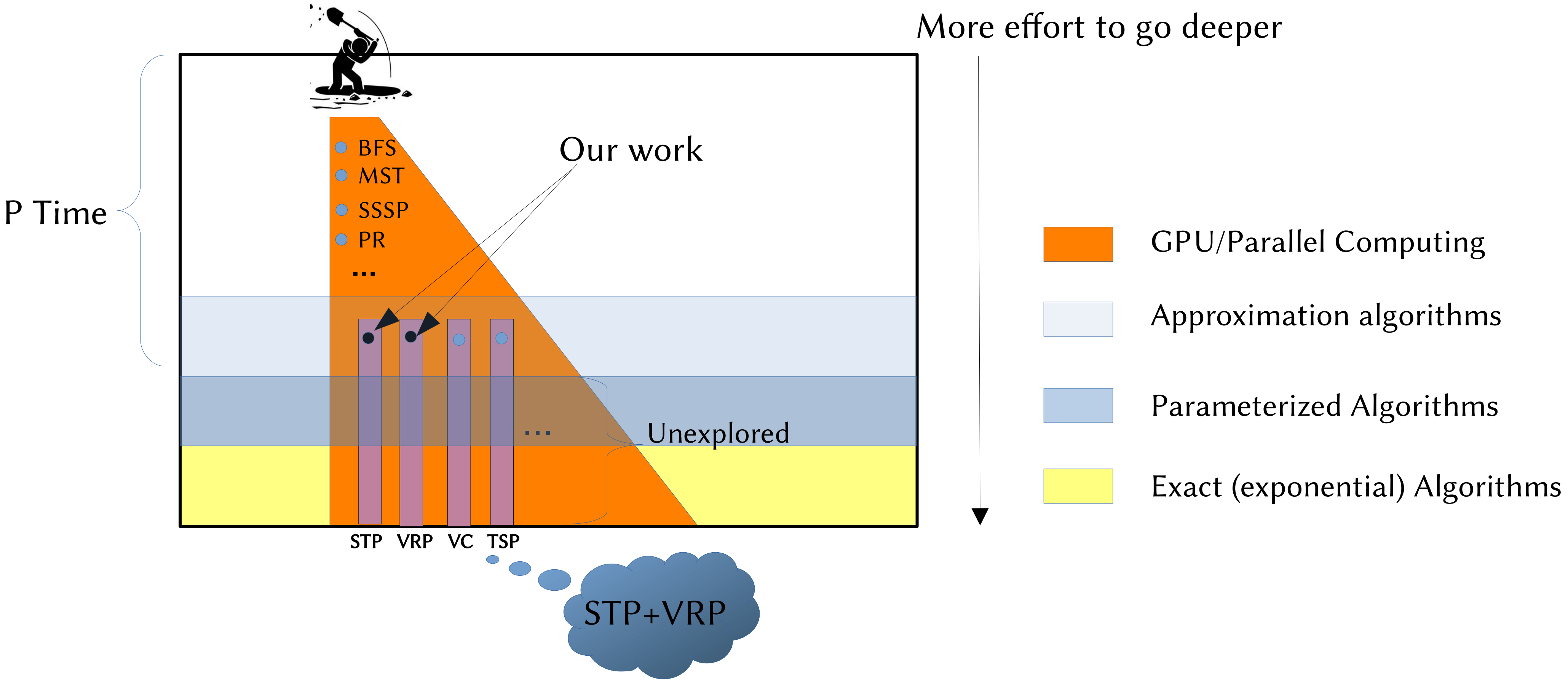
Even more

Peak performance

- Shared memory
- Warp-Intrincics

Is that all?

Landscape of Parallelization



Steiner Tree Problem (STP) – Example

<u>Input</u> : Graph G(V, E, W) $W: E \rightarrow Z^{+}$ and $L \subseteq V$ terminals.

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

// Minimum weighted tree with all terminals.

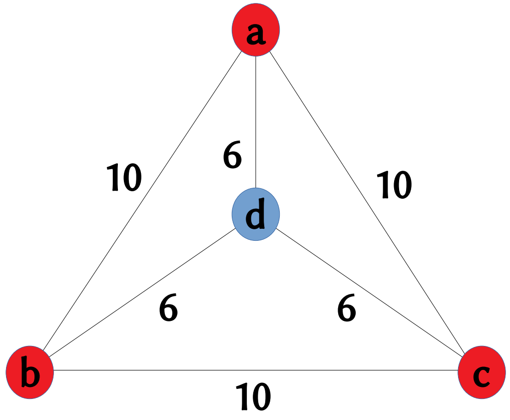


Fig 1 (a)

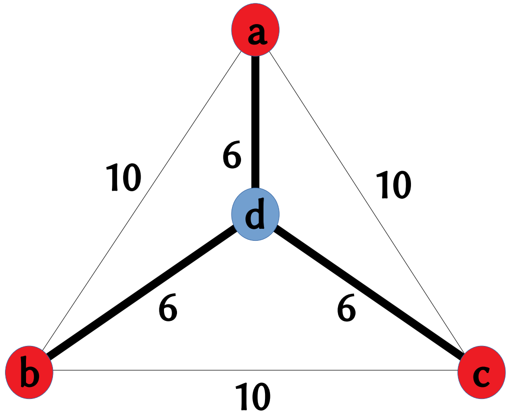


Fig 1 (b)

Isn't MST?

Terminals

Non-terminals

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

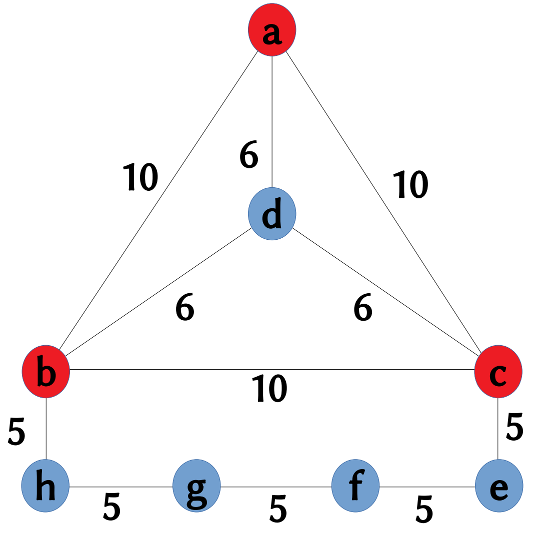


Fig 2 (a)

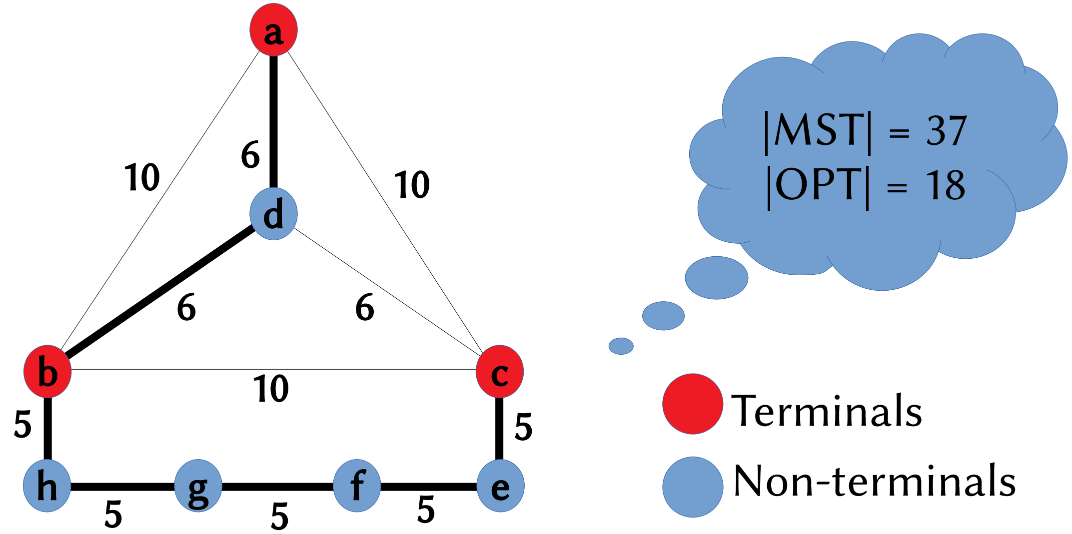


Fig 2 (b)

Steiner Tree Problem (STP) - Hardness

<u>Input</u> : Graph $G(V, E, W)$ $W: E \rightarrow Z^{+}$ and $L \subseteq V$ 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 with respect to 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

Compute 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

For u in L {
  For v in L {
    P_{uv} = ShortestPath(u,v)
    $W'(u,v) = |P_{uv}|$
  }
}

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

Observe:
Two For-loops.
Naive?

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_T, E_T) $V_T \supseteq L$

For s ∈ L {
    SSSP (G, W , L, s)   with Halt
    Compute W' incrementally
}

Single For-loop but runs SSSP to Completion

T' = MST(G' ,W')

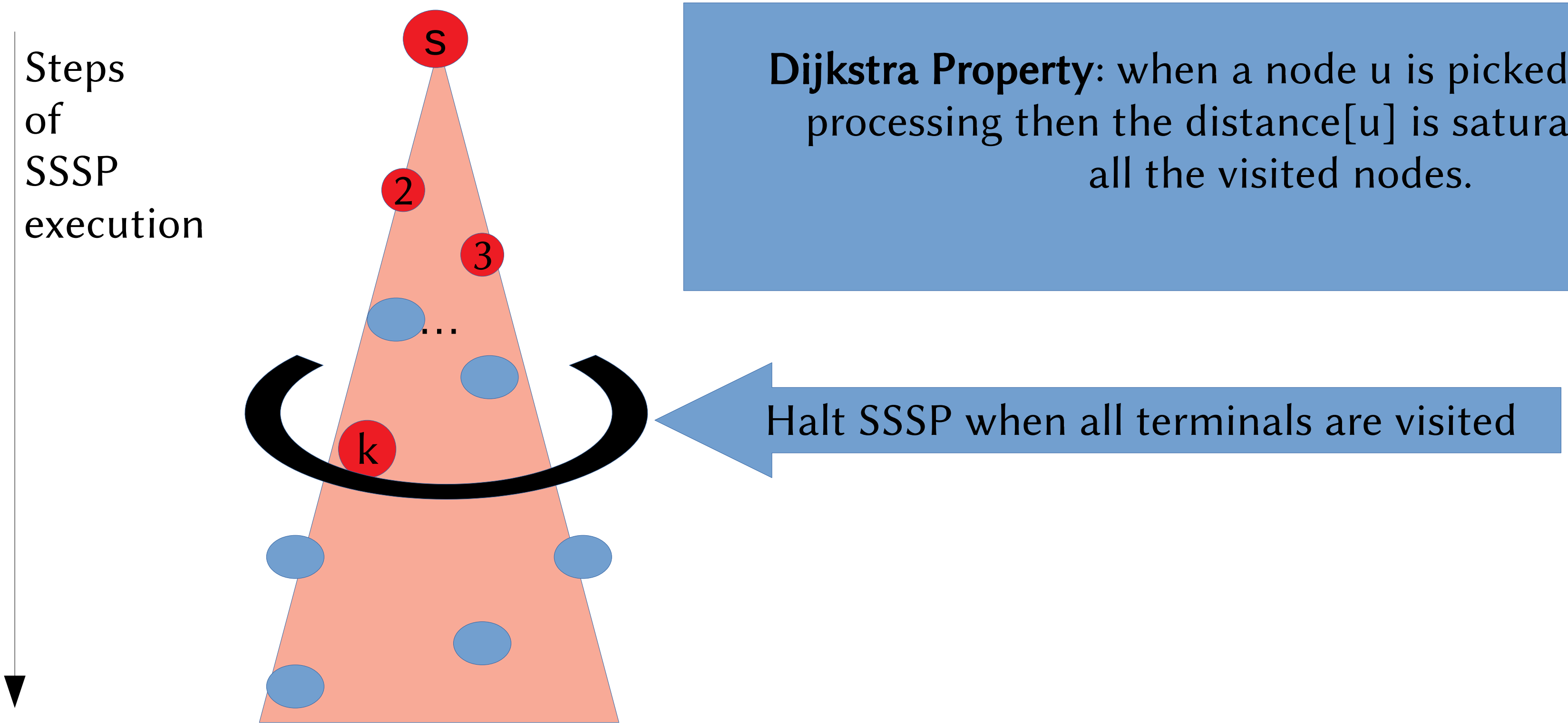
Compute G'' and its vertices, adjList using T'

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

return T''

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.

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 s ∈ L {
  parallel SSSP(G, W , L, s);
  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

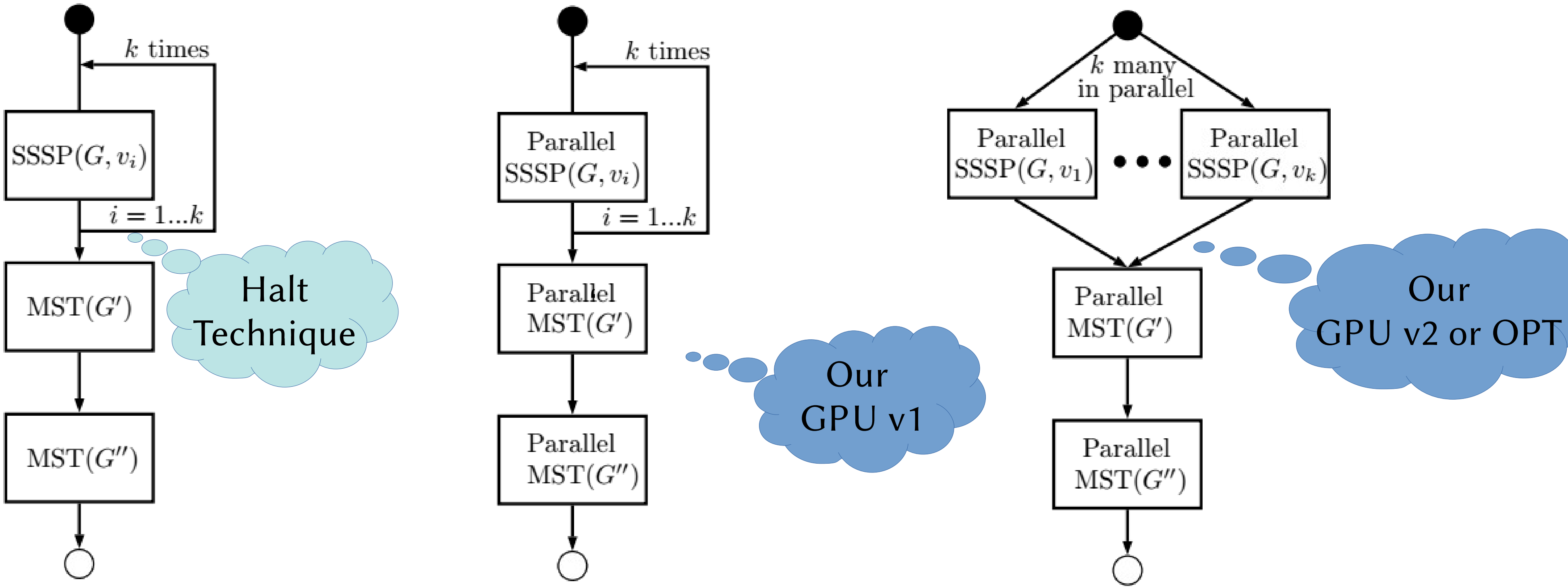


Fig. 5 Sequential vs GPU v1 vs GPU v2

KMBCPU
KMBGPU

GPU Implementation - SSSP

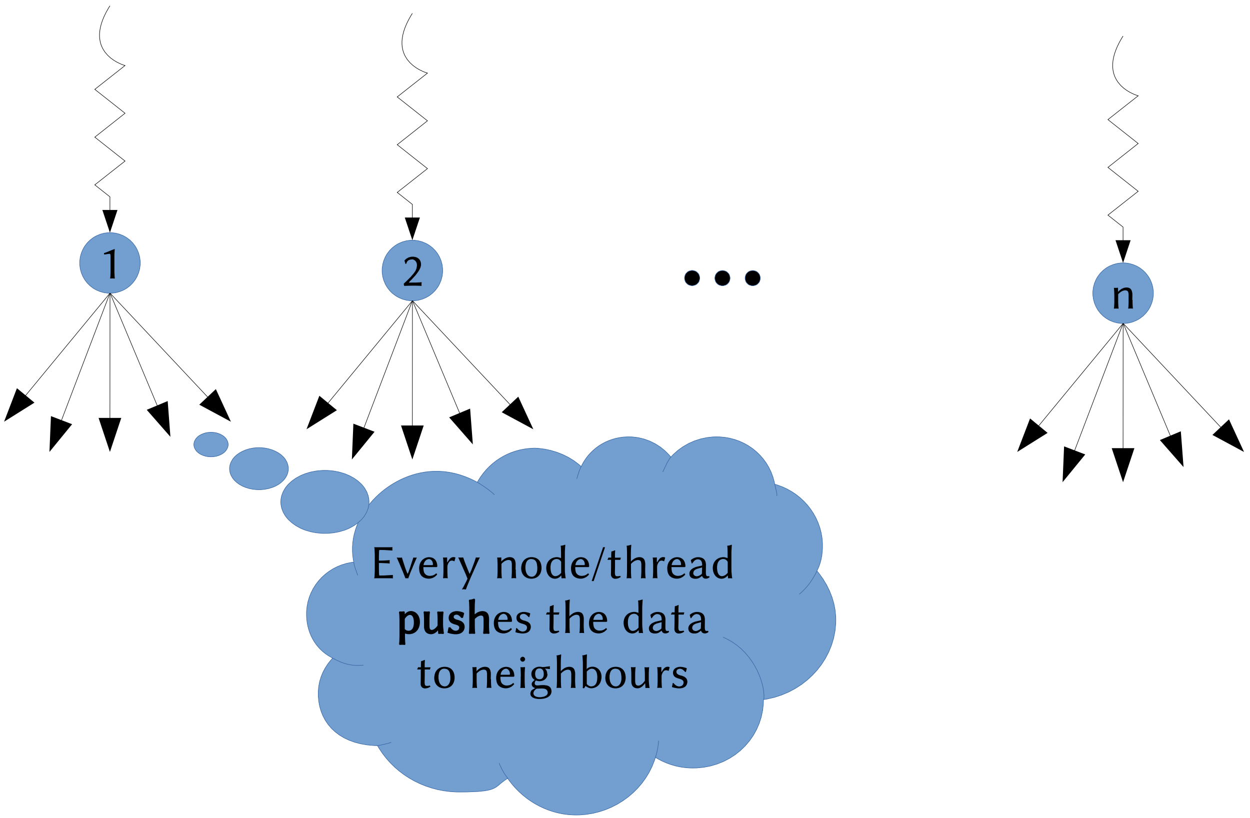


Fig. 6 push-SSSP

- 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)

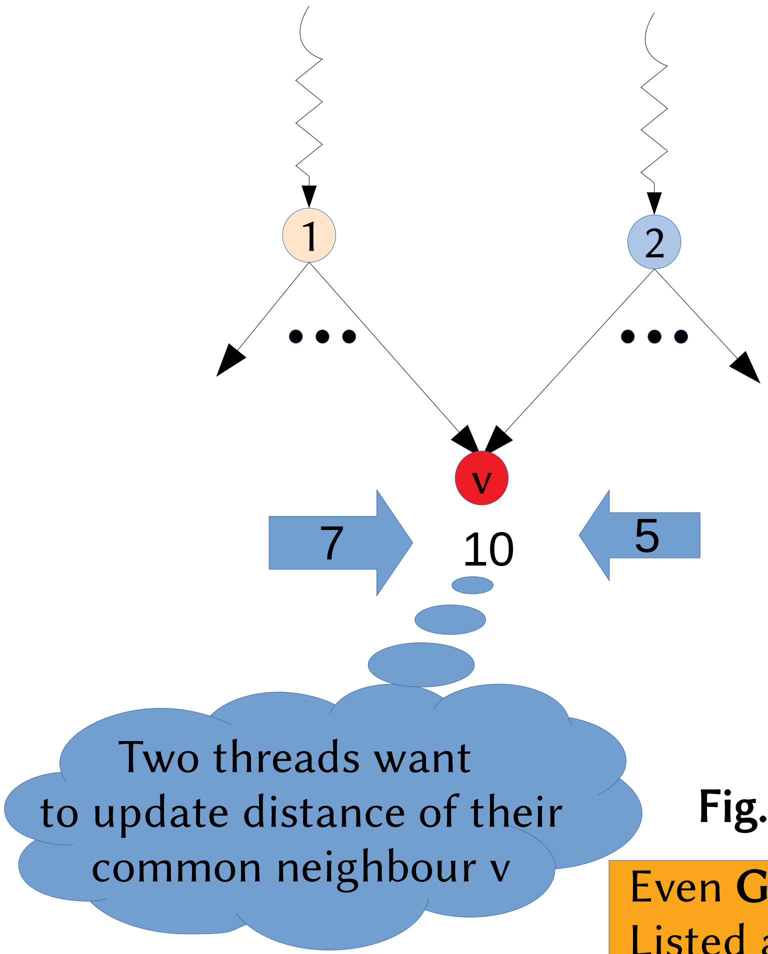
```
RELAX-KERNEL(..,s, d_s , p_s , changed, n) {
u = tid  // compute tid;
If tid < n  {
   For v ∈ adjacent[u] { // Using CSR arrays
      // Relax Operation (u, v, W(u,v))
      newCost = d_s[u] + W(u, v) ;
      old = d_s[v];
      If newCost < old
           Atomic-MIN(d_s[v], newCost);
      // Updates 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 challenge in updating p array consistently.
Listed as known issues https://github.com/gunrock/gunrock/releases/tag/v1.0

Synchronization optimization • Pull

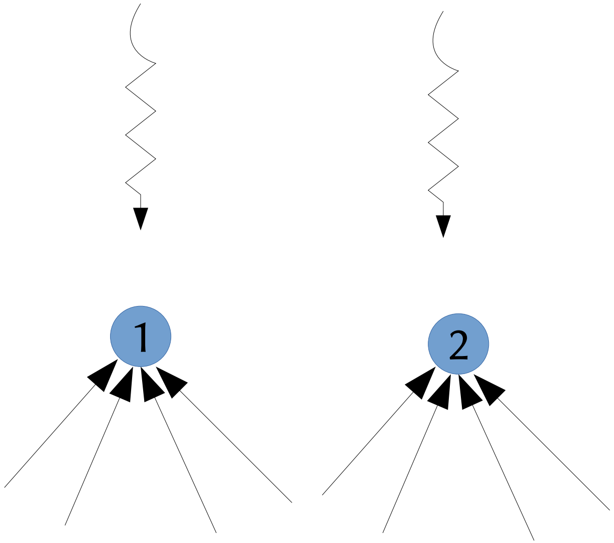


Fig. 8 Pull-SSSP

```
<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

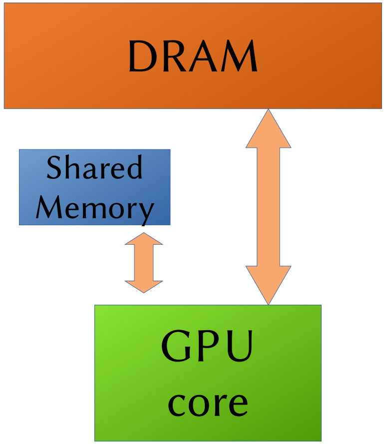
Give more work
or repeat the work?

Memory optimization

- Programmable shared memory can be useful
- When there are multiple reads to DRAM
- We can move data to shared memory

- For example, 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, ...);
}

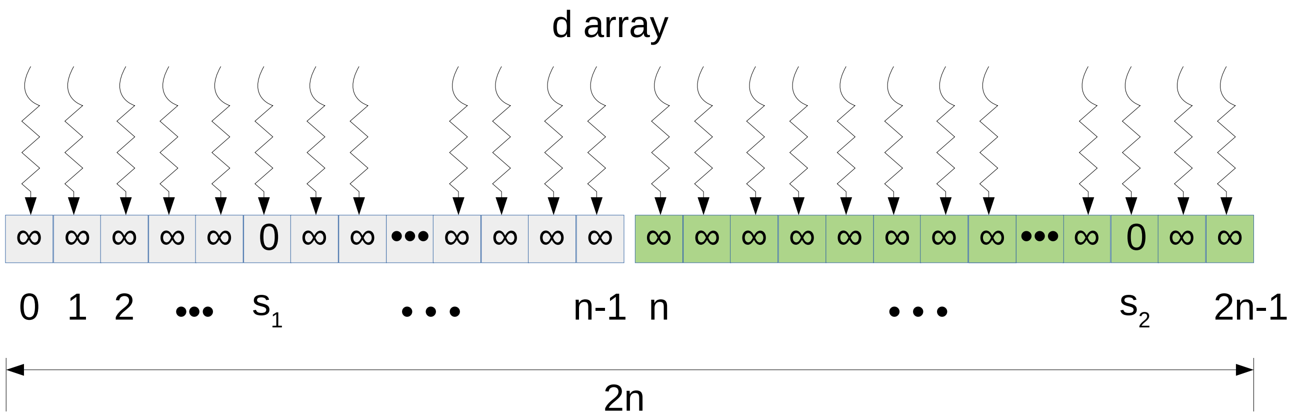


Fig. 9 Double-barrel approach.

Tunable arbitary value

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

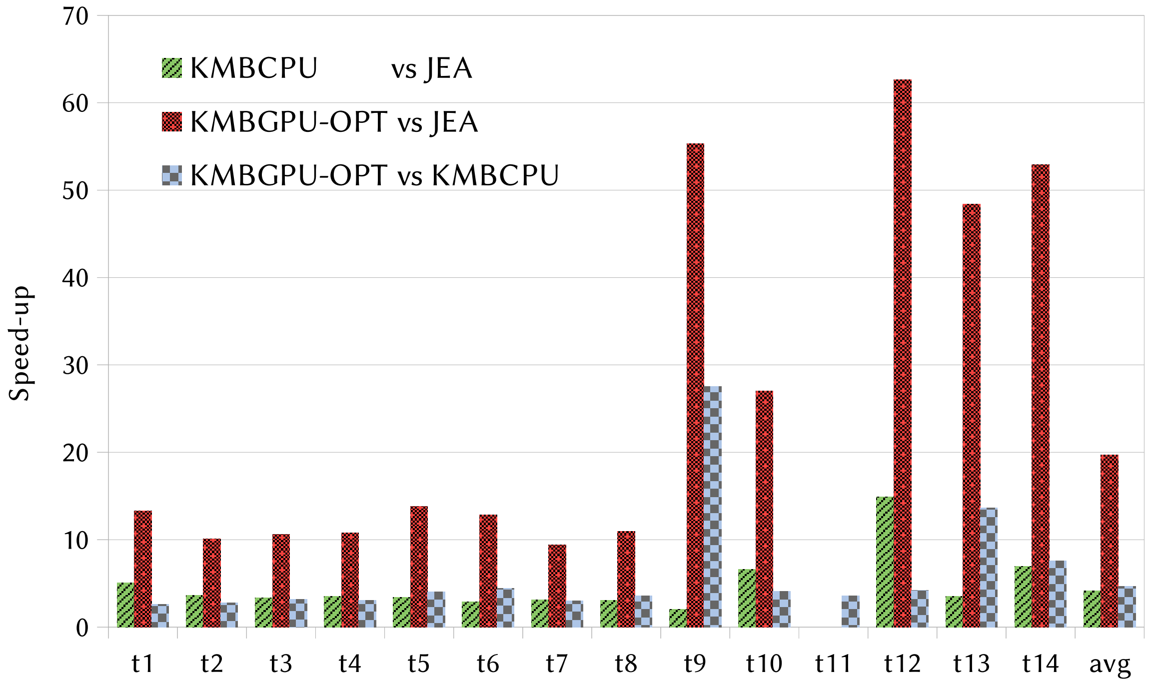


Fig. 10 Speed-up comparisons of the implementations (higher is better). JEA timed-out on t11

Takeaway: KMBCPU and KMBGPU-OPT are better than JEA

Comparison of p-SSSP

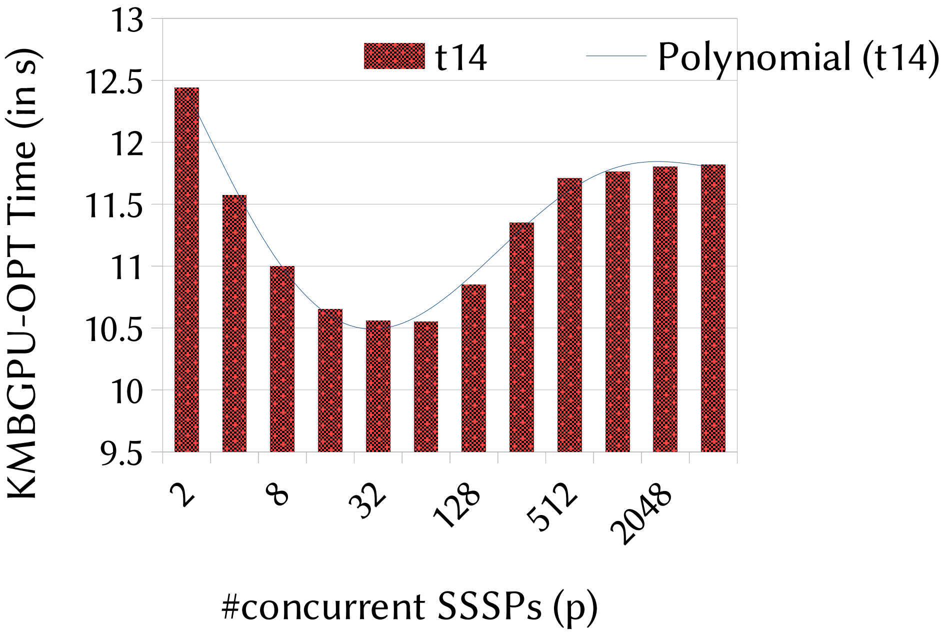


Fig. 12 KMBGPU with varying p-SSSP for the graph t14 (Smaller is better).

Takeaway: As we increase the #parallel SSSPs it reaches peak performance and reduces.

Experiments – Scalability of GPU and CPU

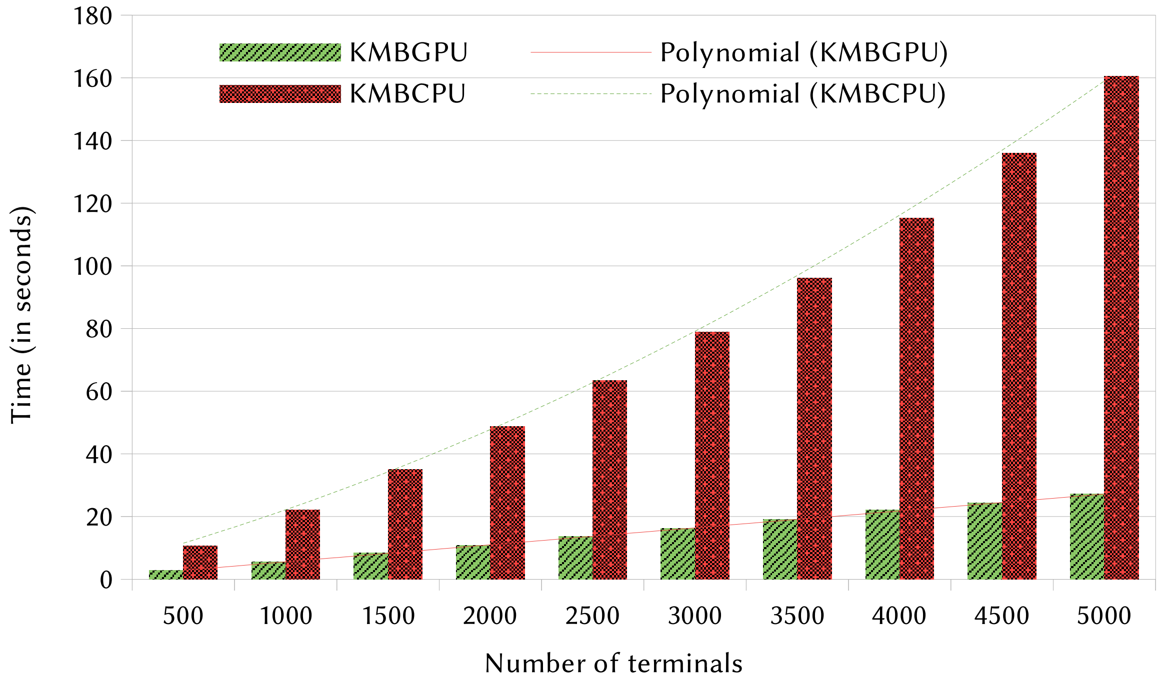


Fig. 13 Scalability plot on **t14** with increasing terminal size (lower is better)

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.

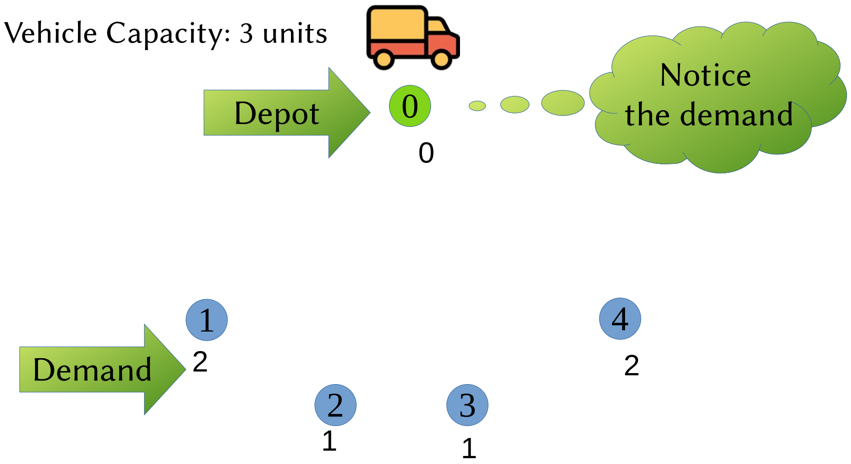
Capacitated Vehicle Routing Problem (CVRP)

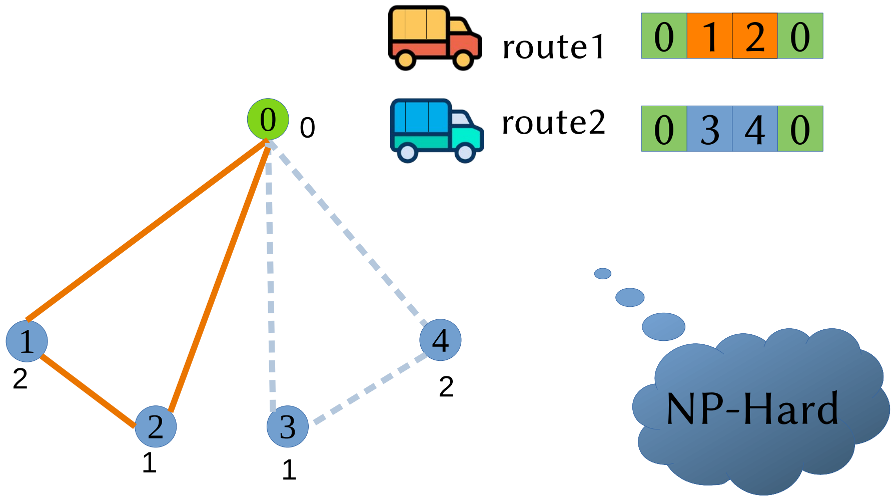
Input : Given n nodes (single Depot and customers) with their coordinates (x_i, y_i) and demands $d_i > 0$ for $i \in n$, Vehicle capacity C. Node 0 is Depot and has zero demand.

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

State-of-the-art

- works 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**

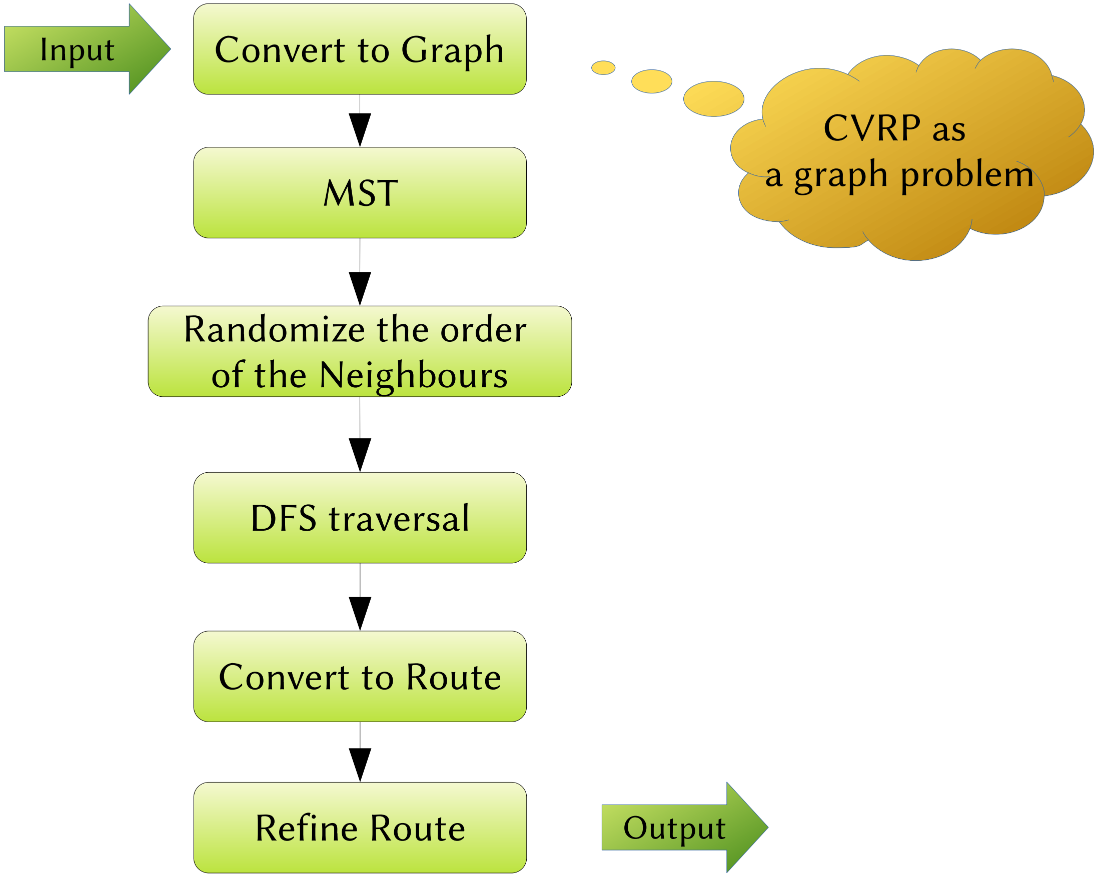
- Serial and Parallel implementation
- Combining MST and DFS
- Uses Local-search approach
- Uses Randomization approach

$$Gap = \left(\frac{Z_S}{Z_{BKS}} - 1\right) \times 100$$

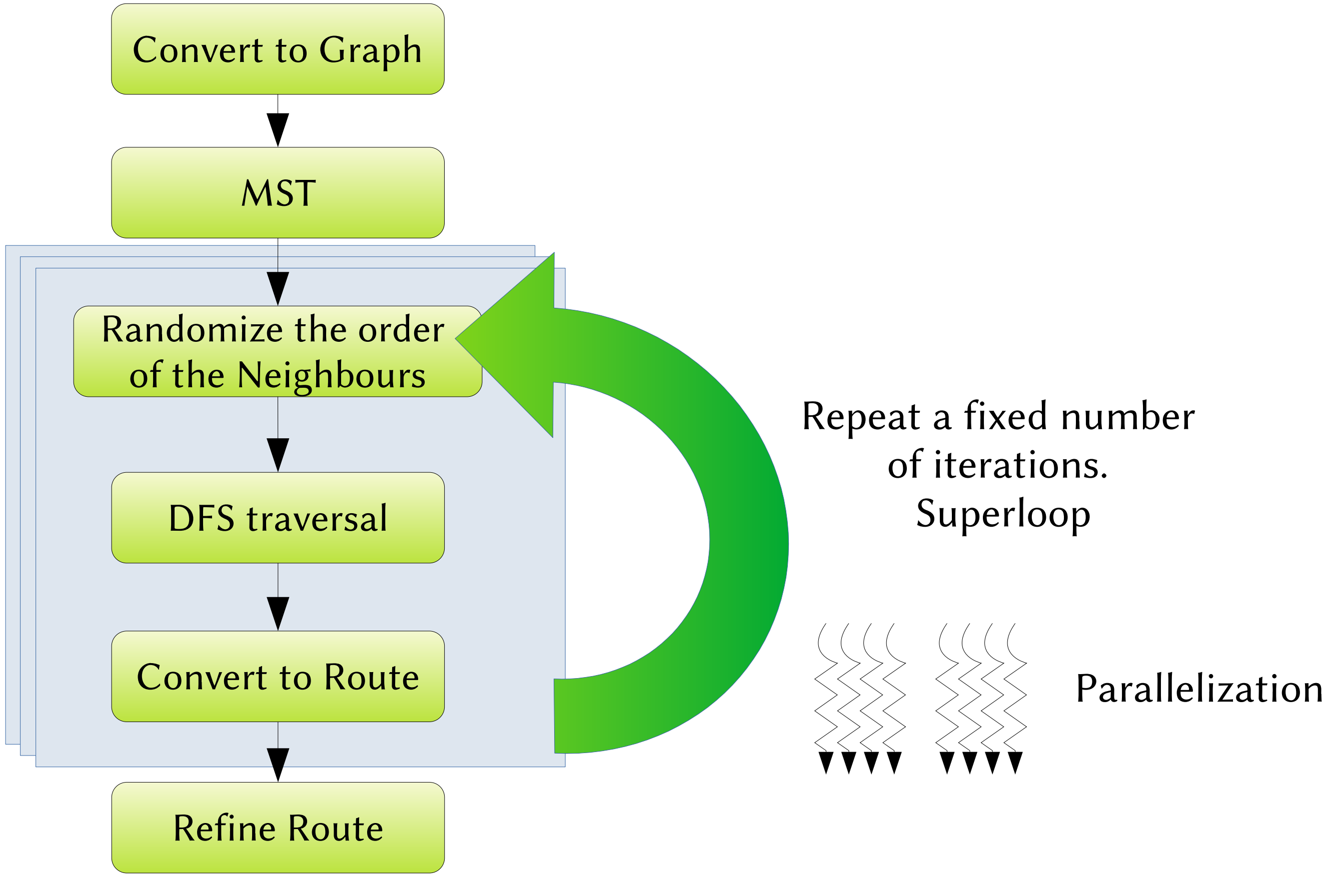
Baseline1: P. Yelmewad and B. Talawar. Parallel Version of Local Search Heuristic Algorithm to Solve Capacitated Vehicle Routing Problem, Cluster Computing, 2021.

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

Overview - ParMDS

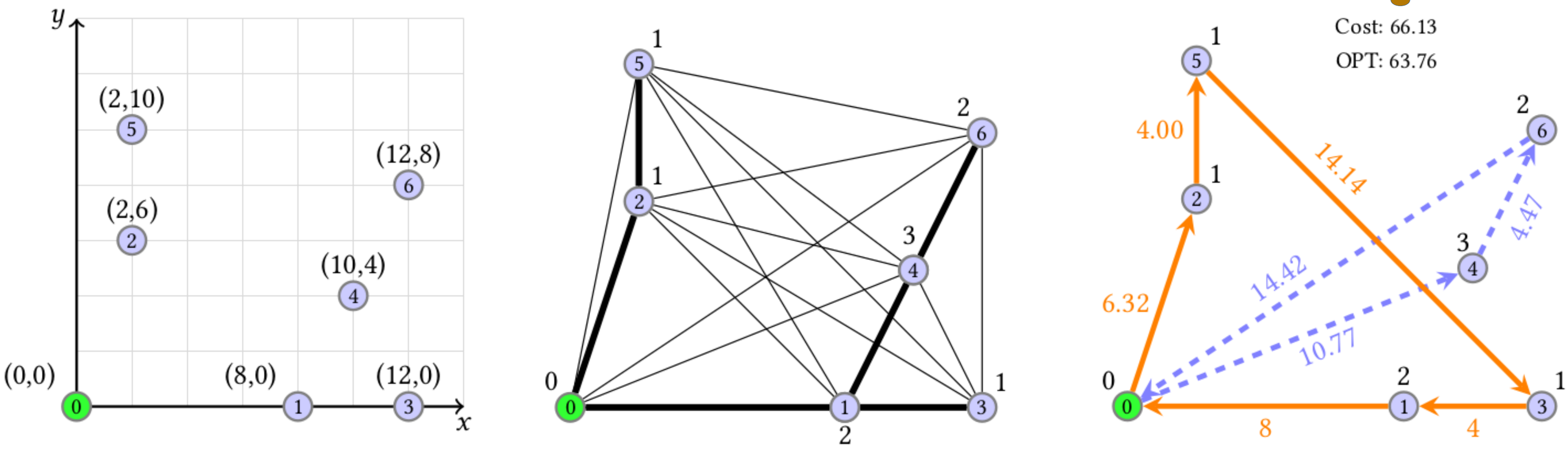


Overview - ParMDS



Example - Overview

Closer to Optimal Cost



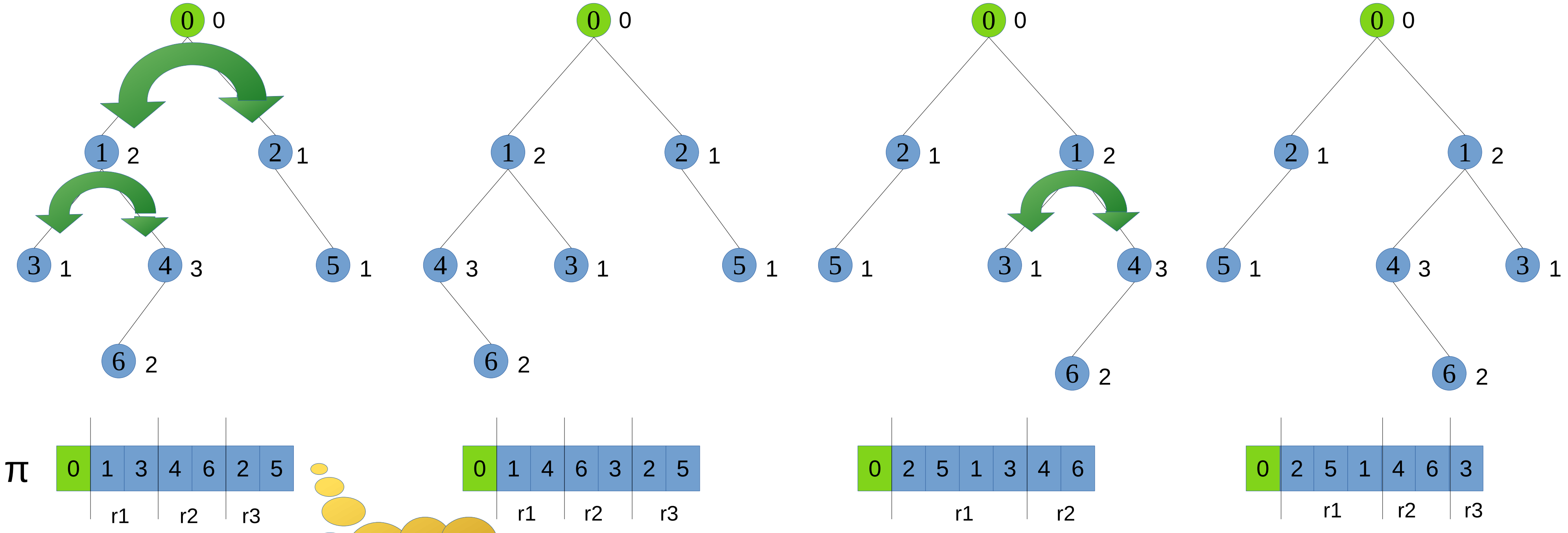
(a) Input instance I

(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

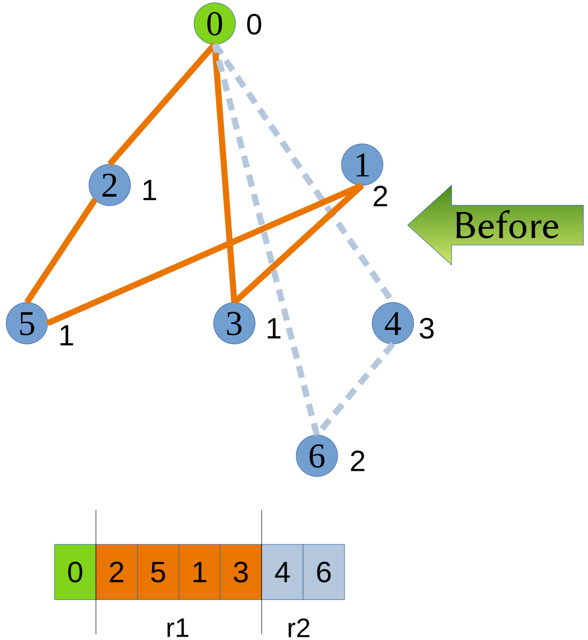


Vehicle Capacity = 5.

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

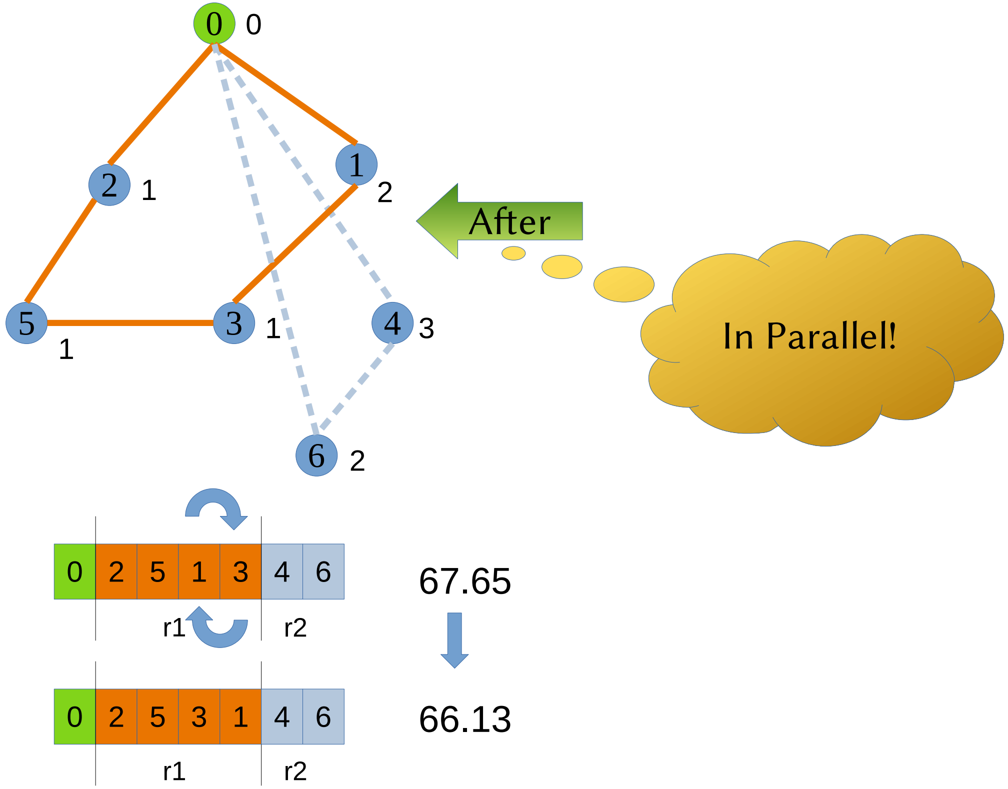
Takeaway: Randomizing neighbours of MST may yield a different DFS ordering. Hence, a different route!

Intra-route optimization - 2Opt



Cost: 67.65

(a)



(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

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

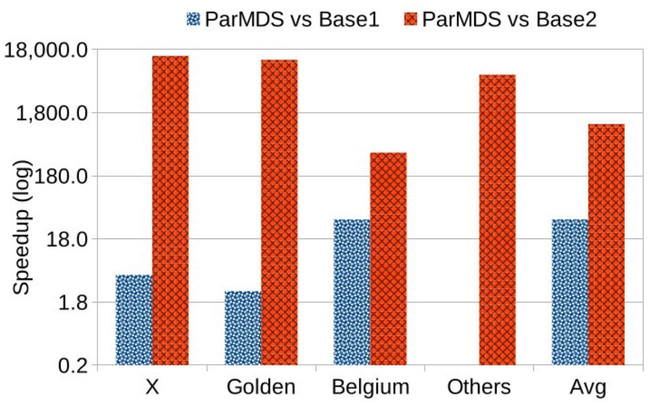
Zoom-in

```
/* Standard: stride = 1;                        */
/* Strided : stride = #CPU cores                */
/* Parallel for loop: Standard/Strided          */
```

for $i \leftarrow 1; i \leq \rho; i = i + stride$ **do**
    for $v \in V$ **do**
        /* seed ← constant or i or rand() */
        SHUFFLE-NEIGHBORS(AdjList(v), seed);
    end
    . . .
end
. . .

Experiments

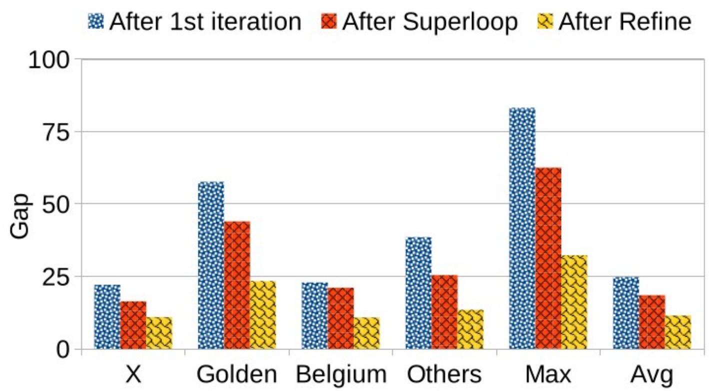
- 130 Instances of CVRPLIB
- Intel Xeon CPU E5-2640 v4
- Baselines on GPU
  - NVIDIA's Tesla P100
  - CUDA 11.5
- Our Code uses
  - **SeqMDS:** GCC 9.3.1
  - **ParMDS:** nvc++ compiler NVIDIA's HPC SDK 22.11



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

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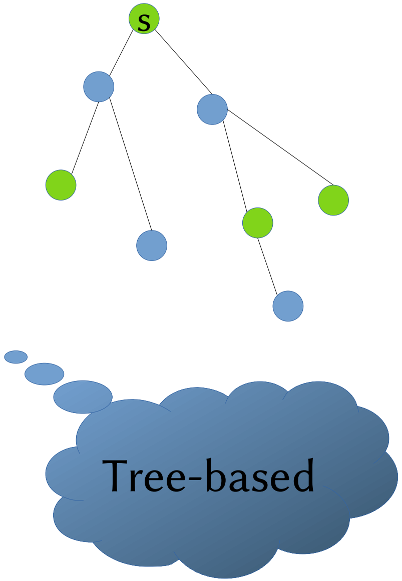
Faster Steiner Heuristics

Algo.	Abbr.	Name
1	DJ	Dijkstra Tree Algorithm
2	DJ-all	Dijkstra Tree from all terminals Algorithm
3	SP	Single Probe Algorithm
4	SP-all	Single Probe from all terminals Algorithm
5	DP	Double Probe Algorithm
6	DP-all	Double Probe from all terminals Algorithm
7	HSD	Hybrid of SP-all and DP-all
Baseline	P18WIN	PACE 2018 Heuristic Track Winner

Table. Our Steiner heuristic algorithms and baseline



Gap and Time comparison

t#	DJ	DJ-all	SP	SP-all	DP	DP-all	HSD	P18WIN
t01	41.21	30.34	6.68	6.09	5.90	5.12	5.12	34.86
t02	45.30	39.78	8.16	7.34	7.12	6.62	6.62	33.91
t03	31.37	29.37	6.96	6.30	5.85	5.48	5.48	30.42
t04	21.77	19.42	5.25	4.74	3.43	3.16	3.43	27.30
t05	2.28	1.83	0.43	0.41	0.43	0.38	0.38	2.34
t06	1.07	0.97	0.18	0.15	TO	TO	0.15	2.76
t07	20.87	17.53	4.28	4.21	3.85	3.49	4.21	32.92
t08	1.90	1.76	0.52	0.31	0.29	0.28	0.28	2.02
t09	51.87	47.50	8.45	8.24	7.57	7.26	7.31	7.10
t10	2.24	2.15	0.38	0.35	0.32	0.32	0.32	5.95
t11	20.99	19.14	4.77	4.48	3.56	3.39	4.48	31.12
t12	153.54	133.48	26.35	20.37	10.49	7.19	7.19	77.07
t13	244.67	154.62	9.00	8.94	9.81	9.59	8.94	36.68
t14	24.42	21.68	1.60	0.98	0.28	0.00	0.04	48.96
avg.	47.39	37.11	5.93	5.21	4.53	4.02	3.85	26.67

t#	DJ	DJ-all	SP	SP-all	DP	DP-all	HSD	P18WIN
t01	0.105		0.162	98.76	9.23			
t02	0.160		0.288	364.80	154.43			
t03	0.220		0.449	944.40	48.56			
t04	0.249		0.453	964.12	32.45			
t05	0.141		0.262	569.96	88.56			
t06	0.115		0.244	573.19				
t07	0.241		0.592	1782.85	139.11			
t08	0.228		0.381	930.70	41.30			
t09	0.083	642.64	0.077	203.42	4.76			
t10	0.239		0.477	1468.10	41.13			
t11	0.466		0.928		137.12			
t12	0.035	813.09	0.055	6.32	2.26	302.12	308.23	
t13	0.050	1176.68	0.084	115.53	4.23			
t14	0.287		0.319	898.93	24.92			
sum	2.618	22432.41	4.769	10721.09	2528.04	23702.12	23708.23	25200
avg.	0.187	1602.32	0.341	765.79	180.57	1693.01	1693.45	1800

Table. Comparison of **(a)** Gap and **(b)** Time (in seconds) for our algorithms vs Baseline

- SP and DP is faster than others
- HSD has the least Gap

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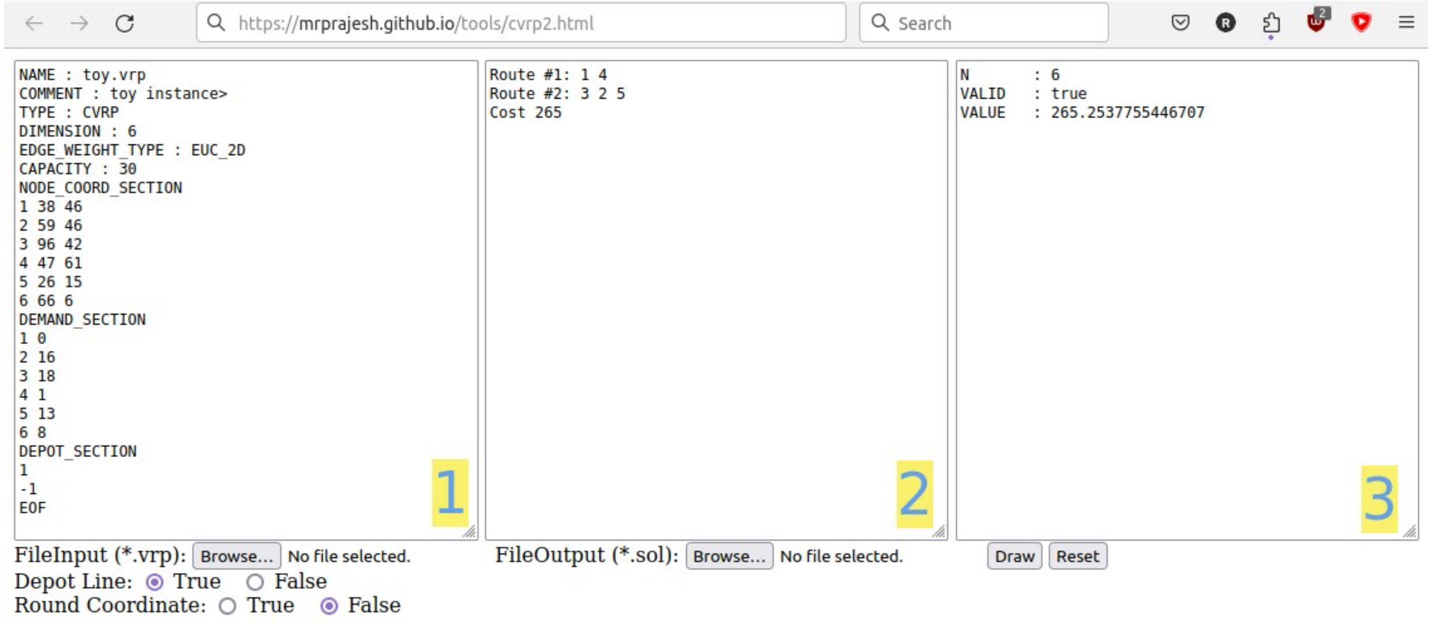
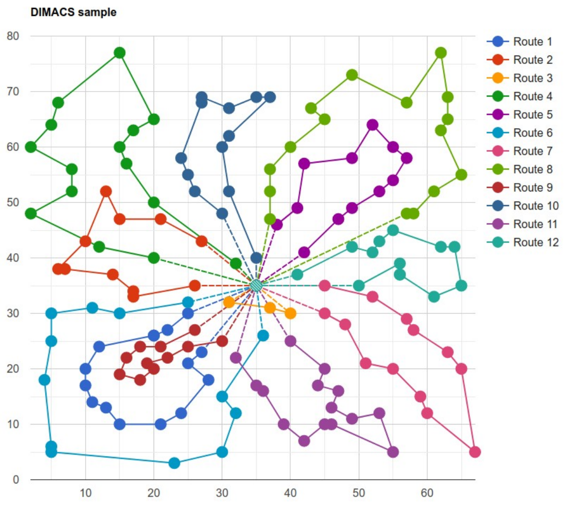
Tools and Visualization

- https://mrprajesh.github.io/tools

- Steiner Tree
- CVRP





Publications

1. Accelerating Computation of Steiner Trees on GPUs. **Rajesh Pandian M**, Rupesh Nasre & N. S. Narayanaswamy. *International Journal of Parallel Programming* (**IJPP**), volume 50, pages152–185 (2022). DOI: https://doi.org/10.1007/s10766-021-00723-0 (Source code)

2. Effective Parallelization of the Vehicle Routing Problem. **Rajesh Pandian M**, Somesh Singh, Rupesh Nasre & N.S.Narayanaswamy. *Genetic and Evolutionary Computation Conference* **(GECCO)**. pgs 1036–1044, 2023. DOI: https://doi.org/10.1145/3583131.3590458 (Source code)

Summary

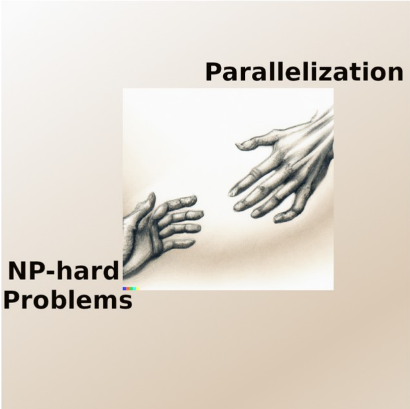
- Fresh perspective to <u>design</u> parallelism-friendly algorithms
- Performance: Algorithmic- and Parallelism- specific Optimizations

- 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