Accelerating Computation of Steiner Trees on GPUs

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Acknowledgements

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- This work evolved after the PACE Challenge 2018 [www.pacechallenge.org] on Steiner Tree

- This work is published in IJPP 2022.

Outline

- Introduction - Steiner Tree Problem
- Definition & Example
- KMB algorithm

Introduction & Algorithm

- Challenges in parallelizing KMB
- Design Choice of KMB
- CPU Optimization

Designing &
CPU Implementation + Optimization

- GPU Implementation
- SSSP Optimization – Sync, Compute, Memory
- Double Barrel and p-SSSP
- Experimental Results
- Summary

GPU Implementation
& Optimization

Steiner Tree Problem (STP)

Informally

Input : Undirected Graph G(V, E, W, L) W is non-negative edge weights; $L \subseteq V$ terminals
Output : A tree with all terminals
Goal : Minimize the weight of the tree

- **Steiner Tree** - tree with all the terminals and zero or more non-terminals.
- **Terminals or** terminal vertices are special vertices which must be present in the tree
- **Non-terminals** or Steiner vertices are optional vertices – generally included in tree to minimize the overall weight of the resulting tree.
- Standard Graph-theoretic notation is used $n=|V|$, $m=|E|$ and additionally $k=|L|$
- Applications[Hwang et. al. 92]: VLSI design, network/vehicle routing, etc.

F.K. Hwang, D.S. Richards, P. Winter, *The Steiner Tree Problem*, Annals of Discrete Mathematics, Elsevier, 1992.

Steiner Tree Problem (STP) – Example

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

Output : Connected subgraph T'(V'⊇L, E'⊆E) of G such that Min W(E')

// Minimum weighted tree with all terminals

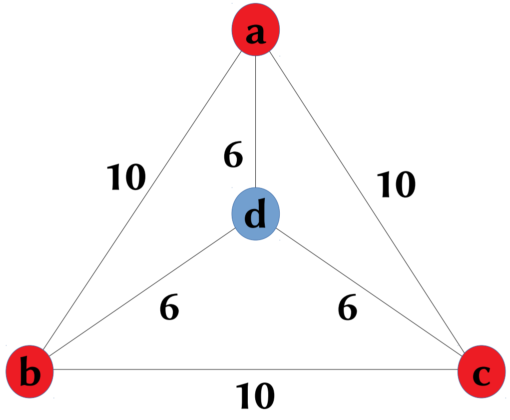


Fig 1 (a)

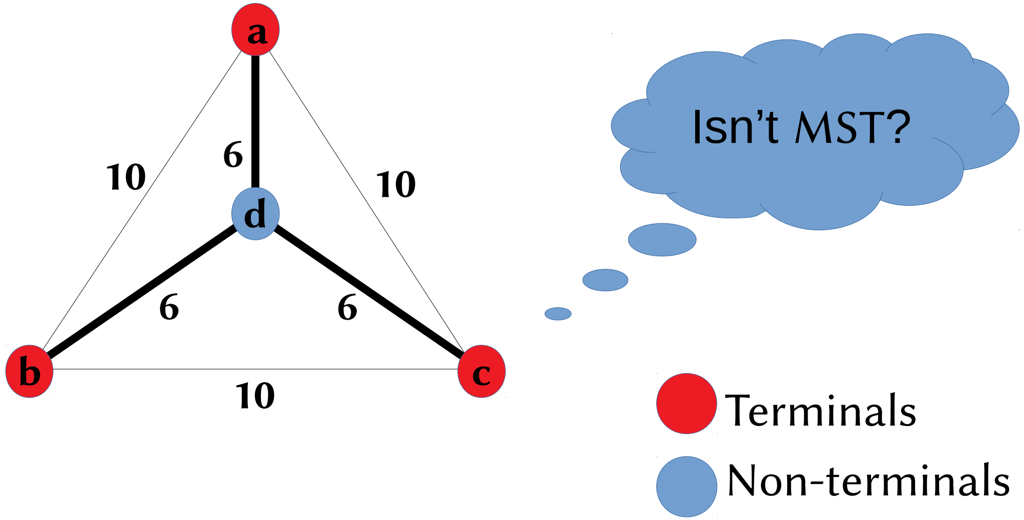


Fig 1 (b)

Steiner Tree Problem (STP) – Example

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

Output : Connected subgraph T’(V’⊇L, E’⊆E) of G such that Min W(E’)

// Minimum weighted tree with all terminals

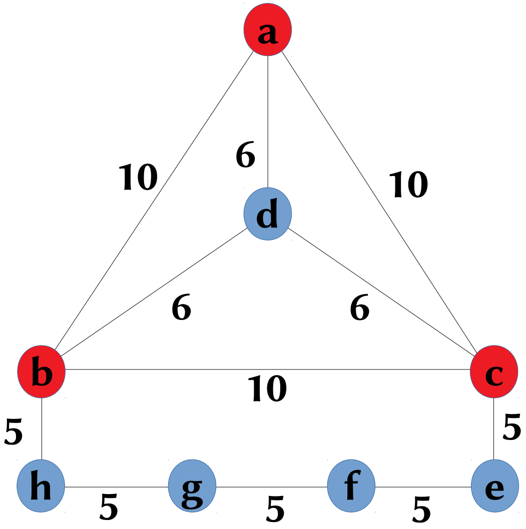


Fig 2 (a)

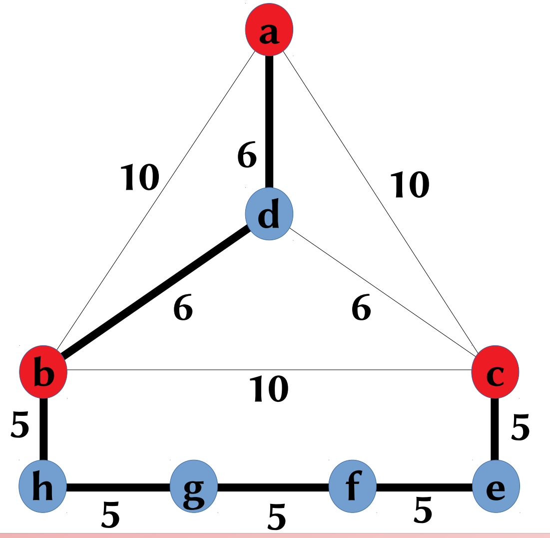


Fig 2 (b)

|MST| = 37
|OPT| = 18

Terminals
Non-terminals

Steiner Tree Problem (STP) - Hardness

Input : Graph G(V, E, W, L) W:E→ Z^+ and L⊆V terminals
Output : 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

Standard Graph-theoretic notation is used n=|V| , m=|E| and additionally k=|L|

How to deal with NP-Hardness

- No Polynomial time algorithm can find optimal solution unless P = NP.
- 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.*

Comparison with related work

Solver	CPU	GPU	k >128	Quality	Time taken
PACE2018 Winner [CIMAT Team]	✓		✓	☆☆	🕒🕒🕒🕒🕒
OGDF's KMB /JEA [BC19]	✓		✓	☆☆☆	🕒🕒🕒
CUDA STAR [MK15]		✓		-	-
Our KMBCPU [MNN22]	✓		✓	☆☆☆	🕒
Our KMBGPU-OPT [MNN22]		✓	✓	☆☆☆	🕒

Table 1 Characteristics comparison with related work and our work.

average

Challenges in parallelizing KMB

- Graph algorithms in general has an irregular access pattern.
  - Defies the scope of parallelizing
- Involvement of multiple primitive algorithms (such as SSSP and MST)
  - Dependence on an algorithm input from the output of previous algorithm
- Maintaining consistent parent information in SSSP along with distances.
  - Individual atomic instructions may not lead to atomic transactions.
- Parallel KMB may output different solutions during different invocations,
  - Makes it difficult to validate the solution,

Our Contributions

- Optimized CPU implementation for KMB algorithm
  - Novel SSSP-halt technique
  - Speed-up upto 15x (average 4x) improvement over JEA/OGDF's KMB[BC19]
- Optimized GPU implementation for KMB algorithm
  - Novel p-SSSP technique (multiple parallel-SSSP in parallel)
  - Speed-up upto 27x (average 4x) over sequential CPU [MNN22]
  - Speed-up upto 62x (average 20x) over sequential JEA/OGDF's KMB [BC19]

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

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

Phase 1

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

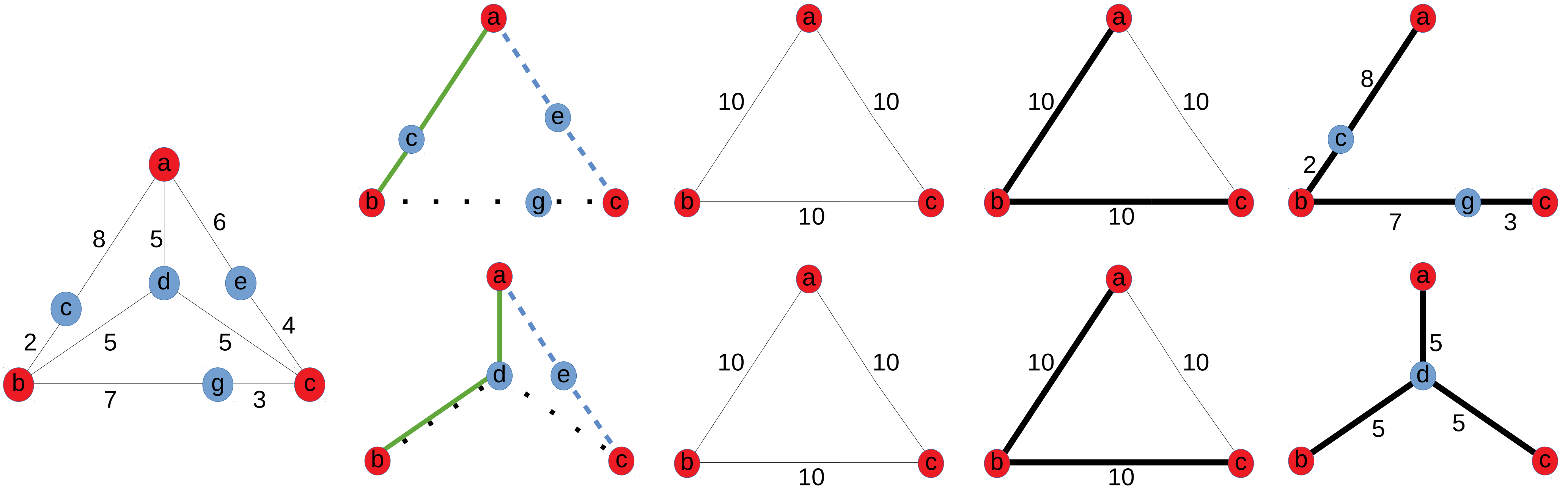
// Construct G''

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'')

KMB Algorithm – Running example



(i) G (ii) SSSP (iii) G' (iv) G'+MST (v) G''+MST

1) A parallel KMB may output a different answer. (2) Last MST may be avoided

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 {
  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_T , E_T) $V_T \supseteq L$

For u ∈ L {
  SSSP(G, W , L, u)
  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

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.

SSSP : Dijkstra vs BellmanFordMoore

- Runs in time O((m+n) log n)
- Uses Fibonacci Min-Heap
- At each iteration,
  - Pick up node from Q
  - RELAXes all its neighbours

In parallel setting it is difficult use Queue

- Runs in time O(nm)
- No heap
- All edges are RELAXed at most (n-1) times

```
For i from 1 to n-1:
   For each edge (u, v) in E
         RELAX(u,v, W(u,v))
```

RELAX all edges
Launched using n threads or m

Dijkstra and its RELAX operations

INPUT: G(V,E,W), src
OUTPUT: d[], p[]

```
INITIALIZE-SINGLE -SOURCE (G, src)
Q = G.V
while(! Q.empty() ) {
   u = ExtractMin(Q);
   For v in Adj[u]
      RELAX(u,v, W)
}
```

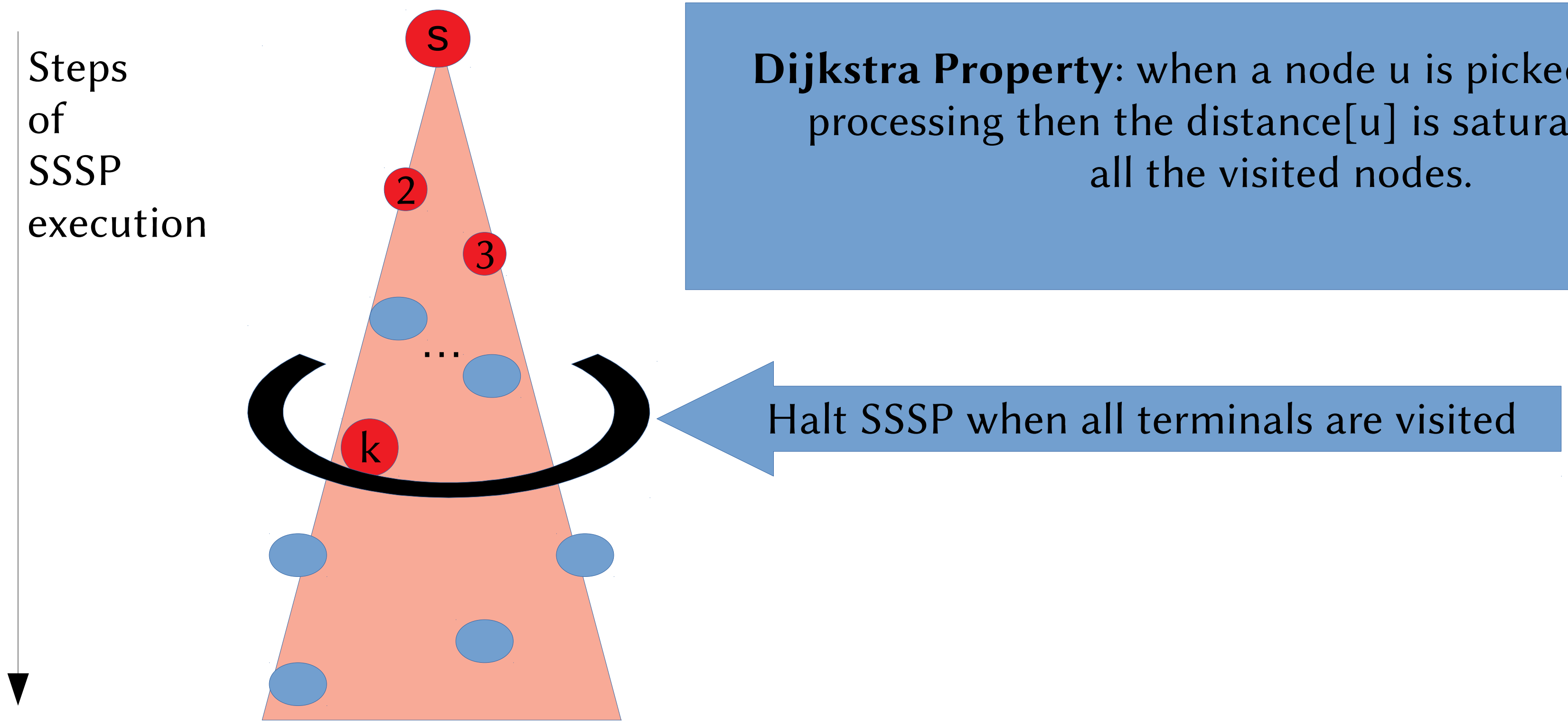
```
RELAX(u, v, W){
   If u.d + W(u,v) < v.d {
      v.d =u.d + W(u,v)
      v.p = u
   }
}
```

```
INITIALIZE-SINGLE -SOURCE(G , src)
   For each v in G.V {
      v.d = ∞
      v.p = NIL
}
src.d = 0
```

Source : CLRS book

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

Design choice for parallelization

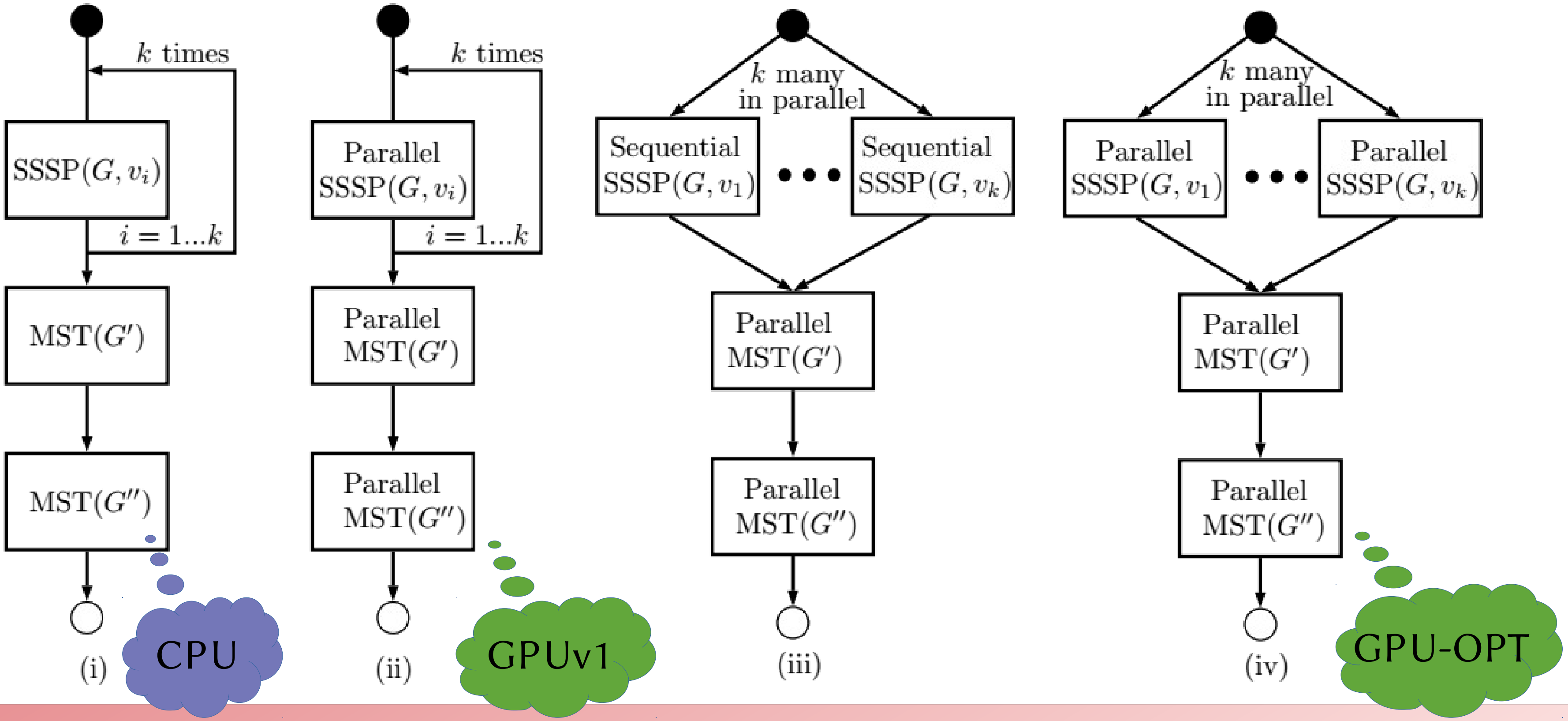
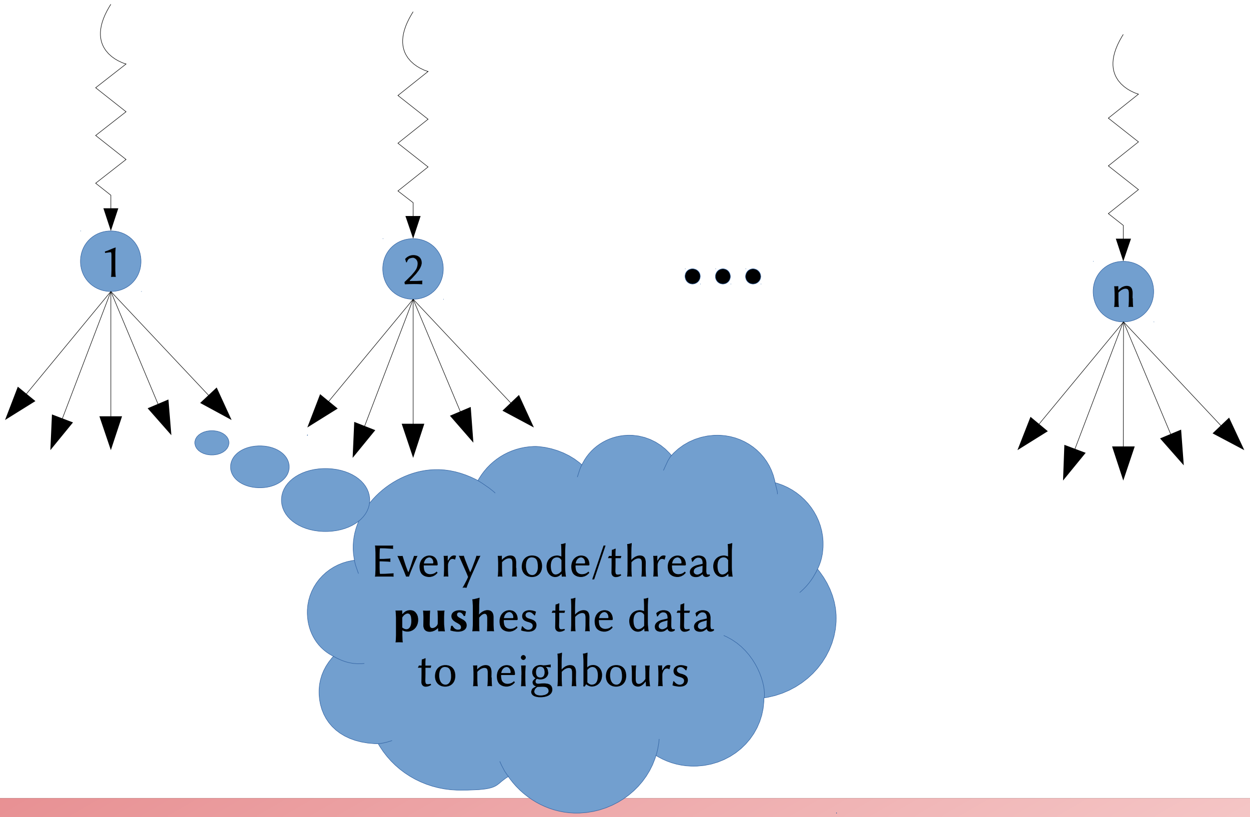


Fig. 5 Design choices.

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

- Note we reuse d[] p[] across iterations
- We need the p[] for knowing the intermediate vertices in the shortest path

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

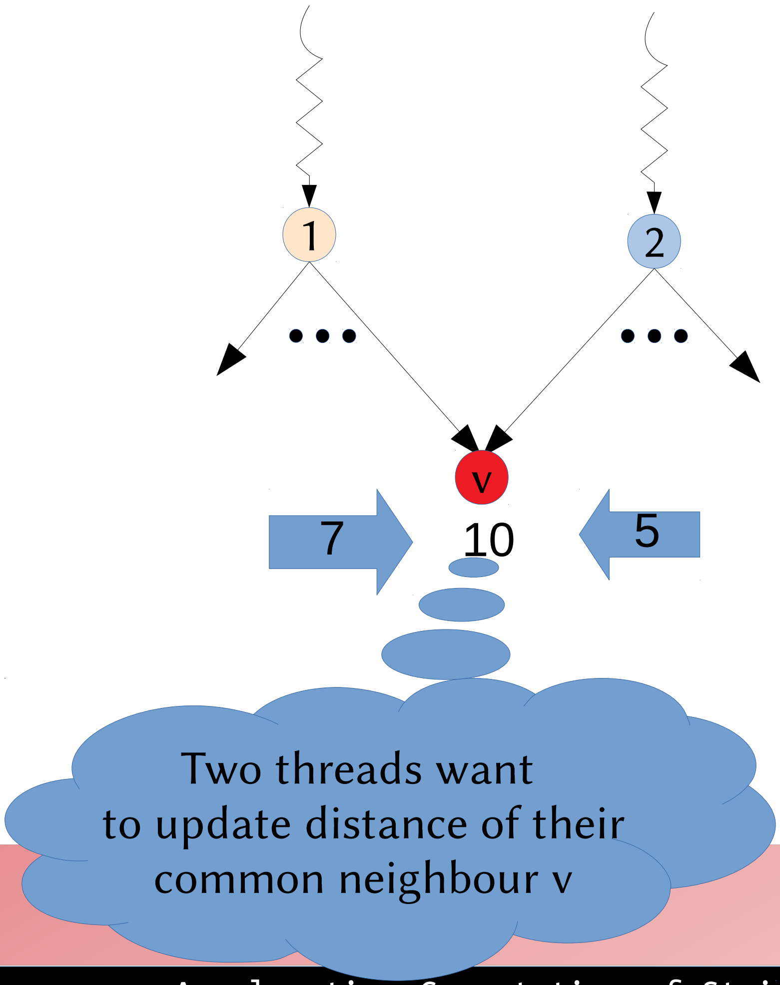
```
SSSP-KERNEL(..,s, d_s , p_s , changed, n) {
u = tid  // compute tid;
If tid < n  {
   For v ∈ adjacent[u] { // Using CSR arrays
      // Relax Operation (u, v, W(u,v))
      newCost = d_s[u] + W(u, v) ;
      old = d_s[v];
      If newCost < old
          Atomic-MIN(d_s[v], newCost);
      // Updates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

Parent update - Challenge

Shared
d[], p[]

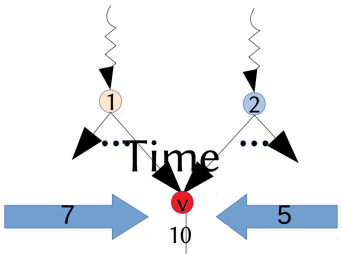
Thread 1

newCost=7
old=10

d[v]=7 //oldA=10

p[v] =1

Wrong!



Thread 2

newCost=5
old=10

d[v]=5 //oldA=7

p[v]=2

```
<snip>
newCost = d[u] + W (u, v) ;
old = d[v];
If newCost < old
  oldA=Atomic-MIN(d[v], newCost);

// Atomic-MIN is Success
If oldA != old {
  // Update's Parent array
   p[v] = u;
   changed = true;
}
```

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? Locks?

Synchronization optimization • Pull

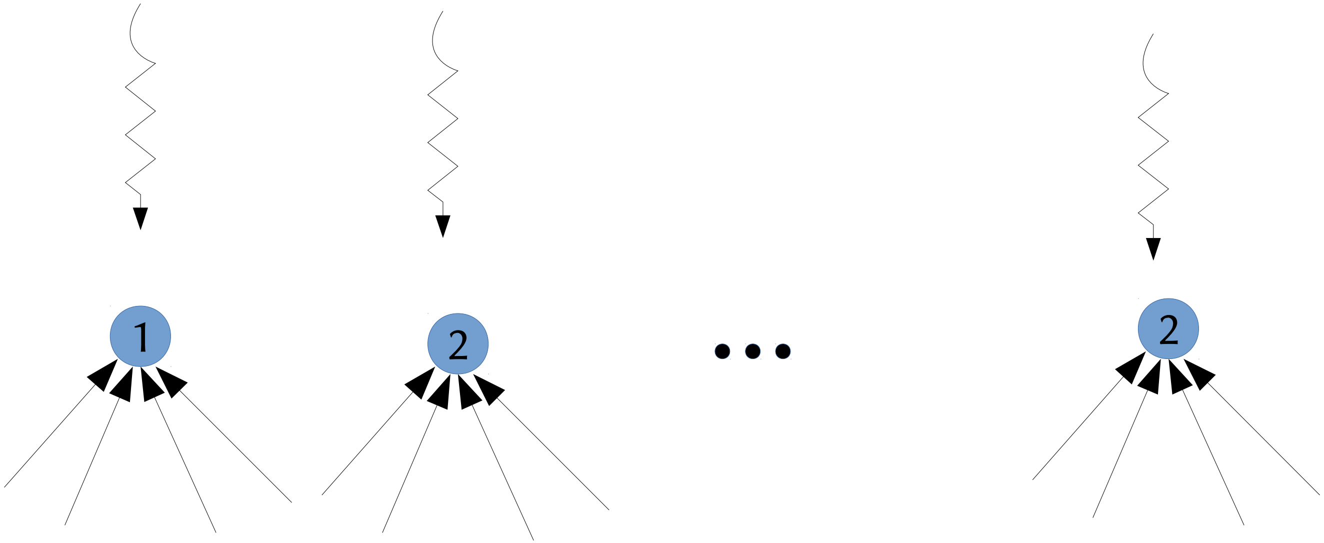


Fig. 8 Pull-SSSP

```
<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
  - **<u>Pull</u>**
- Computation
  - Data-driven
  - Edge-based
  - **<u>Controlled Computation unrolling</u>**
    - Δ^2
    - 2Δ
    - **<u>$t\Delta$</u>**
- 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
  - Empirically, we achieved best performance when t=3
- Data-driven
  - Needs Worklist (WL)
  - Active/Change nodes are inserted into WL
  - Only size of WL many threads launched
  - Need synchronization while inserting nodes in WL
- Edge based optimization
  - m-threads are launched
  - RELAXes one edge or a group of edges
  - Representation needs to be modified.

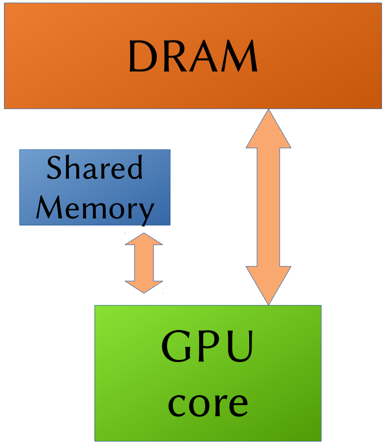
Graph algorithms are memory bounded

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, ...);
}

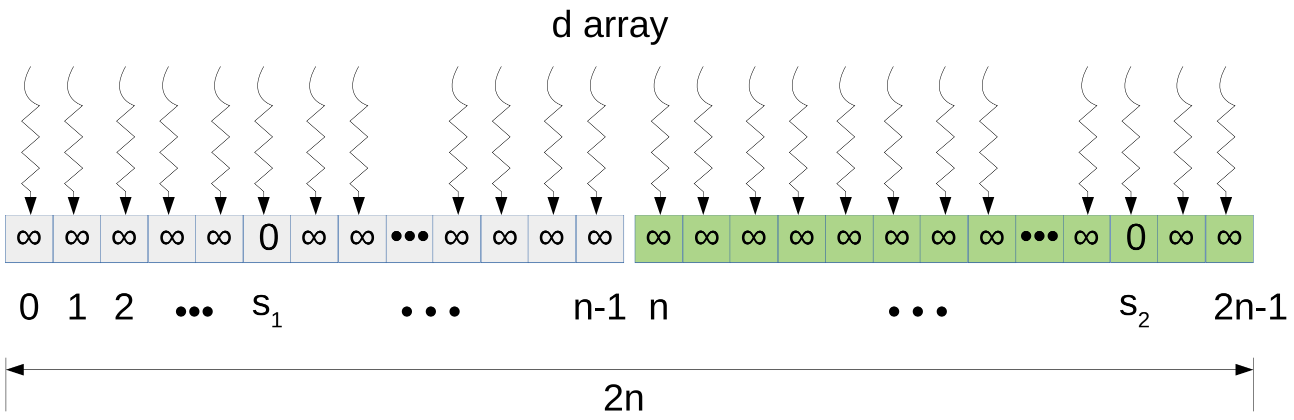


Fig. 9 Double-barrel approach.

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

- CentOS Linux release 7.5
- GCC 7.3.1 with O3
- CUDA 10.2

Graphsuite
- Total 14 Graphs
  - 11 from PACE Challenge [PACE2018]
  - 2 from SteinLib
  - 1 from SNAP
- n : 17K – 235K
- m : 27K – 498K
- k : 0.1K – 6K

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

- PACE 2018 - https://pacechallenge.org/2018/steiner-tree/
- CIMAT Team - https://github.com/HeathcliffAC/SteinerTreeProblem
- S. Beyer and M. Chimani, Strong Steiner Tree Approximations in Practice, JEA 2019.

Experiments – Comparison of solution quality

Why?

STP is an NP-hard,
our algorithm finds a solution
closer to optimum.

Solution Quality

- KMBGPU-OPT, KMBCPU and JEA are similar vs OPT
- KMBGPU-OPT and KMBCPU are better than PACE on all instances

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

Experiments - Speed-up

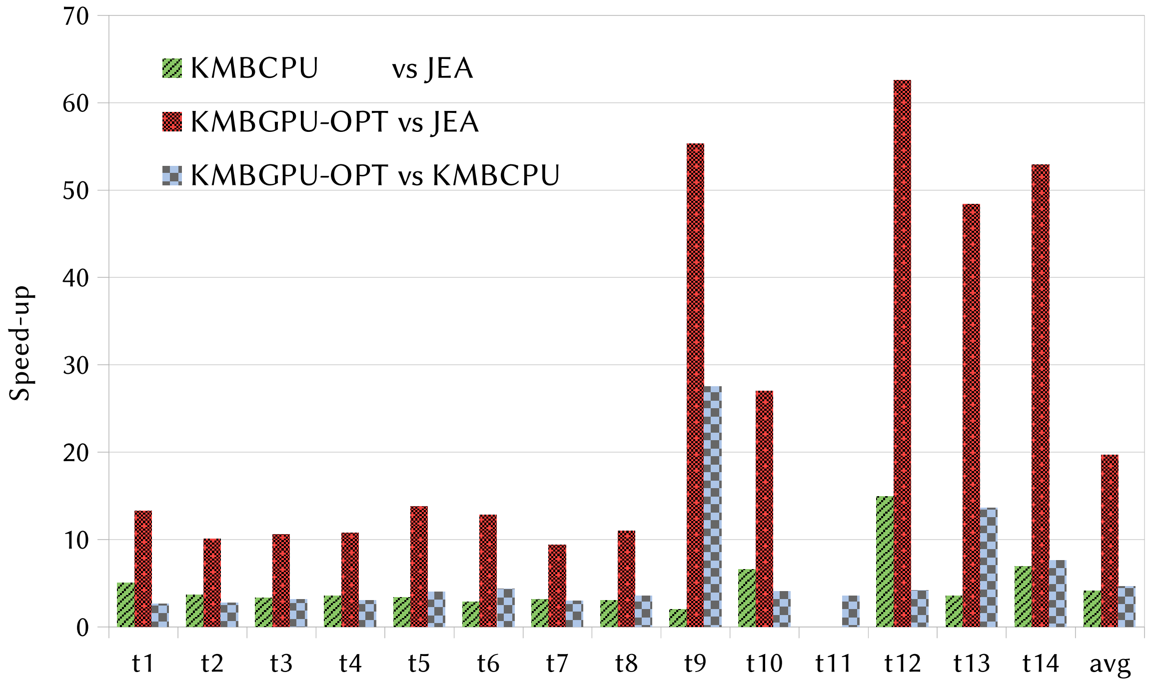


Fig. 10 Speed-up comparisons of the implementations (higher is better). JEA timed-out on t11

Takeaway: KMBCPU and KMBGPUOPT is better than JEA

Comparison of GPU time with Shared memory

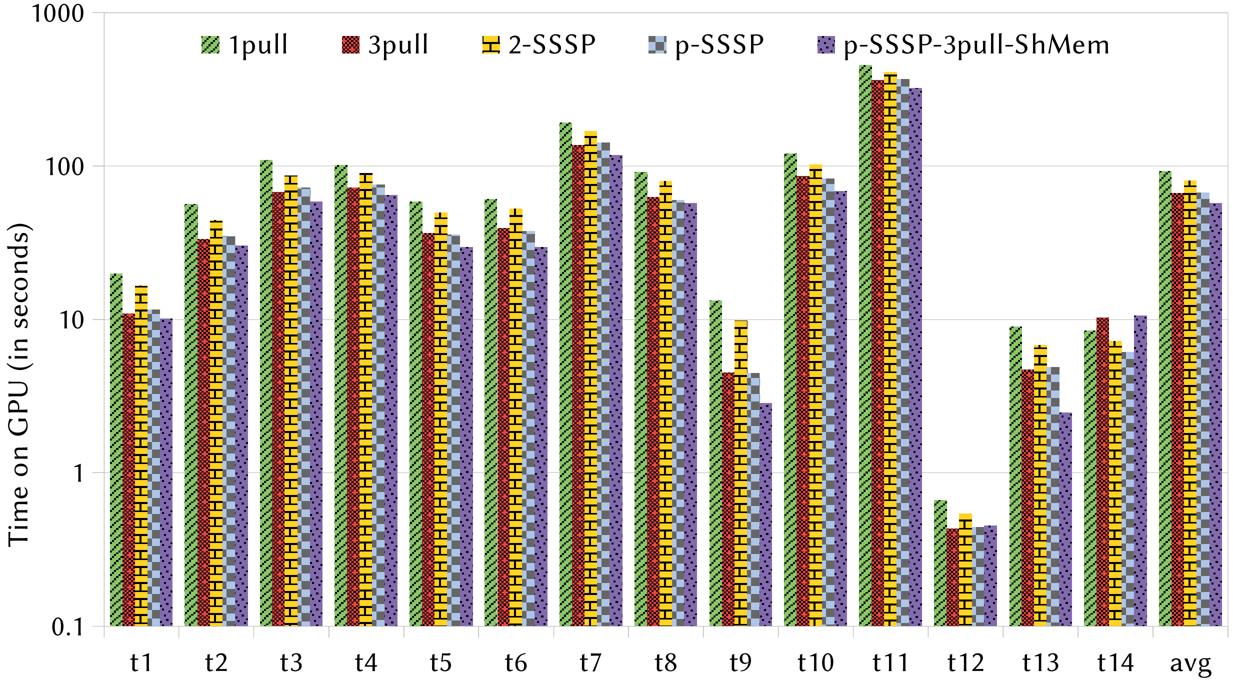


Fig. 11 Comparison of 1-Pull, 3-Pull, Double-barrel & p-SSSP+3-Pull+shared memory (smaller is better). Note: 1-Pull is KMBGPU whereas p-SSSP-3pull-ShMem is KMBGPU-OPT

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

Comparison of p-SSSP

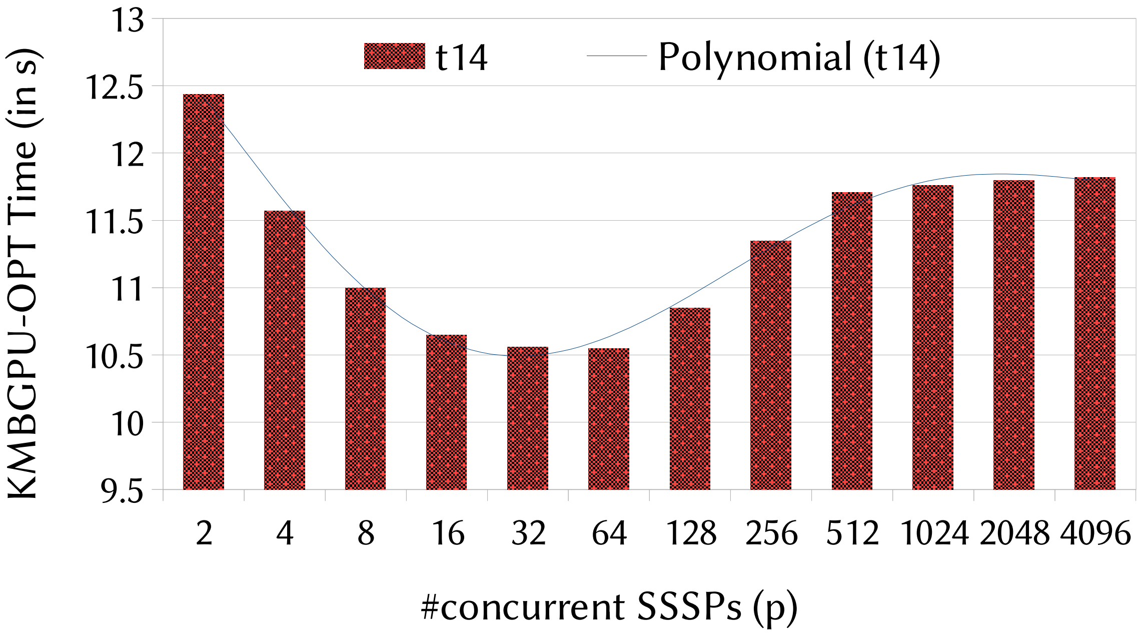


Fig. 12 KMBGPU with varying p-SSSP for the same graphs t14 (Smaller is better).

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

Experiments – Scalability of GPU and CPU

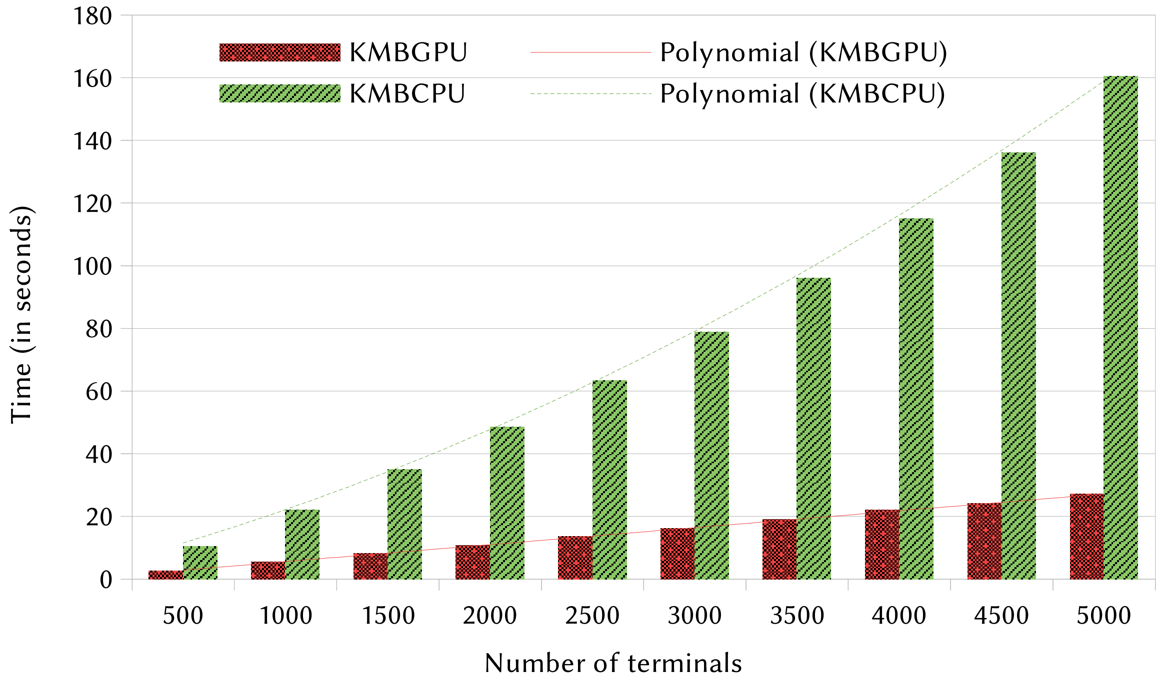
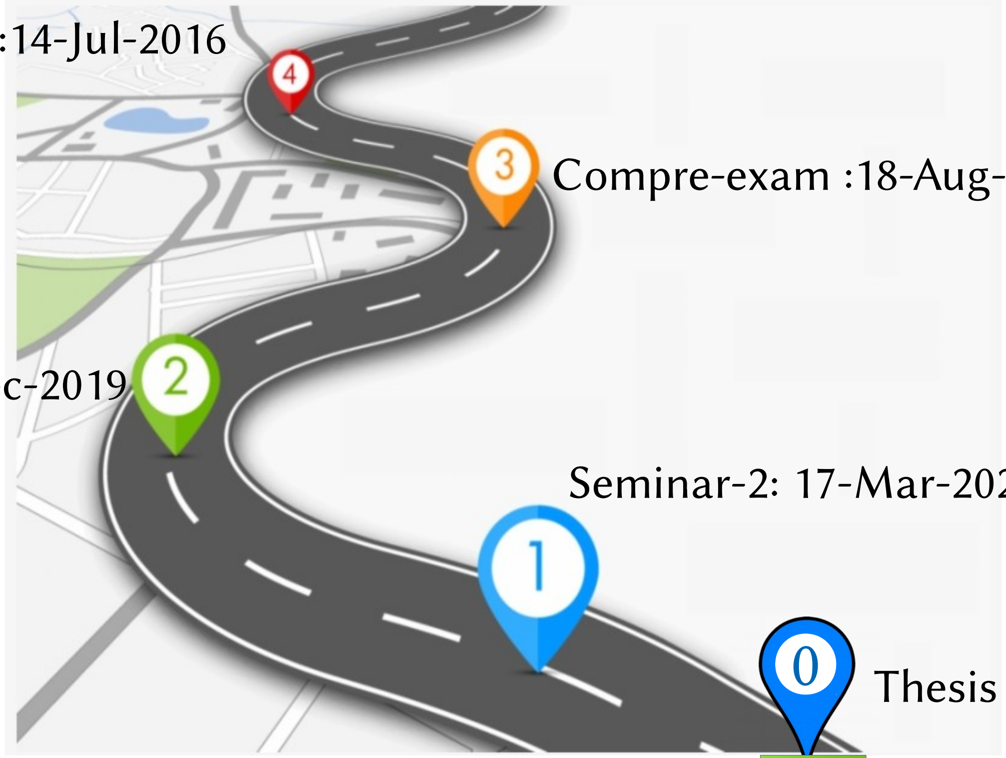


Fig. 13 Scalability plot on **t14** with increasing terminal size (lower is better)

Takeaway: KMBGPU-OPT scales better than KMBCPU

Timeline

Start



Joining:14-Jul-2016

Compre-exam :18-Aug-2018

Seminar-1: 09-Dec-2019

Seminar-2: 17-Mar-2022

Thesis Submission (expected) :30-May-2022

End

Summary

- SSSP halt-optimization benefits CPU.
- Pull and p-SSSP optimization benefits GPU.
- Our output Steiner tree can be used as initial tree for other local search algorithms.
- Our technique is applicable when multiple parallel instances of an operator are used.

Future work

- KMBCPU can be extended to multicore-CPU.
- KMBGPU-OPT can be extended to multi-GPU.

- Capacitated Vehicle Routing Problem
- Build a GPU graph library for aiding NP-Hard problems.

Thank you.