Efficient Maximal Biclique Enumeration on GPUs

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Outline

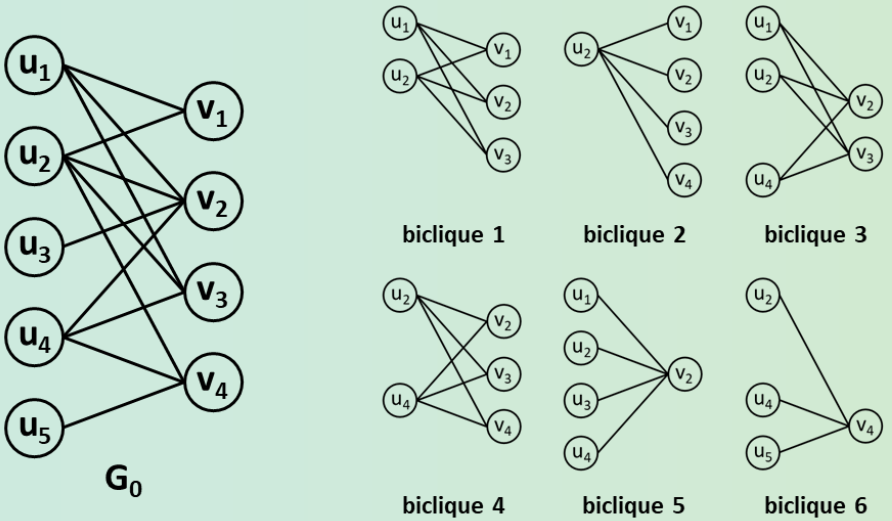
- **Introduction**
  - Problem definition
  - MBE on CPUs
  - Related work comparison
- **Challenges of MBE on GPUs**
  - Large memory requirement
  - Massive thread divergence
  - Load imbalance
- **GMBE : the first highly-efficient GPU solution for the MBE problem**
  - Stack-based iteration with node reuse
  - Pruning using local neighborhood sizes
  - Load-aware task scheduling
- **Evaluation**

Introduction

- Problem definition
- MBE on CPUs
- Related work comparison

Introduction : Problem Definition

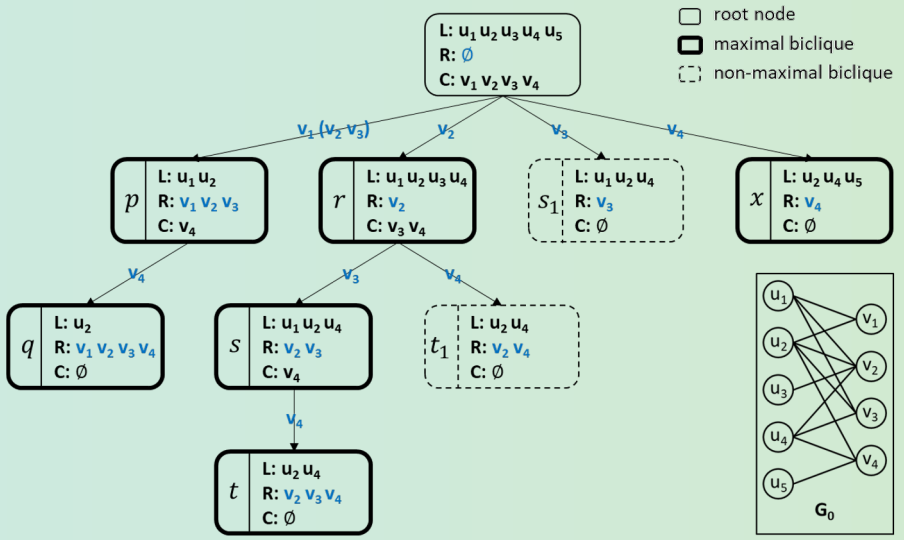
- **Preliminaries**
  - Bipartite graph $G(U,V,E)$: A graph structure contains two disjoint vertex sets U,V and an edge set E. $E \subseteq U \times V$.
  - Biclique : A complete bipartite graph in which every vertex is connected to every vertex in the opposite subset.
  - Maximal biclique : a biclique that can not be further enlarged to form a large biclique.
- **Problem definition**
  - Maximal biclique enumeration (MBE) aims to find all maximal bicliques in G.



A bipartite graph G_0 containing 6 maximal bicliques.

Introduction : MBE on CPUs

- **Set enumeration tree for MBE**
  - Each tree node is a 3-tuple (L, R, C). (L, R) is the corresponding biclique and C stores candidate vertices for expanding R.
- **Baseline solution**
  - Step 1 : Utilize a set enumeration tree to generate the powerset of V.
  - Step 2 : Expand each subset of the powerset of V to a biclique (L, R) and enumerate maximal ones.



Introduction : MBE on CPUs

- **Recent optimizations**
  - Vertex ordering [1, 2, 5]
  - Candidates pruning using pivots [1, 2]
  - Parallelization on multicore CPUs [3] or distributed architectures [4]

Existing solutions for MBE are insufficient because their performance speedup is constrained by the limited parallelism of CPUs.

[1] Lu Chen, Chengfei Liu, Rui Zhou, Jiajie Xu, and Jianxin Li. 2022. Efficient Maximal Biclique Enumeration for Large Sparse Bipartite Graphs. VLDB 2022. 1559-1571.

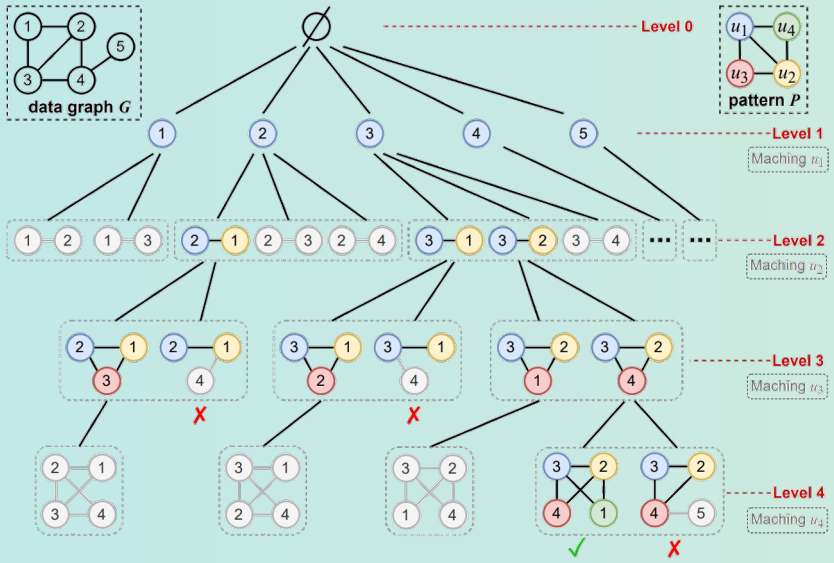
[2] Aman Abidi, Rui Zhou, Lu Chen, and Chengfei Liu. Pivot-Based Maximal Biclique Enumeration. IJCAI 2020. 3558–3564.

[3] Apurba Das and Srikanta Tirthapura. 2019. Shared-Memory Parallel Maximal Biclique Enumeration. HiPC 2019.

[4] Arko Provo Mukherjee and Srikanta Tirthapura. Enumerating Maximal Bicliques from a Large Graph Using MapReduce. IEEE Trans. Serv. Comput. 10, 5 (2017), 771–784.

[5] Yun Zhang, Charles A. Phillips, Gary L. Rogers, Erich J. Baker, Elissa J. Chesler, and Michael A. Langston. BMC bioinformatics 15, 1 (2014), 110.

Introduction : Related Work Comparison



An enumeration tree for mining pattern P in data graph G.

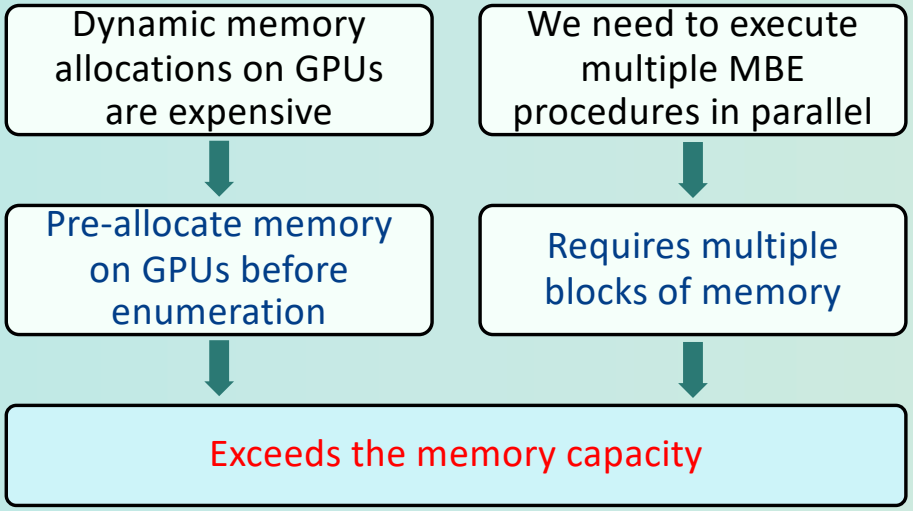
Problem	MBE	Graph pattern mining [1]
Vertex count in enumerated subgraphs	Unfixed number of vertices, can be large.	Fixed number of vertices equivalent to pattern size |P|, typically small.
Enumeration tree height	Unfixed and can be up to $d_{max}(V)$.	Fixed and equal to |P|.
Conclusion	(1) MBE requires **significantly more memory** than GPM to actively maintain up to $d_{max}(V)$ tree nodes for backtracking. (2) MBE generates **more severe imbalanced workloads** than GPM due to the variation in height among its enumeration trees.	

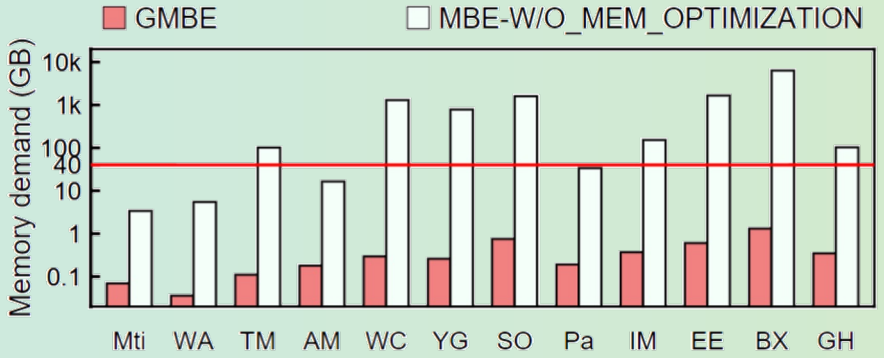
[1] Xuhao Chen and Arvind. Efficient and Scalable Graph Pattern Mining on GPUs. OSDI 2022. 857–877.

Challenges

- Large memory requirement
- Massive thread divergence
- Load imbalance

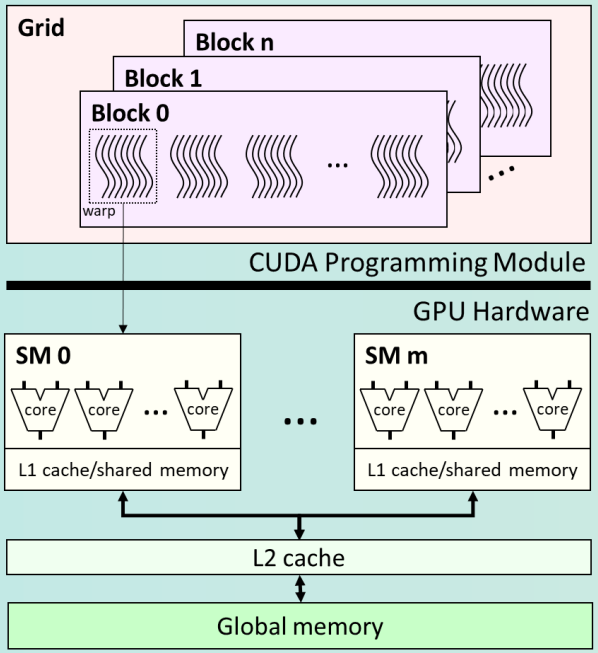
Challenge 1 : Large Memory Requirement





Directly parallelizing existing MBE procedures on an A100 GPU will exceed the memory capacity on multiple datasets.

Challenge 2 : Massive Thread Divergence



GPU architecture.

CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
    code B;
  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
    code F;
  }
}
```

CS 1

```
code A;
code A;
```

CS 0 and CS 1 are GPU code segments where threads with different routines execute 2 sets of codes each.

Challenge 2 : Massive Thread Divergence

CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
    code B;
  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
    code F;
  }
}
```

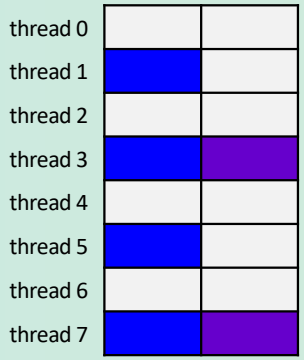
CS 1

```
code A;
code A;
```

Challenge 2 : Massive Thread Divergence

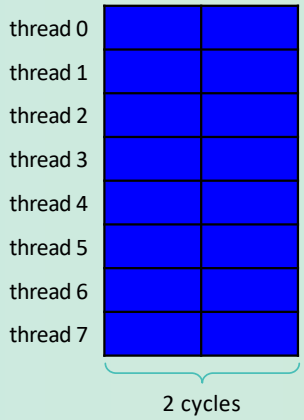
CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
    code B;
  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
    code F;
  }
}
```



CS 1

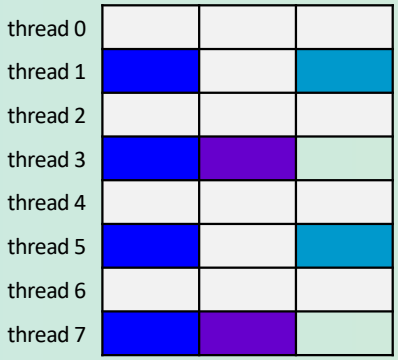
```
code A;
code A;
```



Challenge 2 : Massive Thread Divergence

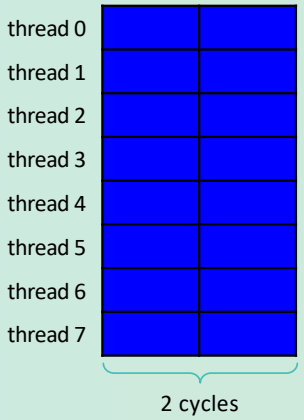
CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
    code B;
  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
    code F;
  }
}
```



CS 1

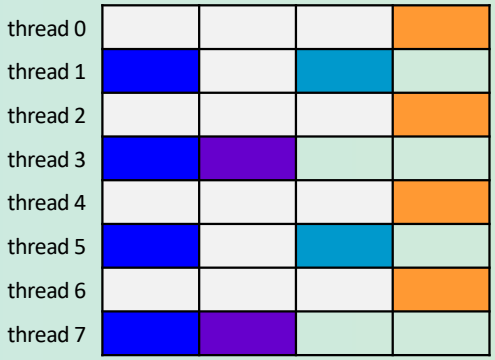
```
code A;
code A;
```



Challenge 2 : Massive Thread Divergence

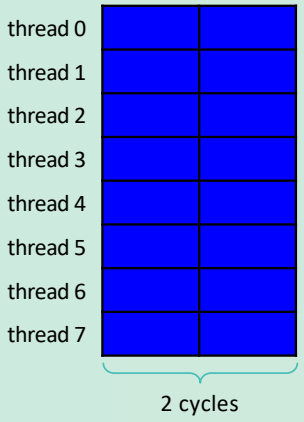
CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
    code B;
  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
    code F;
  }
}
```



CS 1

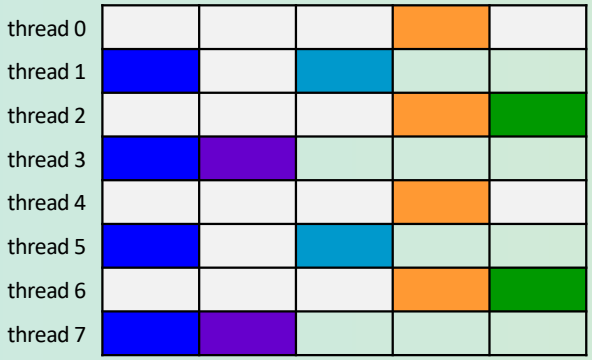
```
code A;
code A;
```



Challenge 2 : Massive Thread Divergence

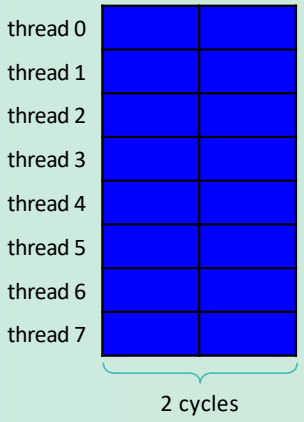
CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
    code B;
  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
    code F;
  }
}
```



CS 1

```
code A;
code A;
```



Challenge 2 : Massive Thread Divergence

CS 0

```
if((threadIdx.x & 1) == 1){
  code A;
  if((threadIdx.x & 2) == 2){
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  } else{
    code C;
  }
}else{
  code D;
  if((threadIdx.x & 2) == 2){
    code E;
  } else{
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  }
}
```
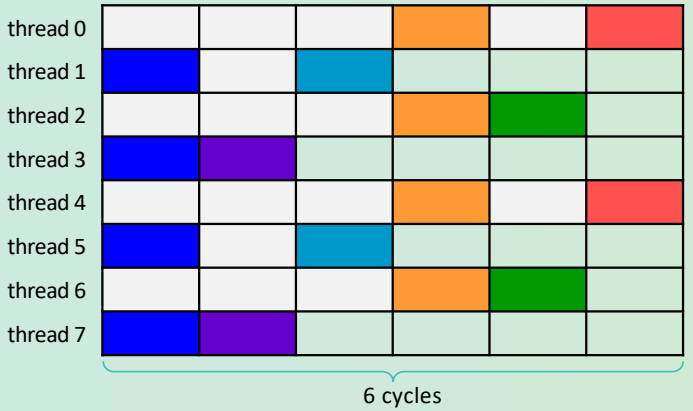
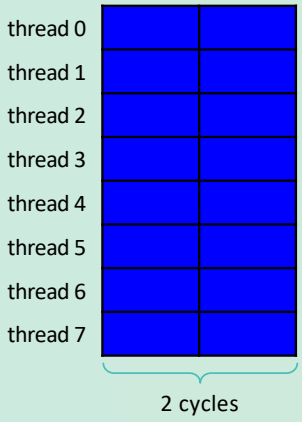



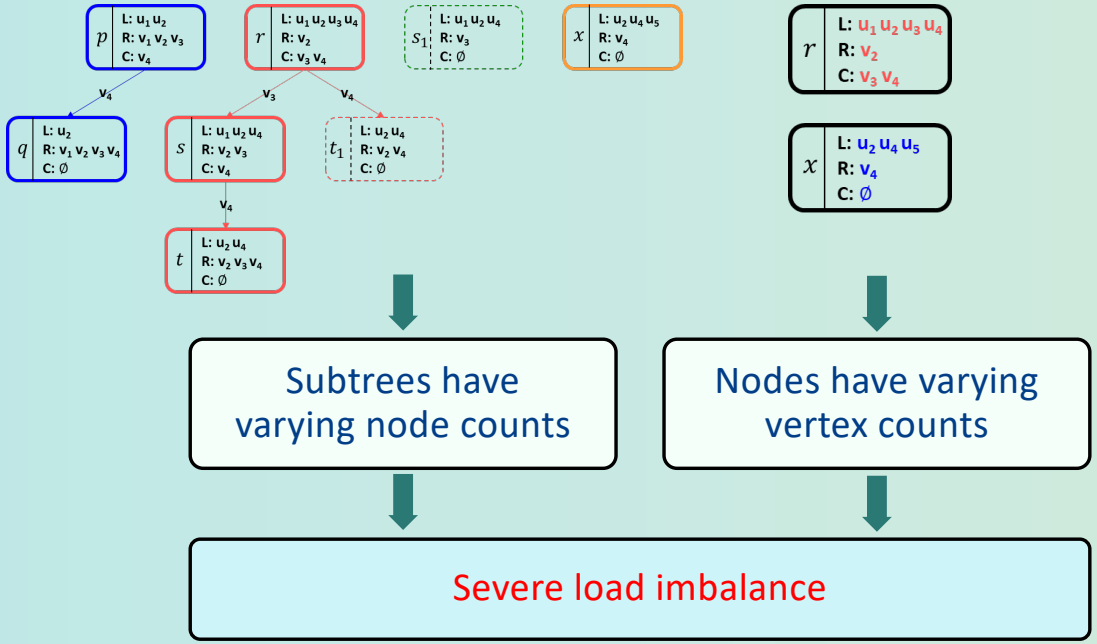
CS 1

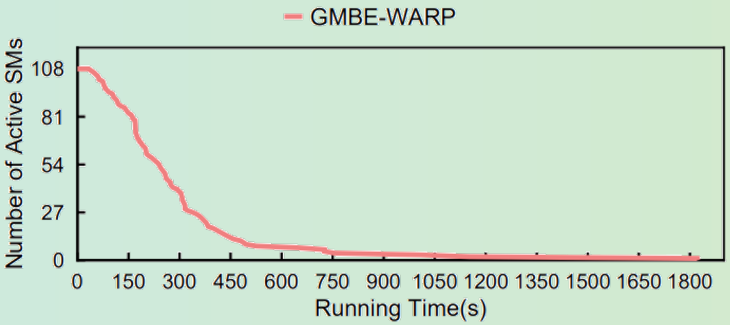
```
code A;
code A;
```



CS 0 requires more time because of the thread divergence.

Challenge 3 : Load Imbalance





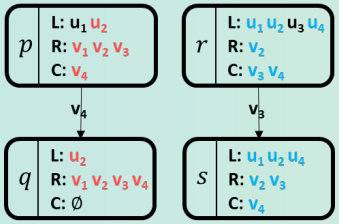
Active SMs rapidly decline over time in a straightforward algorithm.

GMBE

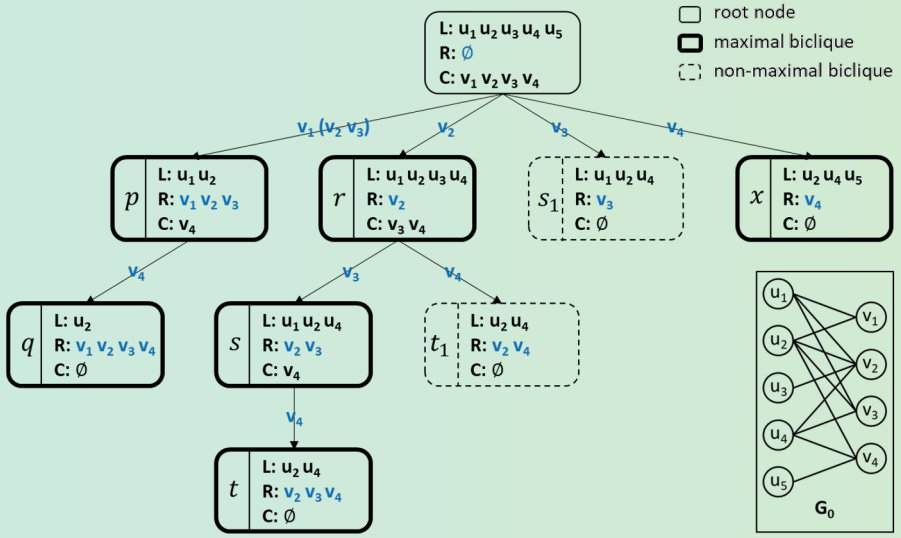
- Stack-based iteration with node reuse
- Pruning using local neighborhood sizes
- Load-aware task scheduling

Idea 1 : Stack-based Iteration with Node Reuse

- **Key Observation**
  - Vertices in the child node are always a subset of vertices in the parent node.



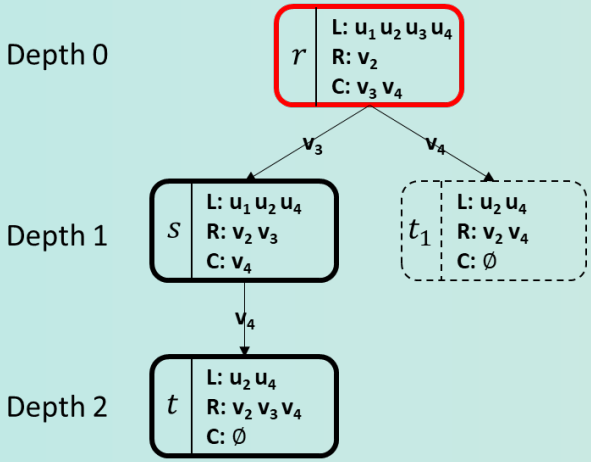
- **Main idea**
  - We allocate memory for the root node and reuse this memory to derive all nodes within the subtree, resulting in a notable reduction in memory usage.



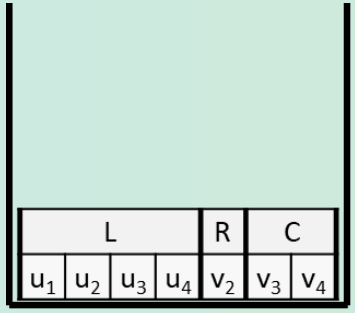
Idea 1 : Stack-based Iteration with Node Reuse

➢ **Step 1 : initialize node r**

Enumeration tree rooted by node r

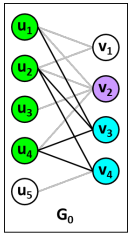


Memory usage for existing approach



Memory usage for GMBE

	L_r				R_r	C_r	
Vertex	u_1	u_2	u_3	u_4	v_2	v_3	v_4
Depth	0	0	0	0	0	∞	∞
Local neighborhood size						3	2

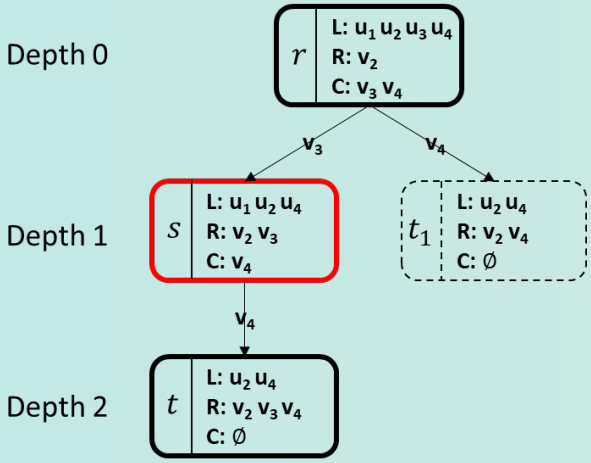


The local neighborhood size for v_3 is 3 because v_3 connect with u_1, u_2, and u_4 in L_r.

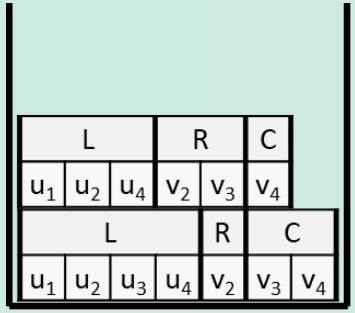
Idea 1 : Stack-based Iteration with Node Reuse

➢ **Step 2 : generate node *s***

Enumeration tree rooted by node r



Memory usage for existing approach



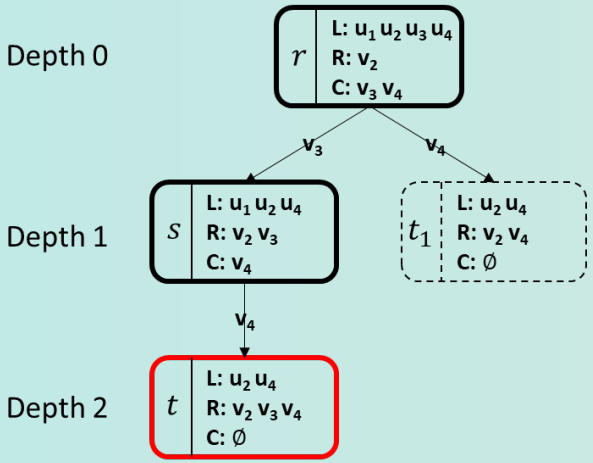
Memory usage for GMBE

	L_r				R_r	C_r	
Vertex	u_1	u_2	u_3	u_4	v_2	v_3	v_4
Depth	1	1	0	1	0	1	∞
Local neighborhood size						3	2

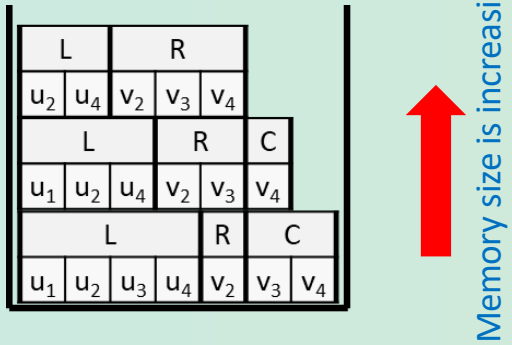
Idea 1 : Stack-based Iteration with Node Reuse

➢ **Step 3 : generate node *t***

Enumeration tree rooted by node r



Memory usage for existing approach



Memory usage for GMBE

	L_r				R_r	C_r	
Vertex	u_1	u_2	u_3	u_4	v_2	v_3	v_4
Depth	1	2	0	2	0	1	2
Local neighborhood size					2	2	

Memory size is fixed

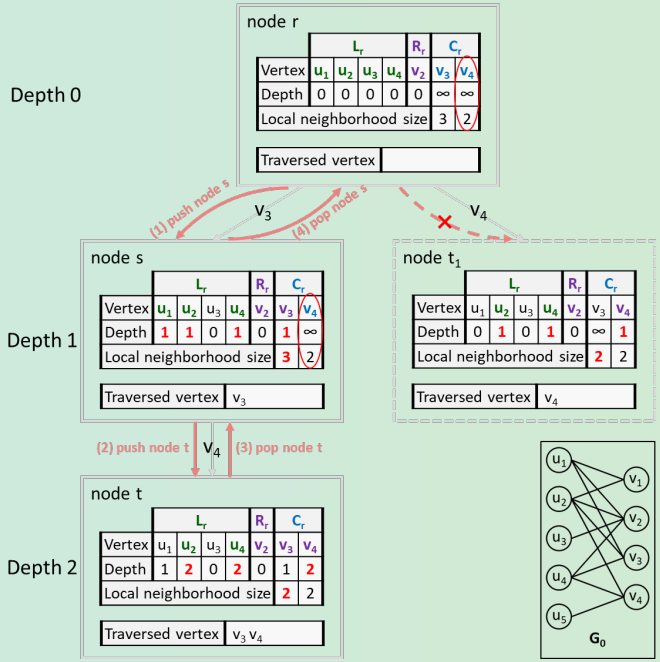
Idea 2 : Pruning Using Local Neighborhood Sizes

➢ Key observation

- Local neighborhood sizes, as a necessary intermediate result, can be utilized for pruning.

➢ Main idea

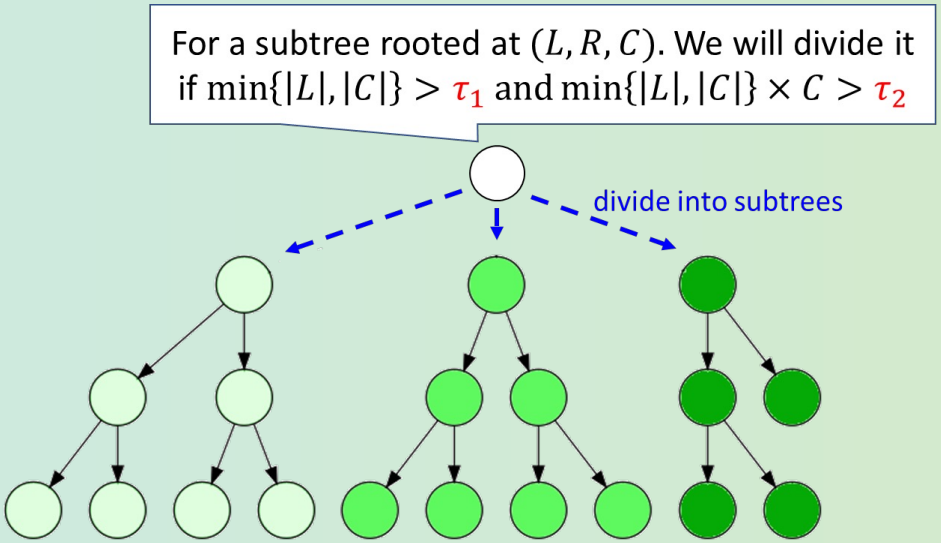
- We prune useless candidates if their local neighborhood sizes do not change after popping a traversed child node. This approach reduces thread divergence by checking multiple local neighborhood sizes simultaneously..



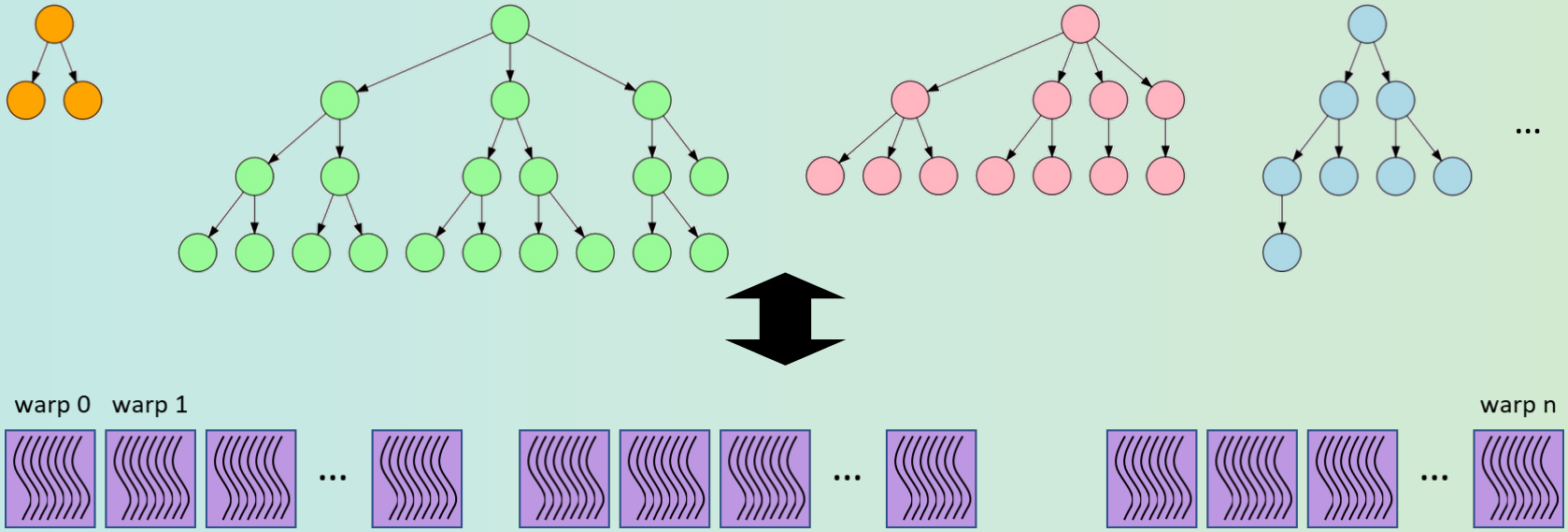
GMBE proactively prunes node t_1 by removing useless candidate vertex v_4 at node r because the local neighborhood size (i.e., 2) for v_4 does not change after popping node s.

Idea 3: Load-aware Task Scheduling

- **Key observation**
  - Due to the imbalance of subtrees in MBE problems, directly mapping subtrees to computational resources leads to significant load imbalance.
- **Main idea**
  - Design two thresholds to detect large subtree.
  - Dynamically divide large trees into multiple subtrees to balance the workloads.

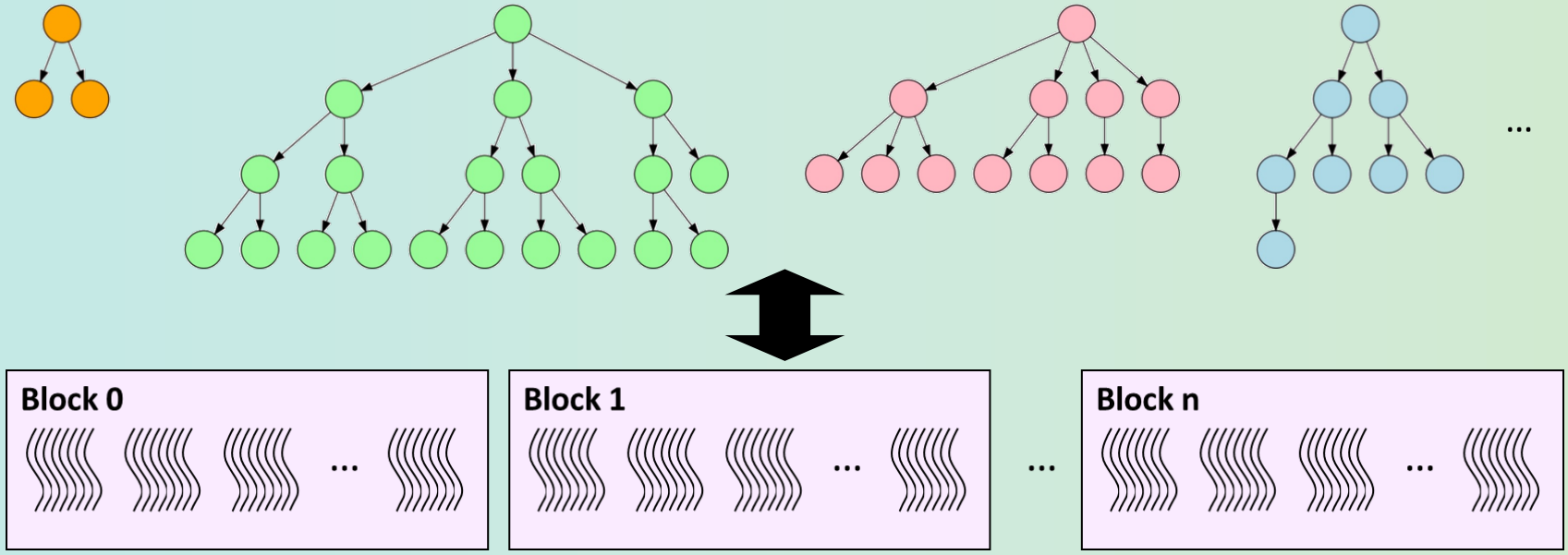


Idea 3: Load-aware Task Scheduling



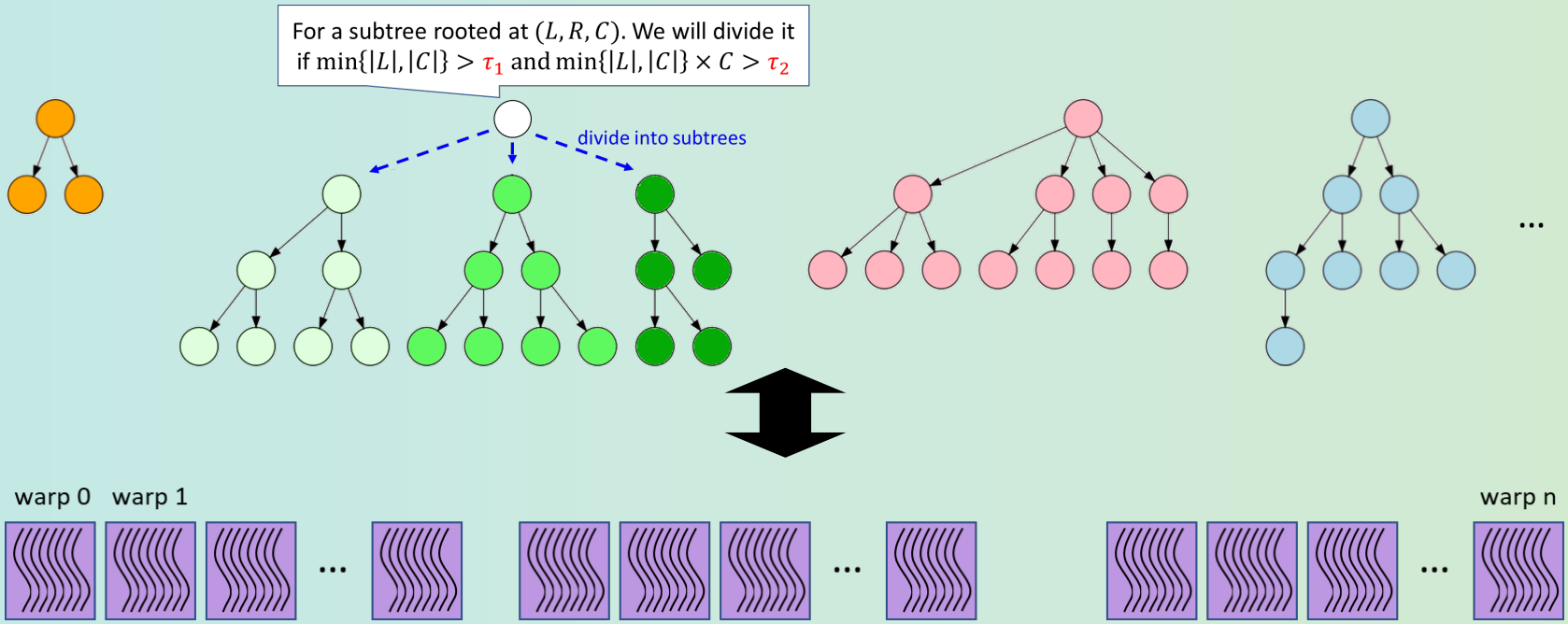
Solution 1 : Map subtrees to warps.

Idea 3: Load-aware Task Scheduling



Solution 2 : Map subtrees to blocks.

Idea 3: Load-aware Task Scheduling



Solution 3 : Dynamically divide large tree into multiple subtrees and map subtrees to warps.

Evaluation

- Overall evaluation
- Effect of optimizations
- Sensitivity Analysis

Evaluation : Overall Evaluation

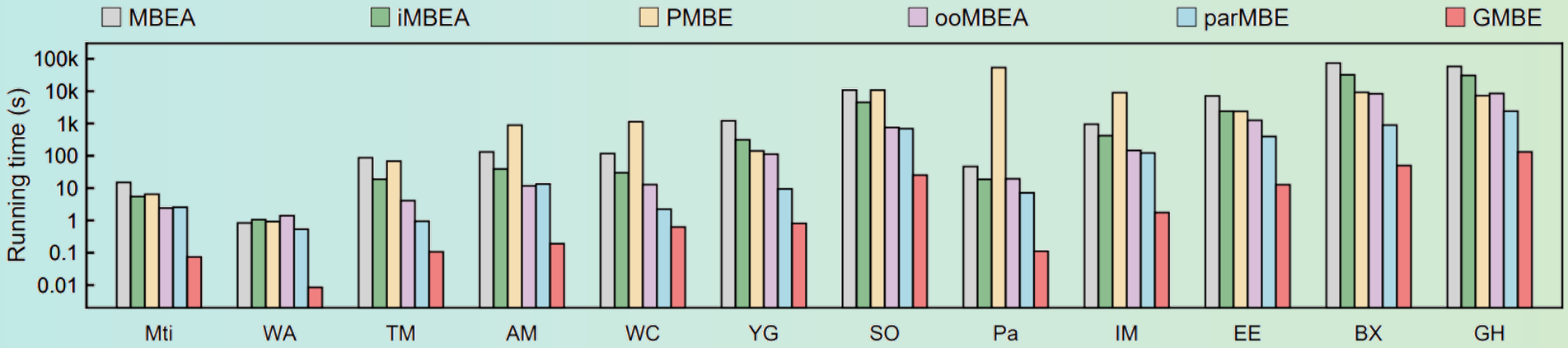


Figure 6: Overall evaluation (log scaled).

GMBE is 3.5×–69.8× faster than any next-best competitor on CPUs on all testing datasets.

Evaluation : Effect of Optimizations

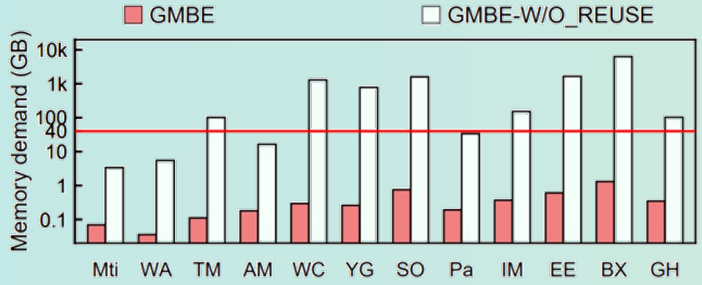


Figure 7: Effect of the node reuse approach (log scaled).

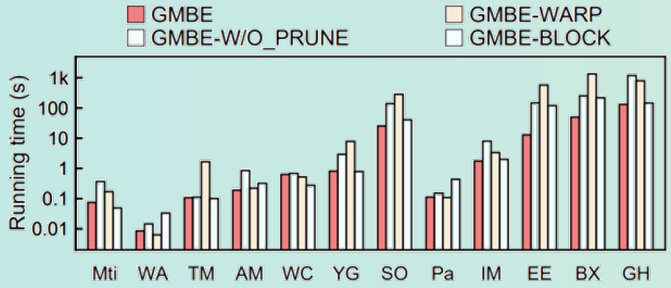


Figure 8: Effect of pruning approach and task scheduling approach (log scaled).

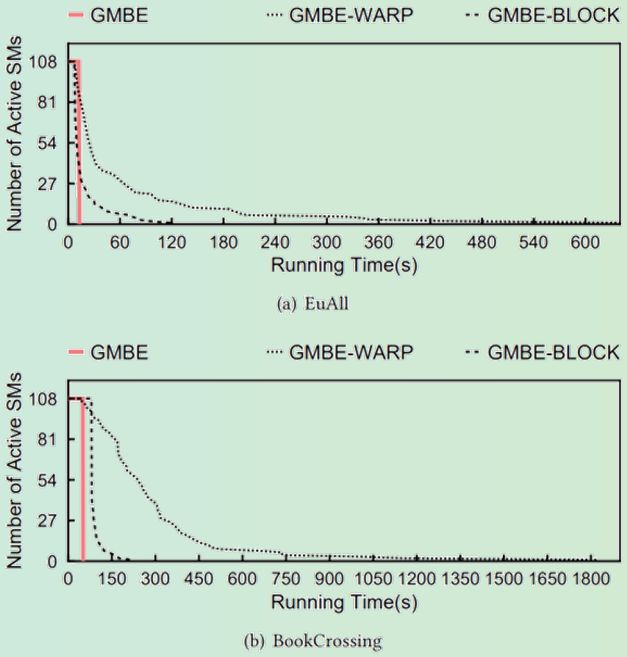
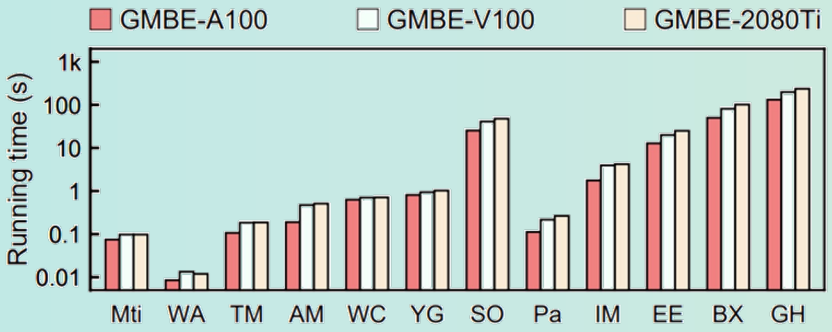


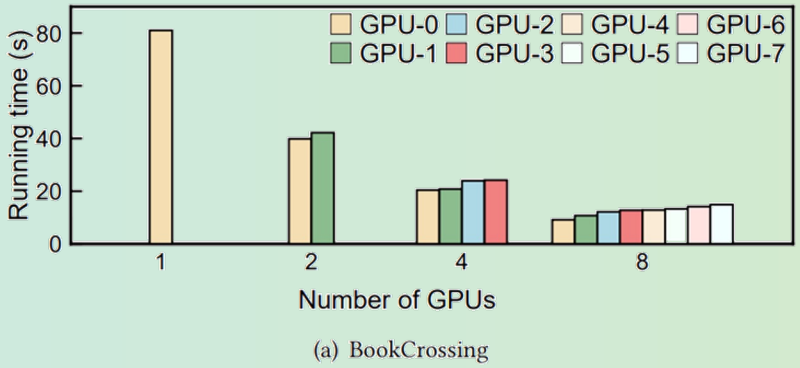
Figure 9: Comparison of runtime loads on SMs among GMBE, GMBE-WARP, and GMBE-BLOCK.

GMBE significantly reduces the memory usage, efficiently reduces the enumeration space, and successfully balance the workloads.

Evaluation : Sensitivity Analysis



Adaptability on different GPU (log scaled).



Scalability of GMBE on a machine with multi-GPU.

Q & A