EUMaster4HPC Challenge: Graph Vertex Coloring

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Objective

Develop a parallel **branch-and-bound algorithm** to compute the **chromatic number** of graphs using the Vega supercomputer.
Vega architecture

CPU CLUSTER: 960 nodes, each with 2 AMD Rome 7H12 CPUs with 64 cores, for a total of 1,920 and 122,880 cores.

GPU CLUSTER: 60 nodes, each 4 Nvidia A100 GPUs and 2 AMD Rome7h12 Cpus240 NVIDIA, for a total of 240 A100 GPUs

Algorithms & Strategies

Zykov Algorithm

G graph with V vertices and E edges.
Given two **non-adjacent** vertices $x, y \in V$ two new graphs defined:

- G'_{xy} where x and y are **contracted** or *merged* into one single vertex xy.
- G''_{xy} where the **edge** $\{x, y\}$ has been added

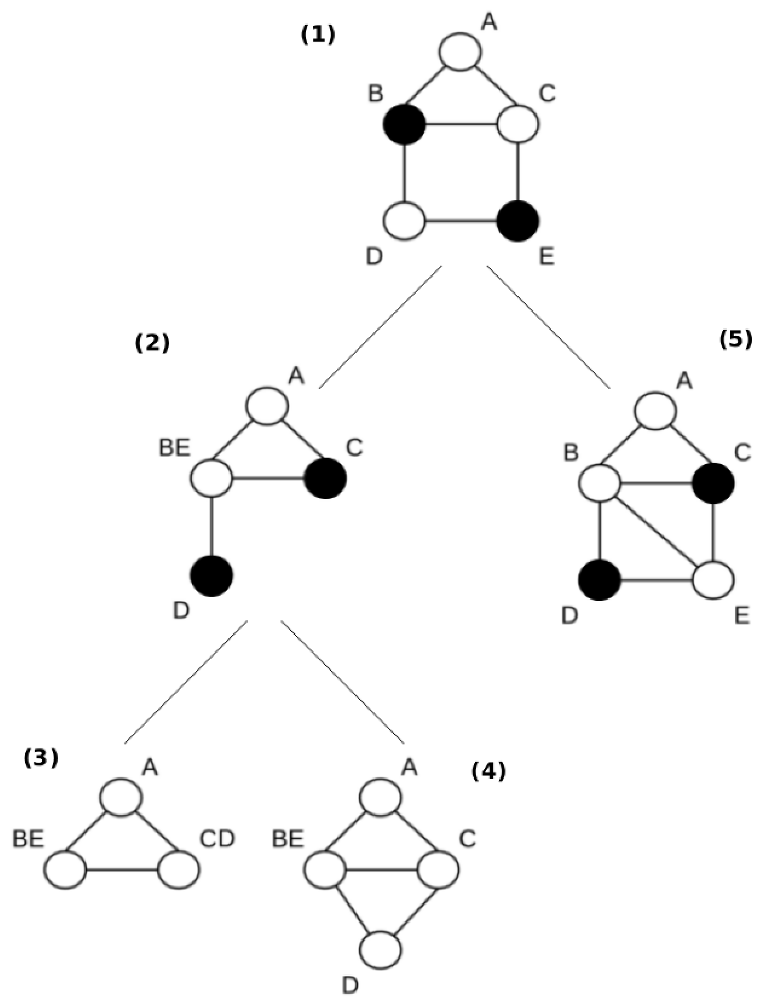
Recursive algorithm, called *Zykov's tree* (Figure 2), built upon following theorem:

Theorem 1. *The chromatic number of G is given by the recurrence*

$$\chi(G) = \min\{\chi(G'_{xy}), \chi(G''_{xy})\}$$

such that $x, y \in V(G)$ and $\{x, y\} \notin E(G)$

Leaf nodes are complete graphs. The chromatic number of the original graph G is the size of the **smallest leaf**.



Graph reduces size at every new branch $\implies$ Problem size decreases as depth increases $\implies$ complexity decreases.

Graph Representation Techniques

Optimize both memory usage and computational efficiency $\implies$ Efficient graph representation crucial.

Operation	Adjacency Matrix	Edge List	CSR	Adjacency List
Add Edge	$O(1)$	$O(1)$	$O(\|E\|)$	$O(1)$
Remove Edge	$O(1)$	$O(\|E\|)$	$O(\|E\|)$	$O(k)$
Add Vertex	$O(\|E\|)$	$O(1)$	$O(1)$	$O(1)$
Remove Vertex	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)$
Merge Vertices	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)$
Get Neighbors	$O(\|V\|)$	$O(\|E\|)$	$O(1)$	$O(1)$

Table 1: Comparison of Graph Representations

Adjacency list great performance in modifying the graph $\implies$ well suited for our application (Zykov).

Coloring Heuristics

Provide an **upper bound** for the chromatic number:

- **Greedy Coloring**: Assigns smallest available color to each vertex.
- **DSatur Algorithm**: Prioritizes vertices with most unique colored neighbors using priority queue.
- **Recoloring Algorithm**: Adjusts colors to minimize total number of colors used.

Clique Strategies

Estimate a lower bound by identifying large cliques in the graph:

- **FastWClq**: Quickly approximates maximum clique using heuristic search.
- **BMS Selection**: Selects vertices that maximize clique growth.
- **Graph Reduction**: Prunes vertices that cannot be part of a maximal clique, improving efficiency.

These heuristics improve pruning efficiency and speed up the search process.

OpenMP & MPI

Parallelization Strategies

Parallelize execution using **MPI** and **OpenMP**.
Work Distribution Models

- Simple Approach: Master orchestrates tasks.
- Scalable Approach 1 and 2: Each process explores its own search space, sharing solutions from time to time.

Multi-Threaded Processing

- Terminator: Monitors execution time and stops processes if needed.
- Gatherer: Collects solutions and updates global best results.
- Employer: Manages work-stealing (Idle workers take over unfinished tasks to balance the load).

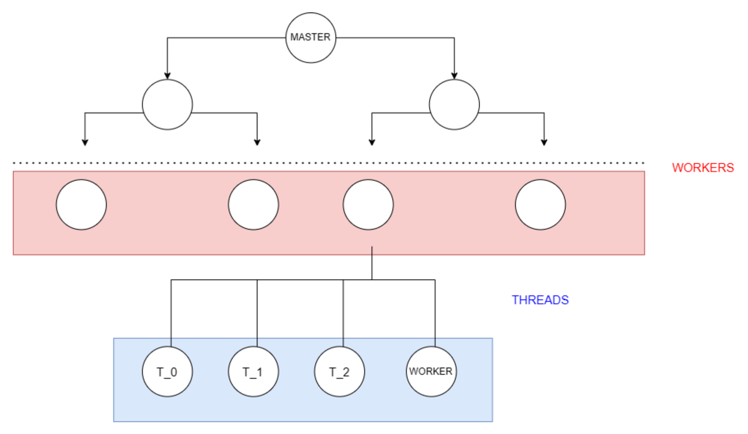


Figure 1: Simple Approach

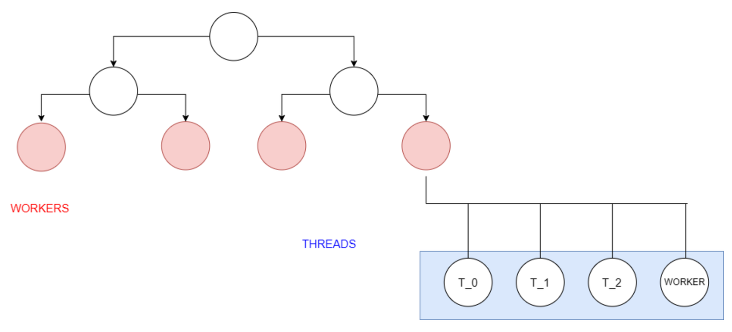


Figure 2: Scalable Approach 1, case 4 cores

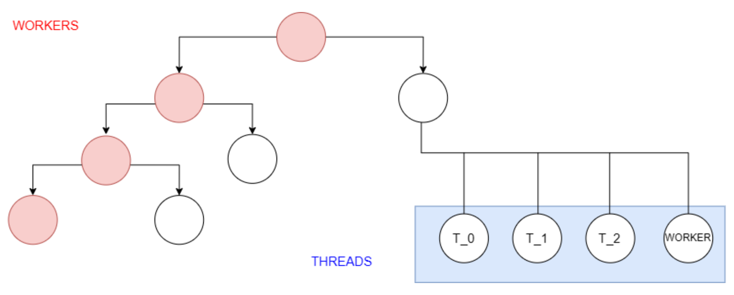


Figure 3: Scalable Approach 2, case 4 cores

Results

Table 2: Strong scaling results for solving the chromatic number of `queen7_7.col`.

Nodes	Time (s)	Total Cores	N processors
1	330.91	32	8
2	100.22	64	16
4	70.78	128	32
8	55.89	256	64
16	46.01	512	128
32	0.23	1024	256

Table 3: Strong Scaling Results (Set 1)

Figure 4: Execution time vs. number of nodes for solving `queen7_7.col`.

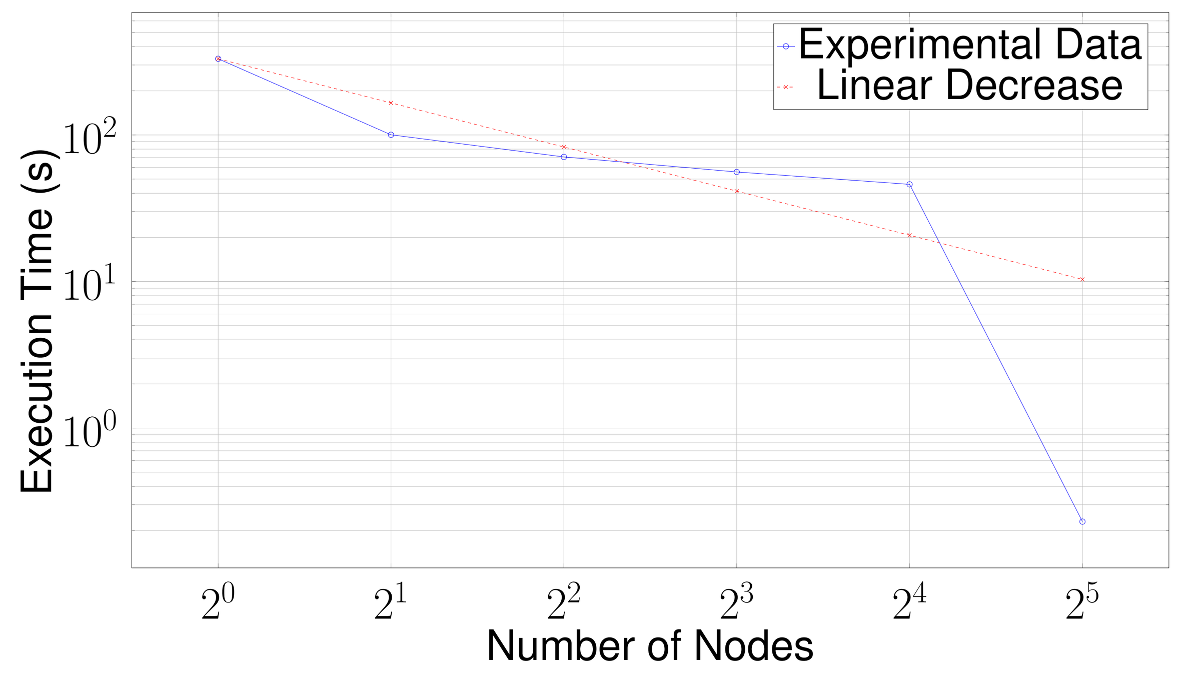
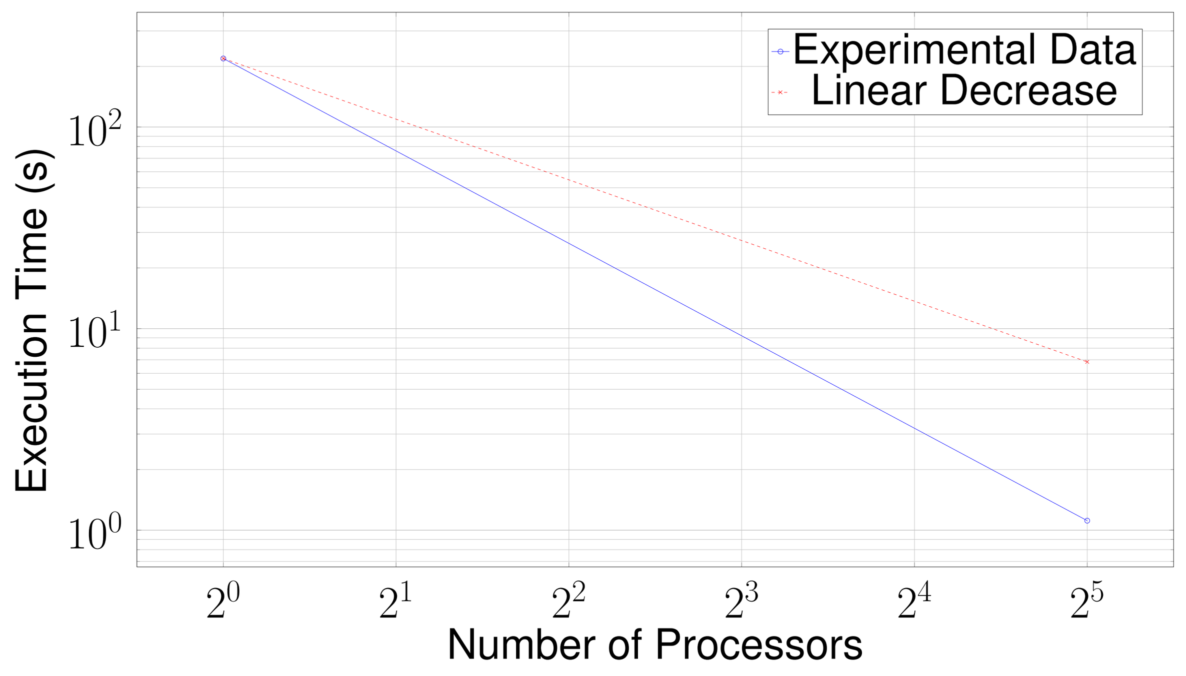


Table 4: Strong scaling results for solving the chromatic number of `queen9_9.col`.

Nodes	Time (s)	Total Cores	N processors
1	218.86	1	1
4	1.115	512	32

Table 5: Strong Scaling Results (Set 2)

Figure 5: Execution time vs. number of nodes for solving `queen9_9.col`.



Conclusion

The proposed parallel branch-and-bound algorithm demonstrates **strong scalability**. Further optimizations for sparse graphs remain an open direction.

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