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 Rome 7h12 Cpus240 NVIDIA, for a total of 240 A100 GPUs

This project aims to leverage HPC capabilities to solve complex combinatorial optimization problems in graph theory.

Zykov algorithm

Given two non-adjacent vertices x, y ∈ V two new graphs can be 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

A recursive algorithm, called Zykov's tree (Figure 1), can be built upon the 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* $\{x, y\} \notin E(G)$

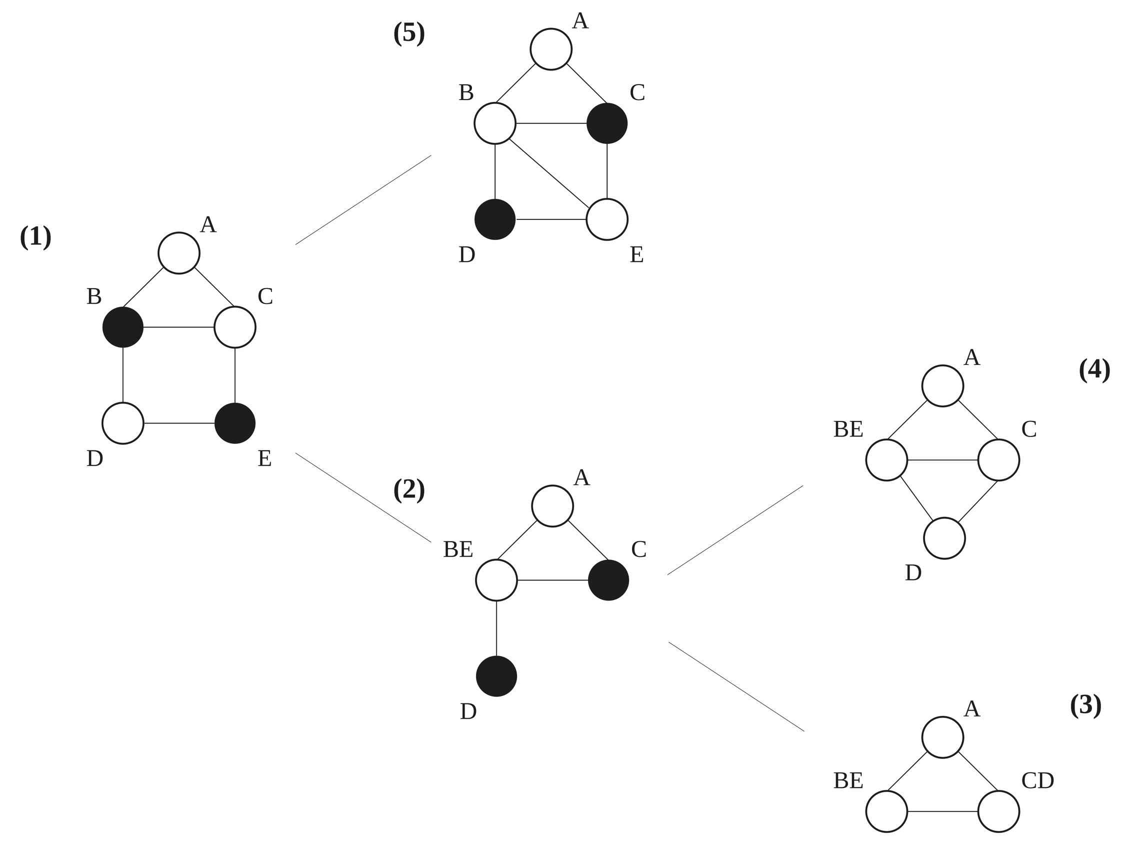


Figure 1: Zykov's tree

Leaf of the graph = complete graph - Size of **smallest leaf** = *chromatic number*.

At each node **lower bound** and **upper bound** computed:

$$lb(\chi) \leq \chi(G) \leq ub(\chi)$$

Bounds are needed for **pruning.** A branch is pruned if:

$$lb(\chi) \leq best\_ub(\chi) \vee lb(\chi) = ub(\chi)$$

where $best\_ub(\chi)$ is the best $ub(\chi)$ ever found

Coloring and clique heuristics

Color heuristics are used for calculating the upper bound. The most remarkable example is **DSatur**, as well as *Greedy* and *Recolor*.

Algorithm 1 DSatur coloring

```
procedure DSATURCOLOR(G)
    Initialize max_color ← 0
    while G not empty do
        v ← GETMAXSATDEGREE(G)
        for i = 1 → max_color do
            if can be assigned color i then
                color[v] ← i break
            end if
        end for
        if not assigned then
            max_color ← max_color + 1
            color[v] ← max_color
        end if
    end while
end procedure
```

Clique heuristics are used for calculating lower bound of the clique number; we adopted **FastWClq** algorithm.

Branching strategy

At each step verteices (u, v) are chosen such that **merging minimizes the graph**:

$$(u, v) = \arg \min_{(u,v)\in V} |N(u) \cap N(v)|$$

where $N(u)$ is the set of neighbors of u

Graph Representation

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	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)^1$
Merge Vertices	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)$	$O(\|E\|)^1$
Get Neighbors	$O(\|V\|)$	$O(\|E\|)$	$O(1)$	$O(1)$

[1]More precisely $O((avg\_neighbors)^2)$, which tipically it is much less

We used **Adjacency list** representation since it is the most flexible

MPI & OpenMPI

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)

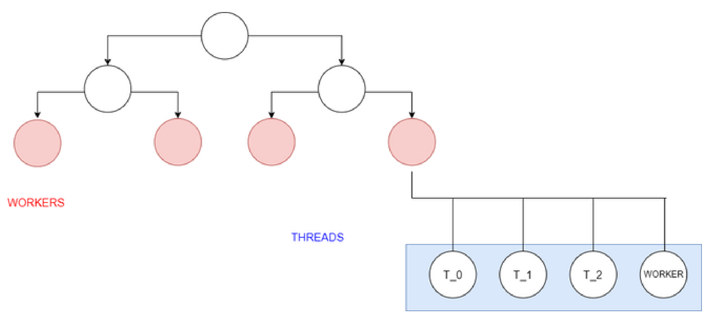


Figure 2: balanced algorithm

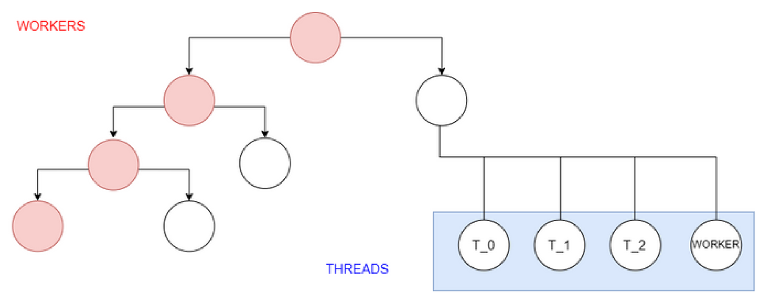


Figure 3: unbalanced algorithm

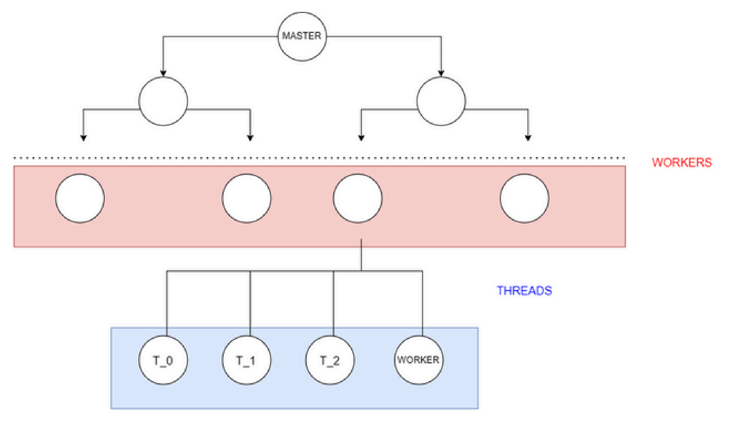
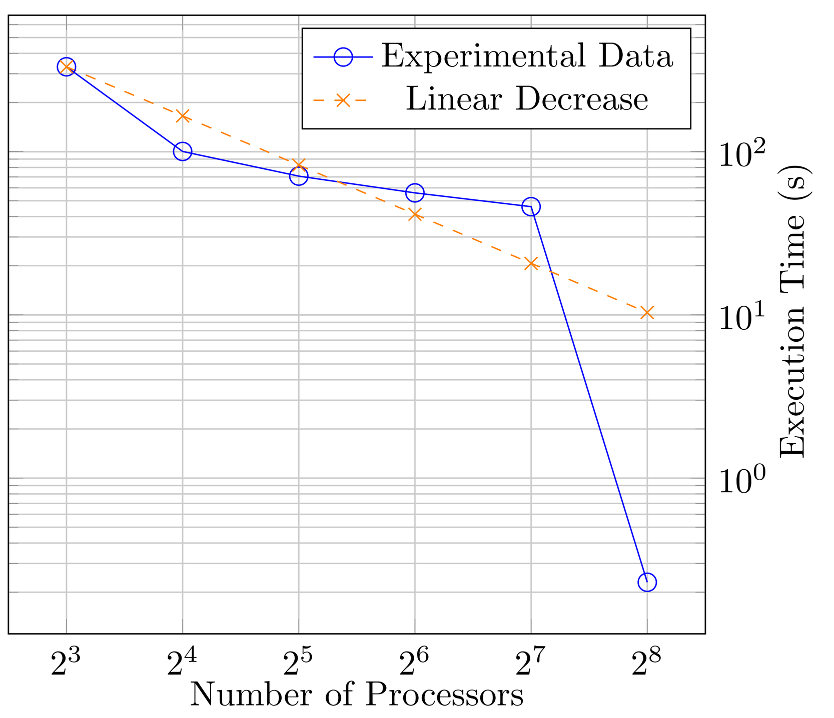


Figure 4: simple algorithm

Results

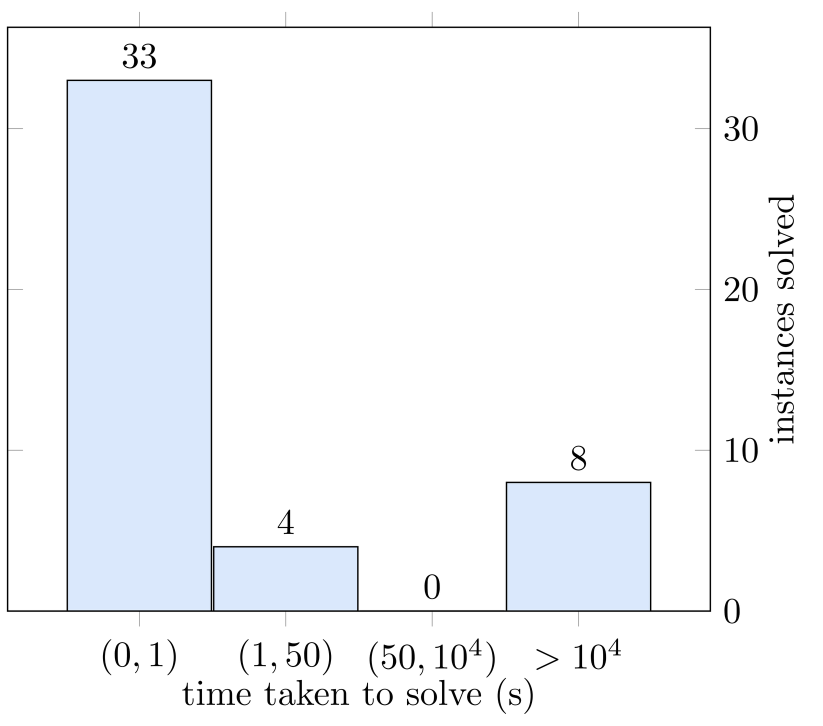
MPI proc	Cores	Time (s)
1	1	> 10000
8	32	330.91
16	64	100.22
32	128	70.78
64	256	55.89
128	512	46.01
256	1024	0.23

Strong scaling (queen7_7.col): **superlinear speedup** due to more pruning



We stopped the execution when a coloring with $\chi(G)$ colors is found, saving further CPUs computation to prove optimality and reducing **energy consumption**. We optimally colored **37** graphs out of the 45 tried.

Non optimal colorings usually use as less as 1 or 2 more colors than optimal solution.



Conclusions

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

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