Construction of Small Diameter/ASPL Graph with GPU

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Graph Golf (Order/Degree Problem)

Graph Golf as optimization problem

- Given:

  Order of graph: n

  Maximum degree of graph: d

- Minimize:

  Diameter of graph

  Average Shortest Path Length(ASPL)

- Note:

  Diameter has higher priority than ASPL.

  Smaller Diameter ≠ Better ASPL.

Difficulties in Graph Golf

- Vast search space

  At least $n!$ optimal solutions exist.
- Objective function is not convex.
- One edge can change many shortest paths.

  Every modification to the graph requires entire recalculation of ASPL/Diameter.
- The calculation time required for ASPL/Diameter is polynomial, but n is so large (up to **1e6**)

My Results

- I found 5 best solutions

Order n	Degree d	Diameter	ASPL	ASPL gap
50	4	4	2.64082	0.04898
1726	30	3	2.47921	0.01834
9344	6	7	5.48822	0.11436
65536	6	9	6.73615	0.18302
100,000	8	7	5.94733	0.20869

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Deepest Improvement

Approach

- Find better solution by **Simulated Annealing** from **multiple** initial solutions.
- Design **symmetric** and **memory-efficient** graph, in order to,
  1. Reduce theoretical calculation time
  2. Avoid memory bandwidth bottleneck
- Make use of **GPU** for ASPL calculation, achieved about **700x faster** than single thread naive CPU implementation

Design of Graph

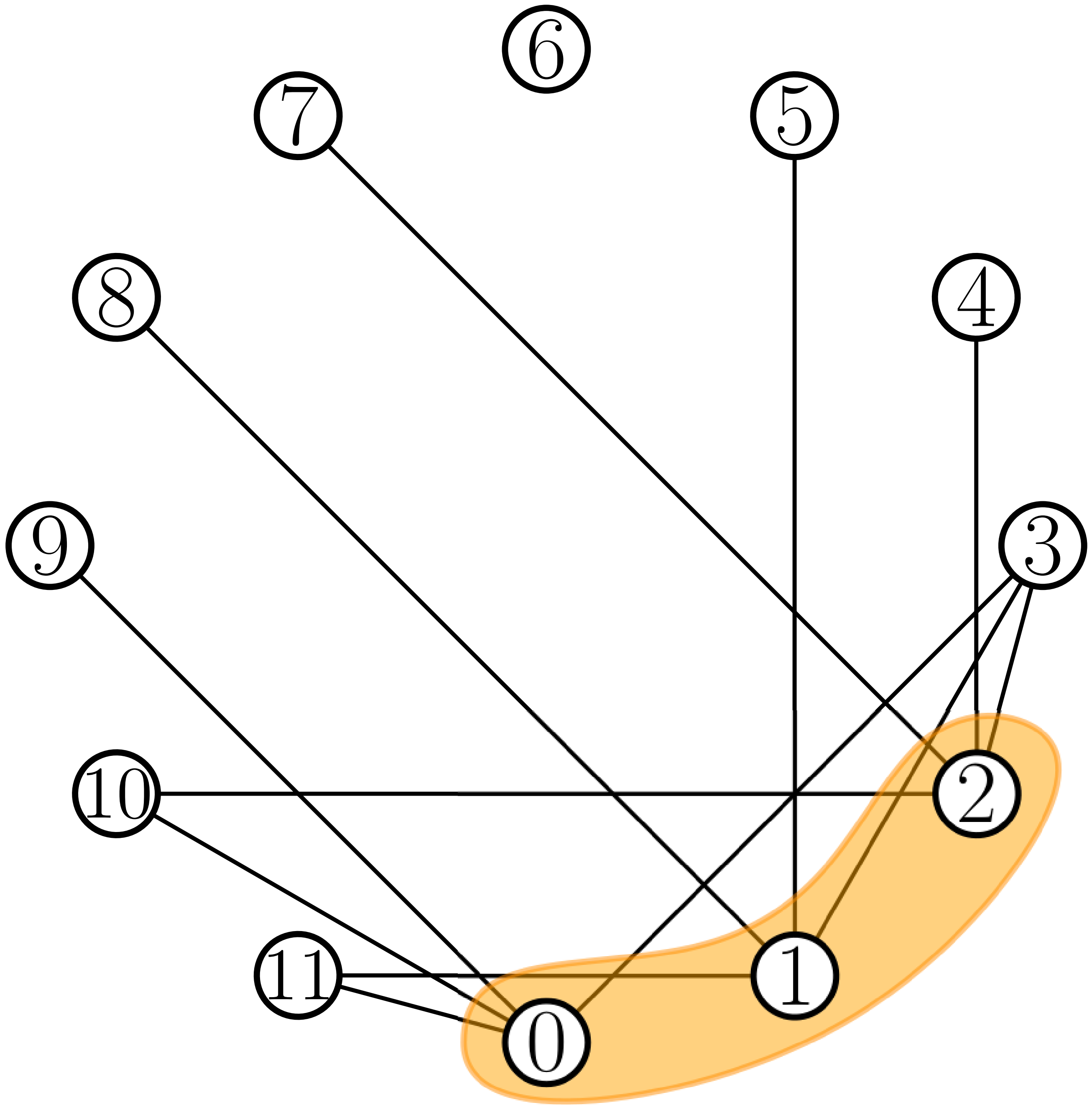
- I designed "part shift graph", similar to Cayley Graph
- Vertices have indices $0 \ldots n-1$

Indices are regarded as elements of cyclic group Z_n

- Show an example of $(n, d) = (12,4)$
- Choose size of "part" $m = 3$ from divisors of n
- Then construct a "part".

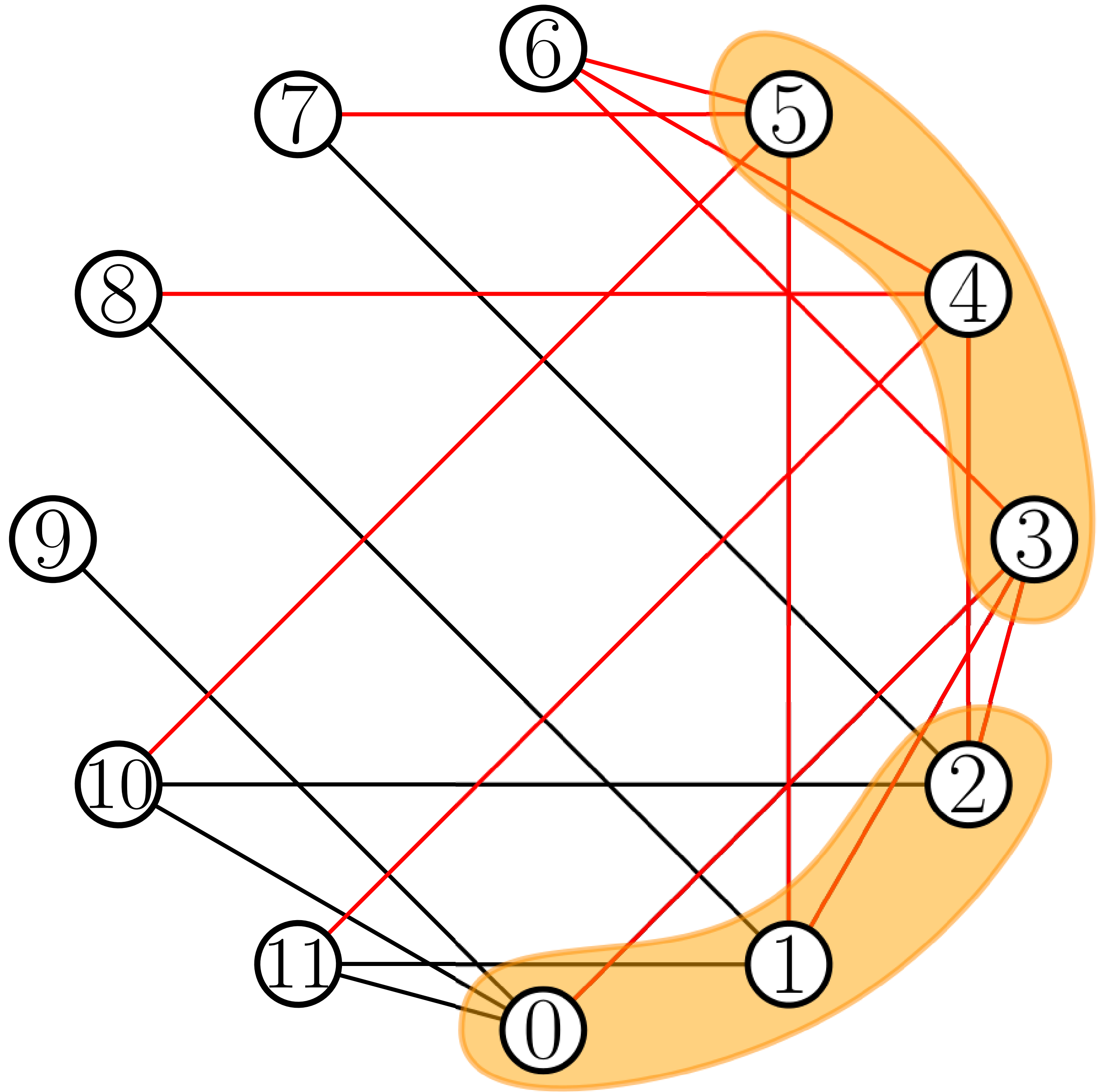
Design of Graph

- "part" is a subgraph, all edges join $0 \ldots m-1$ vertices.



Design of Graph

- Copy & Shift the part by $m(=3)$



Design of Graph

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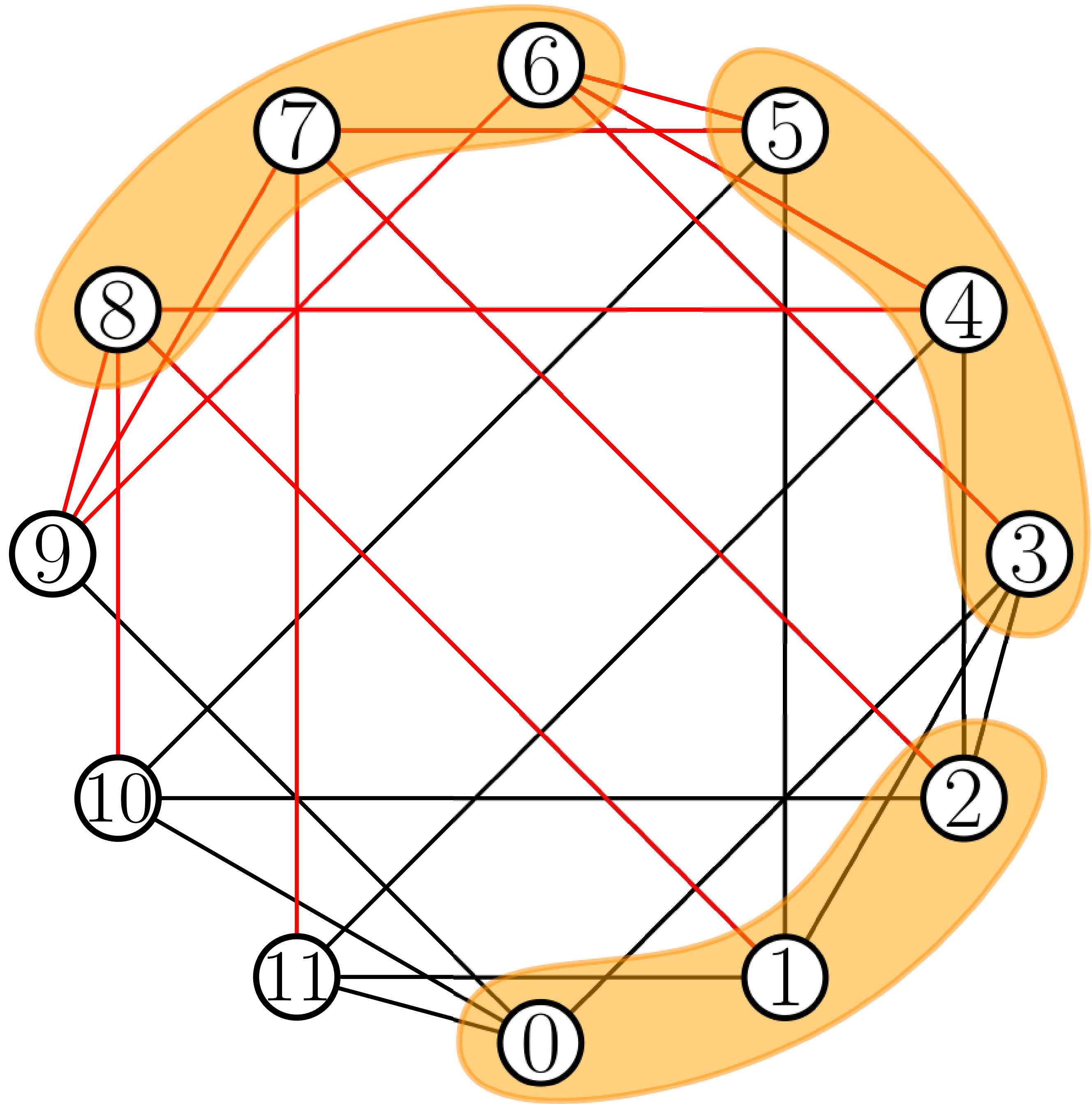

Design of Graph

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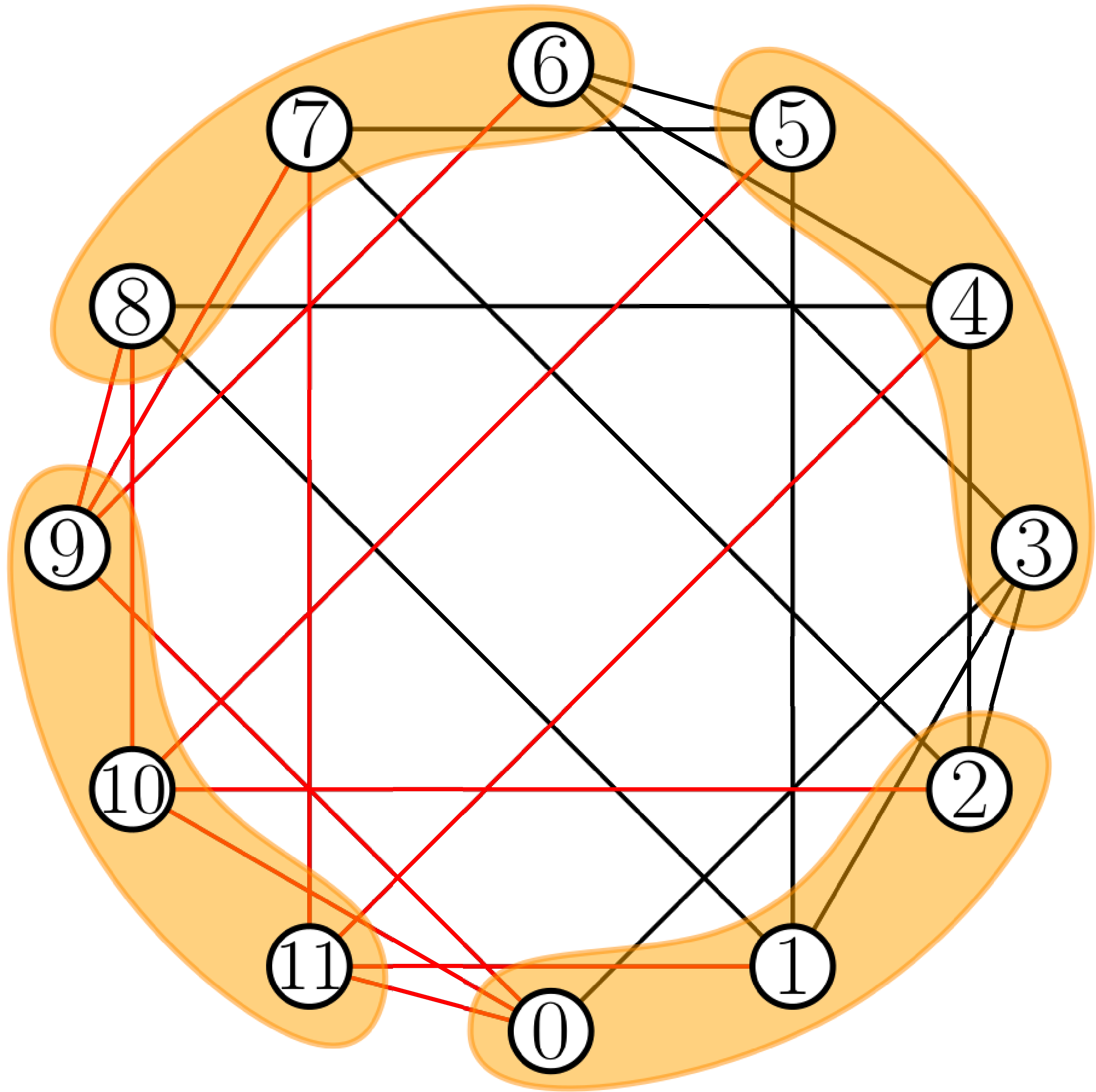
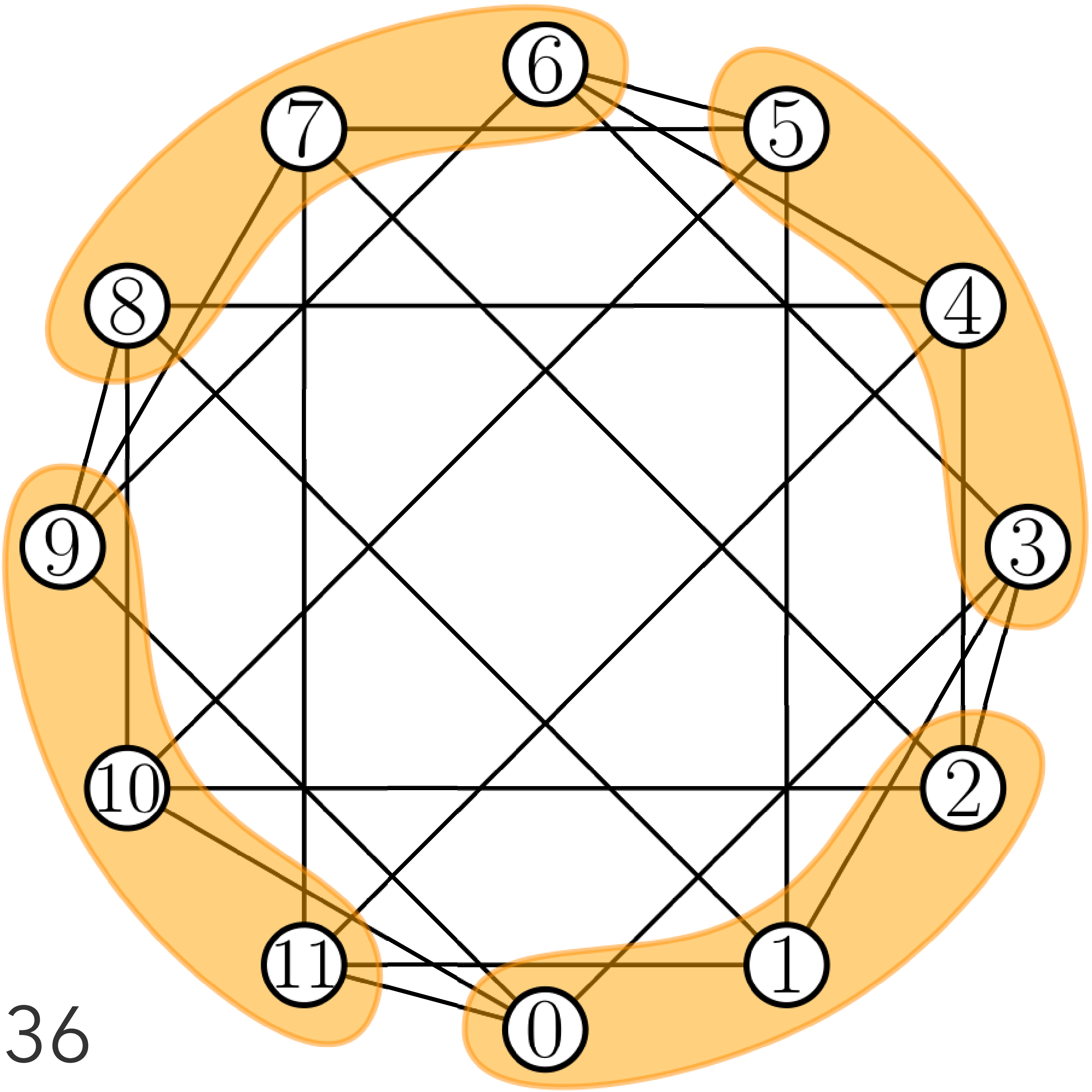


Design of Graph

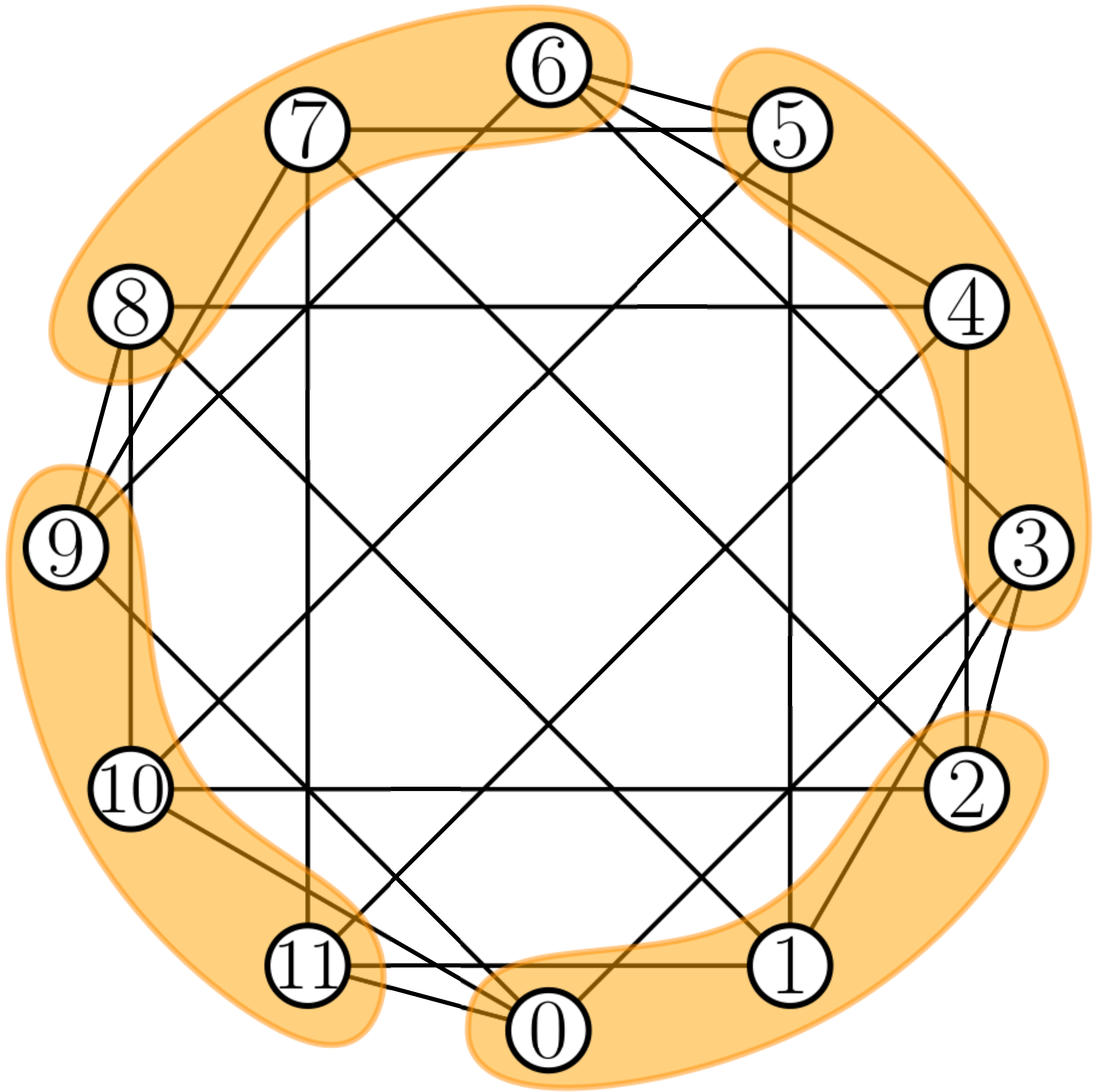
- Erase duplicated edges



Diameter: 2
ASPL: 1.63636

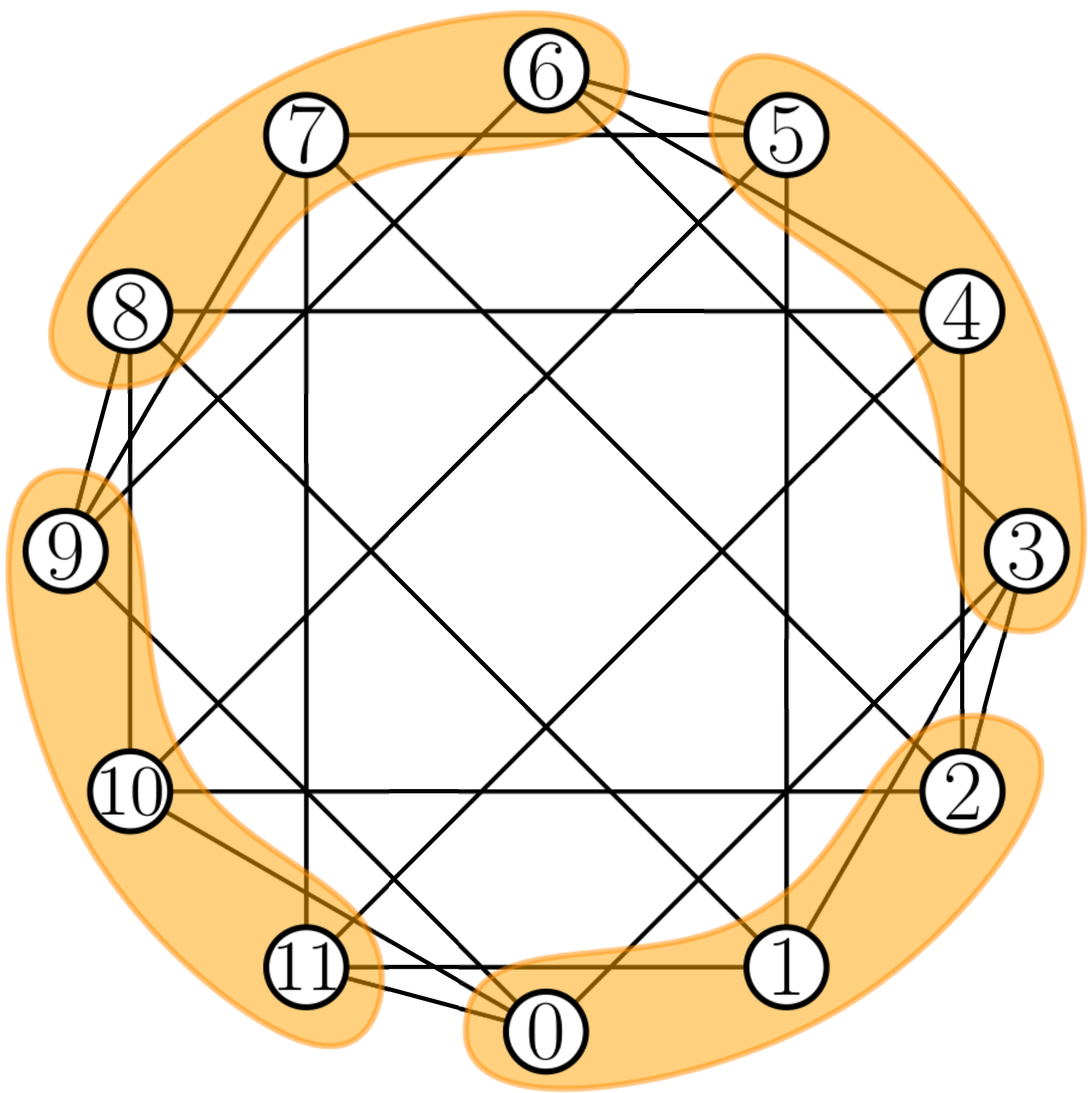
Design of Graph

- This graph is symmetric, thereby All Pairs Shortest Path problem can be solved by Single Source Shortest Path(SSSP) problem m times.



Design of Graph

- This graph is symmetric, thereby edge data requires only $O(md)$ space.



Design of Graph

- m is such a small number that $O(md)$ edge data can be stored in the cache.

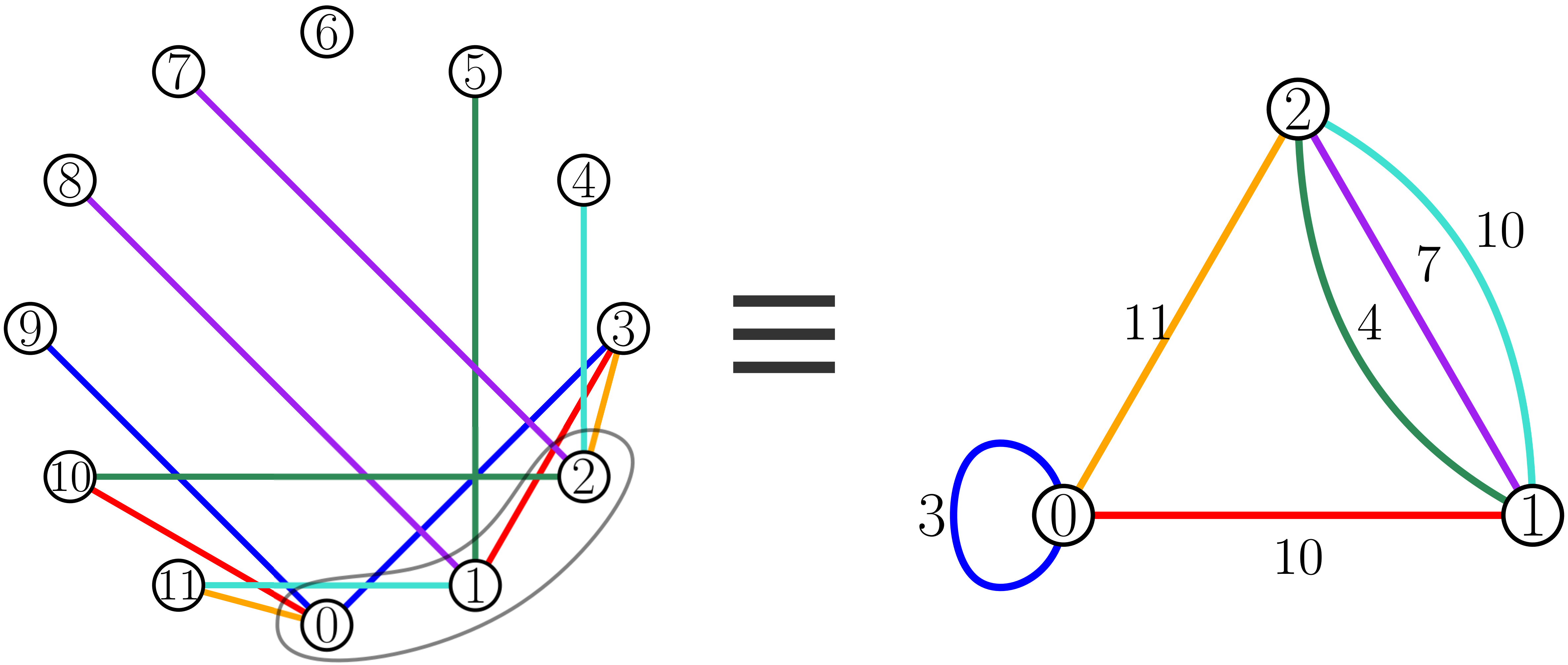
Order n	Degree d	Diameter	ASPL	ASPL gap	m
50	4	4	2.64082	0.04898	**50**
1726	30	3	2.47921	0.01834	**2**
9344	6	7	5.48822	0.11436	**16**
65536	6	9	6.73615	0.18302	**64**
100,000	8	7	5.94733	0.20869	**(4,5)**
4855	15	4	3.42917	0.13066	**5**
1,000,000	32	5	4.33066	0.34858	**64**

Simulated Annealing: Overview

- I'm a beginner of Simulated Annealing
- Representation of solution: "part"
- Cooling Schedule: Exponential Cooling
- Initial Temperature: Determined by experiments
- # of iteration: Determined by experiments (3M~10M)
- Energy: Difference of ASPLs

Simulated Annealing: Initial Solution

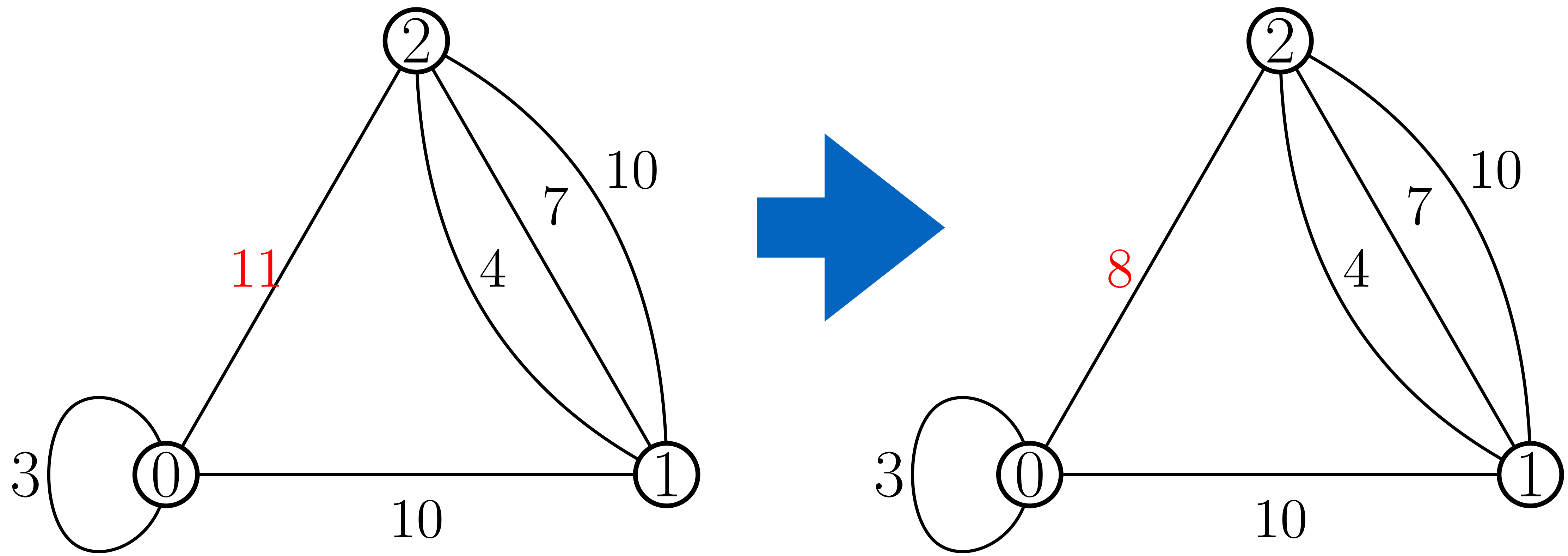
- "part" can be represented as weighted order m graph



- Generate random graph and convert it into a "part"
- Weight is difference of indices.

Simulated Annealing: The Neighbors of State

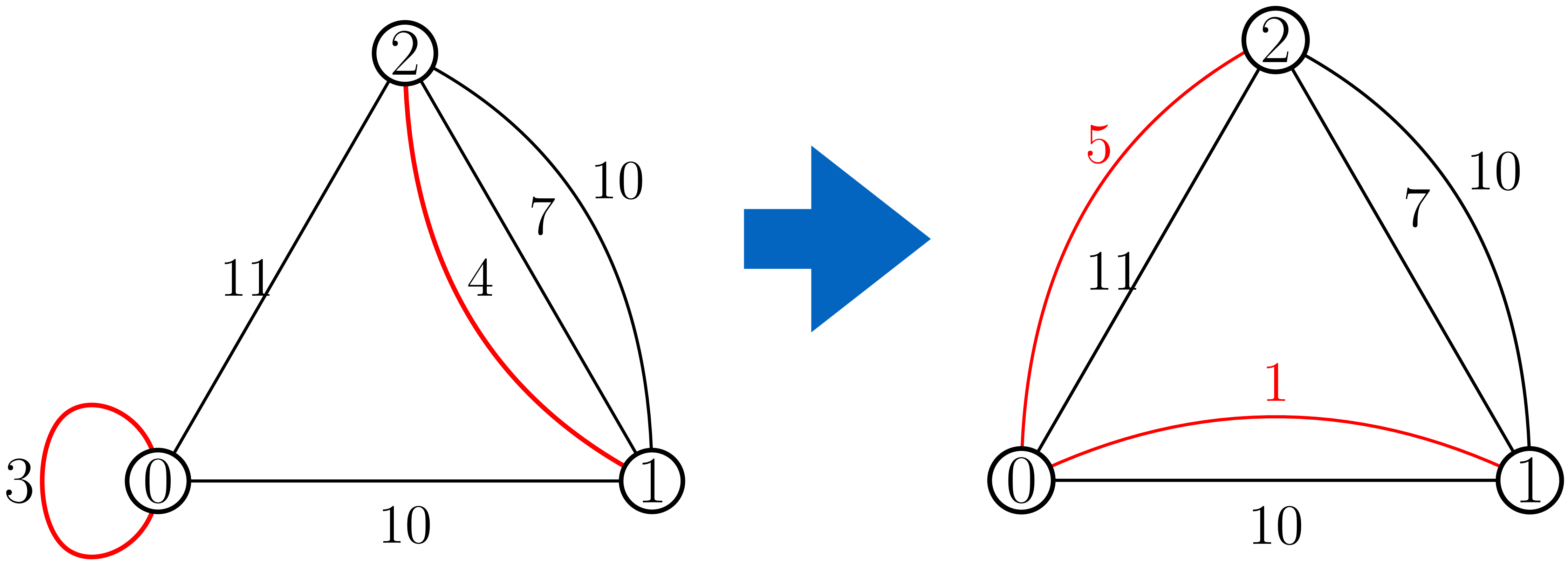
- 2 types of the neighbor
  1. Modify a weight of single edge



(edge weight)%m = (difference of indices)%m

Simulated Annealing: The Neighbors of State

- 2 types of the neighbor
  2. Cut 2 edges and reconstruct 2 edges



(edge weight)%m = (difference of indices)%m

ASPL Calculation

- Average Shortest Path Length(ASPL) of Graph (V, E) is defined as

$$\mathrm{ASPL}(V, E) = \frac{\sum_{u \in V} \sum_{v \in V} d(u, v)}{n(n-1)}$$

- The calculation of All Pairs Shortest Path is needed.
- Calculation time is enormous
  - Floyd–Warshall algorithm: $\mathrm{O}(n^3)$
  - Solving SSSP for all vertices: $\mathrm{O}(n^2 d)$
  - Solving SSSP for all vertices of the “part”: $\mathrm{O}(nmd)$
- **Parallelization** is required

Why GPU Acceleration?

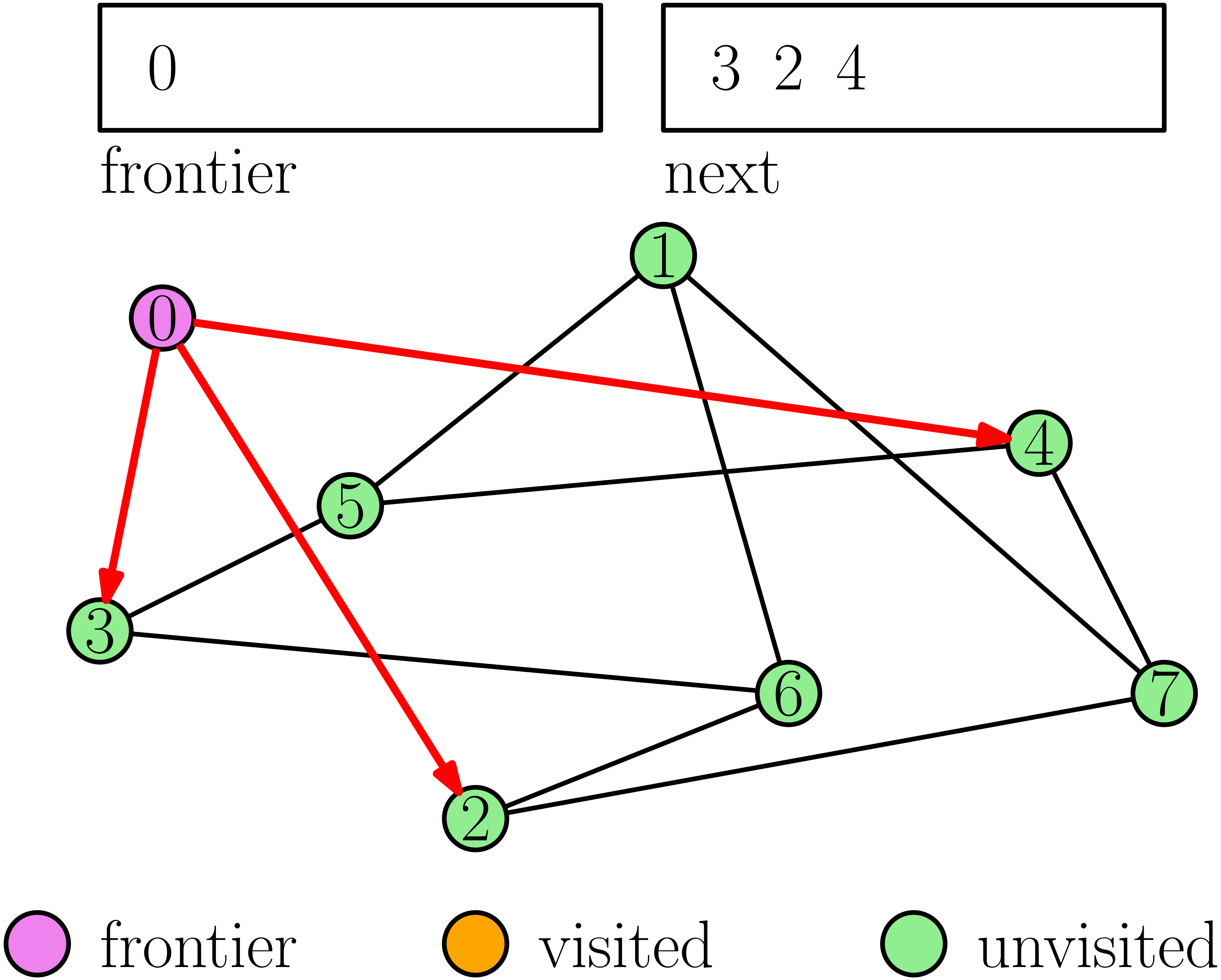
- **Parallelization** is required
- Somehow, my laboratory PC has **<u>two</u>** Geforce GTX 780
- I got **<u>four</u>** PCs equipping Geforce GTX745

OS: Ubuntu18.04
CPU: i7-4790 3.6GHz
RAM: 8GB
GPU: Geforce GTX745

- I implemented CUDA code inspired by Beamer's Bottom-up Algorithm

Parallel Top-Down BFS

Find **unvisited** vertices from each vertex in the **frontier**



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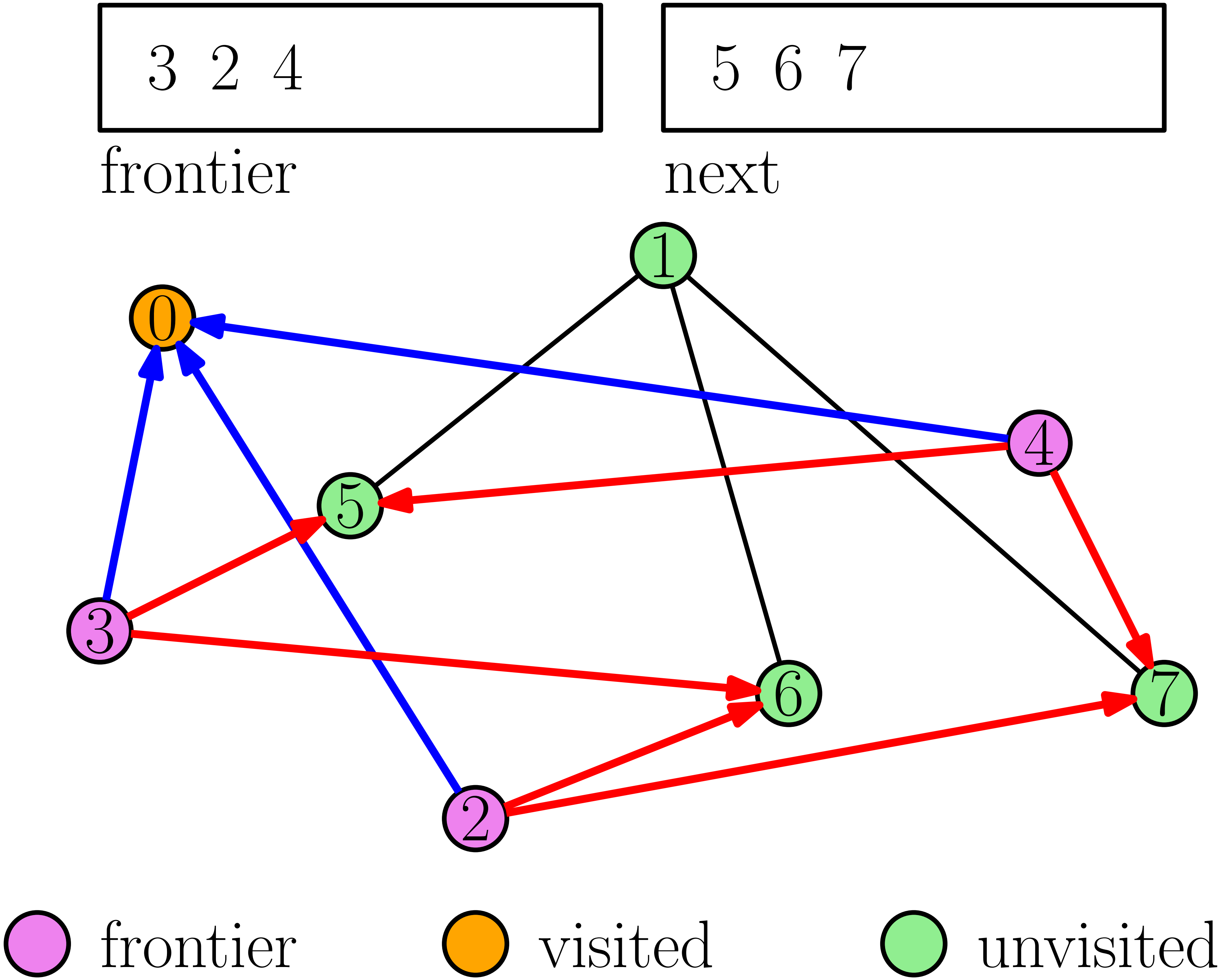

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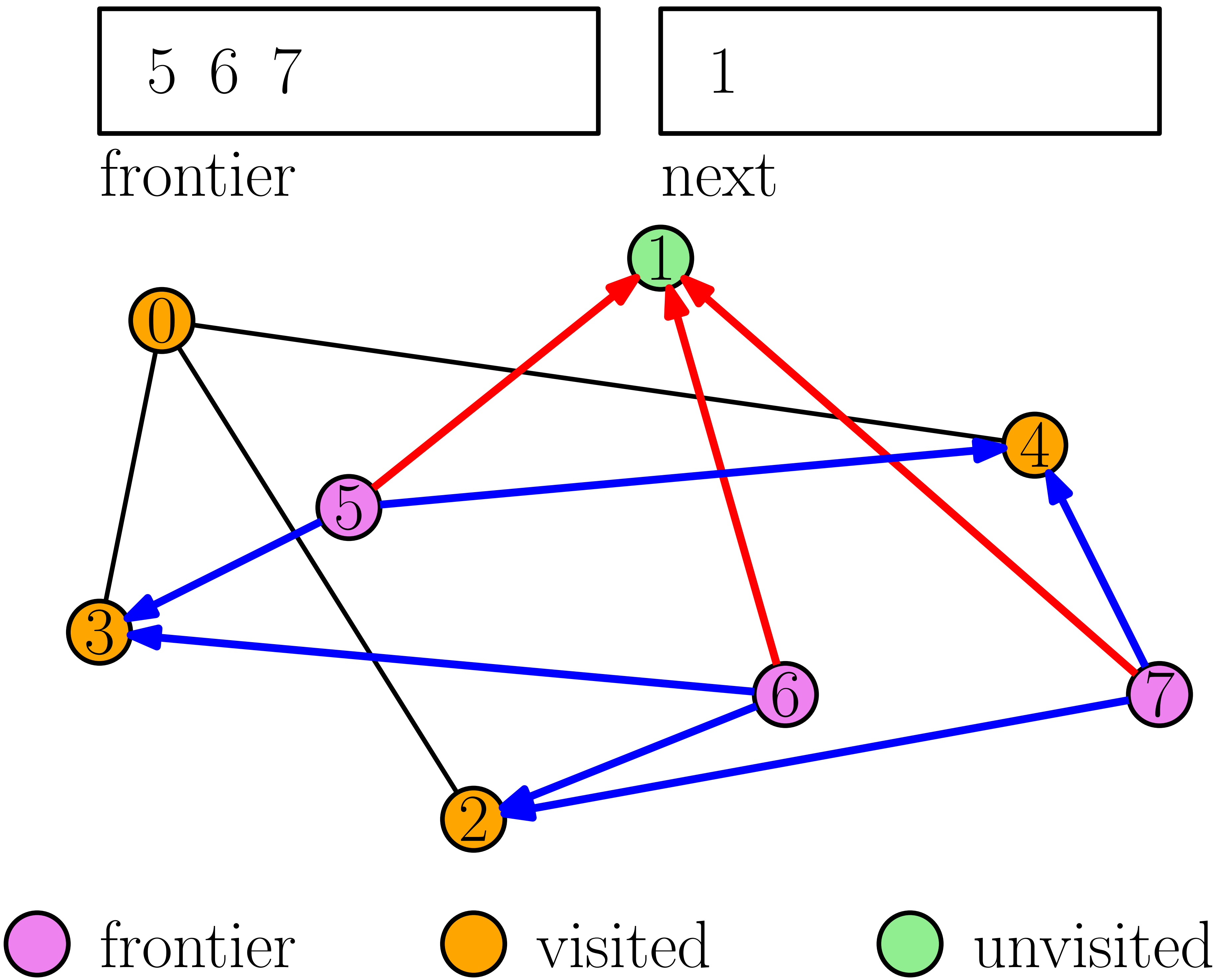

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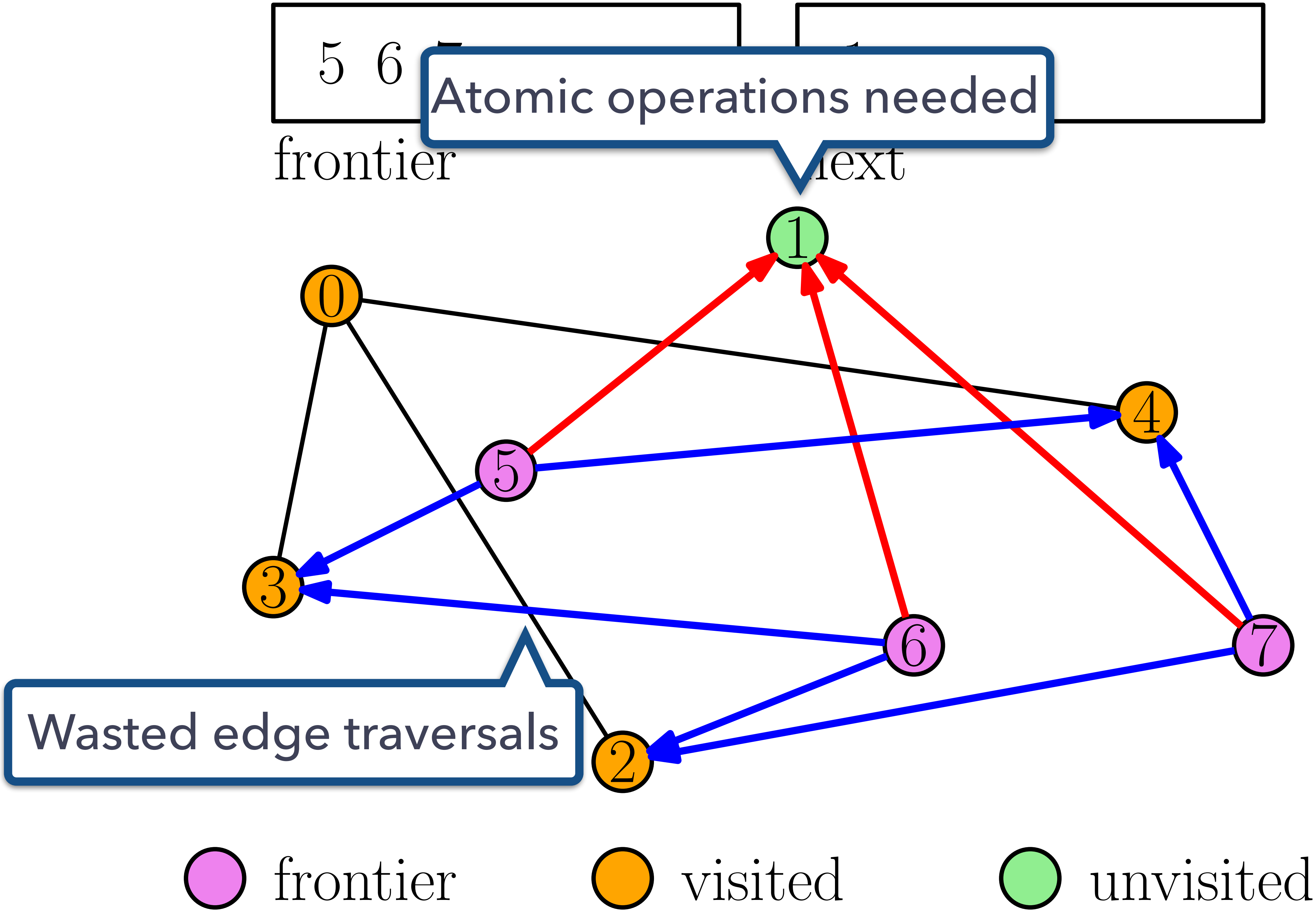
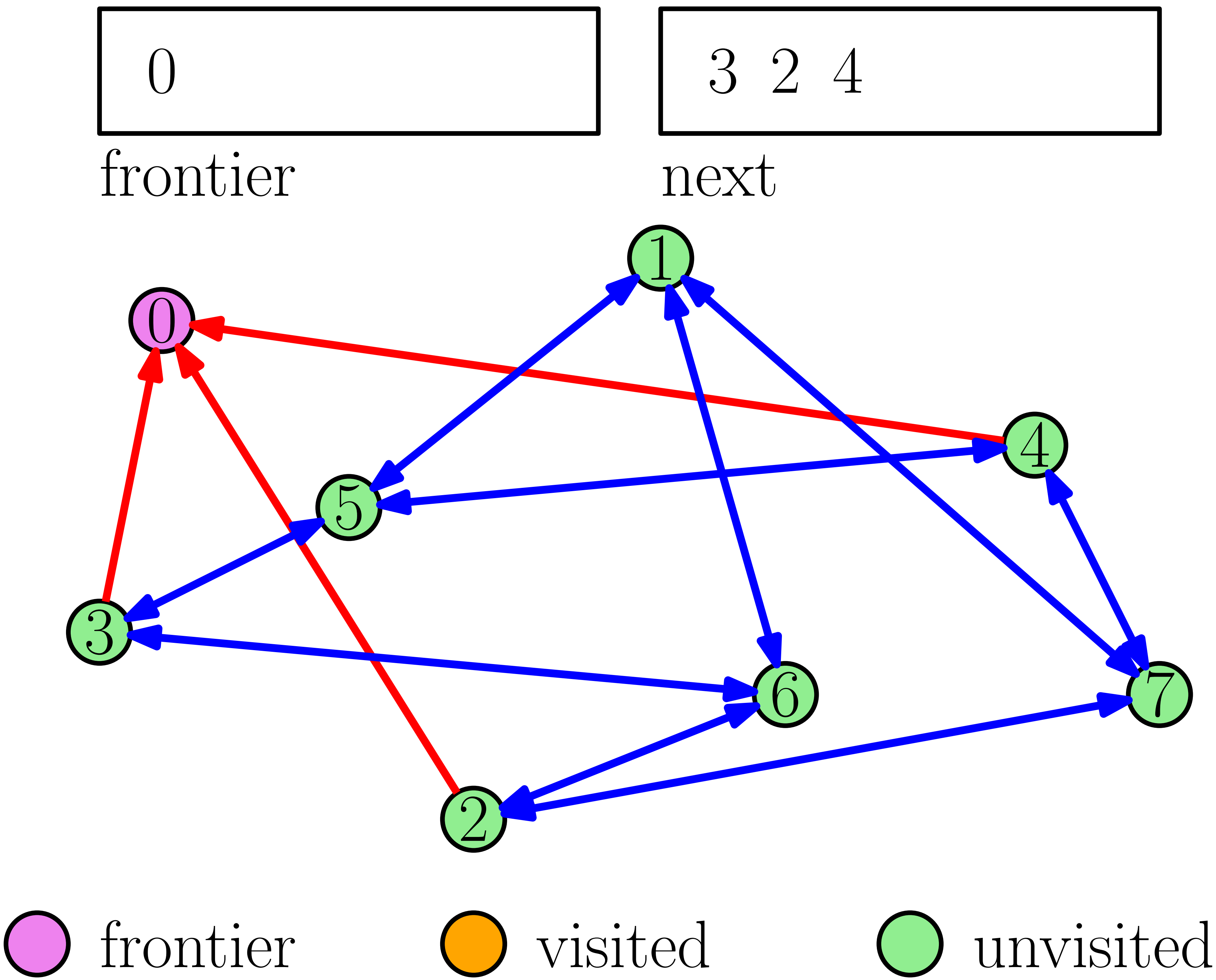


Beamer’s Algorithm (Bottom-up BFS)

Find **frontier** vertices from each **unvisited** vertex



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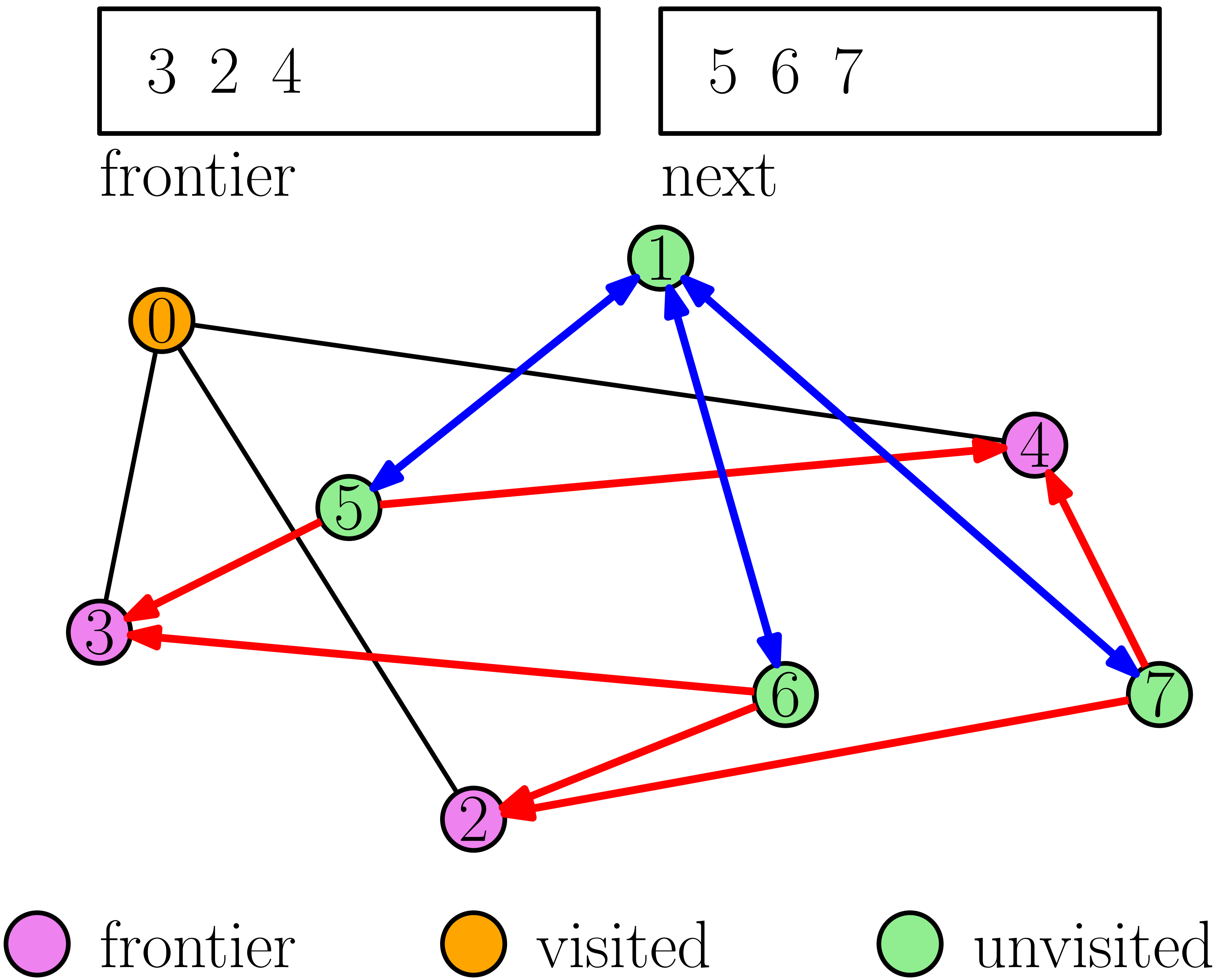

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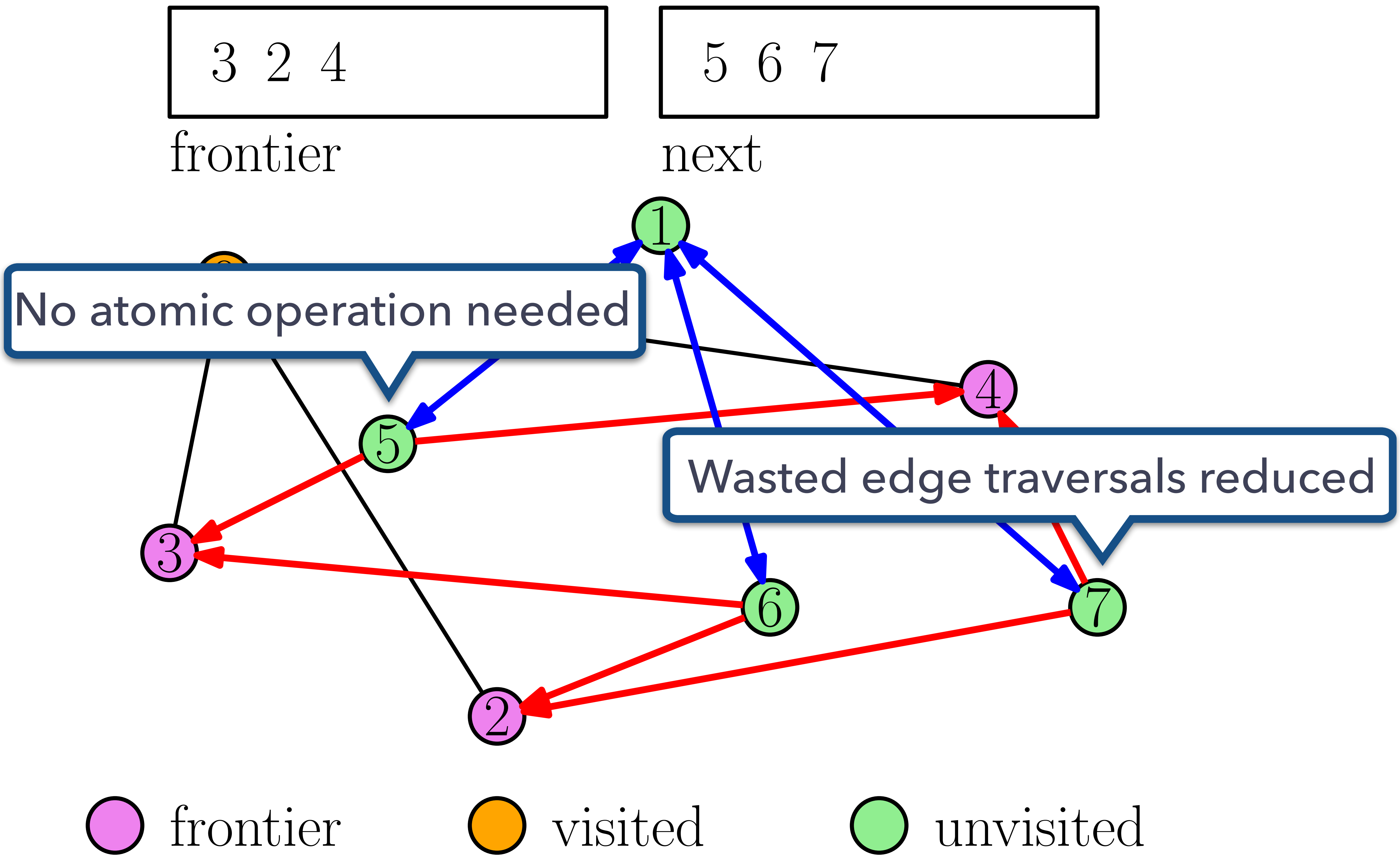

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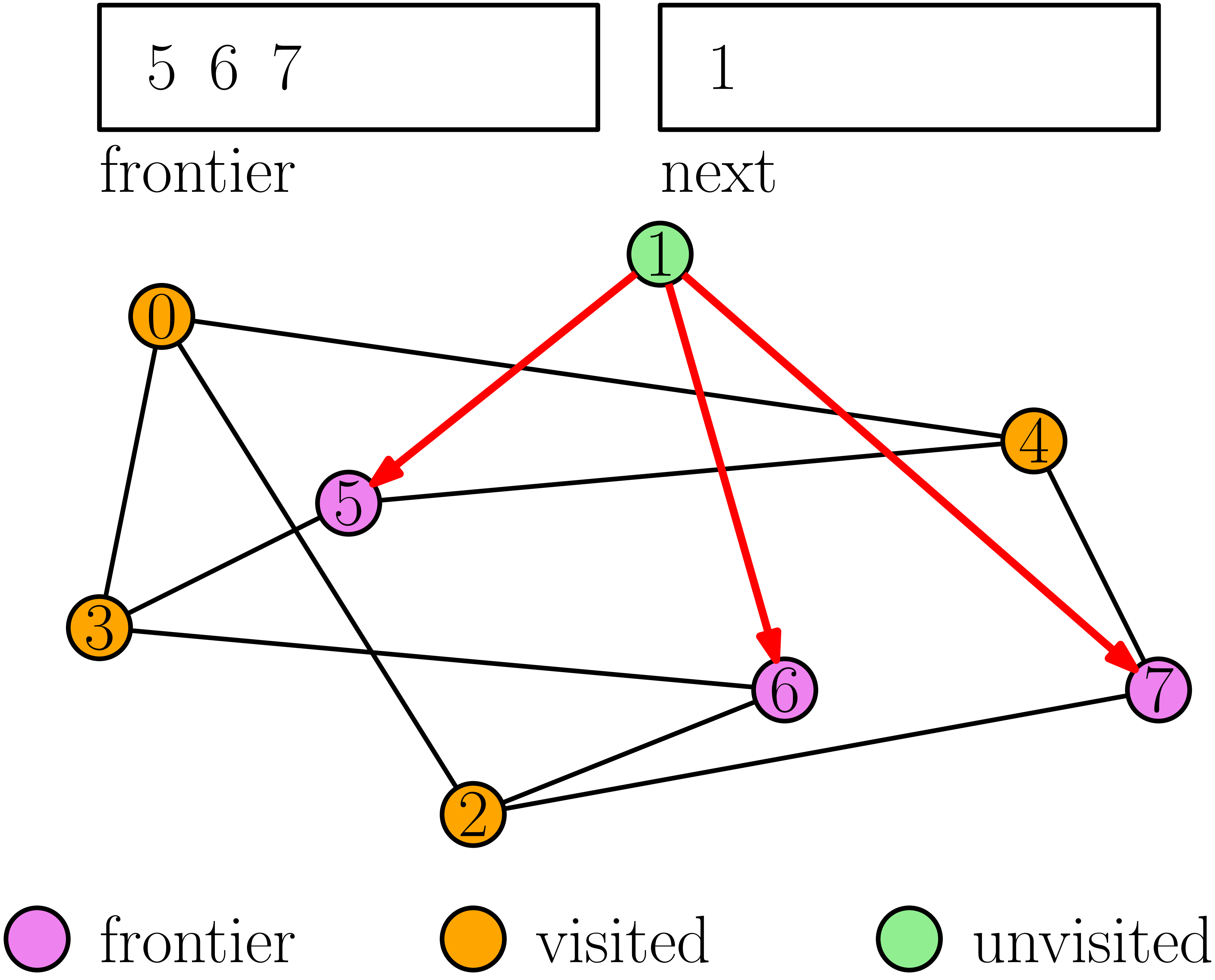
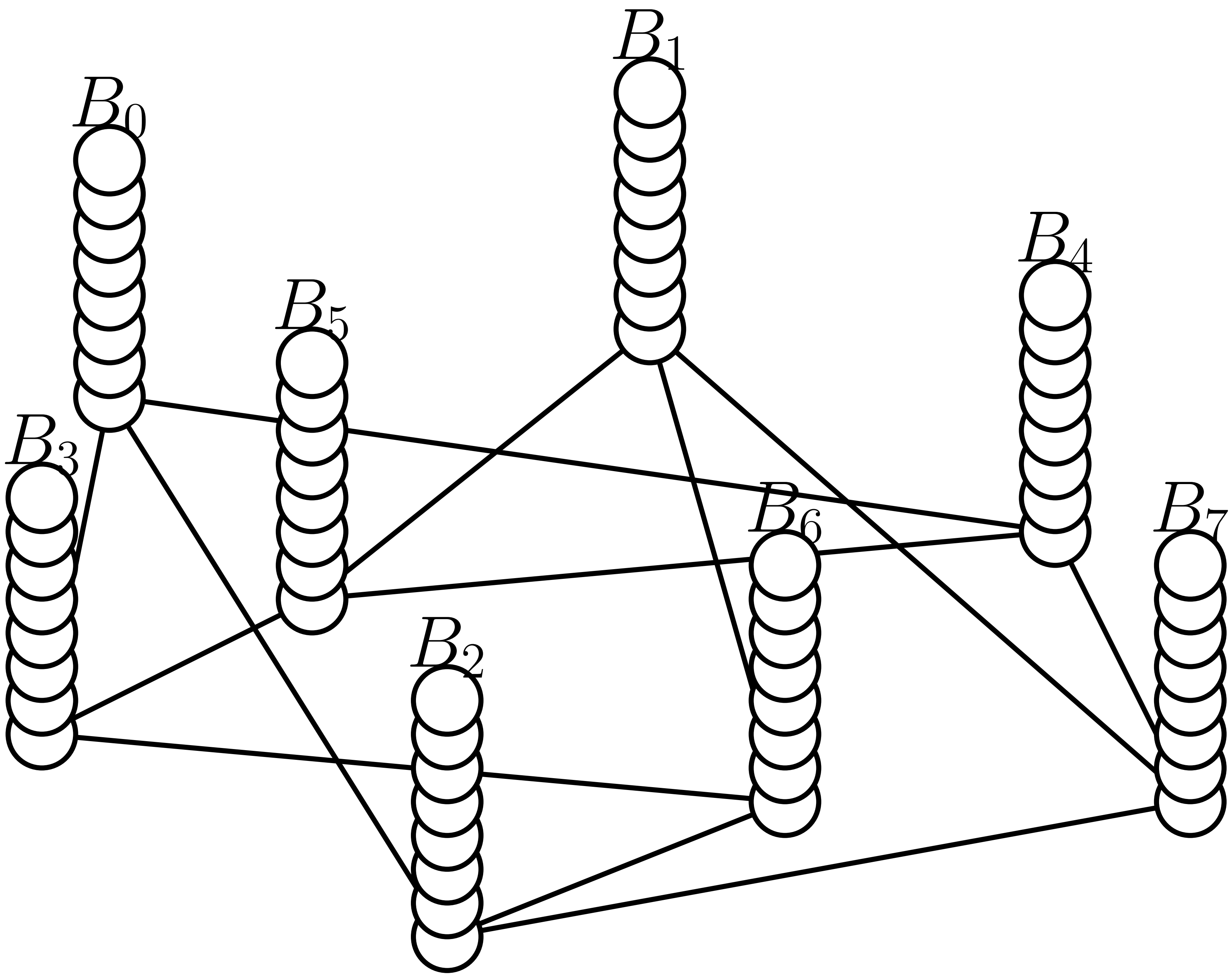


Optimization for CUDA

- Beamer's Bottom-up Algorithm is less efficient for ASPL calculation with CUDA because
  1. visited/unvisited flag is 1 bit information, but each edge traversal cause 32 byte memory access. Memory bandwidth limits performance.
  2. branch divergence gets most of the CUDA cores assigned to vertices idle.
- To maximize efficiency, perform multiple SSSP at once.

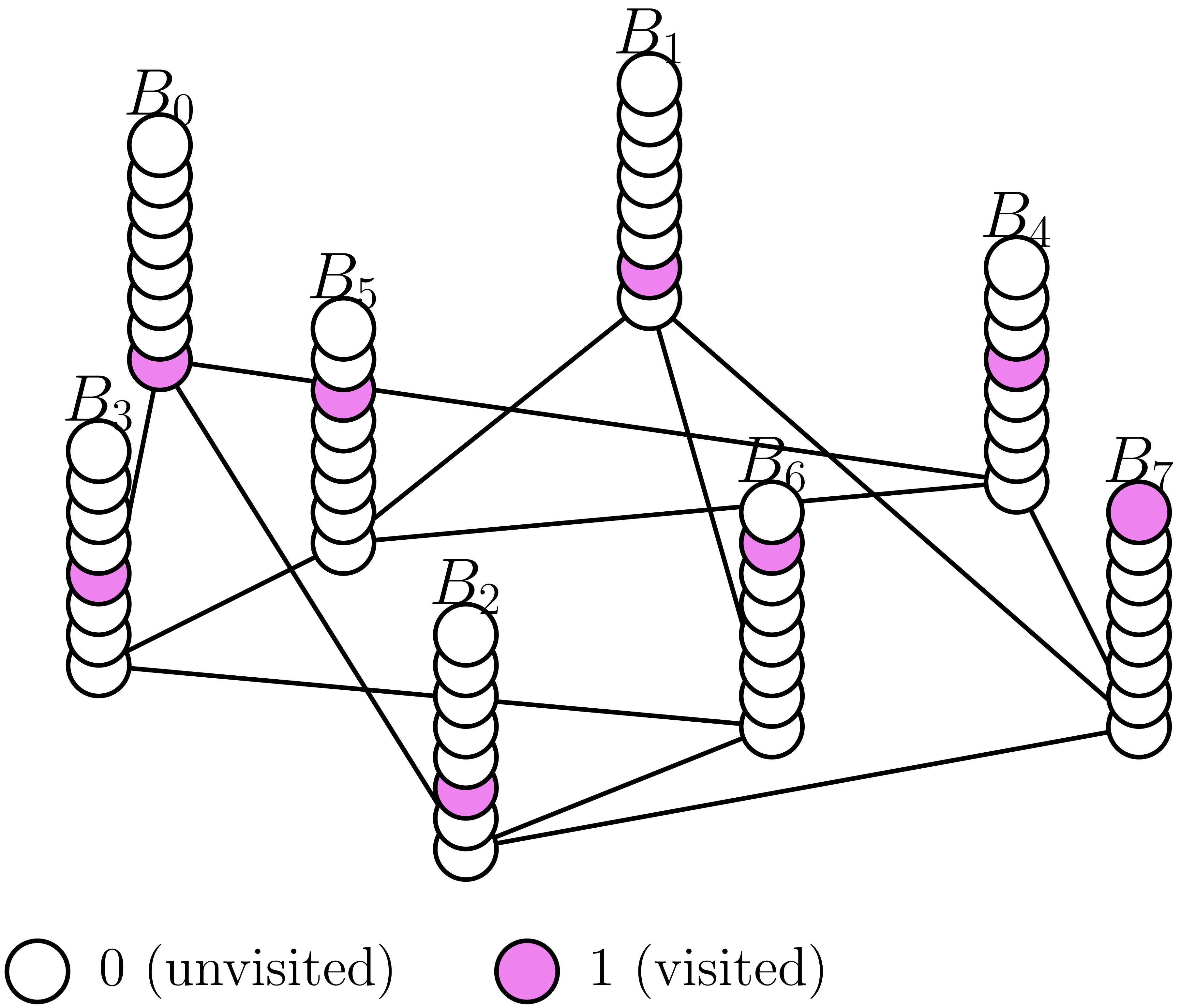
Optimization for CUDA

Assign bit vectors for all vertices



Optimization for CUDA

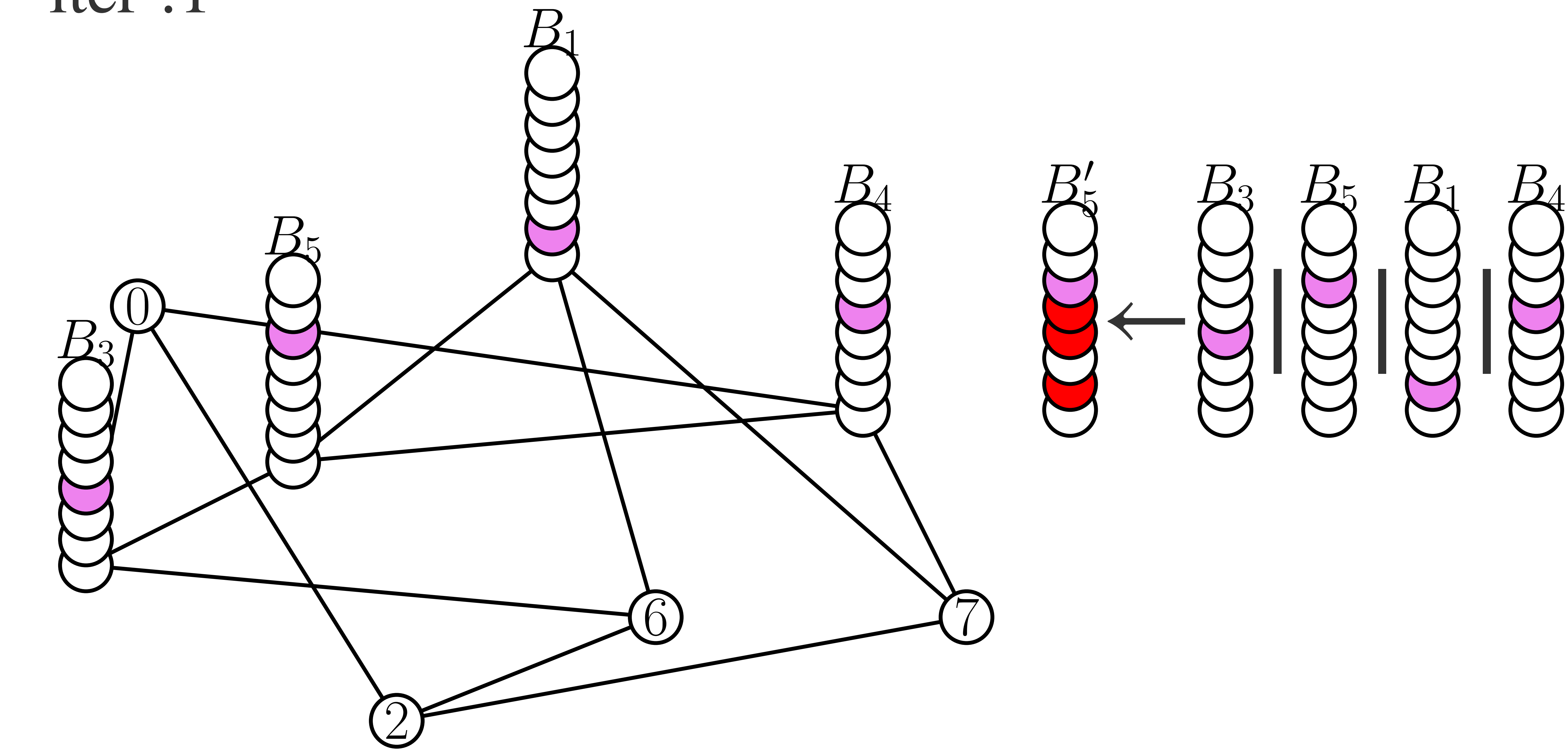
Set i th bit of i th vector "1"



Optimization for CUDA

Update vectors with bitwise OR of neighbors

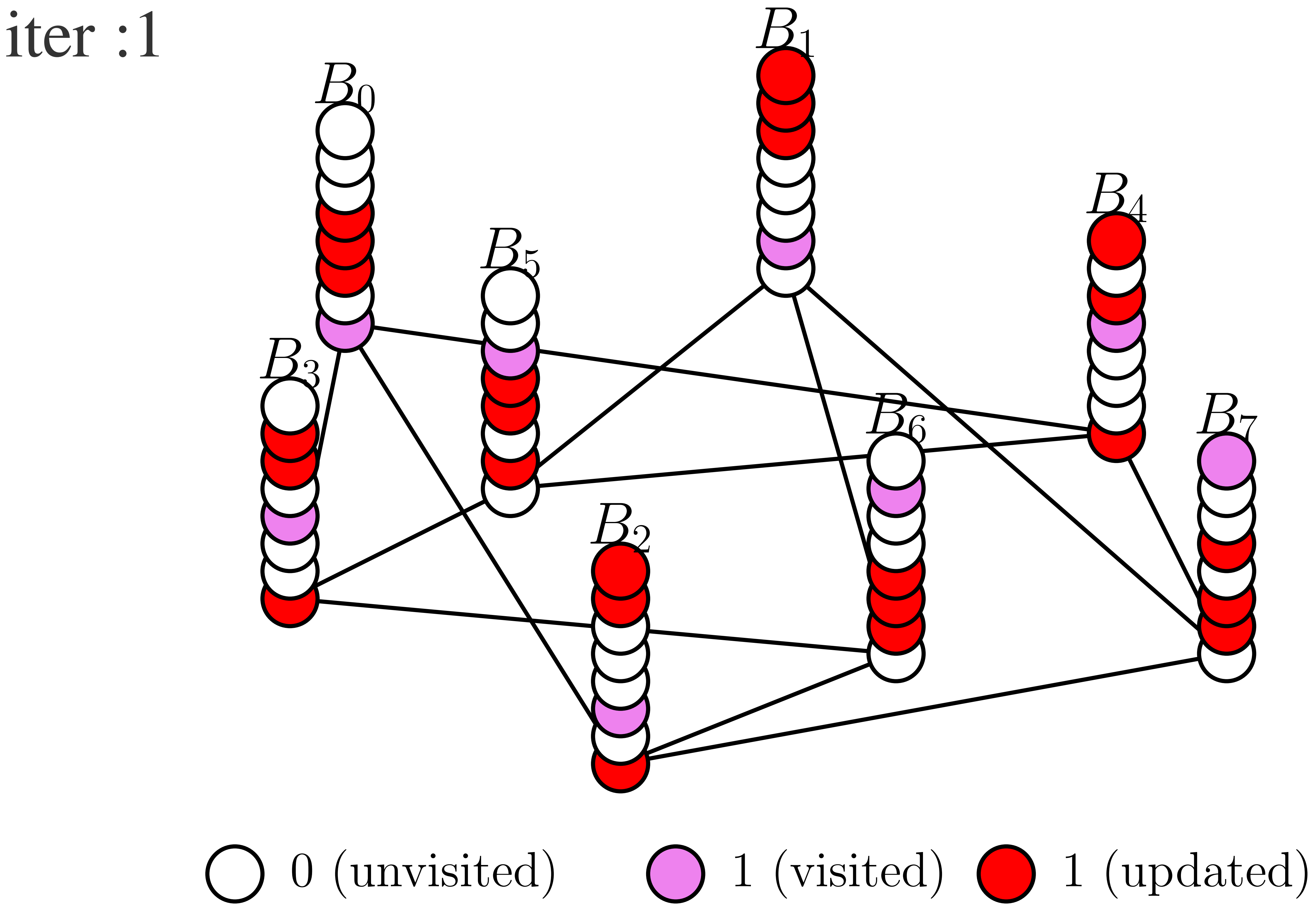
iter :1



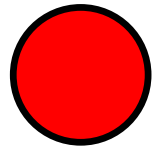
0 (unvisited) 1 (visited) 1 (updated)

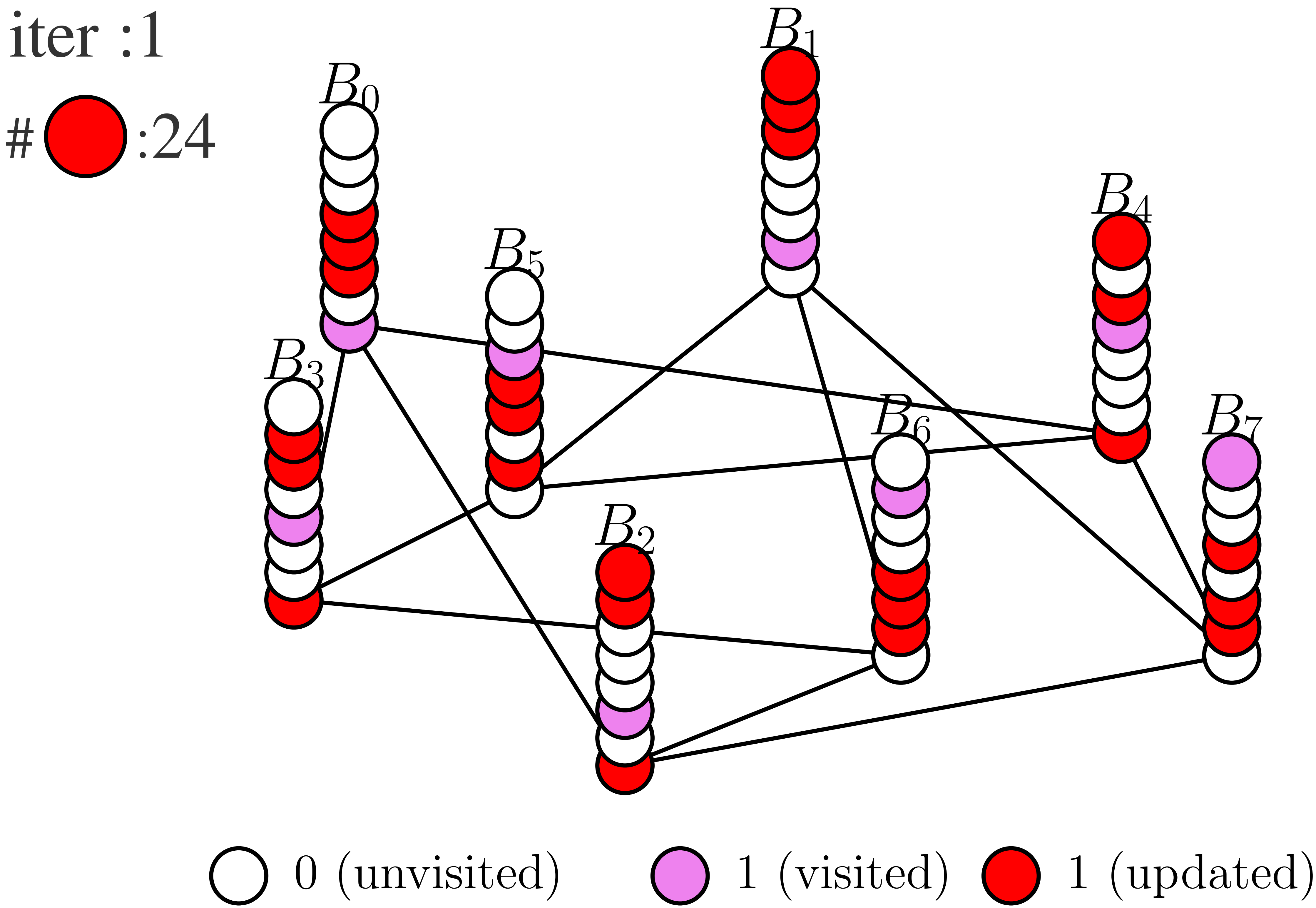
Optimization for CUDA

Update vectors in parallel



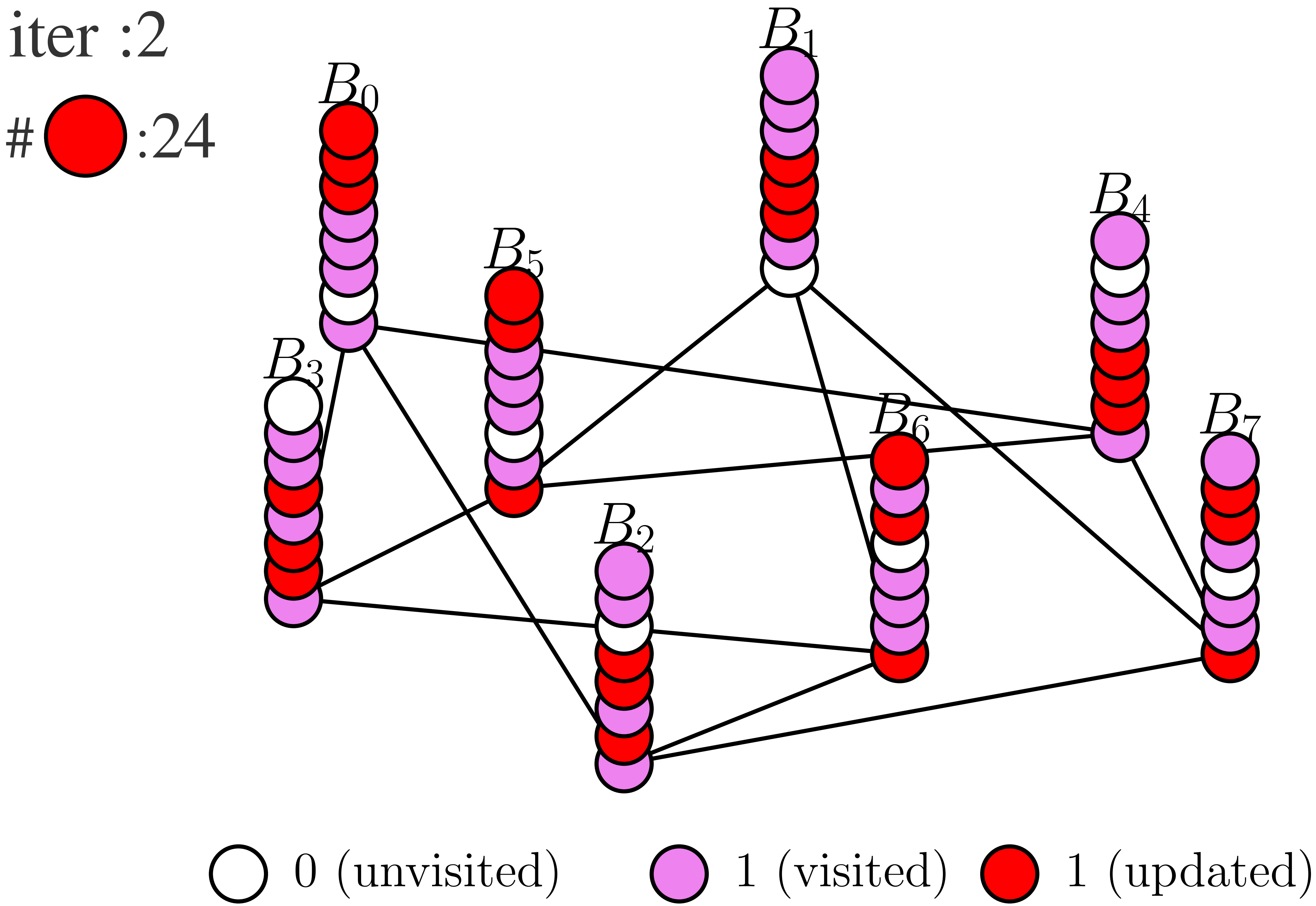
Optimization for CUDA

In t th iteration, # of  corresponds # of distance t pairs



Optimization for CUDA

Update with bitwise OR of neighbors



Optimization for CUDA

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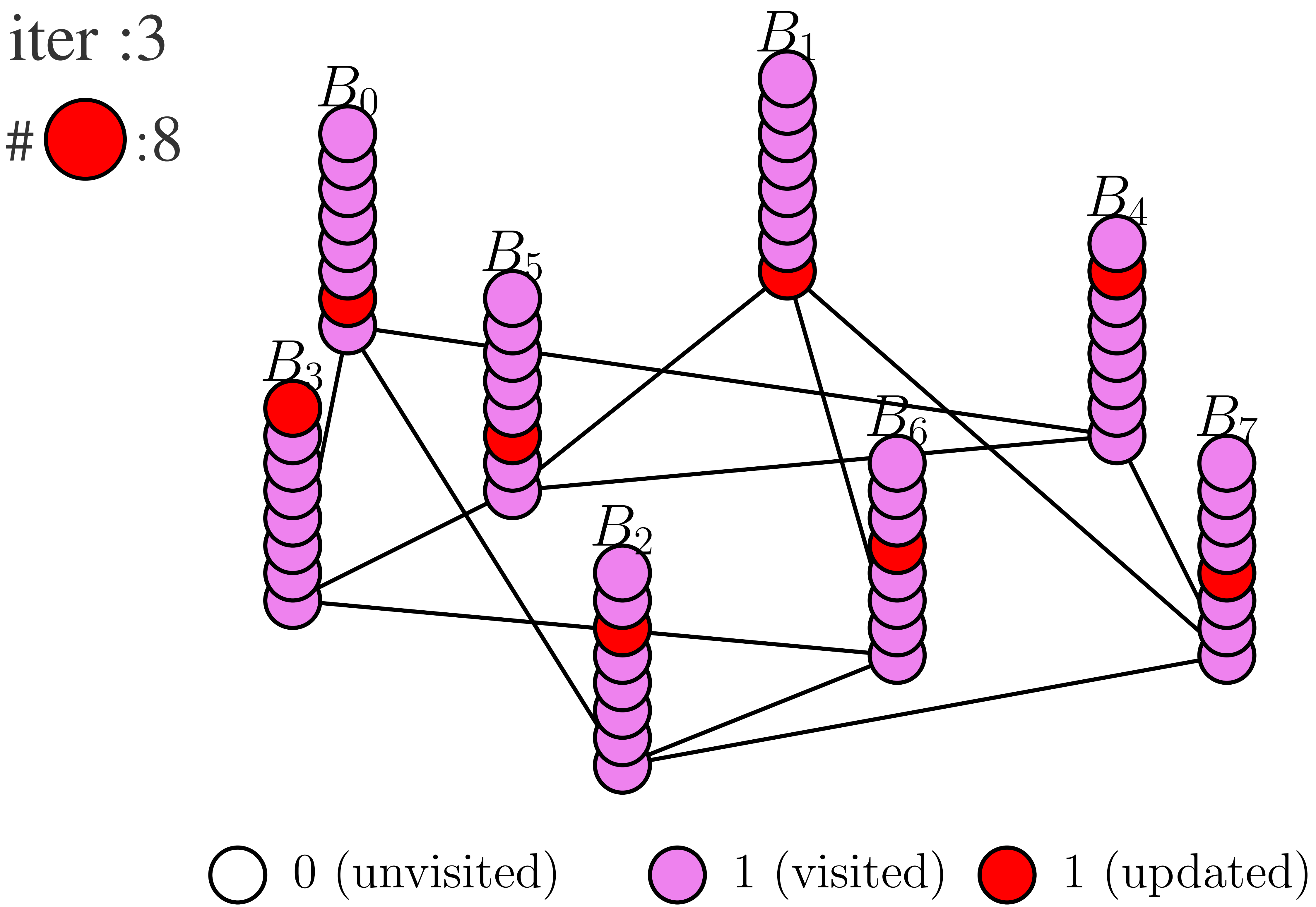
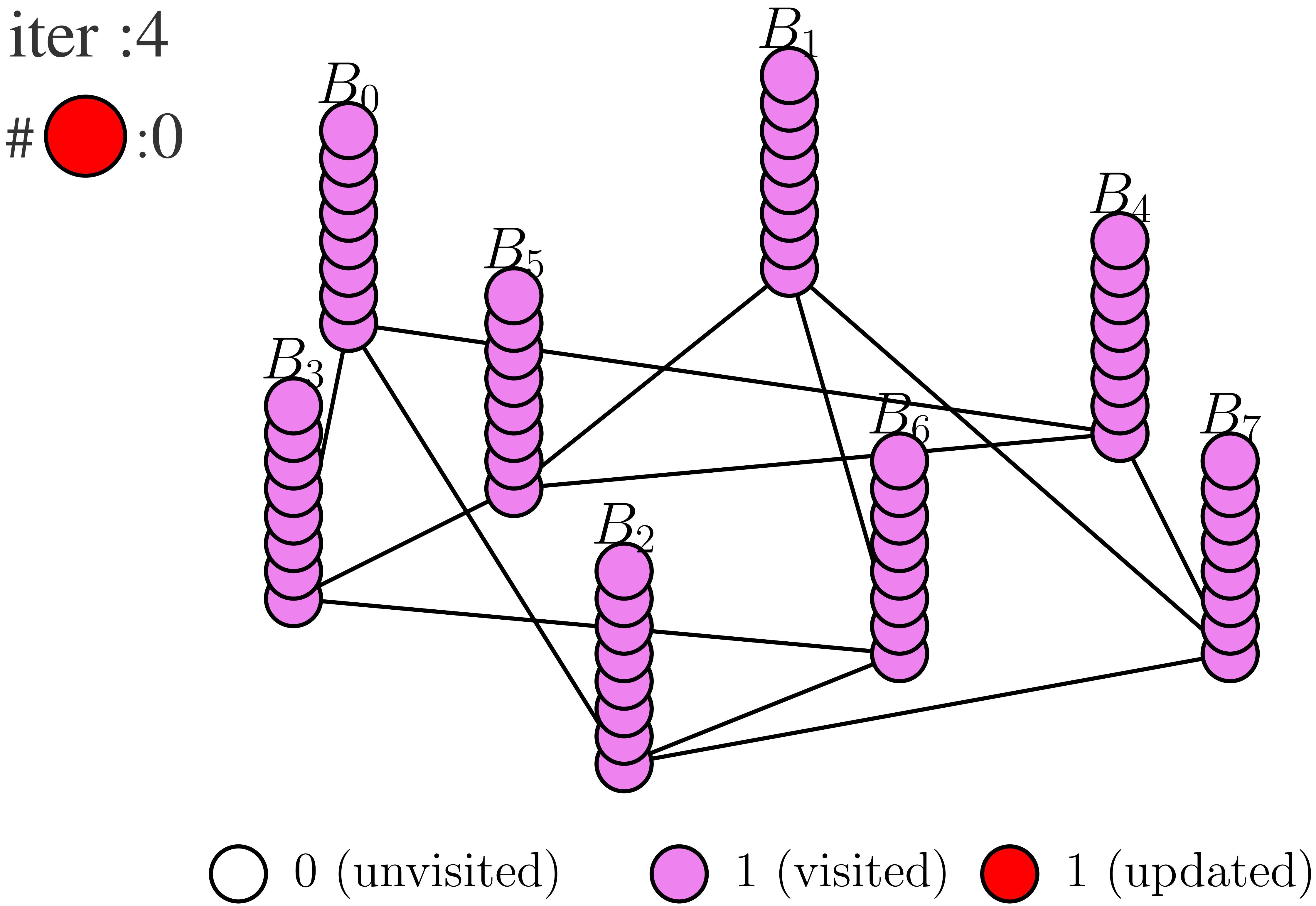


Optimization for CUDA

Terminate iteration when all bit get "1"



Optimization for CUDA

iter :1

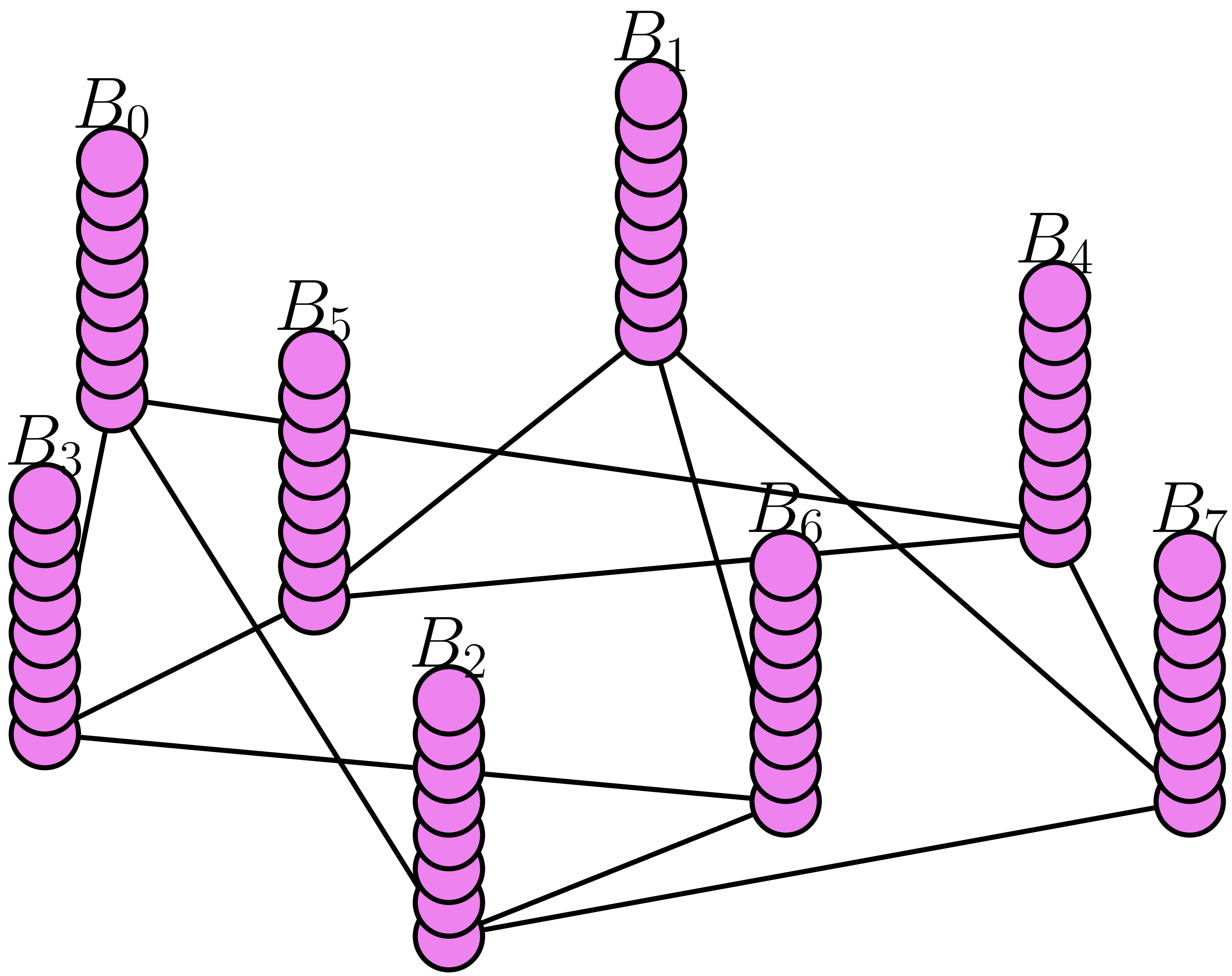
:24

iter :2

:24

iter :3

:8



0 (unvisited) 1 (visited) 1 (updated)

$$\text{ASPL} : \frac{24 \cdot 1 + 24 \cdot 2 + 8 \cdot 3}{8 \cdot 7} = 1.714285\ldots$$

Performance of the implementation

- This implementation reduces memory access drastically.
- ASPL of part shift graph with $(n, d, m) = (1e6, 32, 64)$ can be calculated in 113ms with Geforce GTX780
- ASPL of entire graph with $(n, d) = (1e6, 32)$ is calculated in 160s, 710x faster than native serial BFS implementation with i7-8700.

Conclusion

- "part shift graph" can achieve small Diameter/ASPL.
- GPU acceleration is powerful tool for ASPL calculation of large graphs.

Source Code & References

- Source Code

  https://github.com/confused-uec/graphgolf-cuda

- References

Scott Beamer, Krste Asanović, and David Patterson.
Searching for a parent instead of fighting over children: A fast breadth-first search implementation for graph500. Technical Report UCB/EECS-2011-117, EECS Department, University of California, Berkeley, 2011.

Scott Beamer, Understanding and Improving Graph Algorithm Performance, Technical Report UCB/EECS-2016-153 EECS Department, University of California, Berkeley 2016.