Introduction of fast APSP algorithm and optimization algorithms for grid graphs

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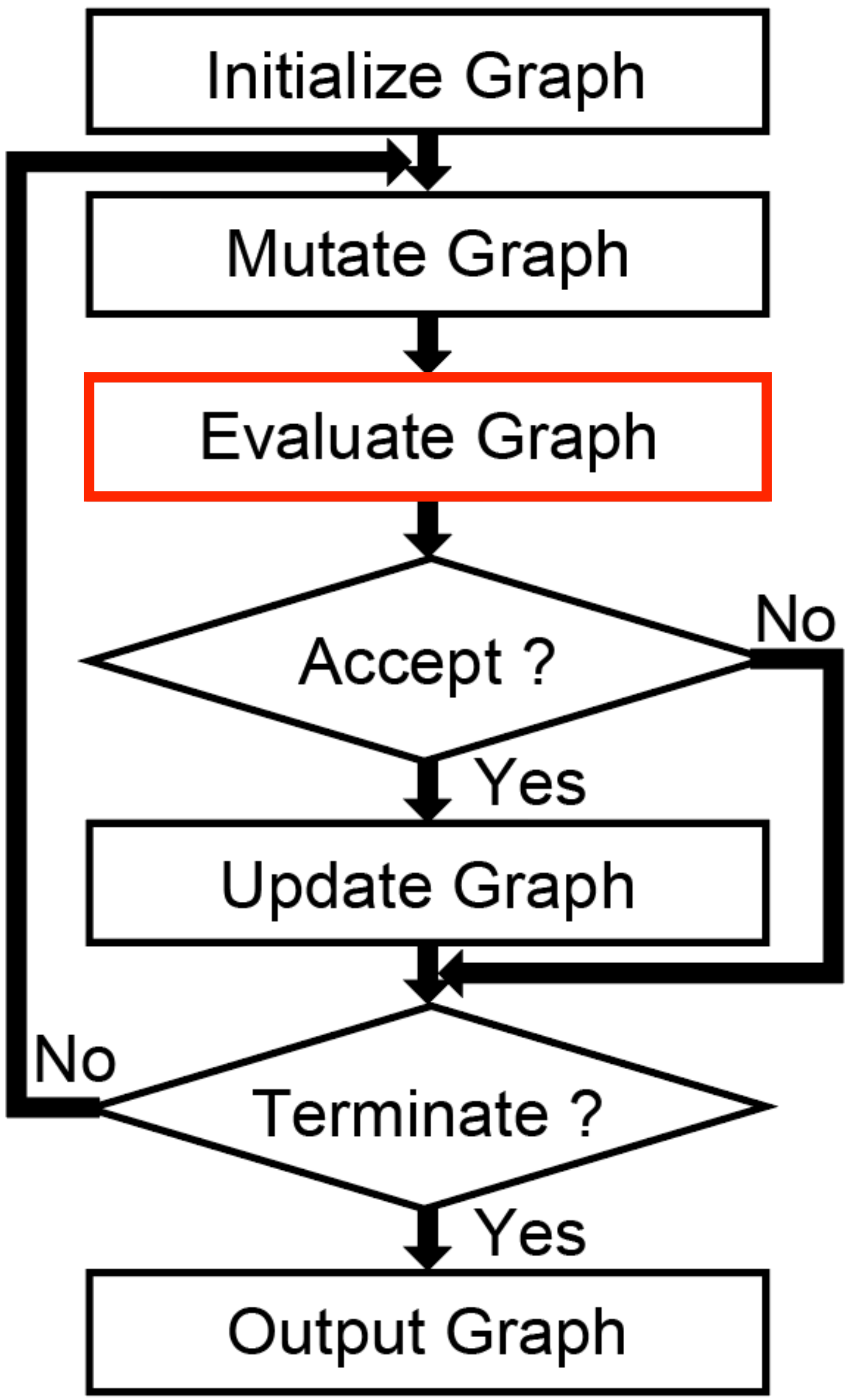
Obtain ASPL and diameter



- Metaheuristic such as SA and GA are often used
- To evaluate a graph, its diameter and ASPL are needed which are calculated by APSP algorithm **many times**
- **It is very important to calculate APSP at high-speed**

e.g. For a problem (n, d) = (1M, 32), the time required for one APSP is about 37 hours by the method based on Breadth-First Search (BFS) on Intel Gold 6126

Our APSP algorithms

- Our previous research provides a parallel APSP algorithm based on BFS (BFS-APSP) [1-3]
- This presentation introduces a new parallel APSP algorithm based on adjacency matrix (ADJ-APSP) [4-5]. The original ADJ-APSP was developed by Ryuhei Mori [6]

You can download our program from
https://github.com/mnakao/APSP/

[1] 中尾昌広ほか. MPI/OpenMP並列によるグラフ対称性とSimulated Annealingを用いたOrder/Degree問題の一解法, HPC研究会. 2018.

[2] Masahiro Nakao et. al. A Method for Order/Degree Problem Based on Graph Symmetry and Simulated Annealing with MPI/OpenMP Parallelization, HPC Asia 2019.

[3] 中尾昌広ほか. 大規模Order/Degree問題に対する最適化アルゴリズムの並列化と解探索性能の評価. 計算工学講演会論文集, 2019.

[4] 中尾昌広ほか. Order/Degree問題のための重みなしグラフにおける全点対間最短経路アルゴリズムの並列化. HPC研究会. 2019.

[5] Masahiro Nakao et al. Parallelization of All-Pairs-Shortest-Path Algorithms in Unweighted Graph, HPC Asia 2020.

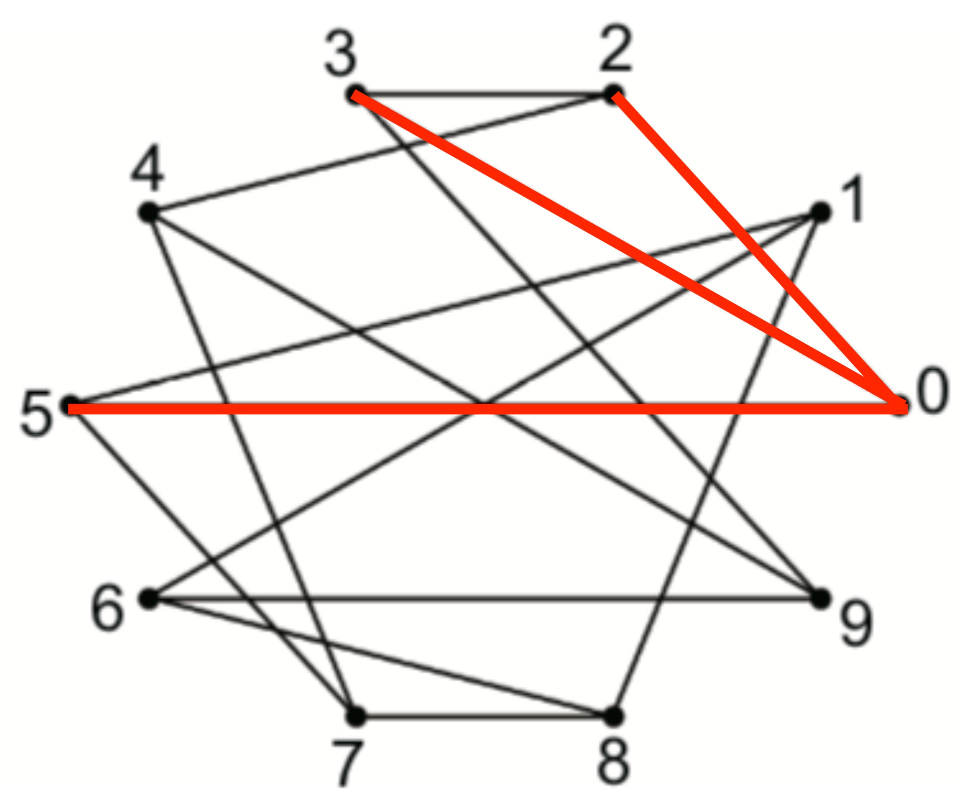
[6] https://github.com/ryuhei-mori/graph_ASPL

ADJ-APSP(1/3)

- Let A be an adjacency matrix of a graph
- If the value of an element a_{i, j} in A^k is 1, it means that the vertex i can reach the vertex j within k hops

```
for(int i=0;i<n;i++)
  A[0][i] |= A[2][i] | A[3][i] | A[5][i];
```

(n, d) = (10, 3)



A	adjlst	A^1
0 0 0 0 0 0 0 0 0 1	2 3 5	0 0 0 0 1 0 1 1 0 1
0 0 0 0 0 0 0 0 1 0	5 6 8	0 1 0 1 1 0 0 0 1 0
0 0 0 0 0 0 0 1 0 0	0 3 4	0 0 0 0 0 1 1 1 0 1
0 0 0 0 0 0 1 0 0 0	0 2 9	1 0 0 0 0 0 1 1 0 1
0 0 0 0 0 1 0 0 0 0	2 7 9	1 0 1 0 0 1 0 1 0 0
0 0 0 0 1 0 0 0 0 0	0 1 7	0 0 1 0 1 0 0 0 1 1
0 0 0 1 0 0 0 0 0 0	1 8 9	1 1 0 1 0 0 0 0 1 0
0 0 1 0 0 0 0 0 0 0	4 5 8	0 1 1 0 1 1 0 0 0 0
0 1 0 0 0 0 0 0 0 0	1 6 7	0 1 1 1 0 0 0 0 1 0
1 0 0 0 0 0 0 0 0 0	3 4 6	1 0 0 1 0 1 1 0 0 0

ADJ-APSP(2/3)

A	adjlst	A^1	A^2	A^3
0 0 0 0 0 0 0 0 0 1	2 3 5	0 0 0 0 1 0 1 1 0 1	1 0 1 0 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 0 1 0	5 6 8	0 1 0 1 1 0 0 0 1 0	1 1 1 1 1 0 0 0 1 1	1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 0 1 0 0	0 3 4	0 0 0 0 0 1 1 1 0 1	1 0 1 0 1 1 1 1 0 1	1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 0 1 0 0 0	0 2 9	1 0 0 0 0 0 1 1 0 1	1 0 0 1 1 1 1 1 0 1	1 1 1 1 1 1 1 1 1 1
0 0 0 0 0 1 0 0 0 0	2 7 9	1 0 1 0 0 1 0 1 0 0	1 1 1 1 1 1 1 1 0 1	1 1 1 1 1 1 1 1 1 1
0 0 0 0 1 0 0 0 0 0	0 1 7	0 0 1 0 1 0 0 0 1 1	0 1 1 1 1 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1
0 0 0 1 0 0 0 0 0 0	1 8 9	1 1 0 1 0 0 0 0 1 0	1 1 1 1 1 1 1 0 1 0	1 1 1 1 1 1 1 1 1 1
0 0 1 0 0 0 0 0 0 0	4 5 8	0 1 1 0 1 1 0 0 0 0	1 1 1 1 1 1 0 1 1 1	1 1 1 1 1 1 1 1 1 1
0 1 0 0 0 0 0 0 0 0	1 6 7	0 1 1 1 0 0 0 0 1 0	1 1 1 1 1 1 0 0 1 0	1 1 1 1 1 1 1 1 1 1
1 0 0 0 0 0 0 0 0 0	3 4 6	1 0 0 1 0 1 1 0 0 0	1 1 1 1 0 1 1 1 1 1	1 1 1 1 1 1 1 1 1 1

- As k is increased in increments of 1, the value of k is the **diameter** when all elements are 1
- Every time k is increased from 1 to the diameter, the total distance is obtained by summing all the elements whose value is 0
  - **ASPL** is calculated by dividing the total distance by the number of elements

ADJ-APSP(3/3)

```
function SERIAL_ADJ_APSP(vertices, nodes)
  diameter ← 1
  distance ← nodes∗(nodes−1)
  elements ← ⌈nodes/E⌉
  A, B ← INITIALIZE(nodes, elements)
  for k=1 ... nodes−1
    for i=1 ... nodes
      for n ∈ neighbors(i, vertices)
        for j=1 ... elements
          B[i][j] ← B[i][j] | A[n][j]

    num ← 0
    for i=1 ... nodes
      for j=1 ... elements
        num ← num+POPCNT(B[i][j])

    if(num = nodes∗nodes) break

    SWAP(A, B)
    diameter++
    distance ← distance+(nodes∗nodes−num)
  average_distance ← distance/((nodes−1)∗nodes)
  return diameter, average_distance
```

← logical sum operation
(the most time-consuming part)

We have developed Serial, Multi-threads GPU, Multi-GPUs versions

Experiment environment

Cygnus system in Univ. of Tsukuba

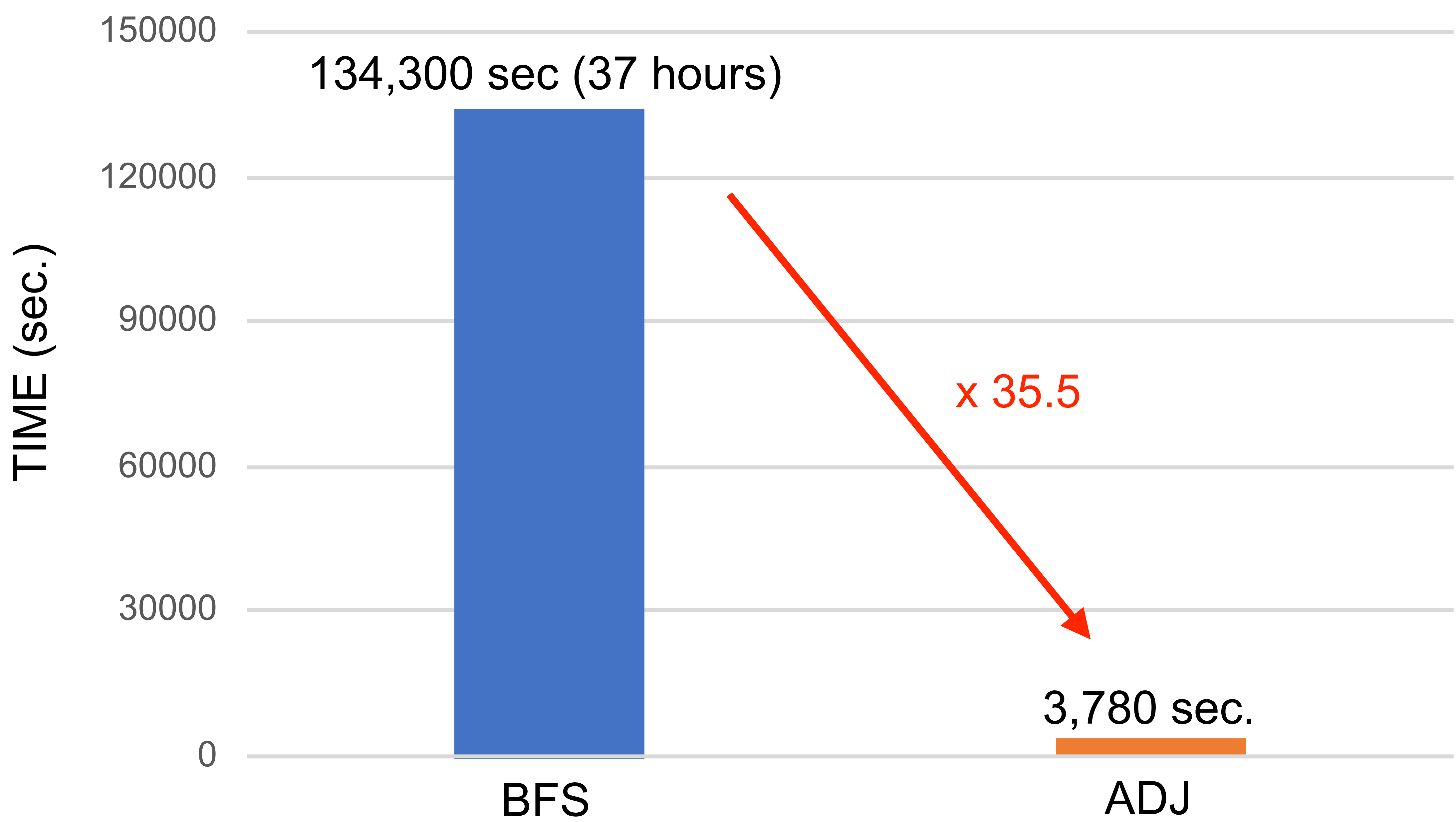
CPU	Intel Xeon Gold 6126 (12Cores, 2.6GHz) × 2
Memory	DDR4 (128GB/s × 2, 192GB)
GPU	NVIDIA Tesla V100 (900GB/s, 32GB) × 4
Network	InfiniBand HDR100 (12.5GB/s) × 4
Software	intel/19.0.3, mvapich/2.3.1, cuda/10.1

- The Cygnus system is provided by Interdisciplinary Computational Science Program in the Center for Computational Sciences, University of Tsukuba
  - Computing resources such as Cygnus and Oakforest-PACS can be used **for free**
  - This entry is held around mid-December

Result (Change from BFS to ADJ)

Speed to calculate APSP for graph with (1M, 32)

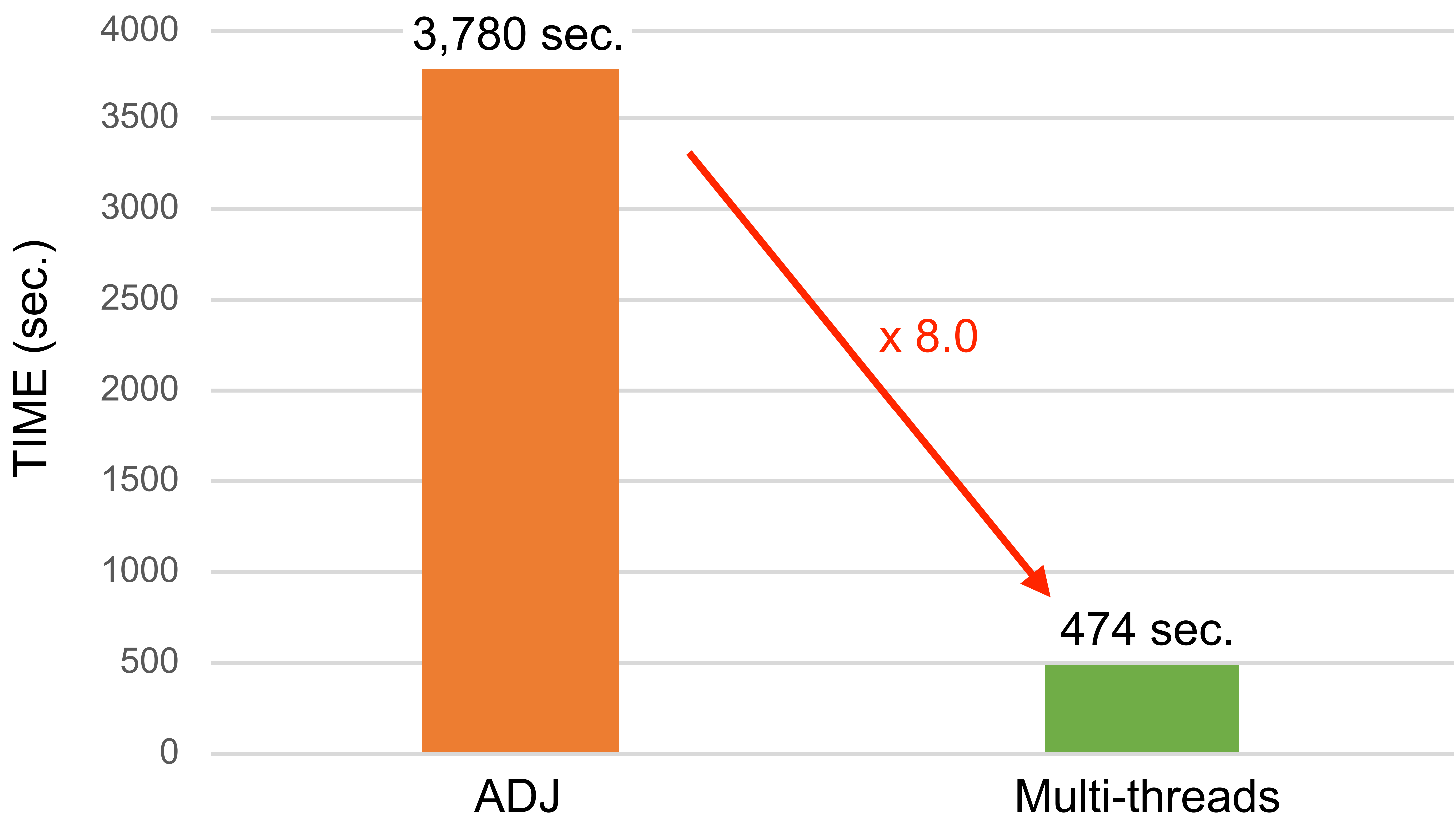
Intel Xeon Gold 6126 2.6GHz



Result (Multi-threads)

Speed to calculate APSP for graph with (1M, 32)

Intel Xeon Gold 6126 2.6GHz (12 cores)



Result (GPU)

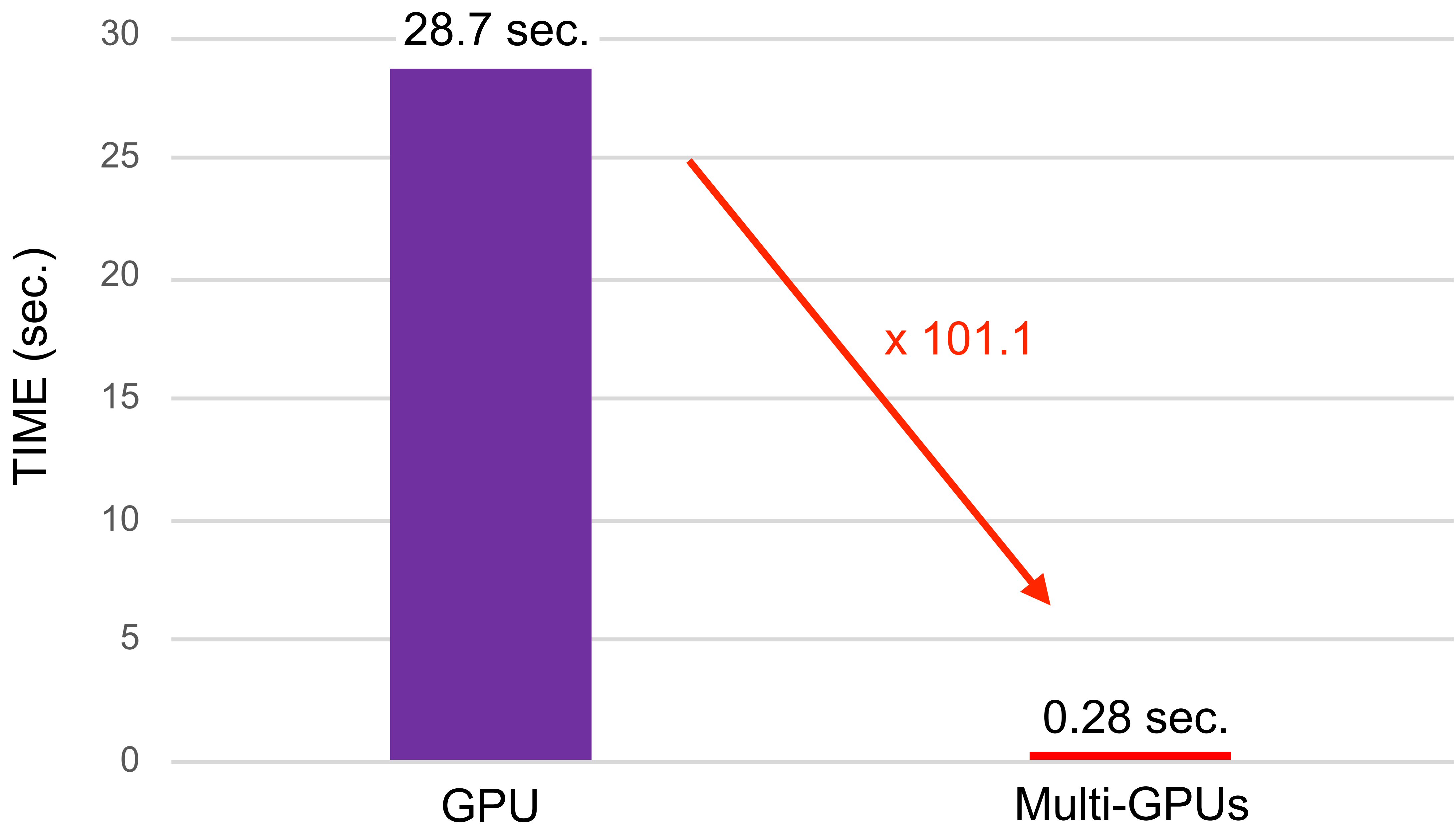
Speed to calculate APSP for graph with (1M, 32)

Intel Xeon Gold 6126 2.6GHz (12 cores) -> NVIDIA V100

Result (Multi-GPUs)

Speed to calculate APSP for graph with (1M, 32)

Intel Xeon Gold 6126 2.6GHz (12 cores) -> NVIDIA V100 x 128

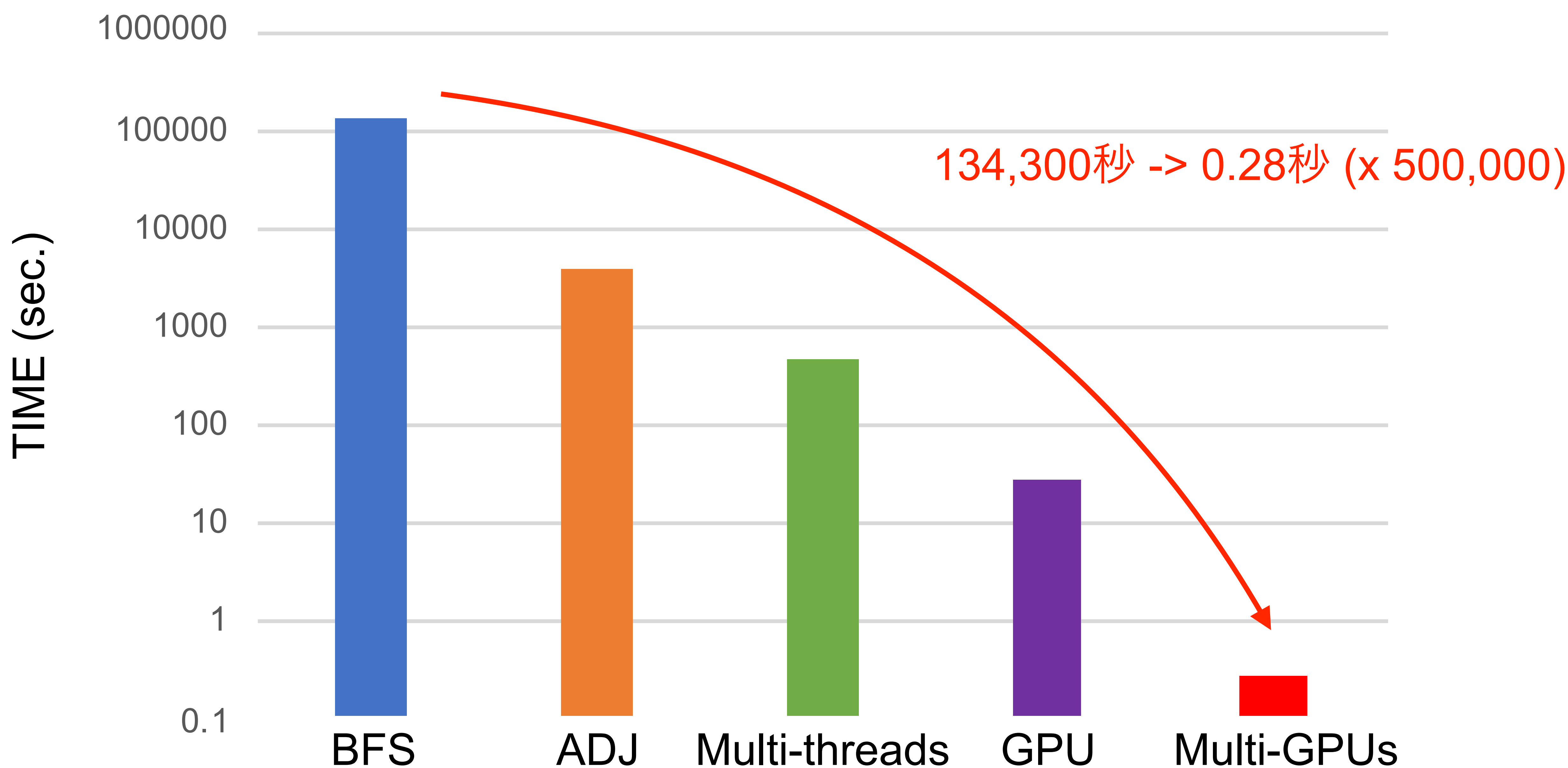


Summary

Of course, when using graph symmetry,
the calculation time can be reduce more greatly.

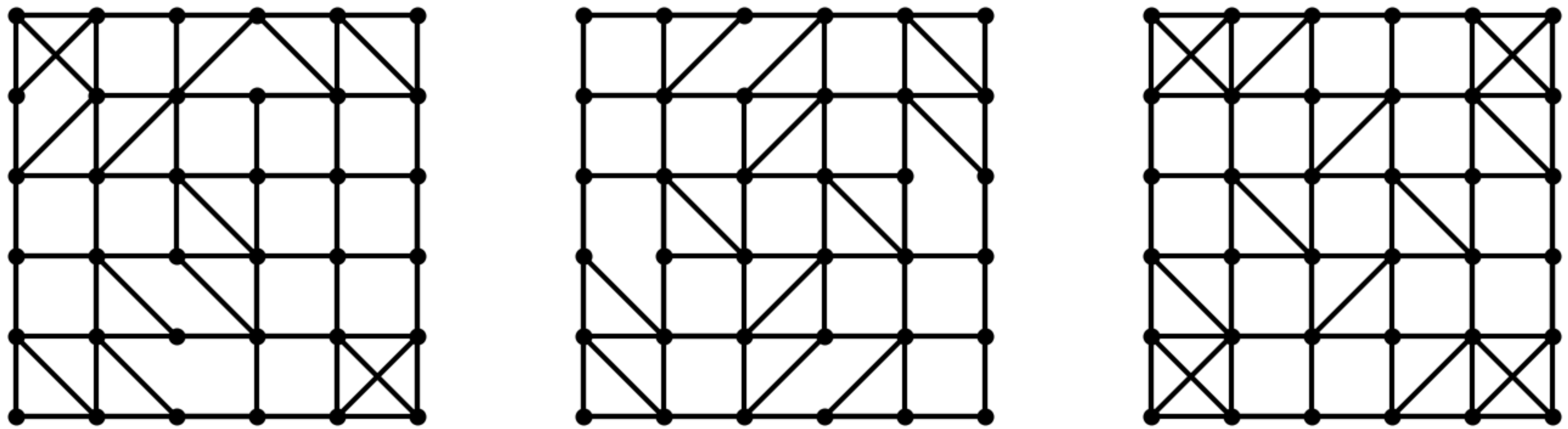
Speed to calculate APSP for graph with (1M, 32)

Intel Xeon Gold 6126 2.6GHz (12 cores) -> NVIDIA V100 x 128



Graph symmetry

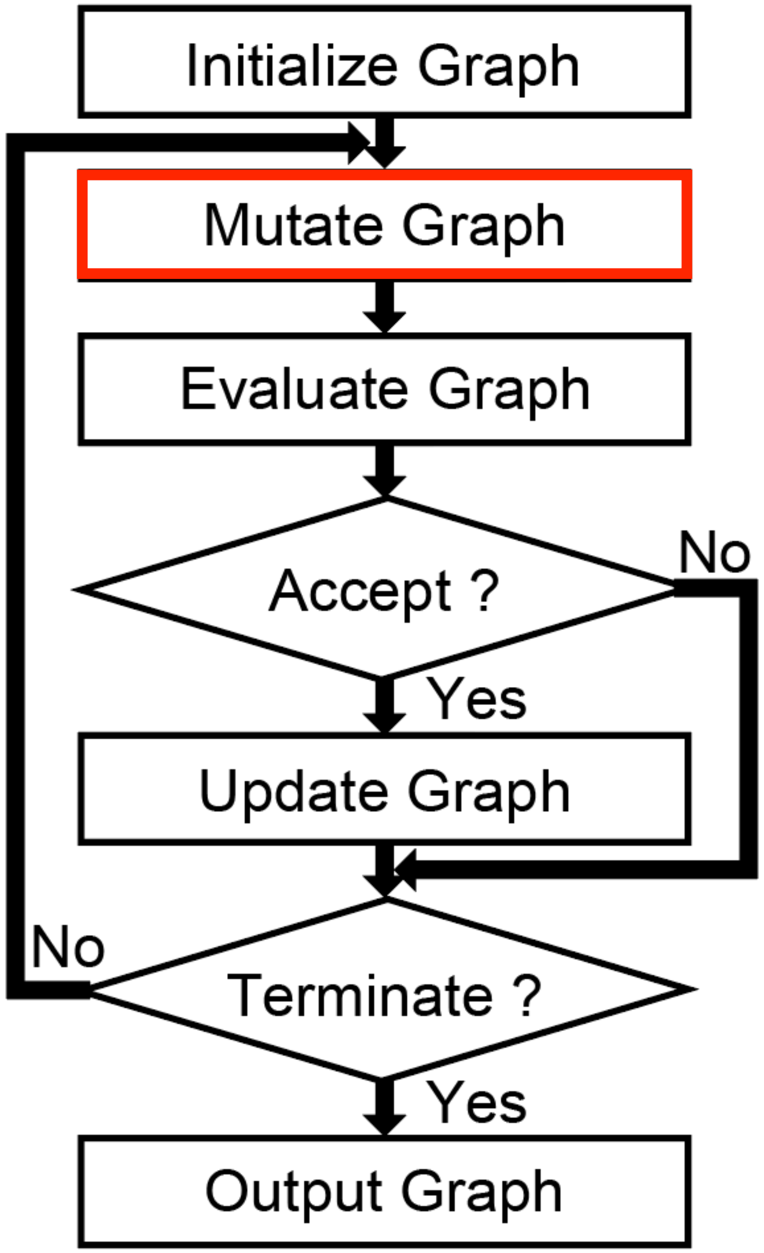
- The algorithm is inherited from mine for general graph last year [1-3]
- Examples of the graph symmetry with (W, H, D, R) = (6, 6, 4, 2)



g=1 (normal graph) g=2 g=4

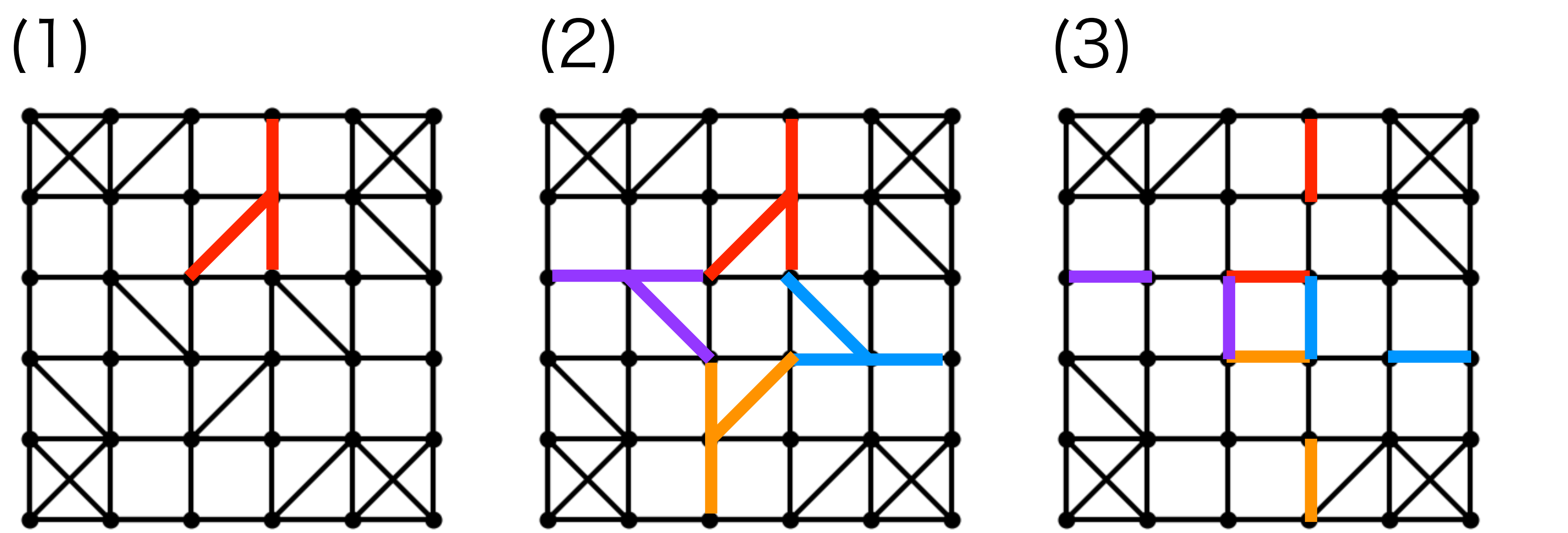
- The variable **g** is the number of groups (g must be 1 or 2 or 4)
- If a graph is rotated by 360/**g** degrees, the connection relationship between the vertex and edge becomes the original one

Edge exchange based on 2-opt



Perform 2-opt method while maintaining symmetry

In case of g=4

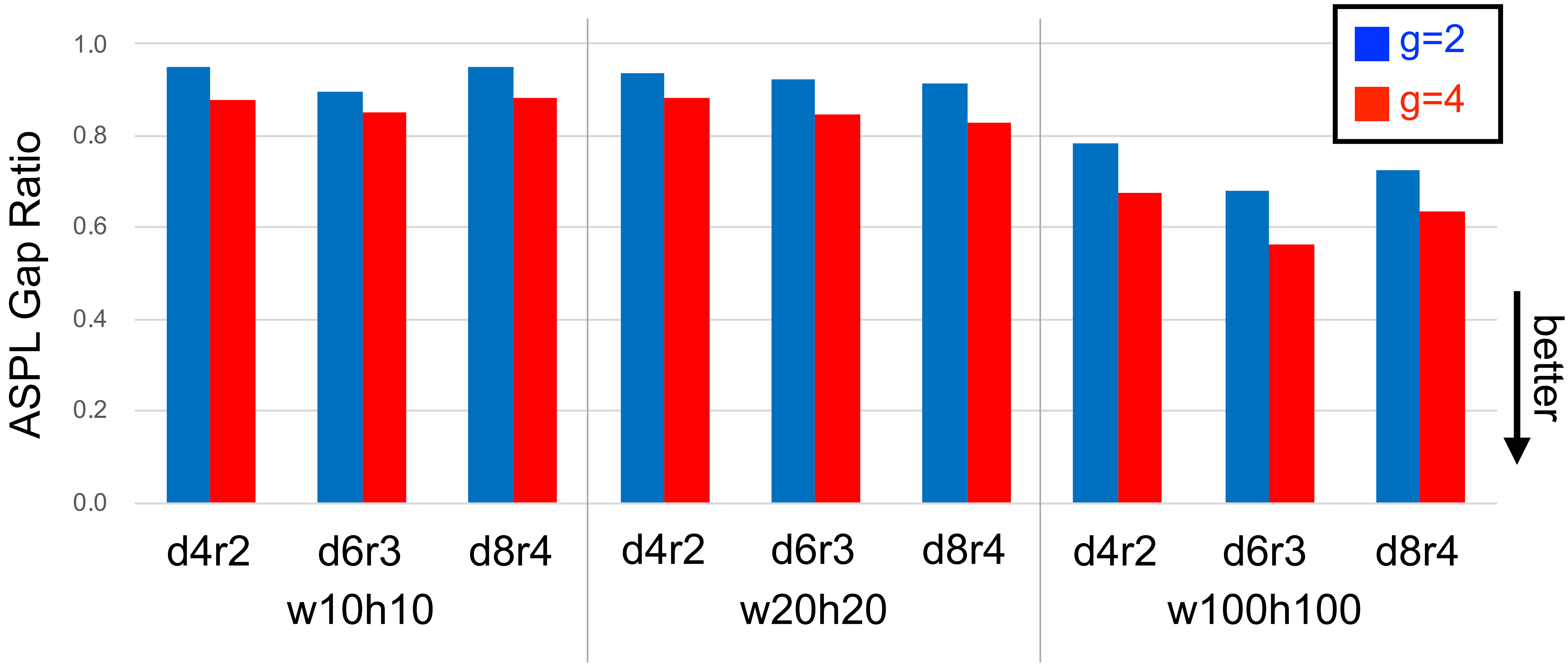


(1) Randomly select two edges from all the edges

(2) Select edges symmetrically related to (1)

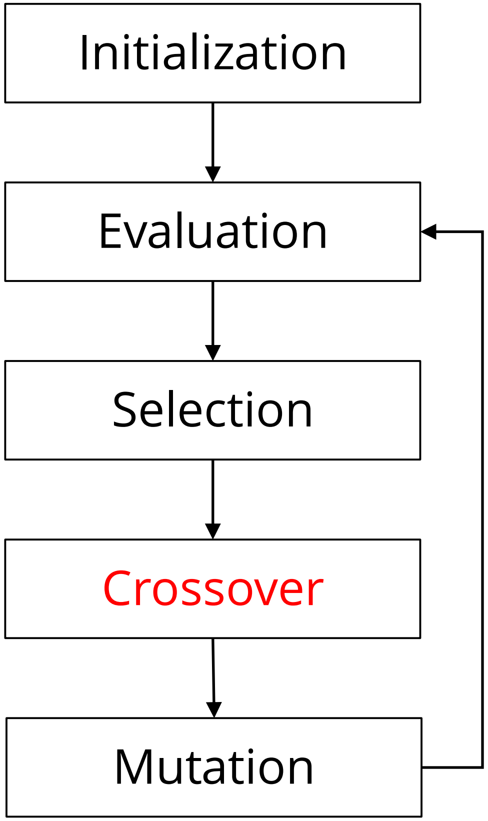
(3) Apply the 2-opt method to above edges each other

Results



- The vertical axis is the ASPL Gap Ratio when the result of g=1 is 1.0
- The larger the value of g is, the smaller the ASPL Gap is
  - Larger problems tend to have larger performance differences
- **The results show that graph symmetry is also useful in grid graphs**

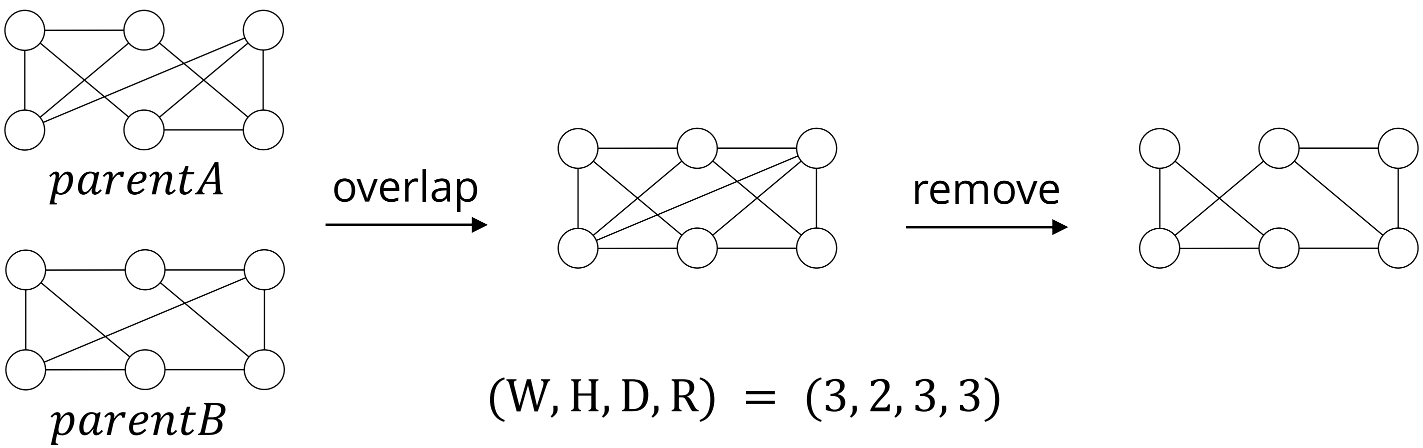
Genetic Algorithm



- GA is a direct search method that can be applied for various complex problems.
- GA shows good performance in large-scale TSP.
- Crossover design is the most important to improve search performance of GA.
  - ➡ Sophisticated crossover that deals with problem-specific features are required.

Crossover Method

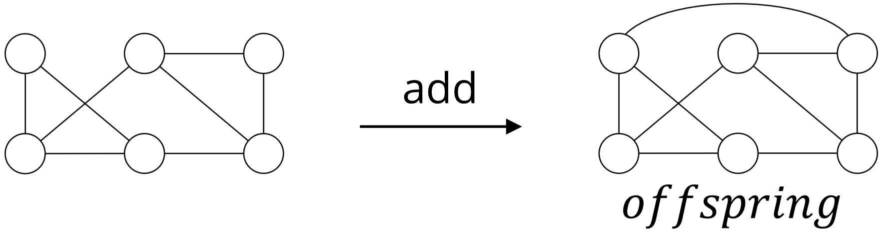
1. Overlap two graphs.
2. Continue removing the edge until the graph satisfy constraint.
   - Select nodes with the highest degree and do not satisfy the degree constraint.
   - Find the edge with the smallest effect on ASPL.



$$(\mathrm{W}, \mathrm{H}, \mathrm{D}, \mathrm{R}) = (3, 2, 3, 3)$$

Crossover Method

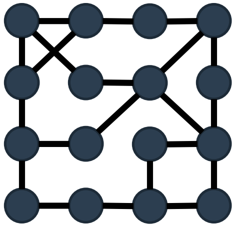
3. Continue adding the edge while edge can be added.
   - Select nodes with the lowest degree that can accept edges.
   - Find the best edge that improves ASPL.



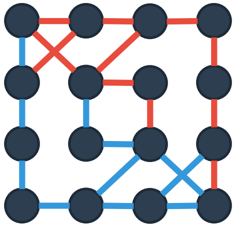
$$(\mathrm{W}, \mathrm{H}, \mathrm{D}, \mathrm{R}) = (3, 2, 3, 3)$$

Numerical Experiments

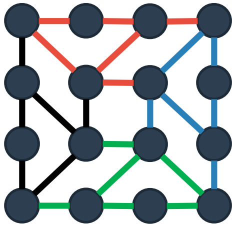
Parameter	
Instance	$(\mathrm{W}, \mathrm{H}, \mathrm{D}, \mathrm{R}) = (10, 5, 4, 2), (10, 10, 4, 2)$
Group size	$1, 2, 4$
Generation alternation model	MGG[1]
Max evaluation count	100M
Population size	100
Offspring size	200
Mutation rate (Shuffle)	0.01



$g = 1$



$g = 2$



$g = 4$

[1] : 佐藤 浩, 小野 功, 小林 重信, 遺伝的アルゴリズムにおける世代交代モデルの提案と評価, 人工知能学会誌, Vol. 12, No. 5, pp734 – 744, 1997

Result using GA

Rectangular Graph

$\mathbf{10, 5, 4, 2}$	Best	Ave	Worst
$g = 1$	3.10694	3.110529	3.11265
$g = 2$	3.1102	3.110445	3.11265

Square Graph

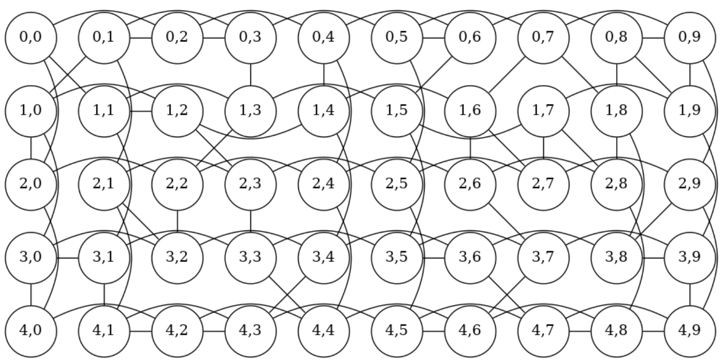
$\mathbf{10, 10, 4, 2}$	Best	Ave	Worst
$g = 1$	4.01434	4.020768	4.02687
$g = 2$	3.99293	3.996365	4.00162
$g = 4$	3.98586	3.993577	3.99596

- For rectangular instance, the symmetric grouping technique makes the performance worse.
- For square instance, grouping technique enhances the performance, and the larger number of grouping is better.

Result using GA

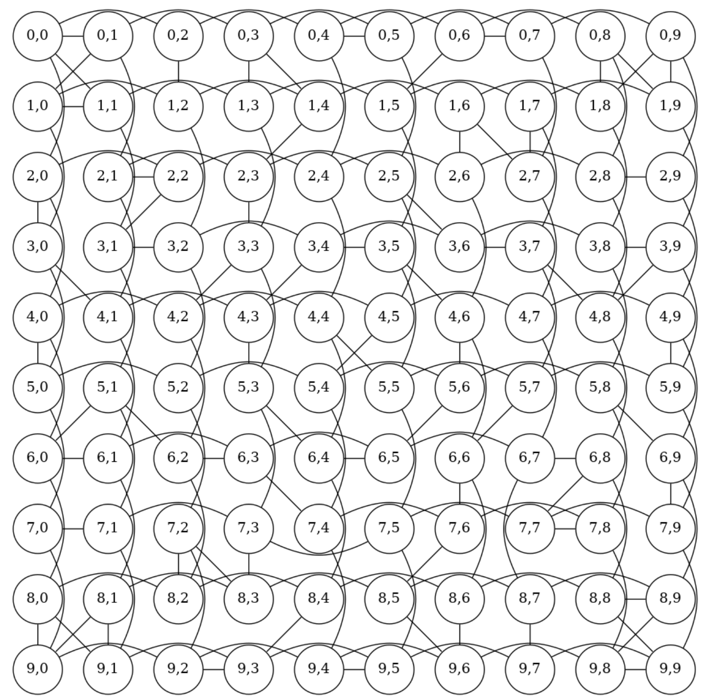
- Remarkable traits that have not been found a conventional approach based on 2-opt were observed.
- Best solutions obtained by GA include non-regular nodes of which degree is less than 4, while best solutions obtained by SA based on 2-opt consist of completely regular nodes.

$d = 3$



$(10, 5, {\color{red}4}, 2)$

$d = 3$



$(10, 10, {\color{red}4}, 2)$

Summary

- We applied GA to solve Graph Golf instances.
- Symmetric grouping technique works well on square instance.
- Remarkable traits that cannot be found in conventional approach were obtained by GA.
- GA requires much computation cost, so that we should improve the efficiency of crossover.