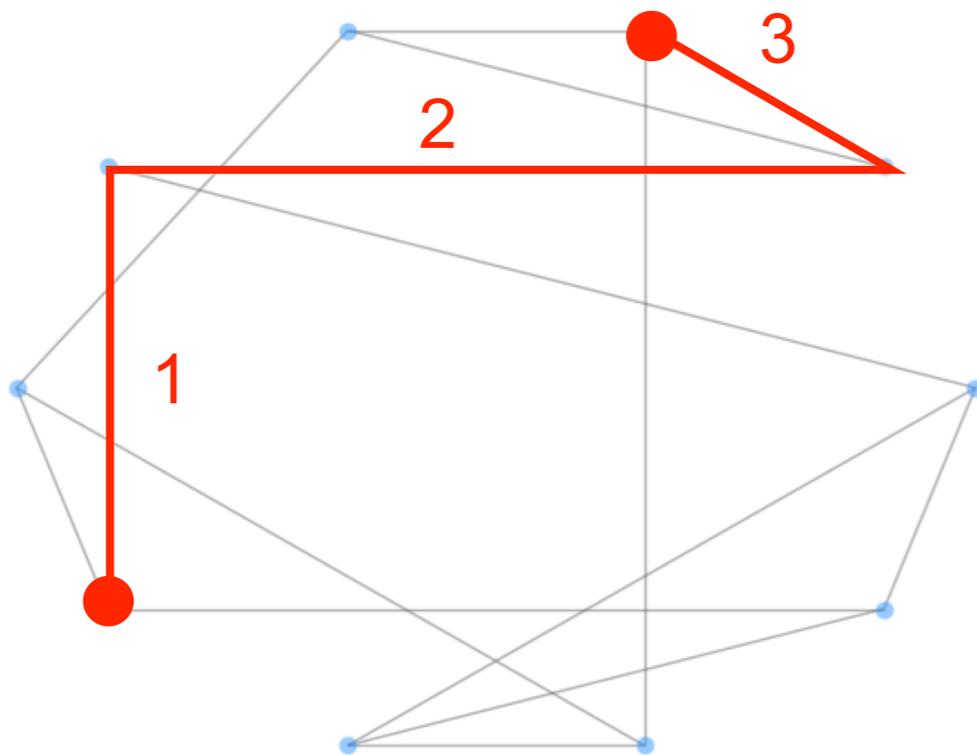


A Method for Order/Degree Problem Based on Graph Symmetry and Simulated Annealing

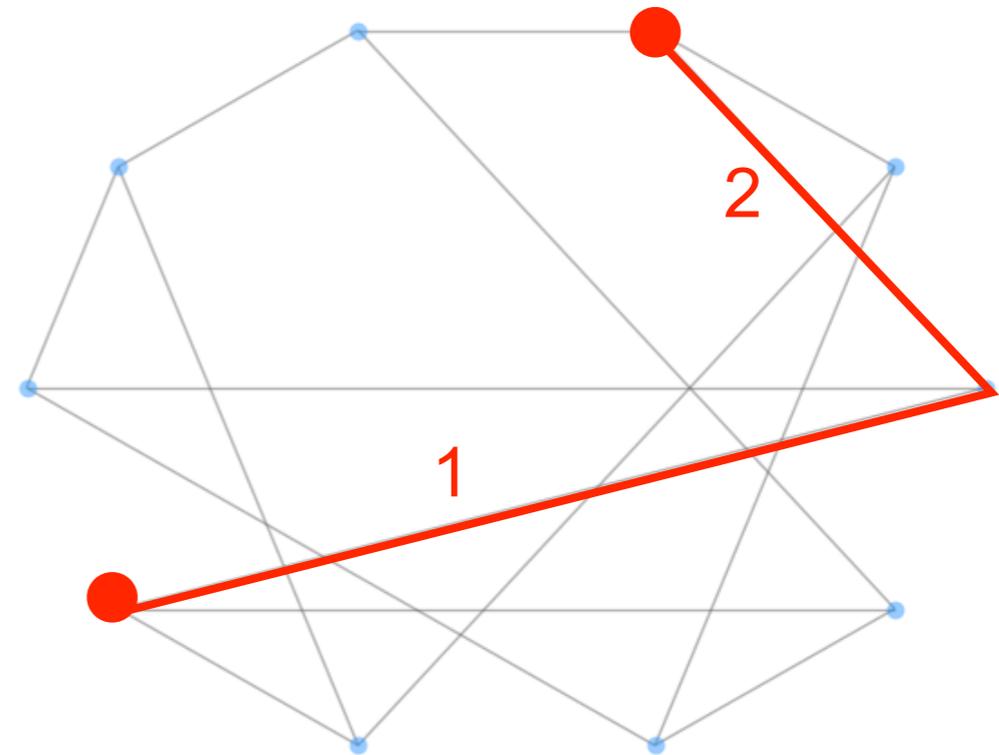
Masahiro Nakao (RIKEN Center for Computational Science)

What is Order/Degree Problem (ODP)?

- Find the graph with the smallest **diameter** and **average shortest path length (ASPL)**
- Given order (n) and degree (d) pairs
 - Examples of the graph with $(n, d) = (10, 3)$



Diameter=3, ASPL=1.89 (Random)

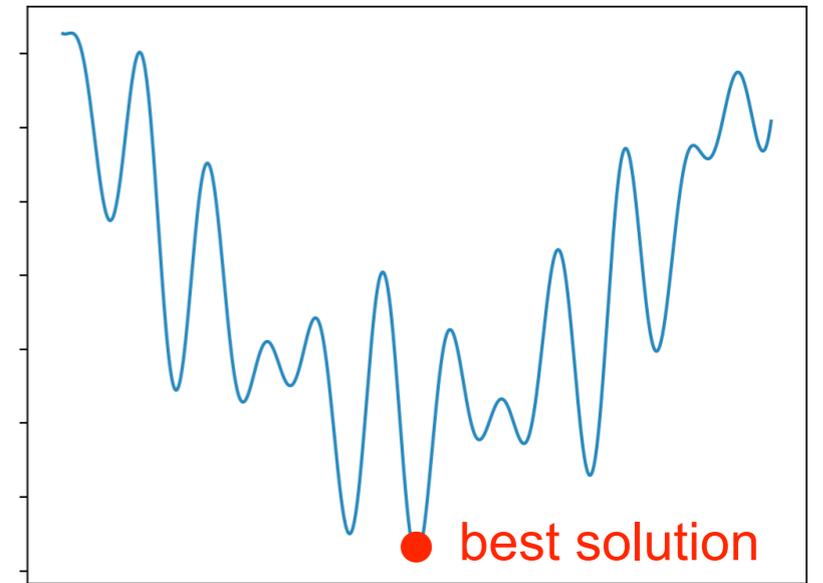


Diameter=2, ASPL=1.67 (Optimal)

What are difficult points in ODP ?

(1) The number of graphs satisfying the given number of vertices and degrees is enormous

- It is difficult to find the **best solution** because the problem has many local optima



(2) The calculation time required for obtaining ASPL is enormous

- The calculation complexity with n vertices and d degrees is $O(n^2 \cdot d)$
- For the graph with $(n, d) = (400,000, 32)$, the calculation time required for obtaining ASPL is **about 5.5 hours** on Xeon Ivy Bridge

Approach

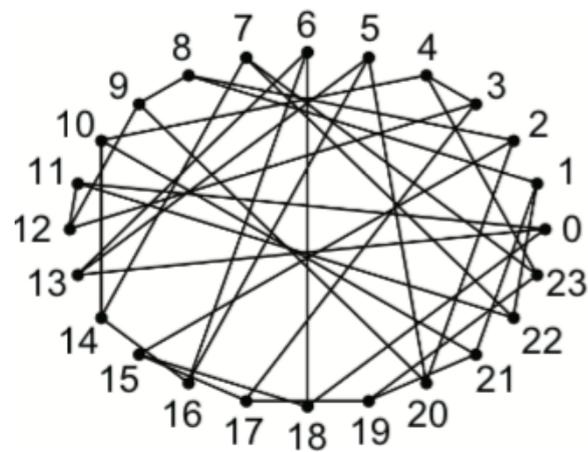
- Make the network topology **symmetrical**, thereby
 - (1) Improving the solution search performance of simulated annealing (SA)
 - (2) Reducing the calculation time of ASPL
- Hybrid parallelization with MPI and OpenMP is applied to further reduce the calculation time on our cluster system

The calculation time of ASPL decreased from 5.5 hours to **0.01 seconds**

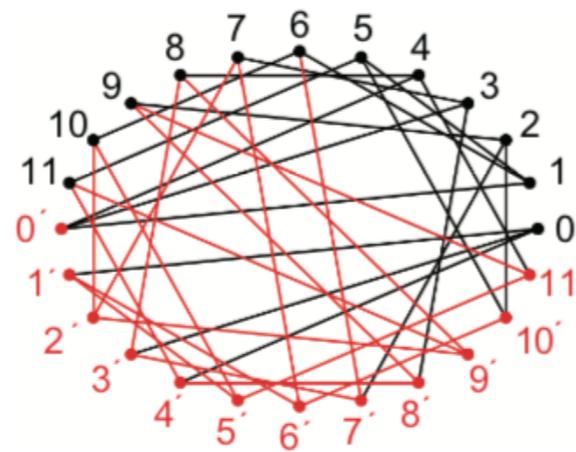

about 2,000,000 times faster

Graph symmetry

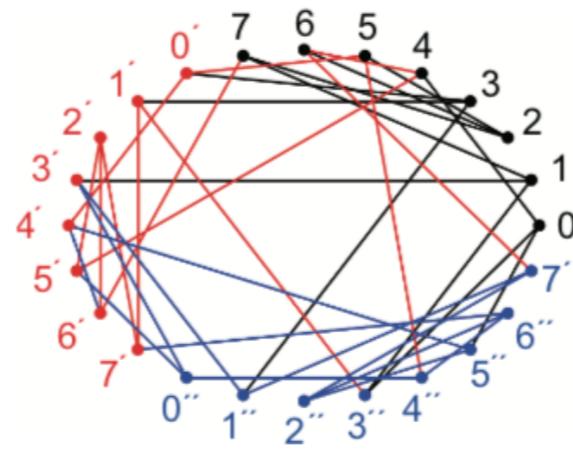
- Examples of the graph symmetry with $(n, d) = (24, 3)$



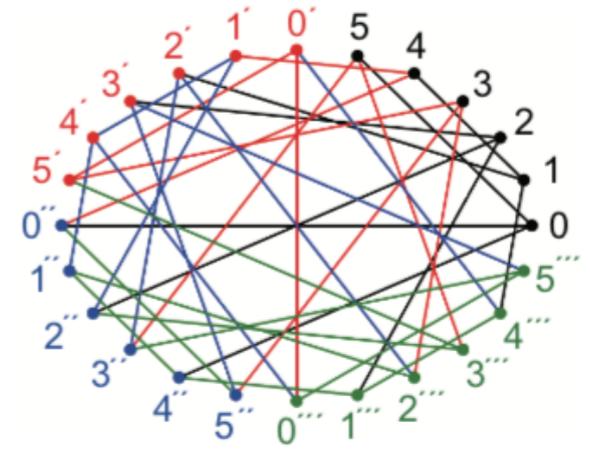
g=1



g=2



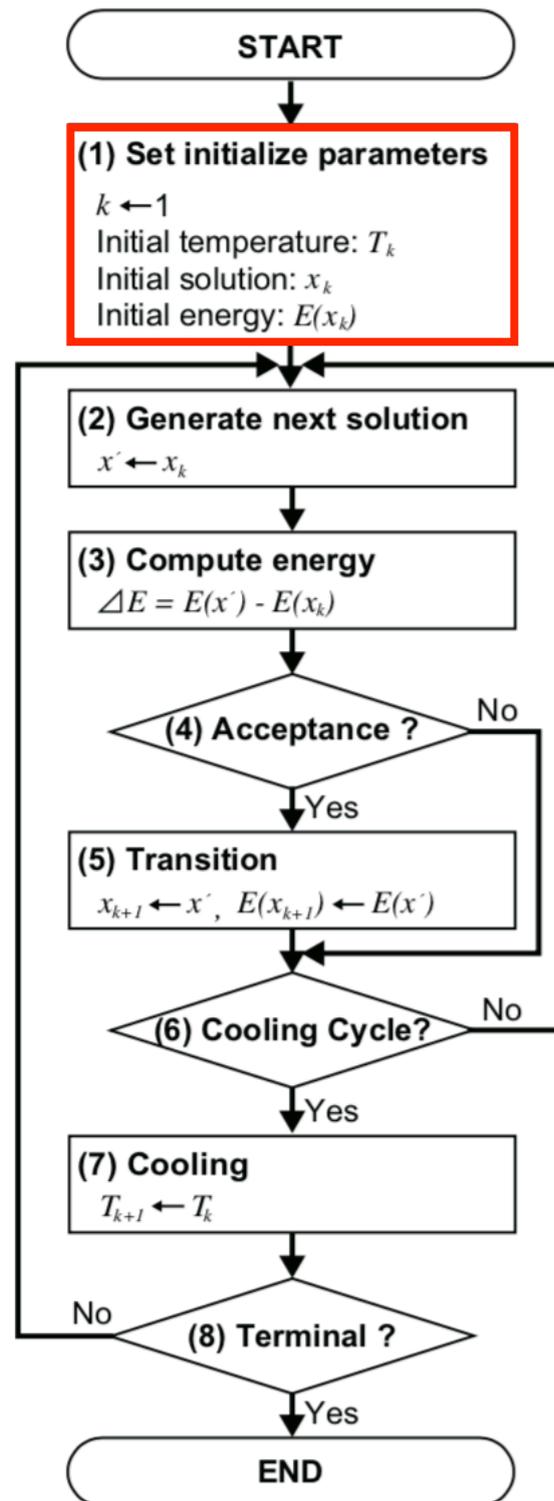
g=3



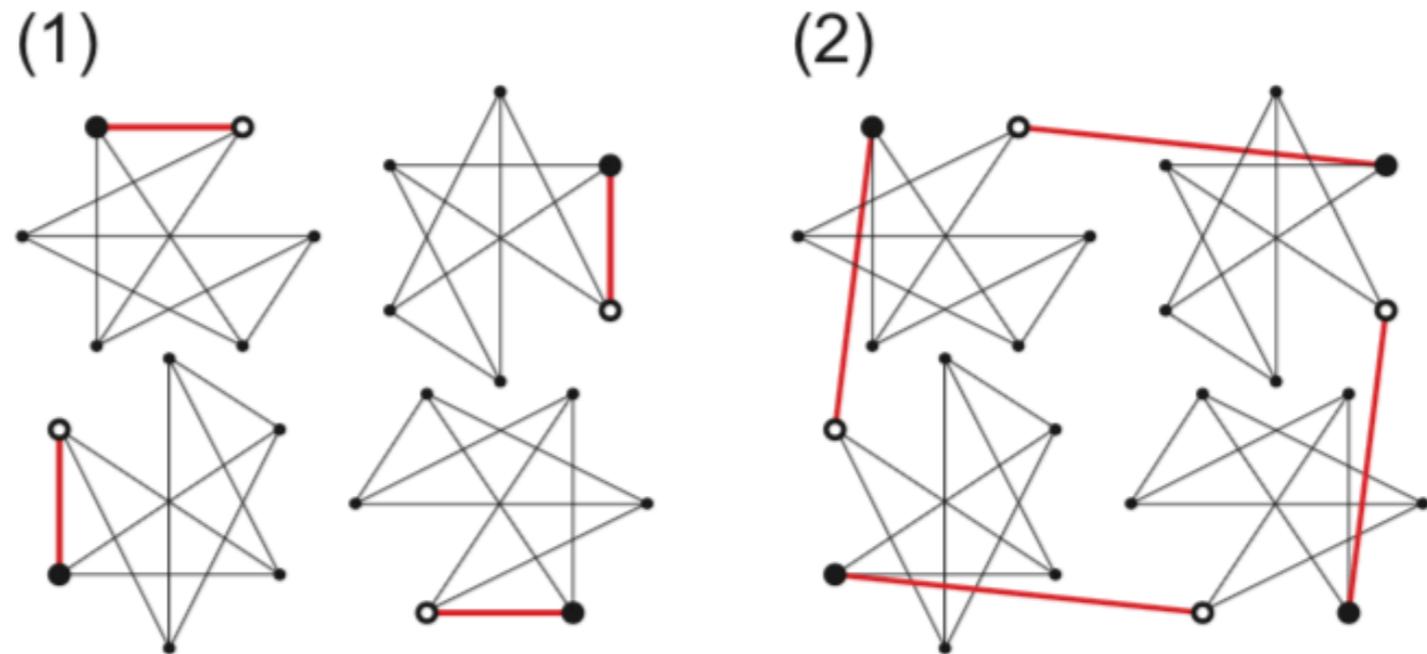
g=4

- The variable **g** is the number of groups (g must be a divisor of n)
- When a graph is viewed as a plane, if it is rotated by $360/g$ degrees, the connection relationship between the edge and the vertex becomes the same graph
- For the case of **g = 1**, a normal graph (not symmetrical) is obtained

SA with Graph symmetry



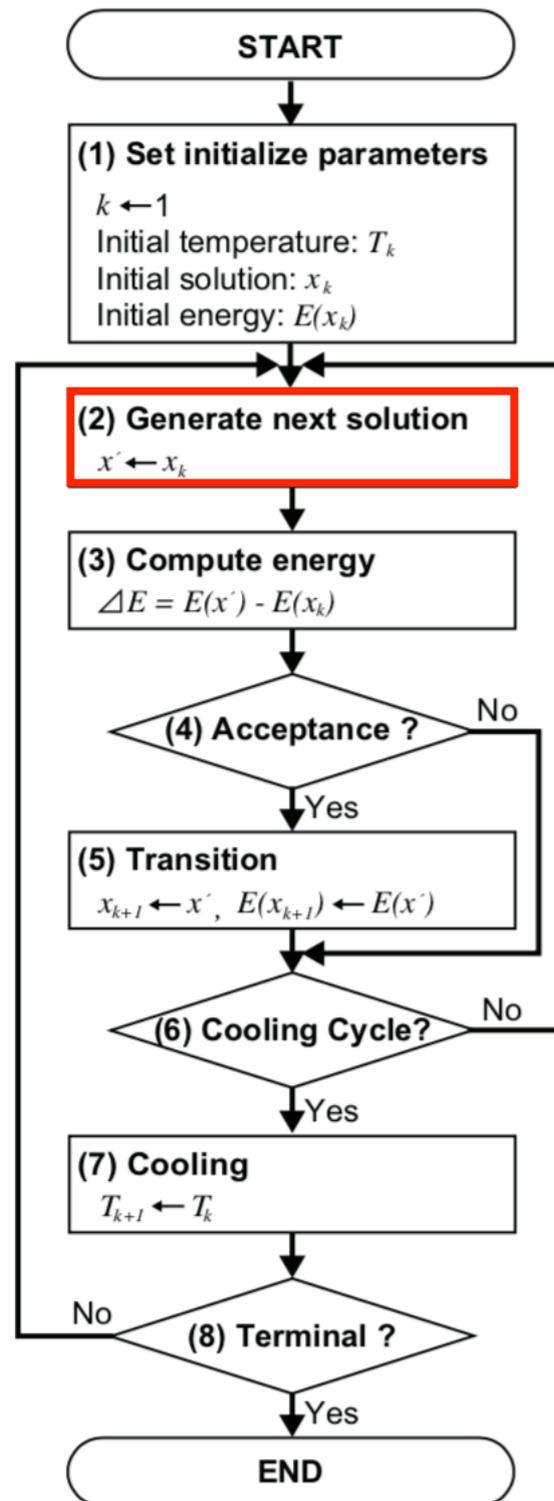
- Generate initial solution $(n, d, g) = (24, 3, 4)$



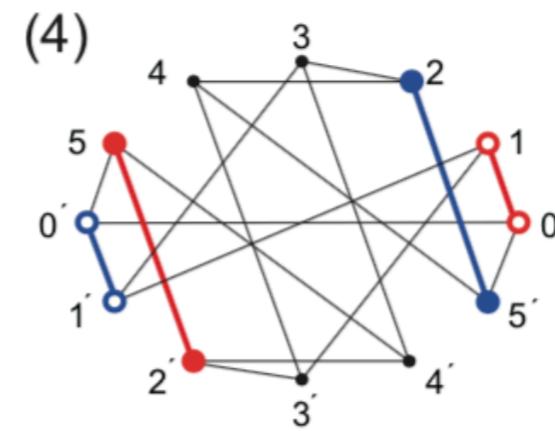
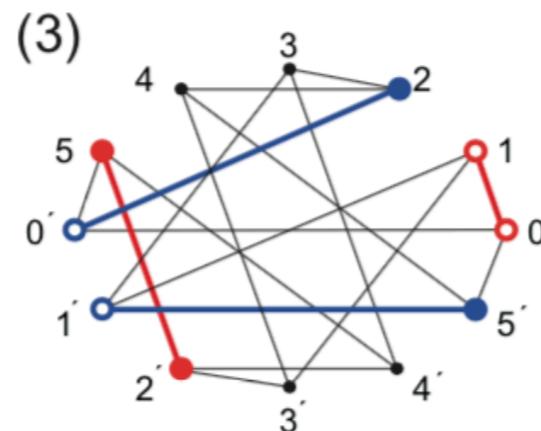
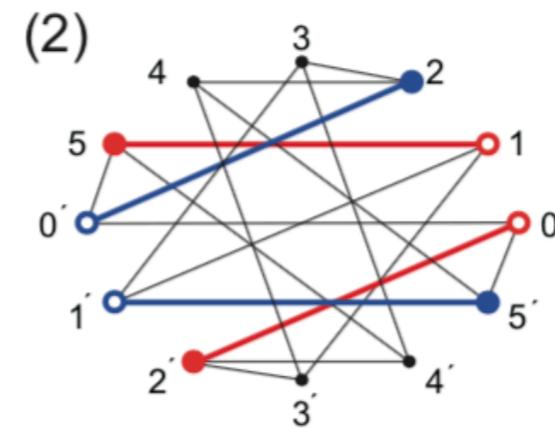
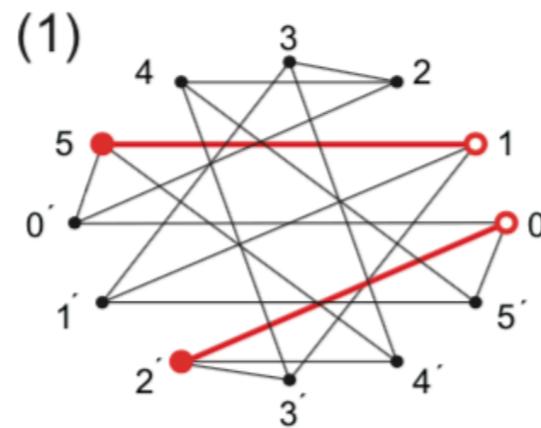
- (1) Create a random graph with the number of vertices of the target graph divided by g , and duplicate g the graphs (the graph with $(n, d) = (6, 3)$ is created $\times 4$). And select one edge from each graph.

- (2) Connect both sides so that it becomes symmetrical

SA with Graph symmetry

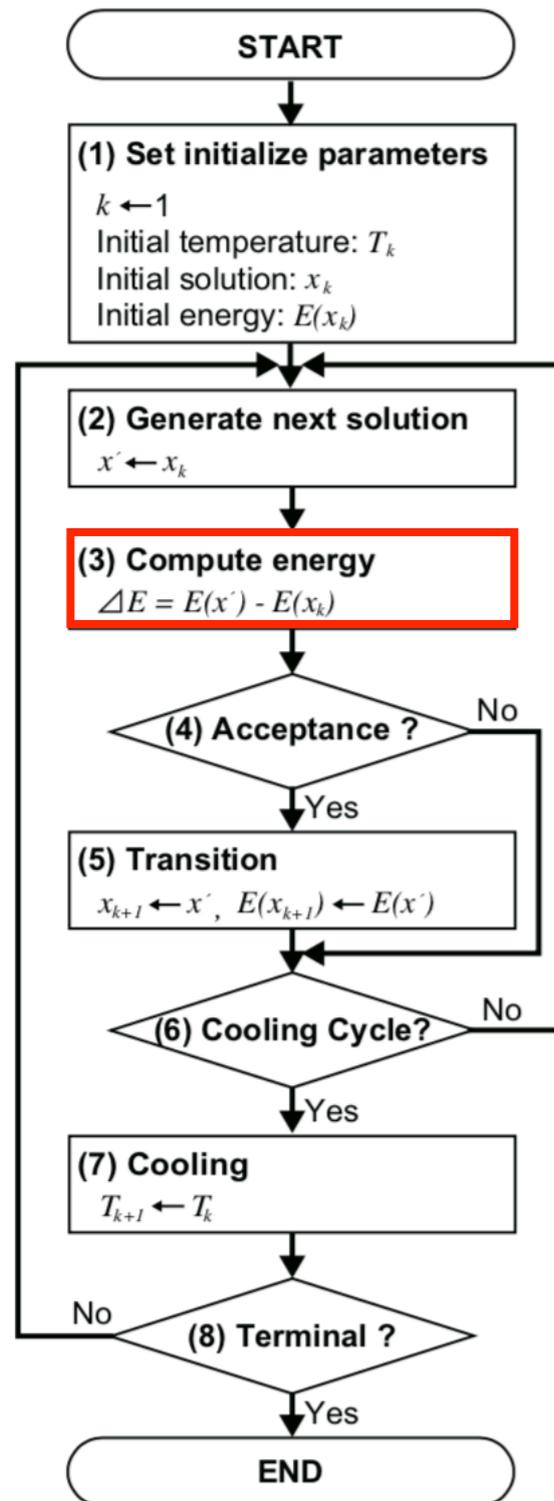


- Generate new solution $(n, d, g) = (24, 3, 2)$

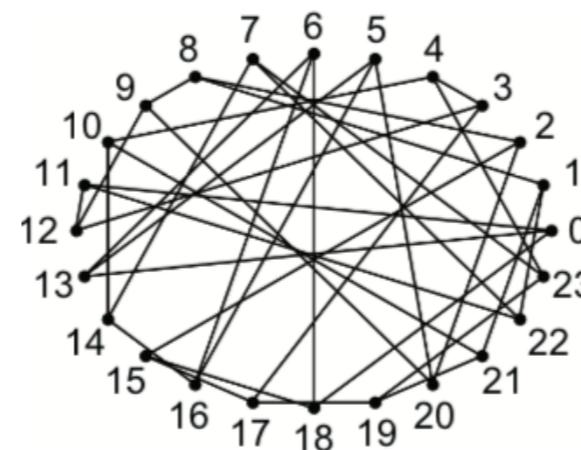


- (1) Randomly select two edges from all the edges
- (2) Select edges symmetrically related to (1)
- (3) Apply the 2-opt method to the edges selected in (1)
- (4) Apply the 2-opt method to (2) in the same way as (3)

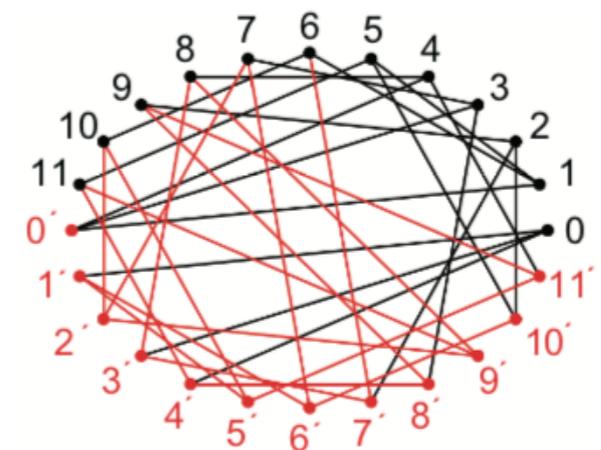
SA with Graph symmetry



- Reduction the calculation time for ASPL
 - In general, it is necessary to calculate the distance from all vertices to all other vertices using BFS
 - However, with graph symmetry, the distances from the vertex to all other vertices are the same for all symmetrically related vertices
 - Thus, the complexity becomes $O(n^2*d/g)$ from $O(n^2*d)$

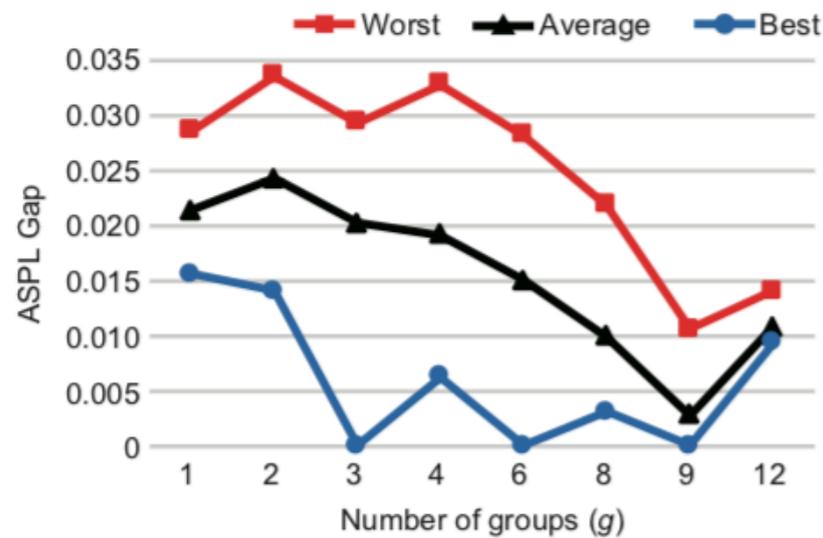


$g=1$

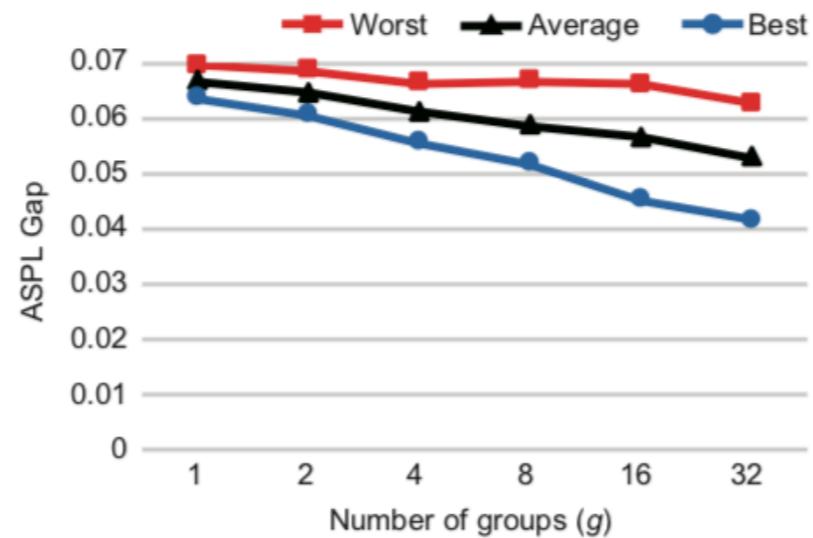


$g=2$

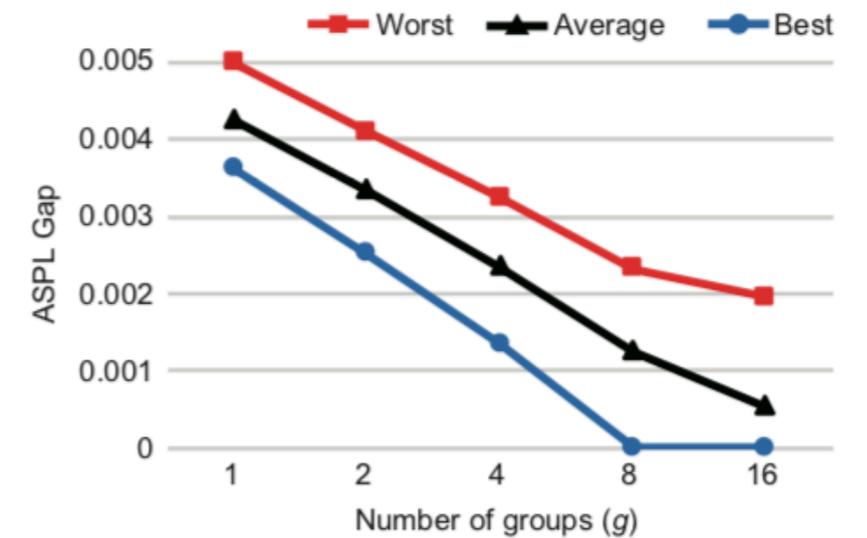
Search Performance



$(n, d) = (72, 5)$



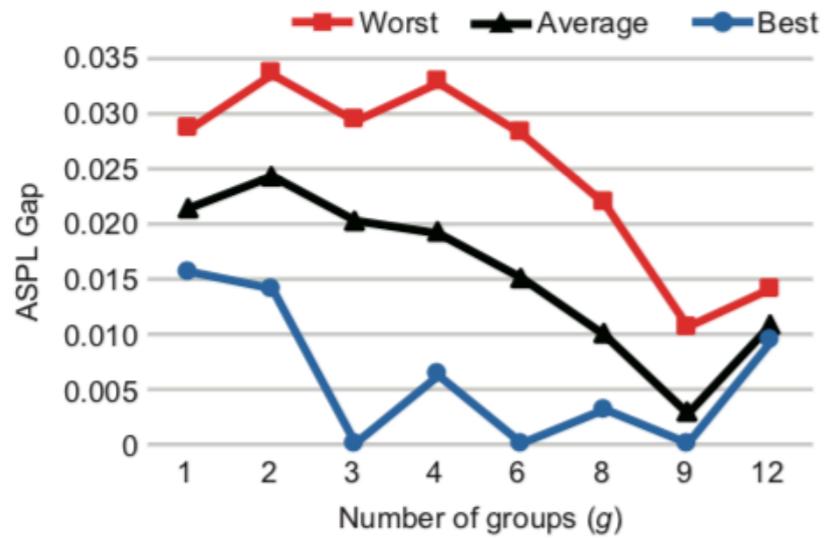
$(n, d) = (256, 5)$



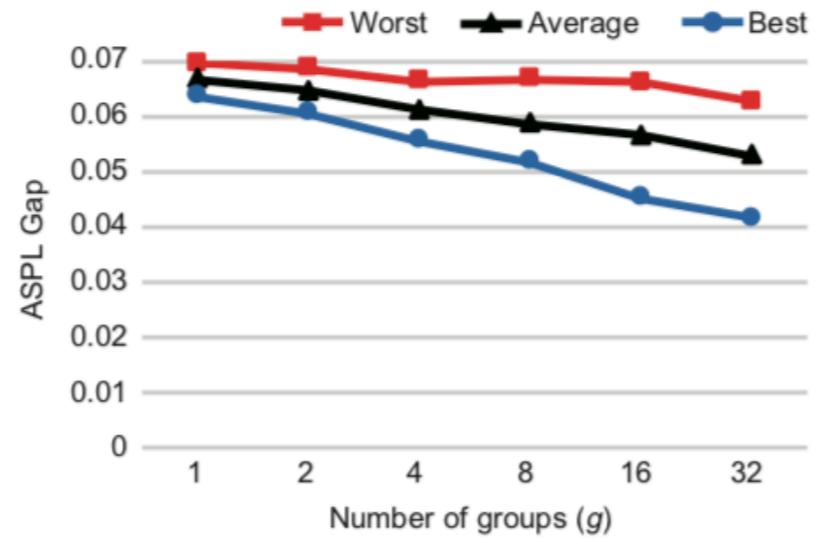
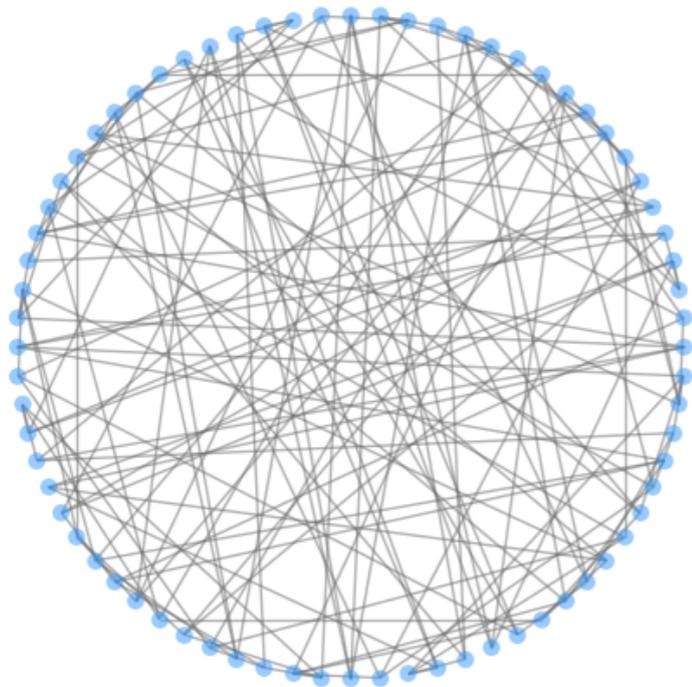
$(n, d) = (256, 10)$

- Proposed method is executed 100 times with different g
- The solution search performance tends to increase as the g increases
- However, the problem $(n, d) = (72, 5)$, the solution search performance is better for $g=9$ than for $g=12$, indicating that solution search performance may deteriorate if the value of g is too large
 - The g expresses the strength of regularity of a graph; regularity becomes stronger as g increases

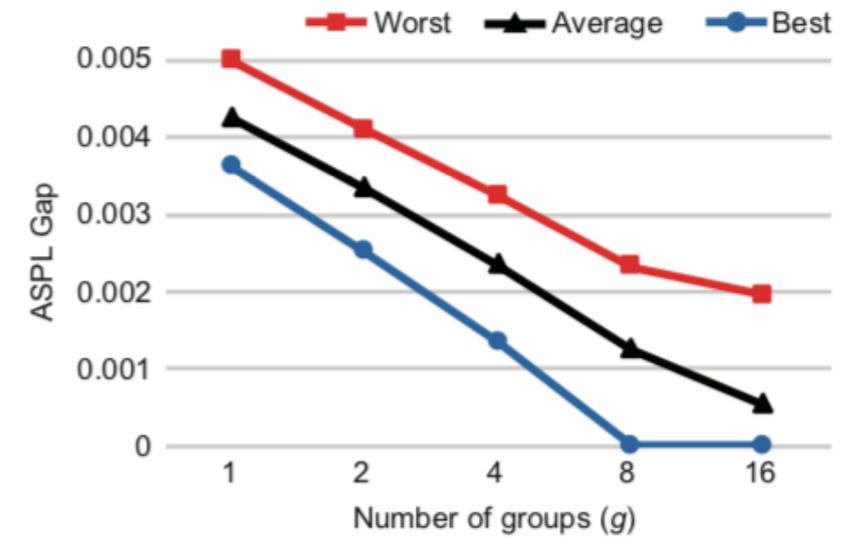
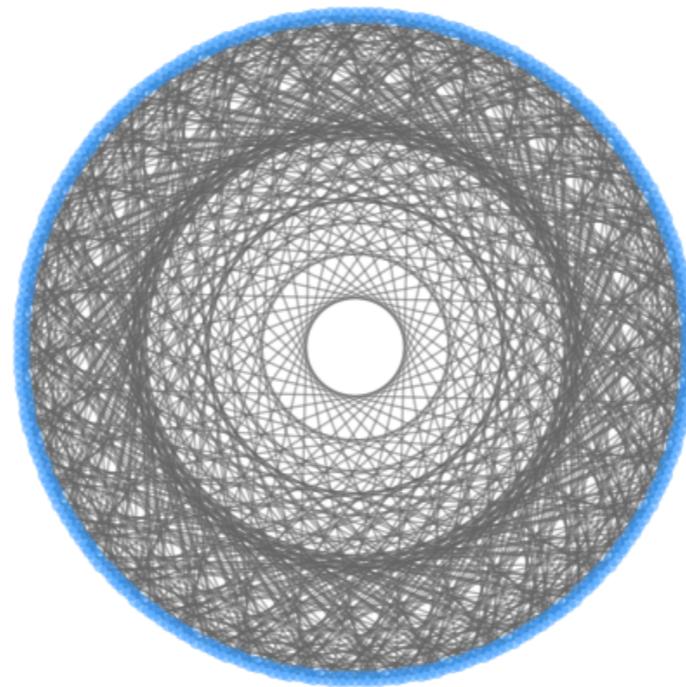
Search Performance



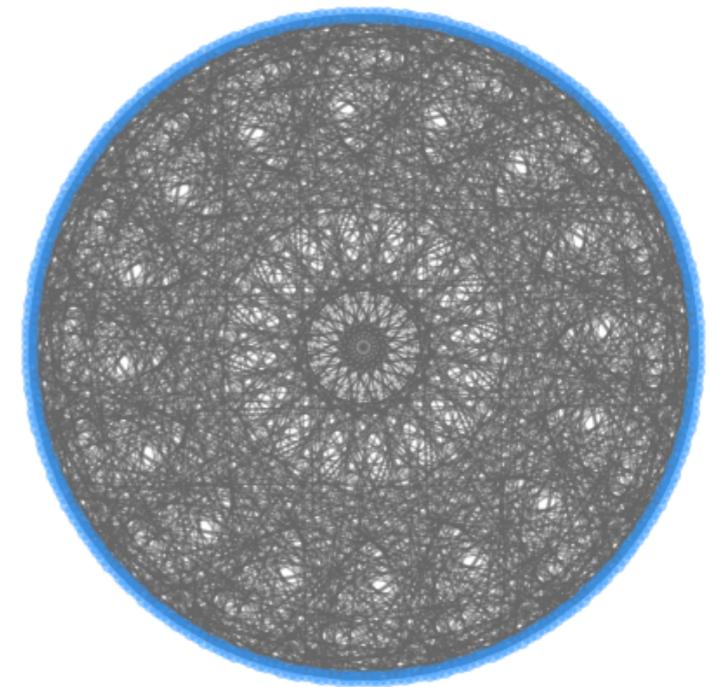
$(n, d) = (72, 5)$



$(n, d) = (256, 5)$

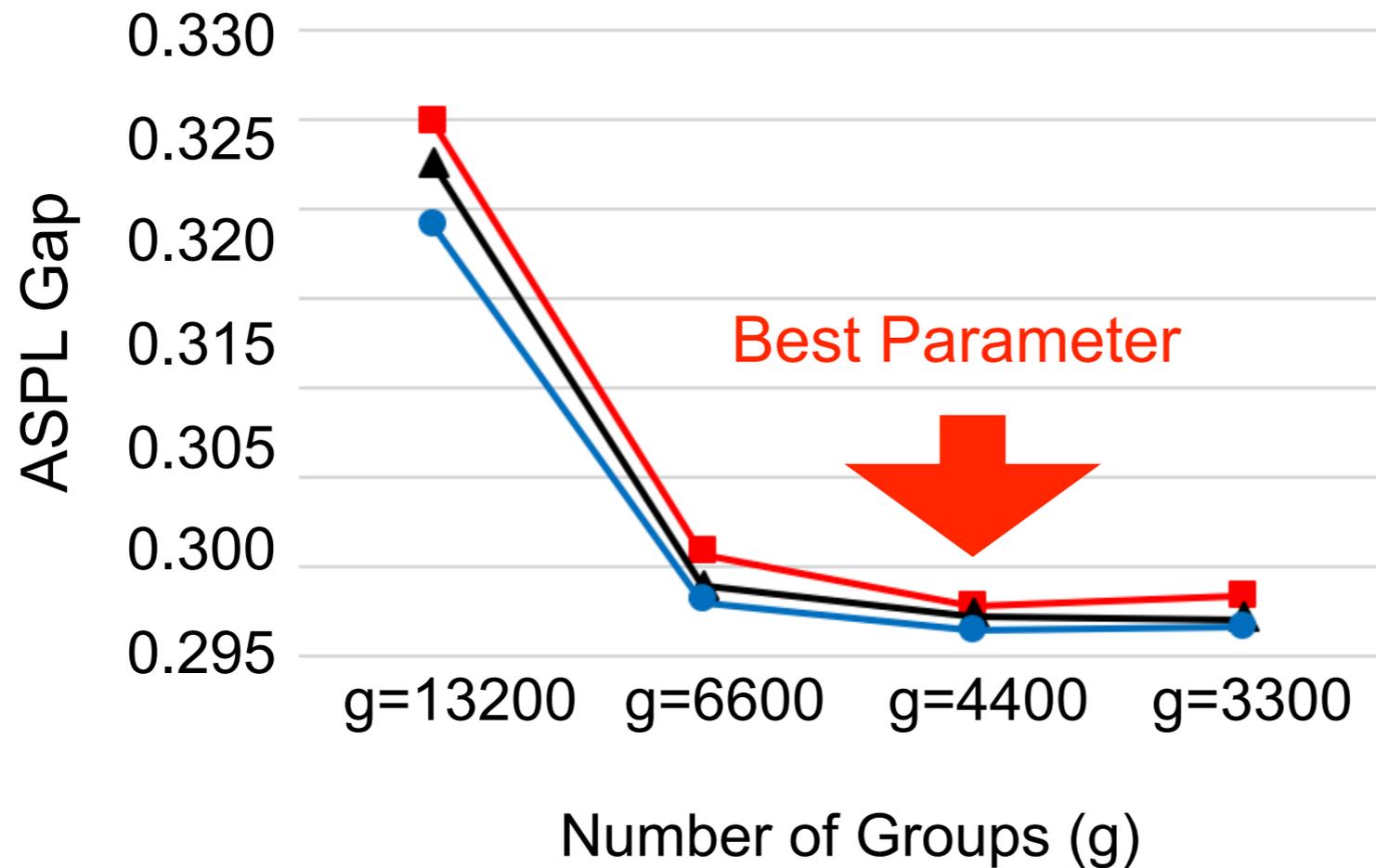


$(n, d) = (256, 10)$



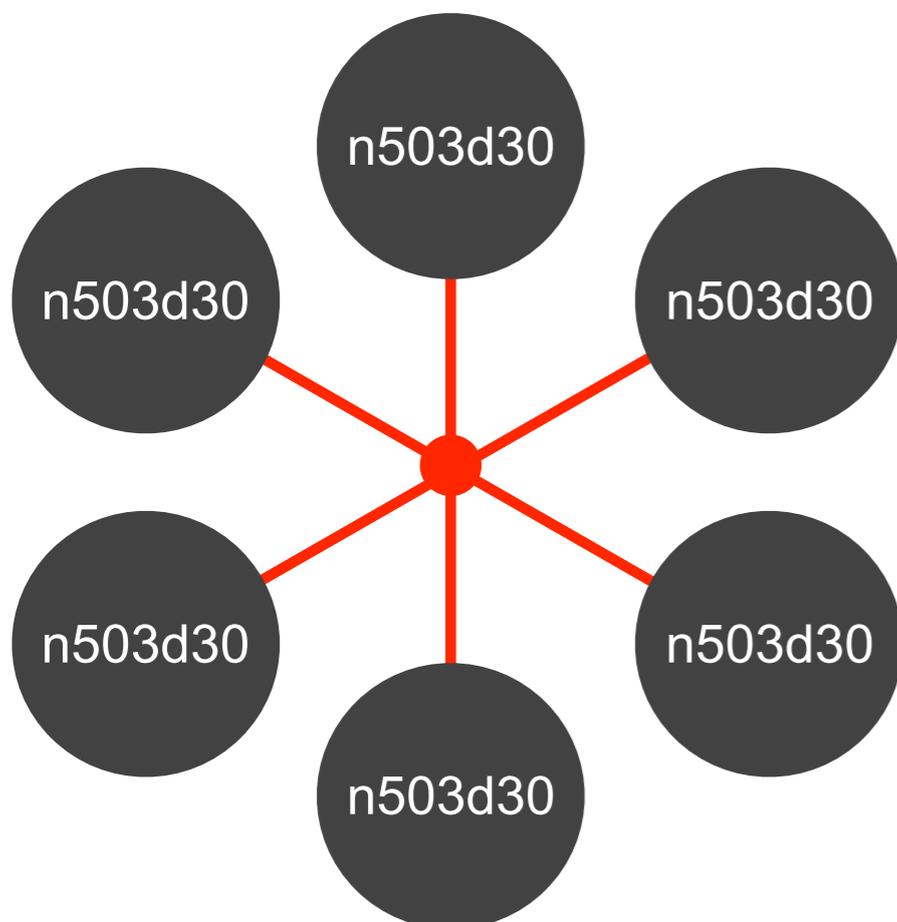
How do I set the value of g ?

- Firstly, set a value of g which is as large as possible
- Next, gradually reduce the value of g
- $(n, d) = (132000, 8)$



When n is a prime number

- In GraphGolf 2018, there is a problem with $(n, d) = (3019, 30)$
- When n is a prime number, g cannot be set in the method explained so far
 - Extend the method to deal with cases where n is a prime number
 - Add **center points** to the graph



$$\underline{n503d30} \times \underline{g6} + \underline{c1} = n3019d30$$

$$\text{groups} = 6 \quad \text{centers} = 1$$

$$(n, d) = (503, 30)$$

$$503 \times 6 + 1 = 3019$$

In addition, the following combinations are possible.

$$n301d30 \times g10 + c9 = n3019d30$$

$$n200d30 \times g15 + c19 = n3019d30$$

$$n100d30 \times g30 + c19 = n3019d30$$

Speed Performance

- COMA cluster system at University of Tsukuba

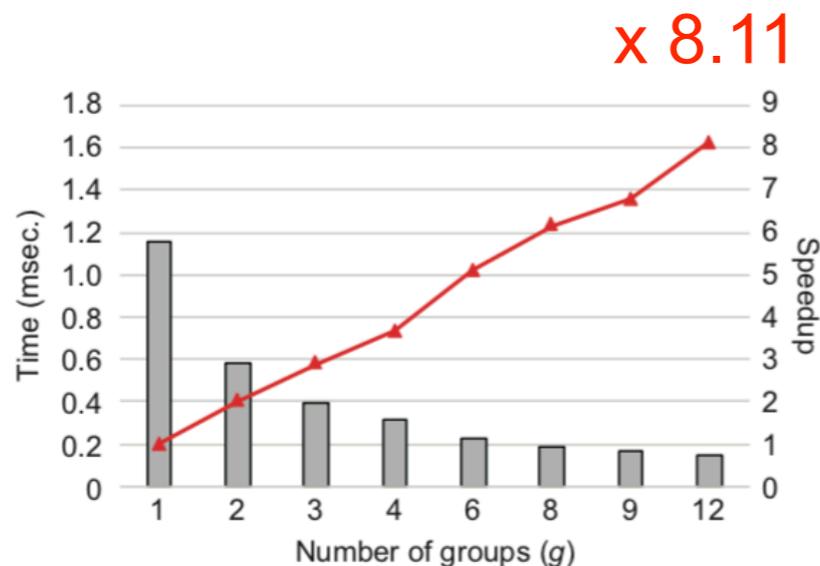
CPU	Intel Xeon-E5 2670v2 2.8 GHz x 2 Sockets
Memory	DDR3 1866MHz 59.7GB/s 64GB
Network	InfiniBand FDR 7GB/s
Software	intel/16.0.2, intelmpi/5.1.1, Omni Compiler 1.2.1 Python 2.7.9, networkx 1.9



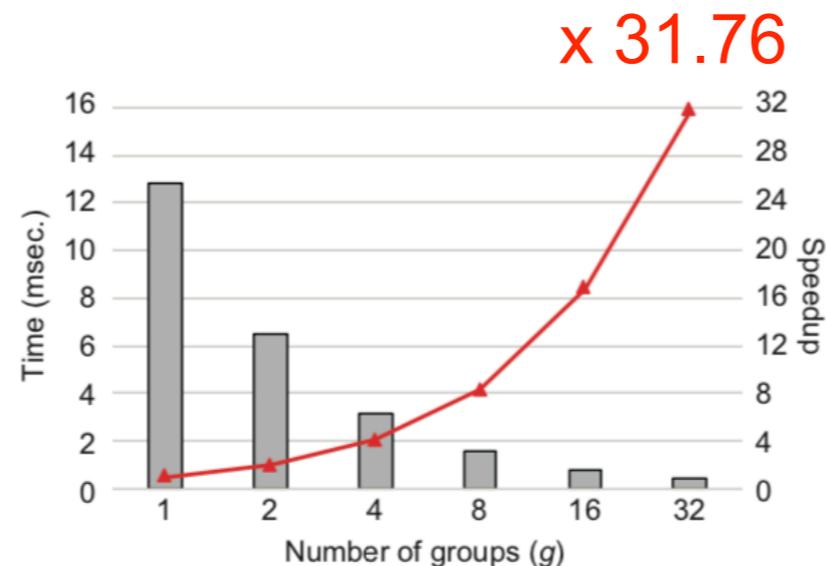
- Speed-up techniques
 - Graph symmetry
 - Hybrid parallelization with MPI and OpenMP
- The COMA system provided by Interdisciplinary Computational Science Program in the Center for Computational Sciences, University of Tsukuba
 - Computing resources such as COMA and Oakforest-PACS can be used **for free**
 - Entries are held every December

Performance results by Graph Symmetry

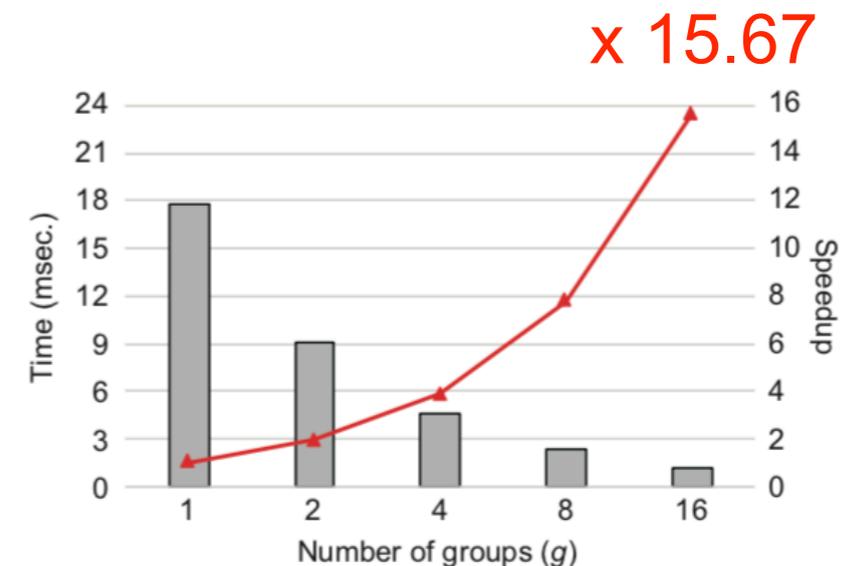
- Measure time to calculate ASPL 100 times



$(n, d) = (72, 5)$



$(n, d) = (256, 5)$



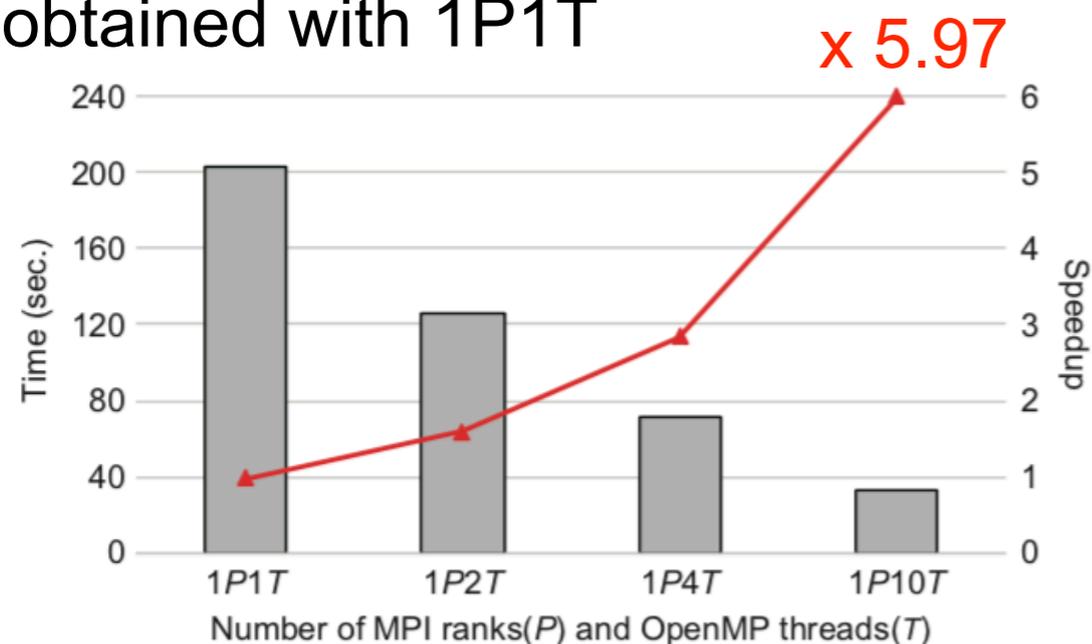
$(n, d) = (256, 10)$

- The bar graph shows the time on the left vertical axis, and the line graph shows the speed up ratio with $g = 1$ on the right vertical axis
- Speed ups of **8.11**, **31.76**, **15.67** times, respectively, were achieved for $(n, d, g) = (72, 4, 12)$, $(256, 5, 32)$, and $(256, 10, 16)$

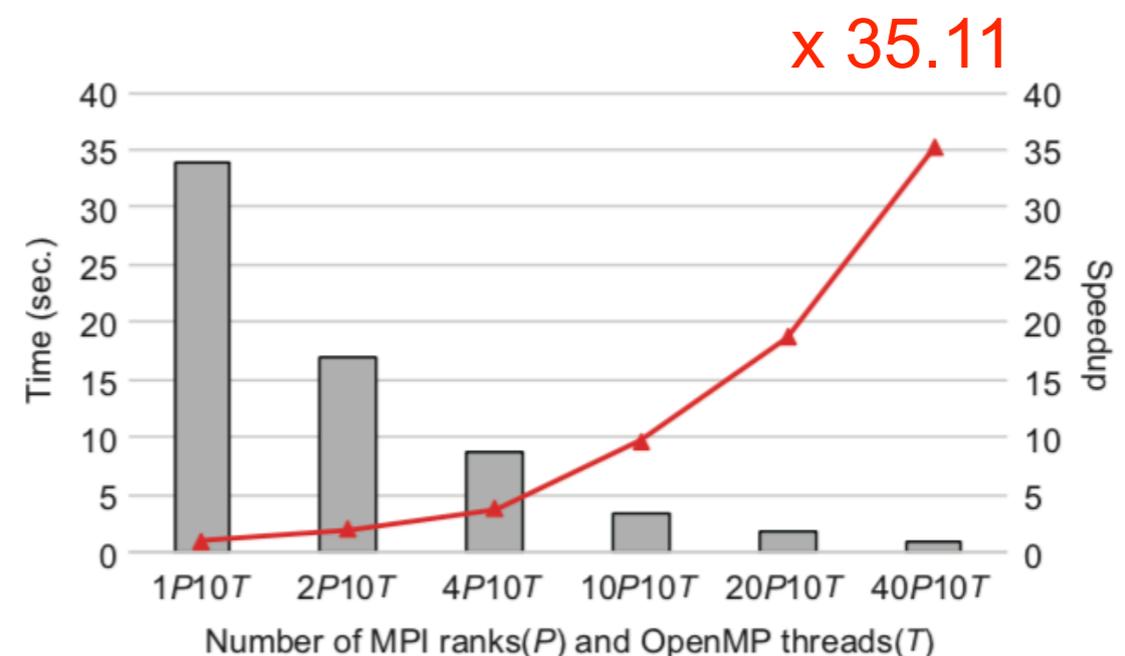
Performance results by Hybrid Parallelization

- Multiple BFS are simultaneously executed using MPI, and each BFS is executed in parallel using several OpenMP threads
- The calculation complexity for the ASPL becomes $O(n^2 \cdot d / (g \cdot P \cdot T))$ from $O(n^2 \cdot d / g)$ when the number of MPI ranks is P and the number of threads is T
- The largest problem $(n, d, g) = (400000, 32, 10000)$ in Graph Golf 2018 is used
- The performance obtained with 40P10T is **209.80** times higher than that

obtained with 1P1T



Thread parallelization with OpenMP



Hybrid parallelization with MPI and OpenMP

Results

 : Awarded

No	Problem (n, d)	Groups	ASPL Gap
1	72, 4	9	0
2	256, 5	32	0.02255
3	256, 10	16	0
4	2300, 10	115	0.03132
5	3019, 30	15	0.00237
6	4855, 30	15	0.00057
7	12000, 7	1000	0.26531
8	20000, 11	1000	0.12263
9	40000, 8	1600	0.12066
10	77000, 6	2200	0.22312
11	132000, 8	4400	0.29266
12	200000, 32	5000	0.01362
13	200000, 64	2500	0.25707
14	400000, 32	10000	0.07890



**Proposed method won
8 problems in 14 problems**

For more information

- Source Code
 - <https://github.com/mnakao/GraphGolf>
- Publication
 - 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, 第167回HPC研究会, 沖縄, 2018年12月
 - A Method for Order/Degree Problem Based on Graph Symmetry and Simulated Annealing with MPI/OpenMP Parallelization, HPC Asia 2019, Guangzhou, China, Jan. 2019

Conclusion

- In the proposed method, the topology is made **symmetrical**, making it possible to efficiently find a good solution
- Making the topology of the graph symmetrical reduced the calculation time required for the ASPL
 - Moreover, by utilizing hybrid parallelization with MPI and OpenMP, the calculation time for the ASPL was further reduced
 - A performance improvement of 209.80 times was achieved for the problem $(n, d, g) = (400000, 32, 10000)$ using only the hybrid parallelization
 - In addition, since graph symmetry was also applied, the performance improvement was about **2,098,000** times compared to that obtained with $g=1$
 - The calculation time of ASPL decreased from 5.5 hours to **0.01 seconds**