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

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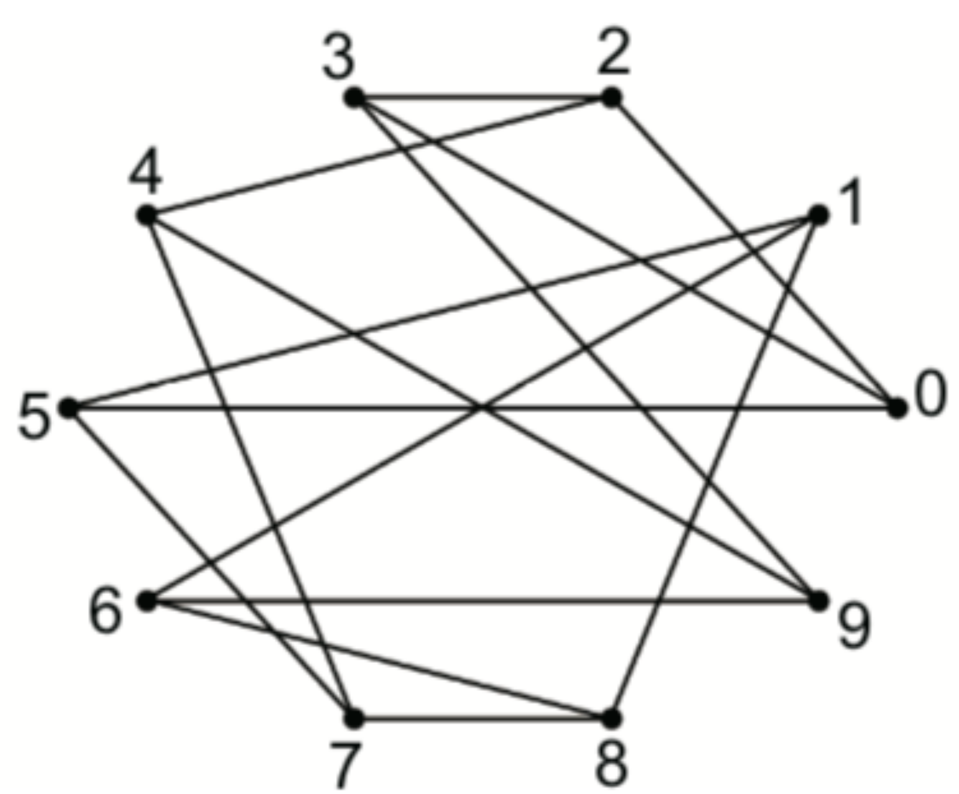
Background (1/3)

- **Order/Degree Problem (ODP) in graph theory**
  - Find a graph with smallest **diameter** and **average shortest path length (ASPL)** given an order (n：頂点数) and a degree (d：次数)
  - Degree is a number of edges connected to one node
  - ASPL is an average of the distances between all nodes
  - Examples of the graph with (n, d) = (10, 3)



	0	1	2	3	4	5	6	7	8	9
0		2	1	1	2	1	3	2	3	2
1	2		3	3	3	1	1	2	1	2
2	1	3		1	1	2	3	2	3	2
3	1	3	1		2	2	2	3	3	1
4	2	3	1	2		2	2	1	2	1
5	1	1	2	2	2		2	1	2	3
6	3	1	3	2	2	2		2	1	1
7	2	2	2	3	1	1	2		1	2
8	3	1	3	3	2	2	1	1		2
9	2	2	2	1	1	3	1	2	2	

distance matrix

Diameter = 3 (maximum value in distances)

ASPL = 85/45 = 1.88...

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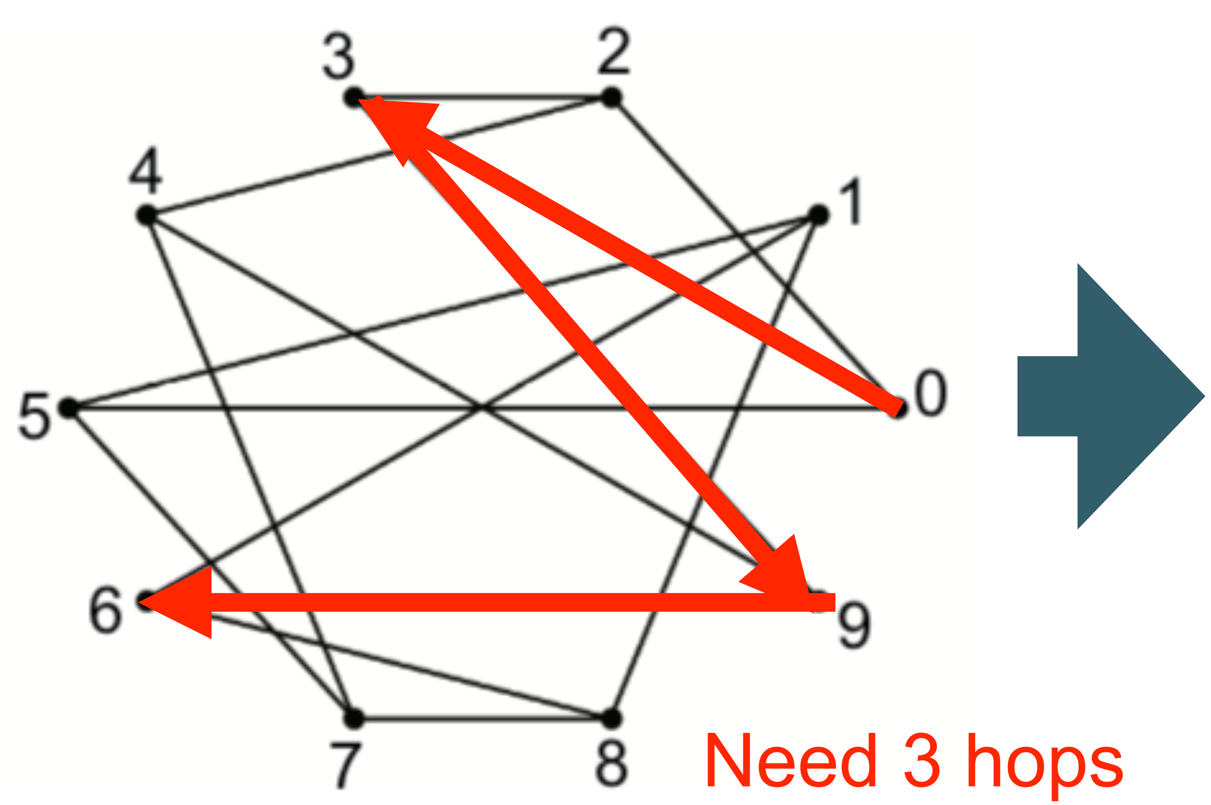

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0		2	1	1	2	1	3	2	3	2
1	2		3	3	3	1	1	2	1	2
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4	2	3	1	2		2	2	1	2	1
5	1	1	2	2	2		2	1	2	3
6	3	1	3	2	2	2		2	1	1
7	2	2	2	3	1	1	2		1	2
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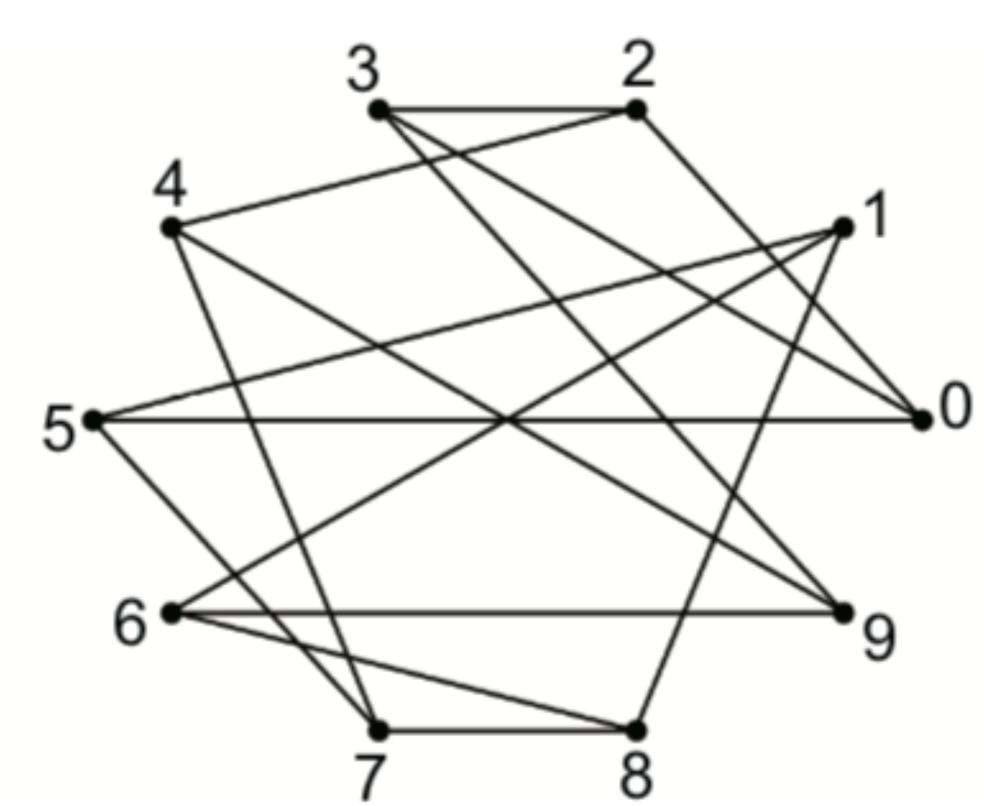

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1	2		3	3	3	1	1	2	1	2
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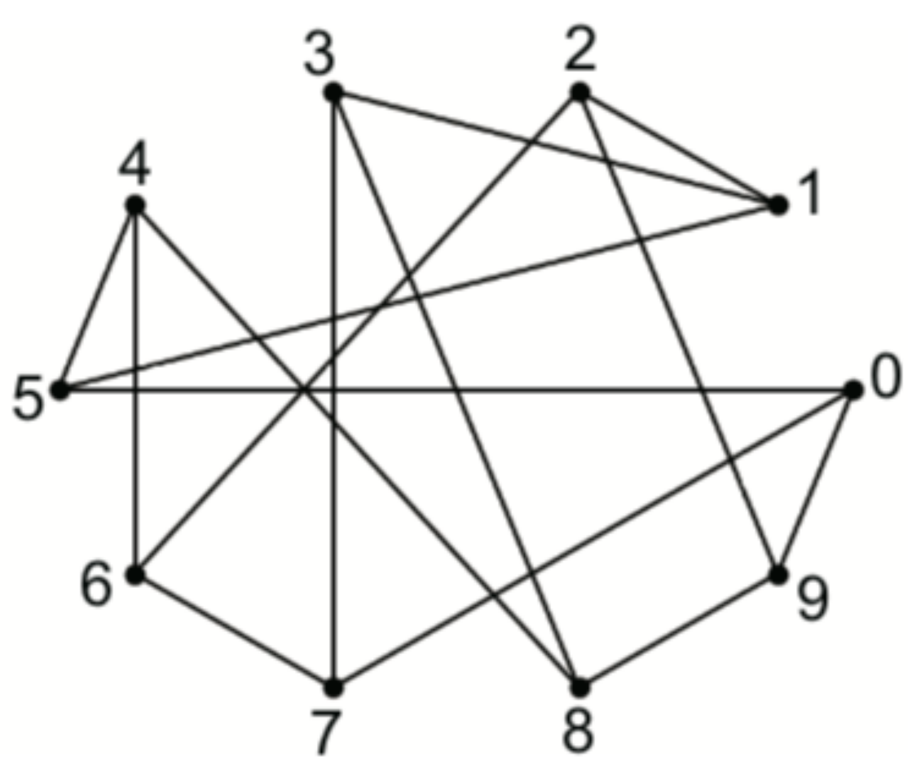

	0	1	2	3	4	5	6	7	8	9
0		2	2	2	2	1	2	1	2	1
1	2		1	1	2	1	2	2	2	2
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4	2	2	2	2		1	1	2	1	2
5	1	1	2	2	1		2	2	2	2
6	2	2	1	2	1	2		1	2	2
7	1	2	2	1	2	2	1		2	2
8	2	2	2	1	1	2	2	2		1
9	1	2	1	2	2	2	2	2	1	

distance matrix

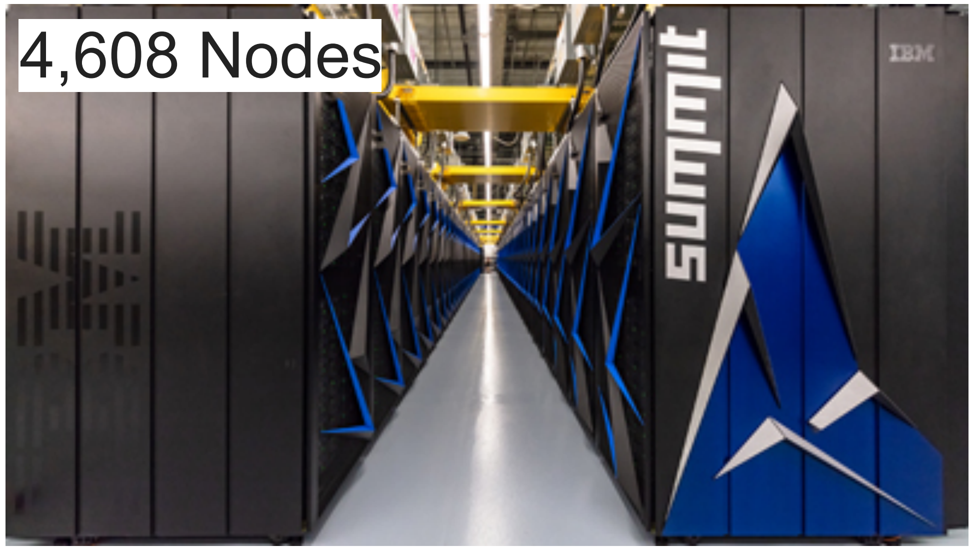
Diameter = **2**
(maximum value in distances)

ASPL = **75**/45
= **1.67**...

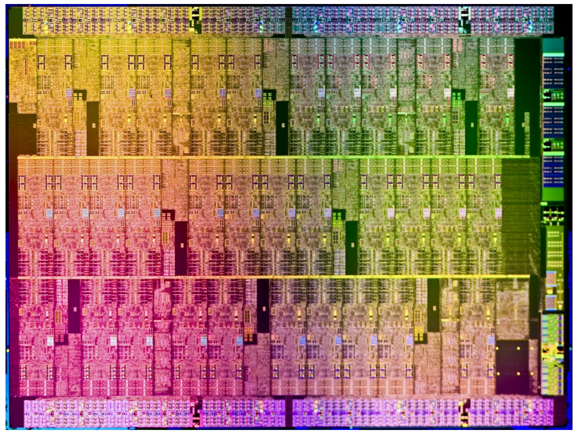
Better !!

Background (2/3)

- ODP is useful for design of network topology with low latency
  - Network topology in HPC systems affects its performance
  - Supercomputers



  - Data centers in Google, Amazon etc.
  - Processor chip (e.g. Knights Landing has 72 cores)
    - Packet network in many core processor



https://www.extremetech.com/extreme/171678-intel-unveils-72-core-x86-knights-landing-cpu-for-exascale-supercomputing

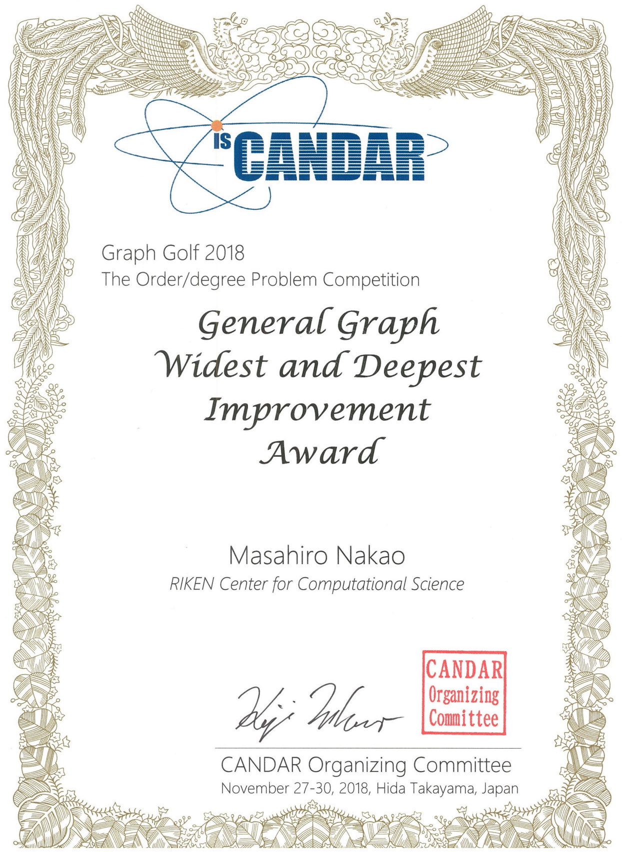
Background (3/3)

- **Graph Golf Competition for ODP**
  - **http://research.nii.ac.jp/graphgolf**
  - Held by National Institute of Informatics, Japan since 2015
  - Rule
    - Find each graph with the smallest **diameter** and **ASPL** in 14 problems in 2018
    - Problems are changed every year
    - Participants uploads their graphs on the official website within a limited period (May 14 to Oct. 14, 2018)

No	Problem (n, d)
1	72, 4
2	256, 5
3	256, 10
4	2300, 10
5	3019, 30
6	4855, 30
7	12000, 7
8	20000, 11
9	40000, 8
10	77000, 6
11	132000, 8
12	200000, 32
13	200000, 64
14	400000, 32

Objective

- Proposes an algorithm for efficiently solving ODP
  - Based on "graph symmetry" and "simulated annealing (SA)"
  - **Evaluate "search performance" and "speed performance"**
  - Won award of Graph Golf 2018



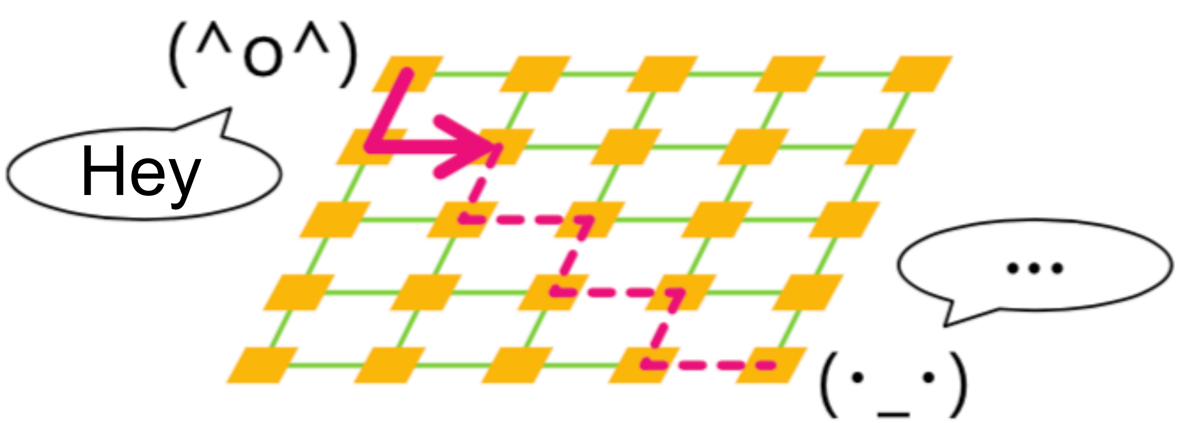
Award ceremony, CANDAR'18, Takayama, Gifu, Japan

Agenda

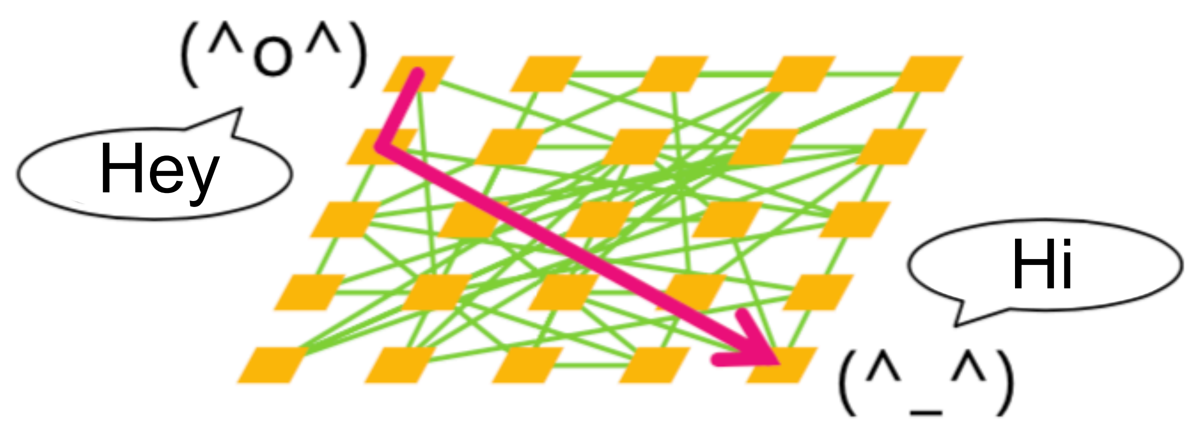
- Background
- Related works
- Explain our algorithm
- Evaluation of search and speed performances
- Summary

Related Works (2/3)

- Randomized topology [Koibuchi2012, Koibuchi2013, Singla2012]
  - When connecting nodes randomly, the distance shrinks due to the **small world effect**, and its latency decreases
    - Extensibility and failure resistance
  - For cases where the cable length becomes long, it can be relaxed by rack placement optimization



Regular Topology
(It takes a long time for the message to arrive)



Randomized Topology
(Shortcut allows a message to arrive soon)

https://www.nii.ac.jp/userimg/openhouse/2015/B11.pdf (Partial modification)

Related Works (3/3)

- Are randomized topologies best ? -> No

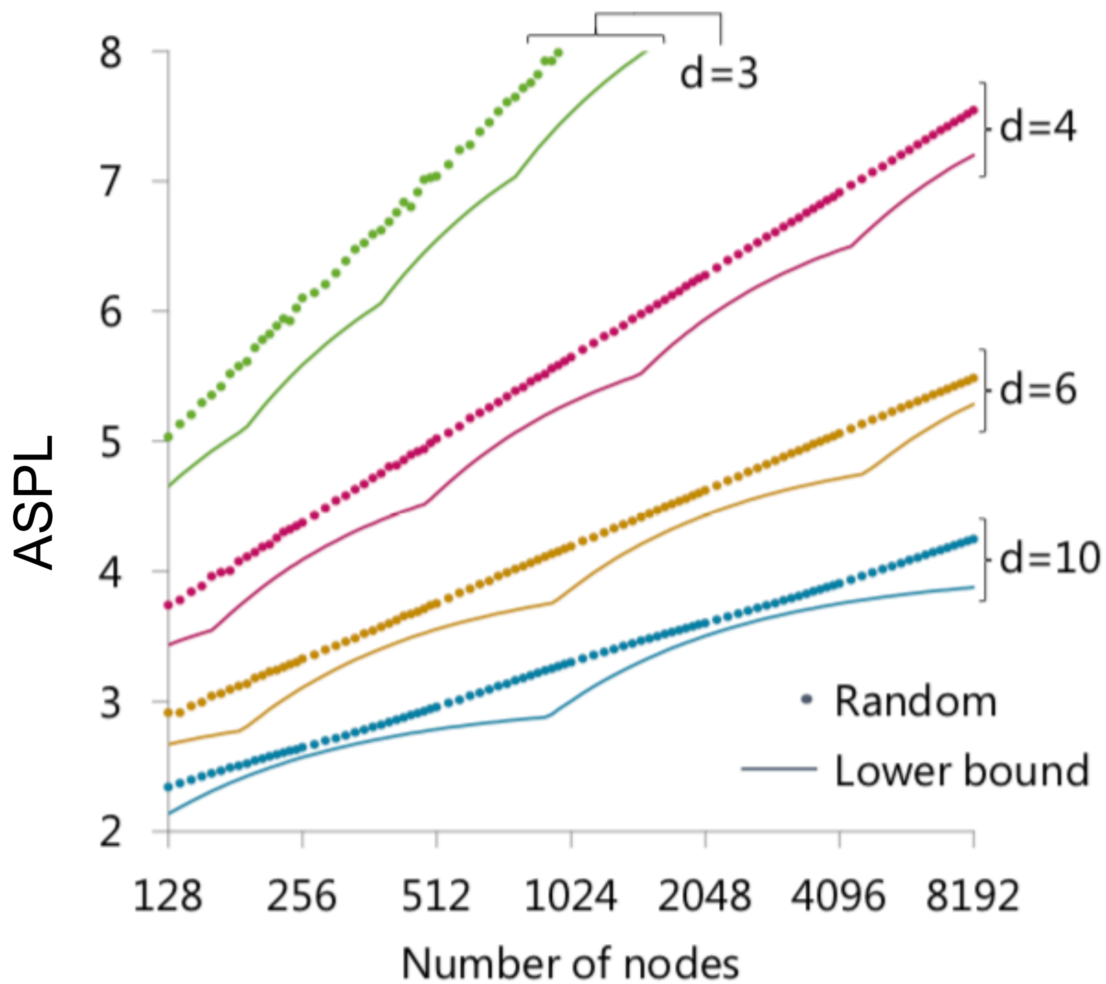
From the numbers of nodes n and degrees d,
the theoretical diameter lower bound K_{n,d}
and the ASPL lower bound L_{n,d} are calculated

$$K_{n,d} = \begin{cases} \left\lceil \frac{n-1}{2} \right\rceil & \text{if } d = 2 \\ \left\lceil \log_{d-1}\left(\frac{(n-1)(d-2)}{d}\right) + 1 \right\rceil & \text{if } d > 2 \end{cases}$$

$$L_{n,d} = \begin{cases} 1 & \text{if } K_{n,d} = 1 \\ \frac{S_{n,d} + K_{n,d} R_{n,d}}{n-1} & \text{if } K_{n,d} \geq 2 \end{cases}$$

$$S_{n,d} = \sum_{i=1}^{K_{n,d}-1} id(d-1)^{i-1}$$

$$R_{n,d} = n - 1 - \sum_{i=1}^{K_{n,d}-1} d(d-1)^{i-1}$$



http://research.nii.ac.jp/graphgolf/2016/candar16/graphgolf2016-fujiwara.pdf

Difference between ASPL and theoretical lower bound is large

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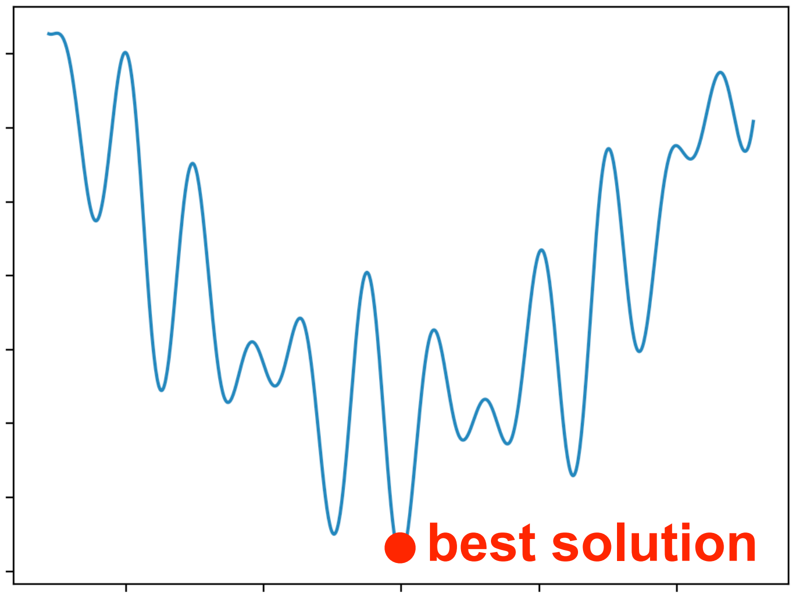
What are difficult points in ODP ?

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

- Number of graphs satisfying (n, d) = (12, 4) is about 480 Billions
- It is difficult to find the **best solution** because the problem has many local optima



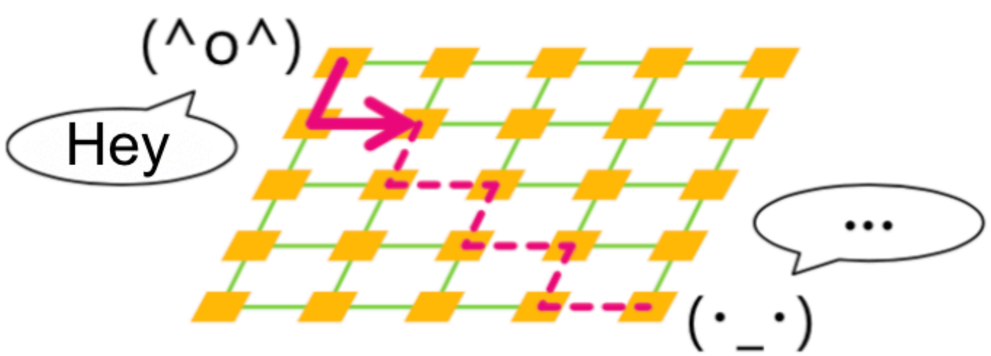
(2) The calculation time required for obtaining ASPL is enormous

- The calculation complexity with n nodes and d degrees is **O(n^2*d)**
- For the graph with (n, d) = (400000, 32), the calculation time required for obtaining ASPL is **about 5.5 hours** on Xeon Ivy Bridge

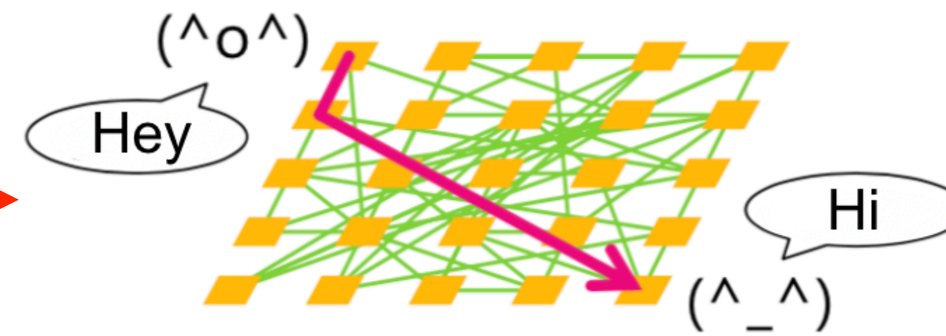
(Diameter can be calculated simultaneously with ASPL)

Origin of idea

- What kind of topology does small diameter and ASPL have ?
  - Randomized topology is better than regular topology for latency
  - But, randomized topology is not best



Regular Topology
(It takes a long time for
the message to arrive)



Randomized Topology
(Shortcut allows a message
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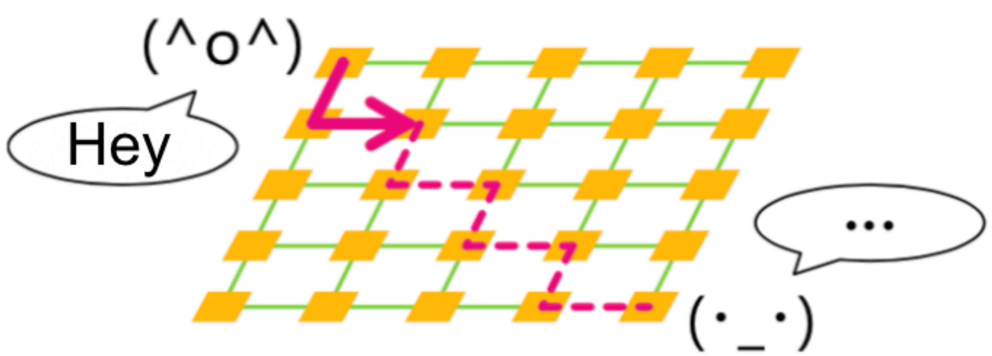

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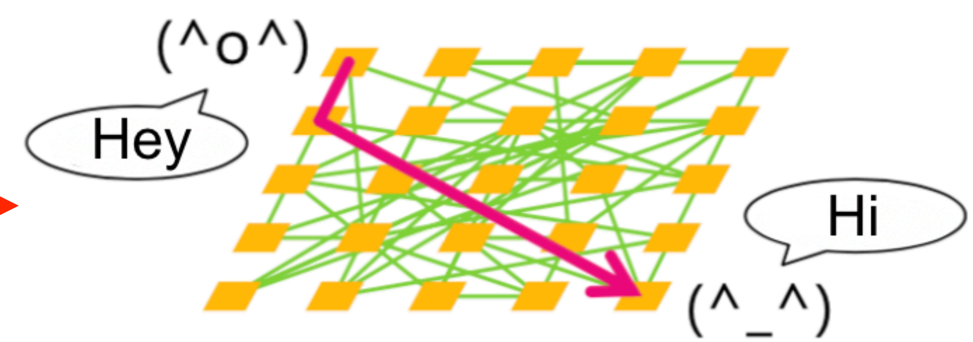


Randomized Topology
(Shortcut allows a message
to arrive soon)

Topology with both regular and randomized properties may be better

Approach

(1) Make the network topology **symmetrical**

- SA's search performance may be improved due to reduce search space
- The reason for using SA is that it doesn't easily fall into local optima

(2) Reducing the calculation time of ASPL

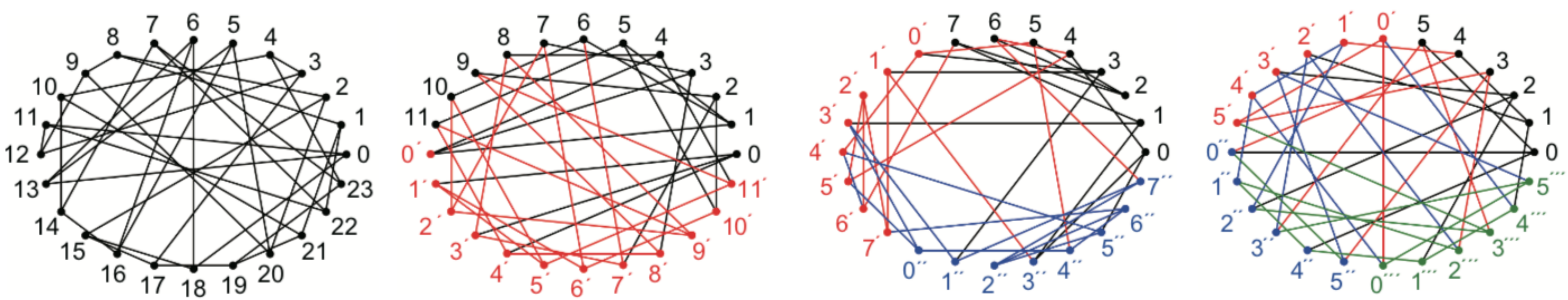
- Reduce calculation time of ASPL by the network topology symmetrical (**Up to 10,000 times**)
- Hybrid parallelization with MPI and OpenMP on our cluster system (**Up to 200 times** on 400 CPU cores)
- Calculation time of ASPL decreased from 5.5 hours to 0.01 sec.

about 2,000,000 times faster (= 10,000 x 200)

Our source code is available at
https://github.com/mnakao/GraphGolf

Graph symmetry

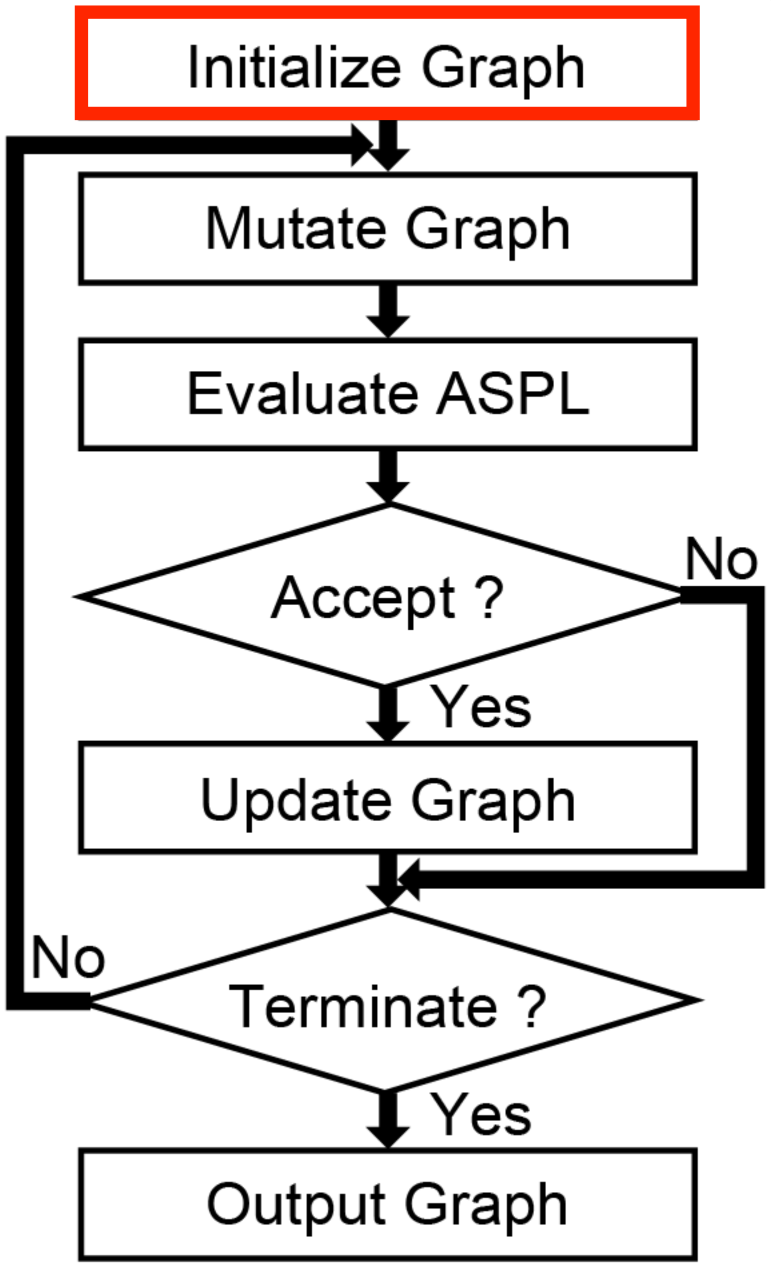
- Examples of the graph symmetry with (n, d) = (24, 3)



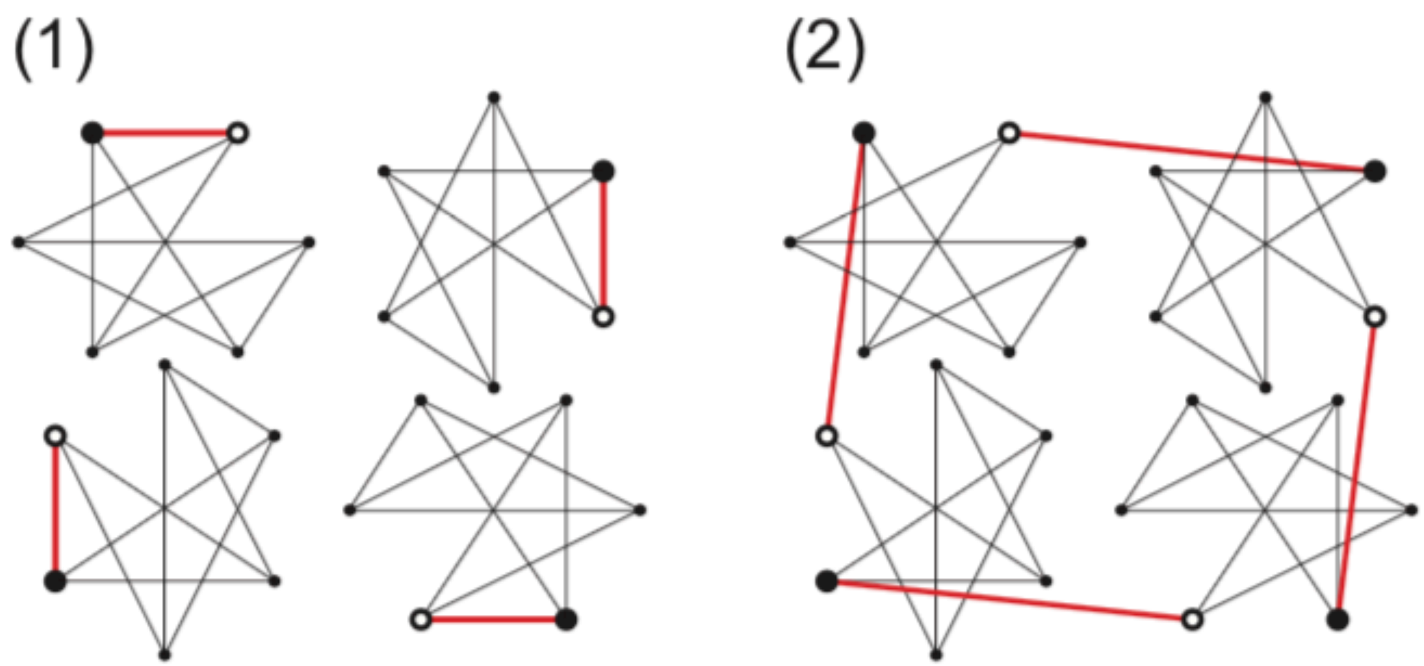
g=1 **g=2** **g=3** **g=4**

- 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 node becomes the same graph
- For the case of **g = 1**, a normal graph (not symmetrical) is obtained

SA with Graph symmetry



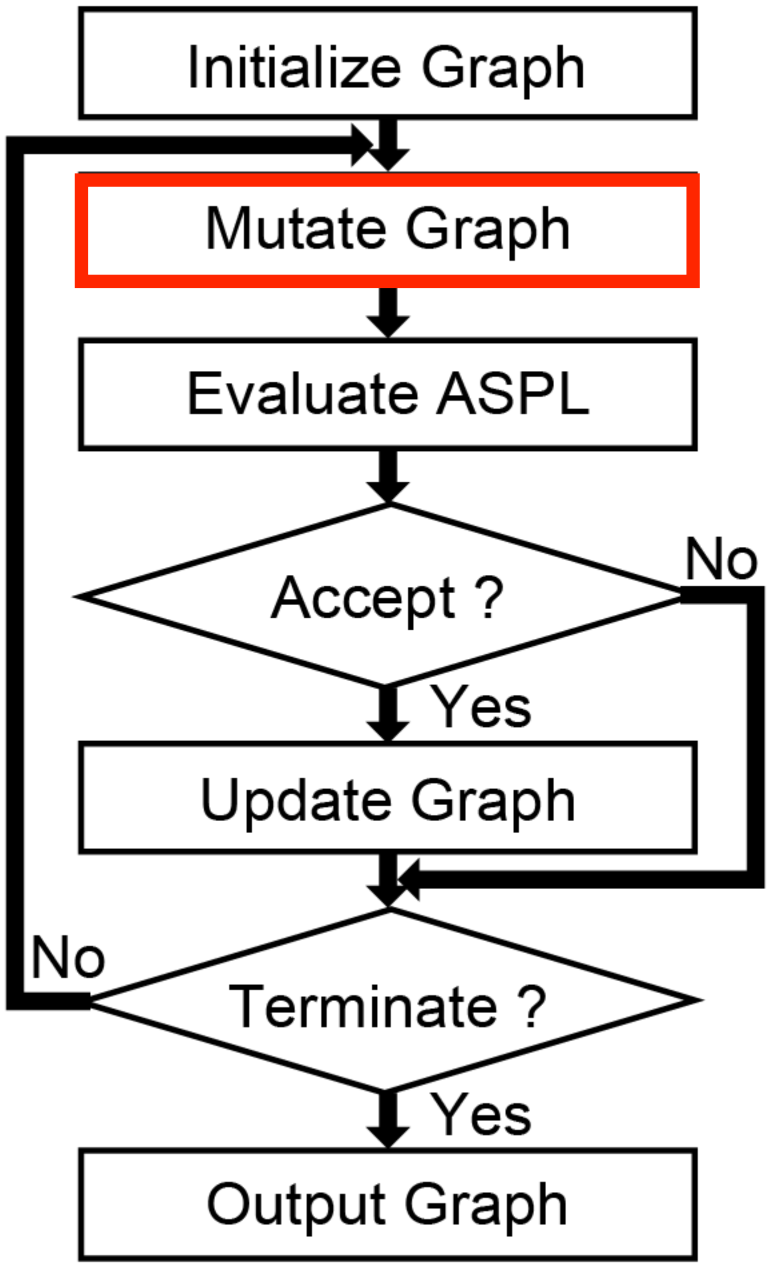
- Initialize a solution (n, d, g) = (24, 3, 4)



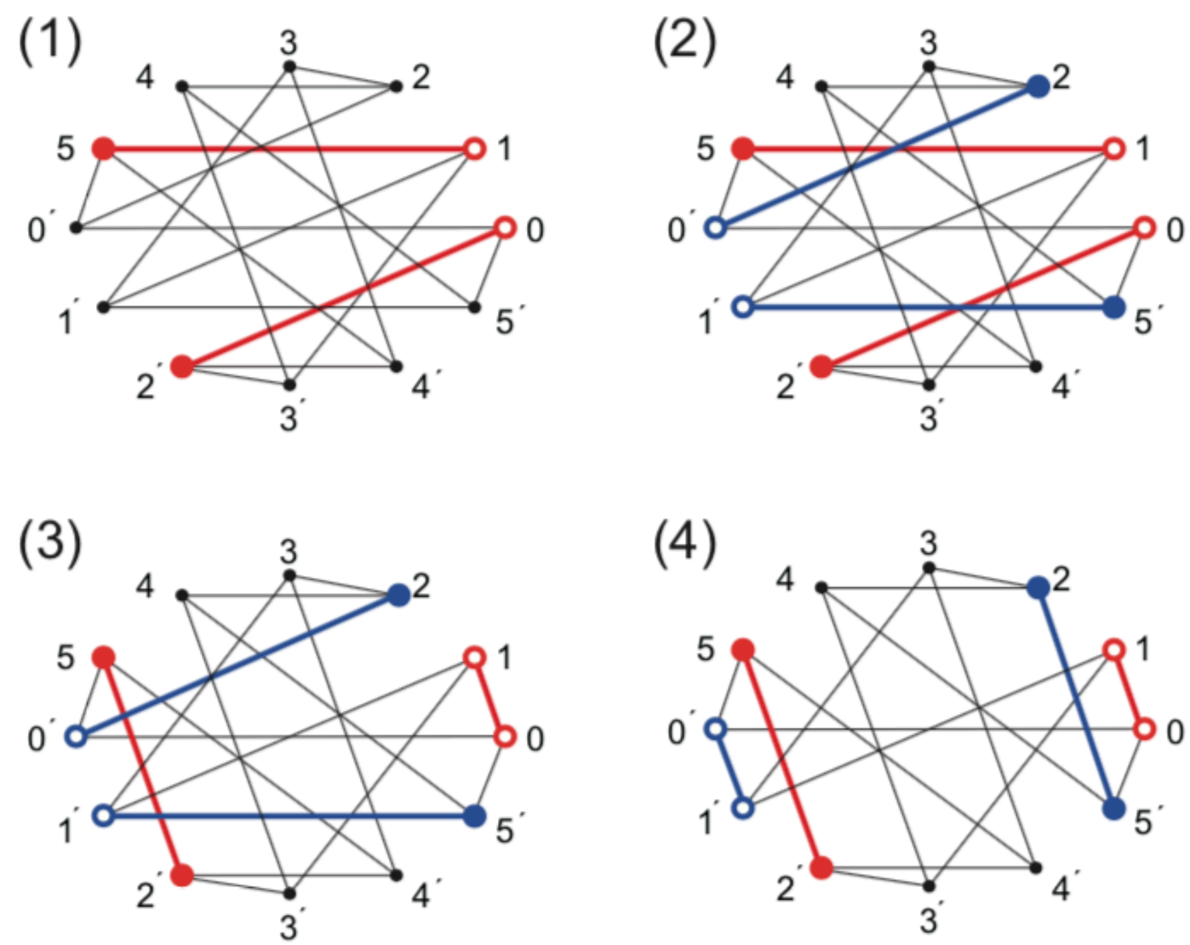
(1) Create a random graph with the number of nodes of the target graph divided by g, and duplicate g the graphs (the graph with (n, d) = (6, 3) is created x 4). And select one edge from each graph.

(2) Connect both sides so that it becomes symmetrical

SA with Graph symmetry

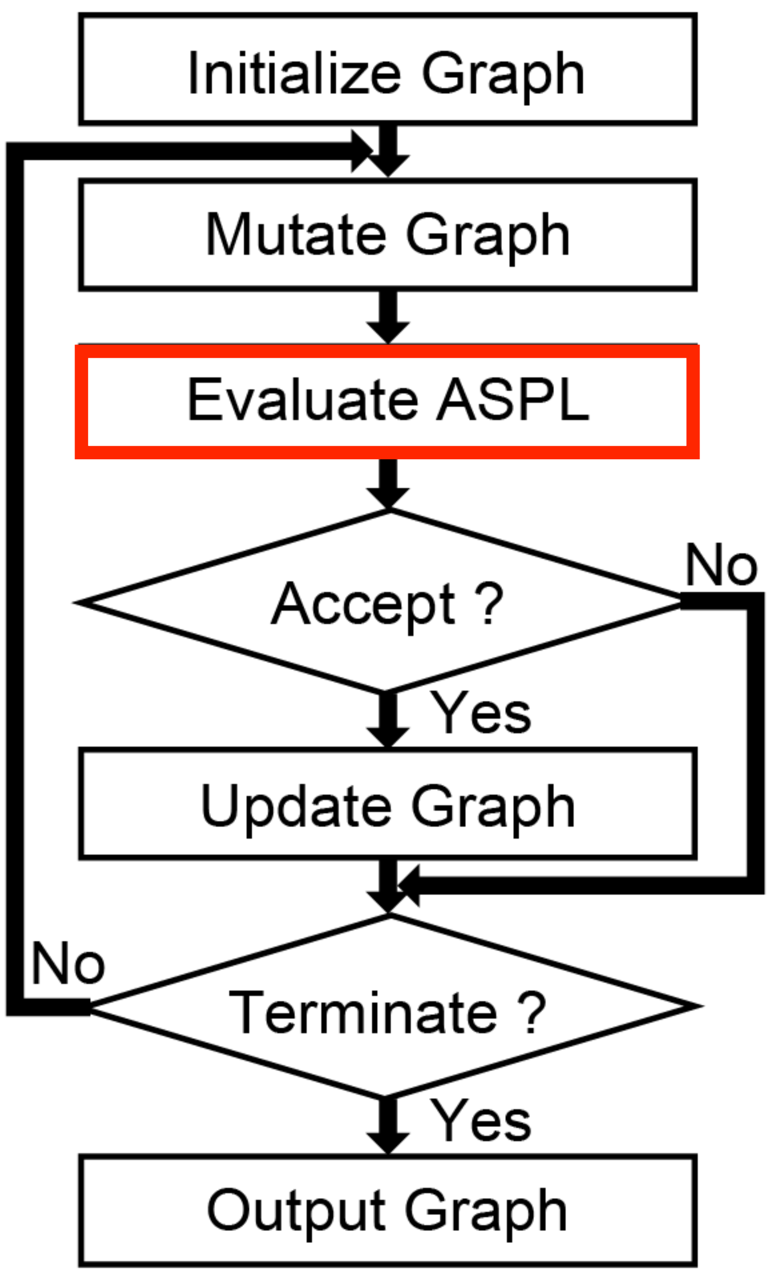


- Mutate a new solution (n, d, g) = (24, 3, 2)

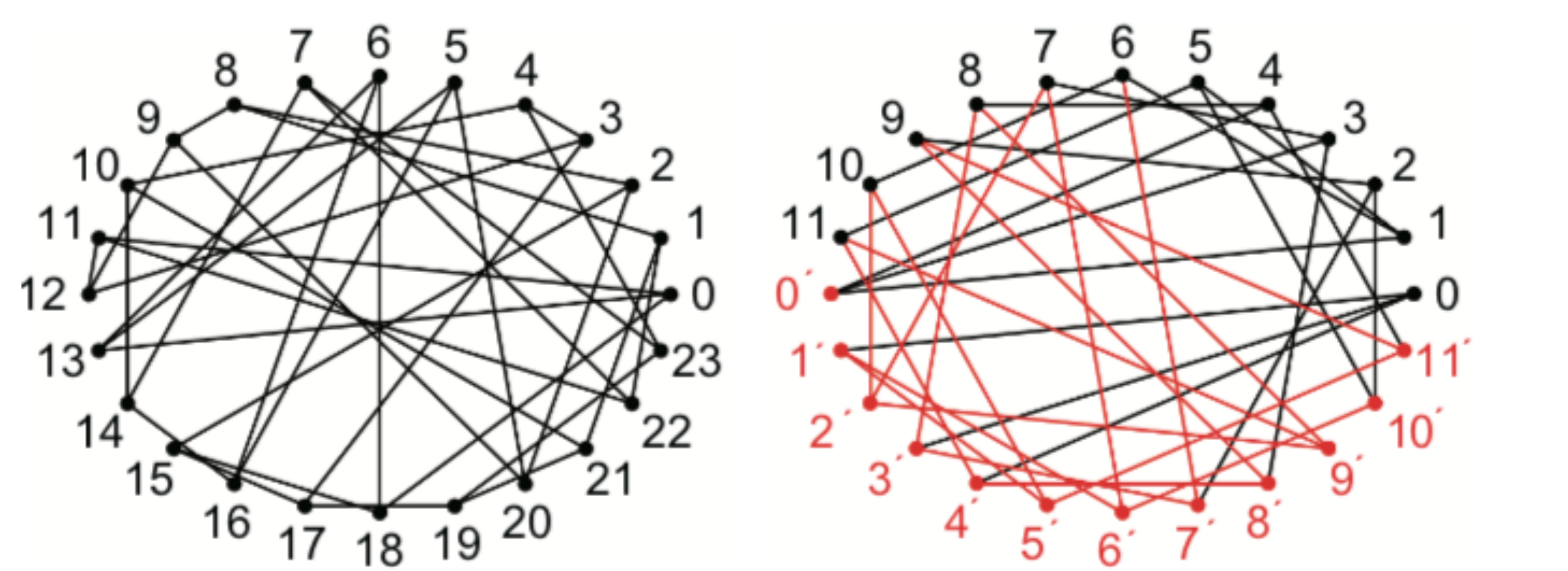


(1) Randomly select two edges from all the edges
(2) Select edges symmetrically related to (1)
(3) Apply the 2-opt method to the edges selected in (1)
(4) Apply the 2-opt method to (2) in the same way as (3)

SA with Graph symmetry



- Reduce the calculation time for ASPL
  - In general, it calculates the distance from all nodes to all other nodes using BFS
  - However, with graph symmetry, the distances from the node to all other nodes are the same for all symmetrically related nodes
  - Thus, the complexity becomes **O(n^2*d/g)** from O(n^2*d)



g=1 **g=2**

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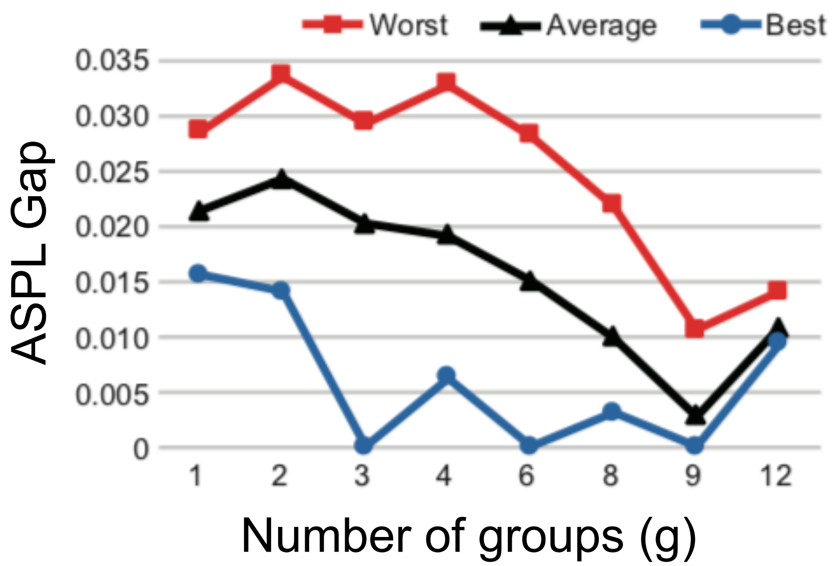
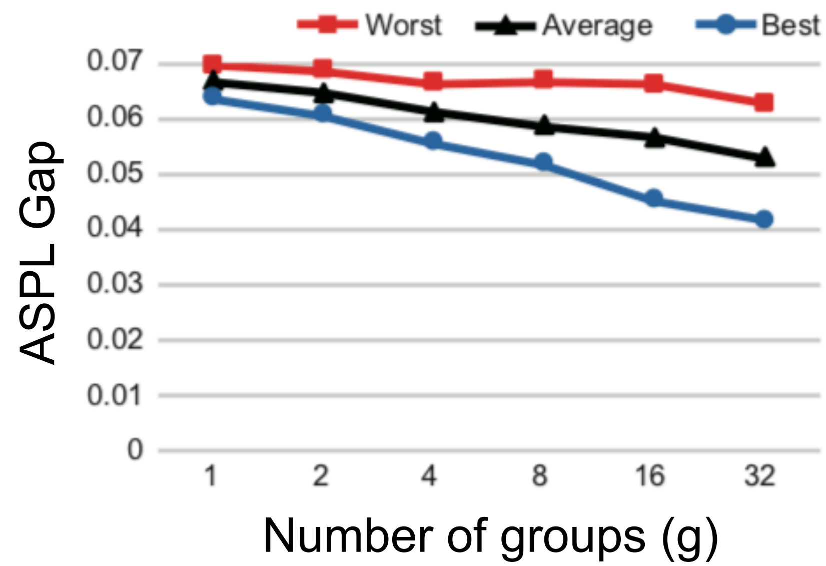
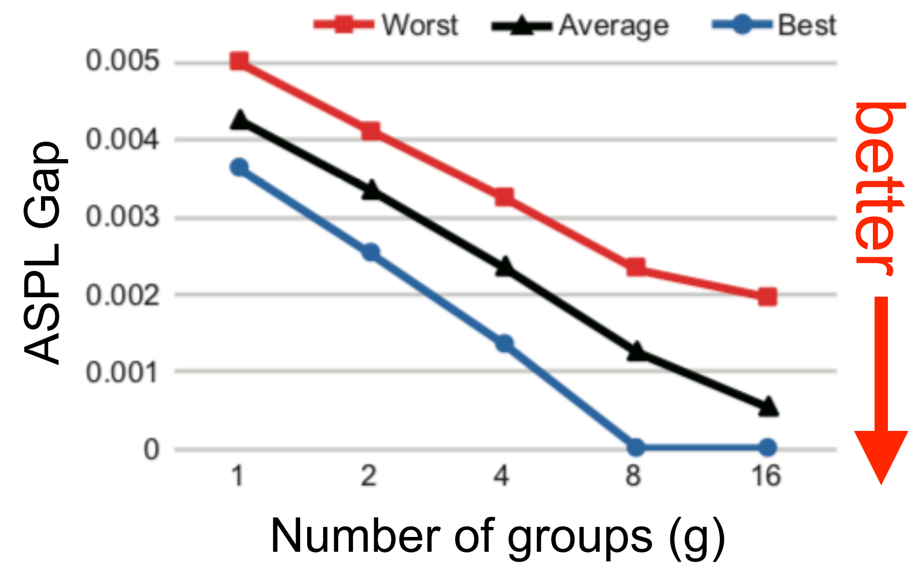
Search Performance



(n, d) = (72, 5)



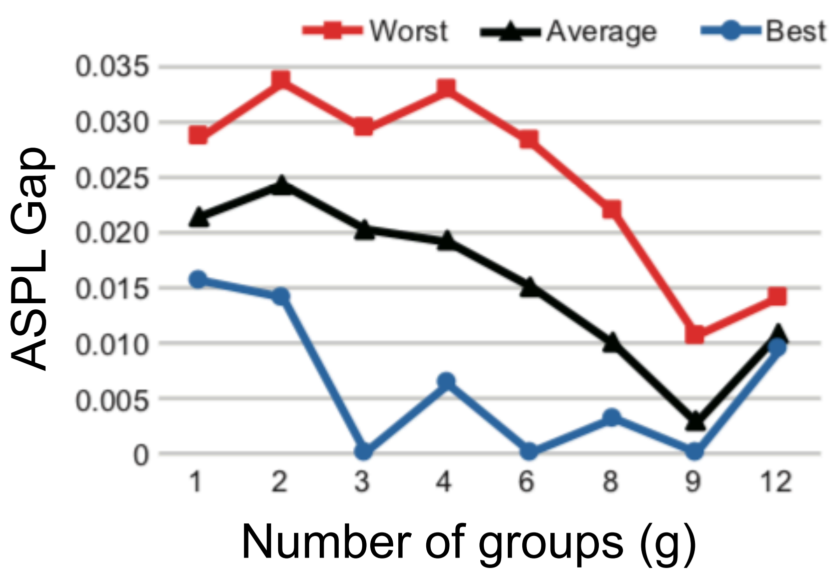
(n, d) = (256, 5)



(n, d) = (256, 10)

- In vertical axis, **ASPL Gap** is a difference from theoretical lower bound
- Proposed method is executed 100 times with different g
- Search performance tends to increase as the g increases
- However, the problem (n, d) = (72, 5), the search performance is better for g=9 than for g=12, indicating that the solution 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



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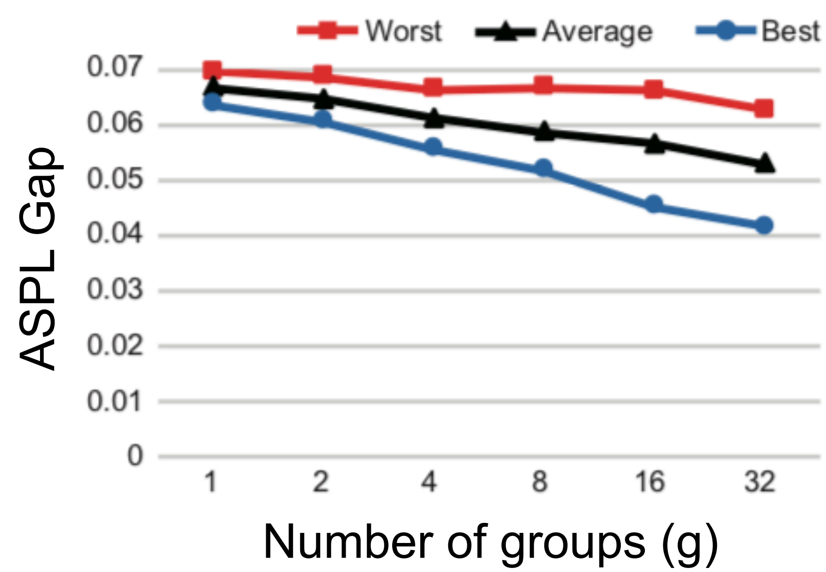

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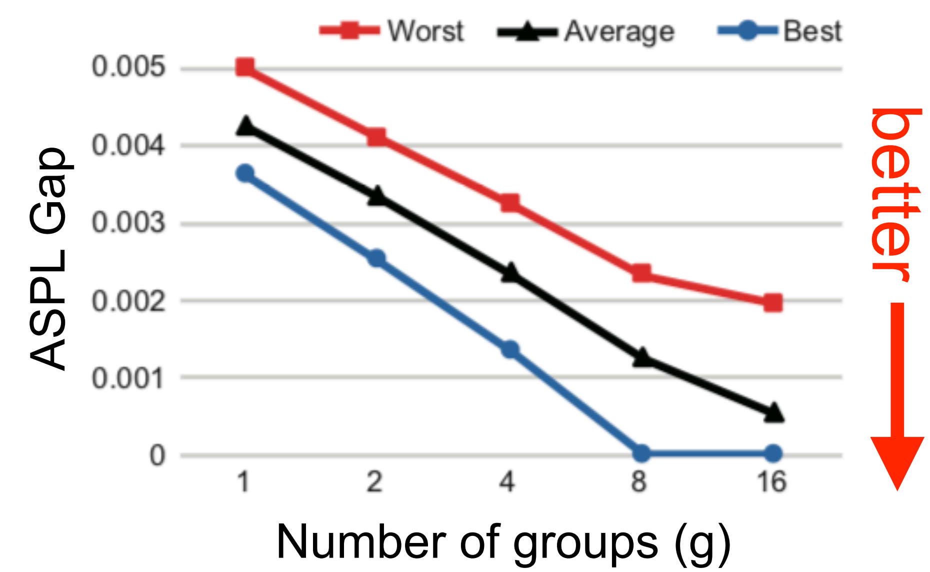
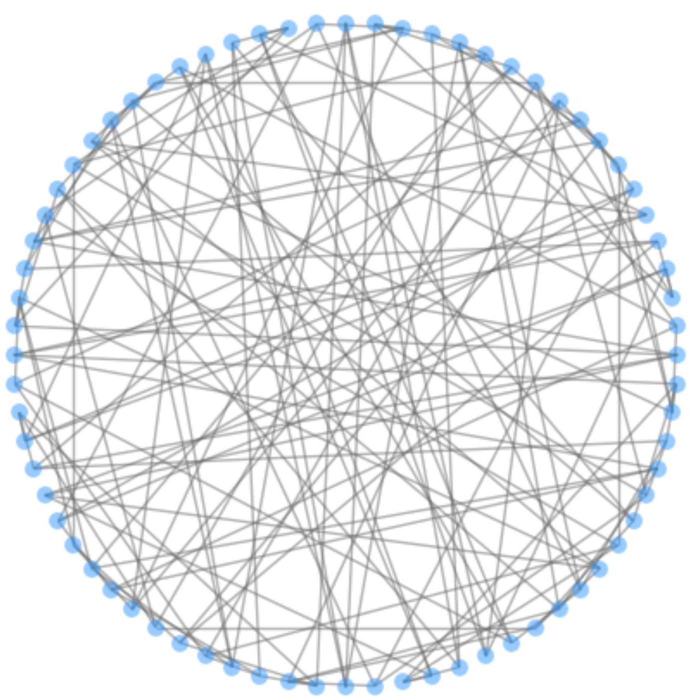
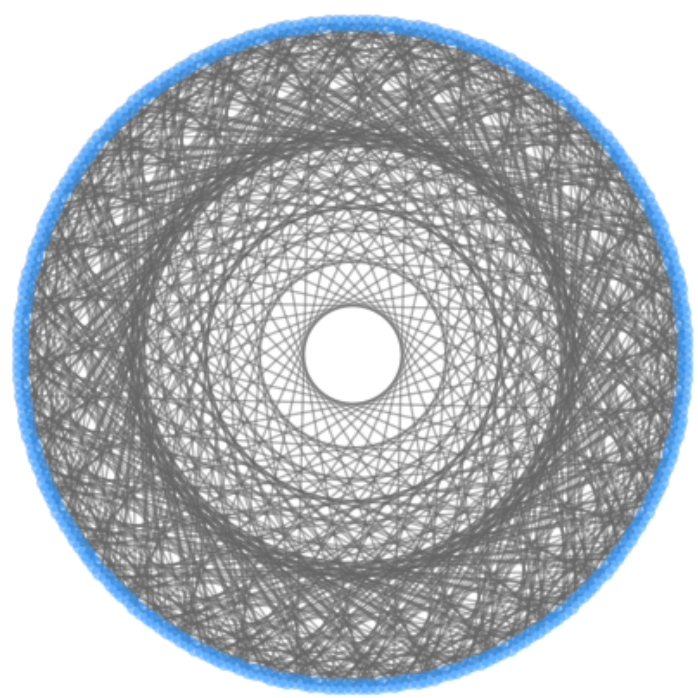


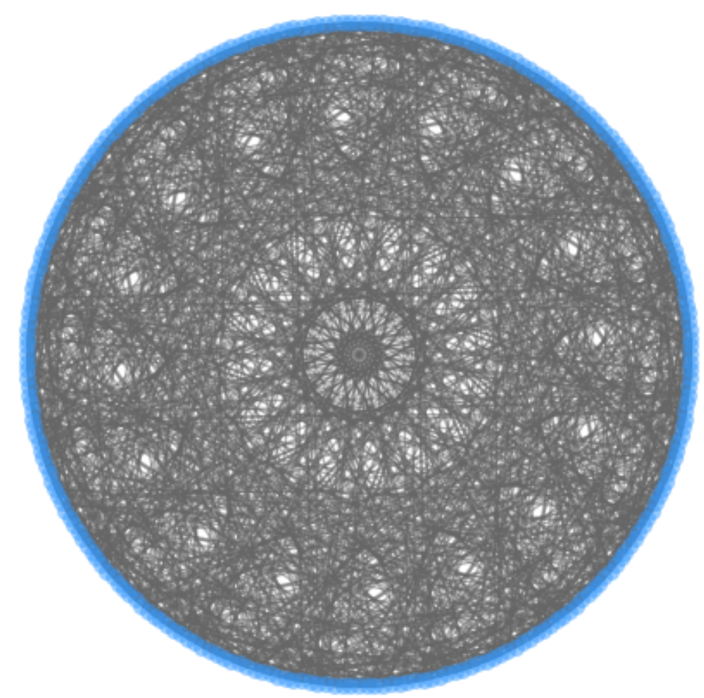
(n, d) = (256, 10)



Theoretical lower bound



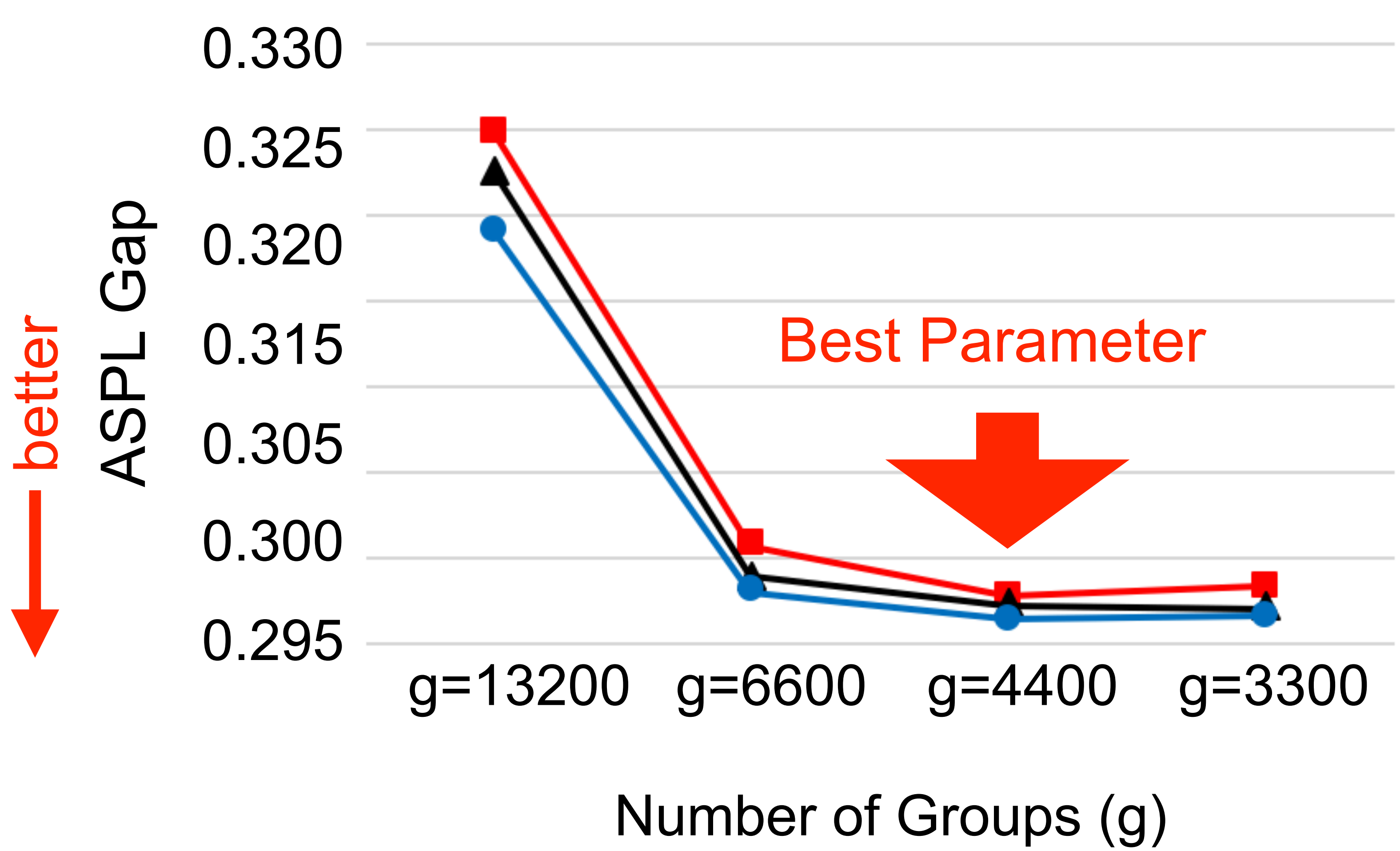
Best solution in Graph Golf



Theoretical lower bound

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)



Speed Performance

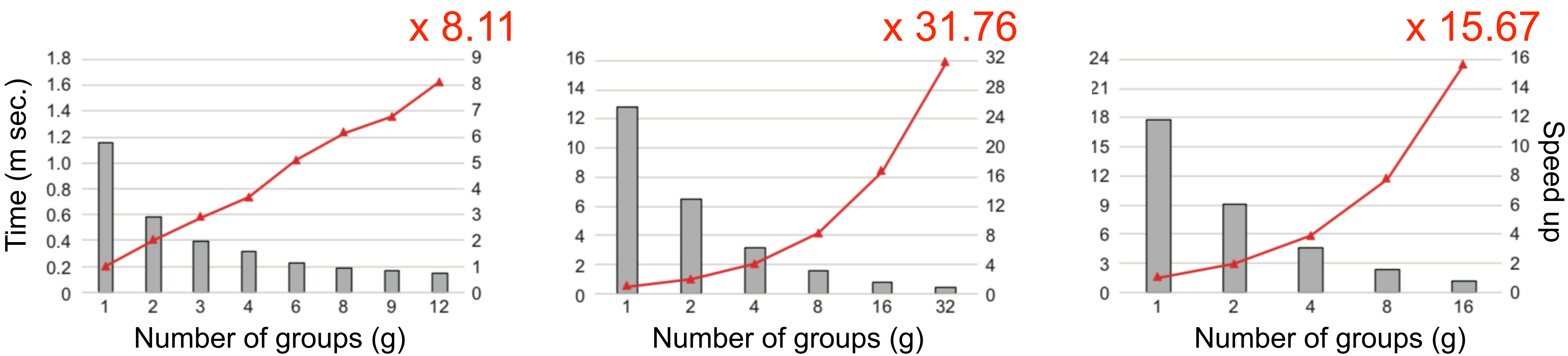
- COMA cluster system at University of Tsukuba

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

Performance results by Graph Symmetry

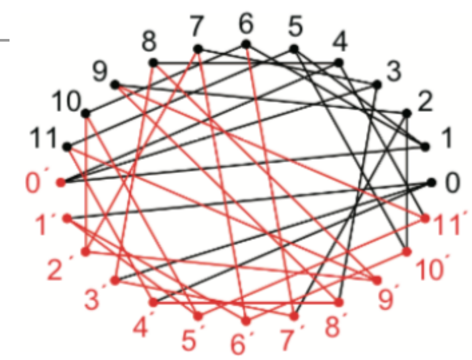
- Measure time to calculate ASPL 100 times



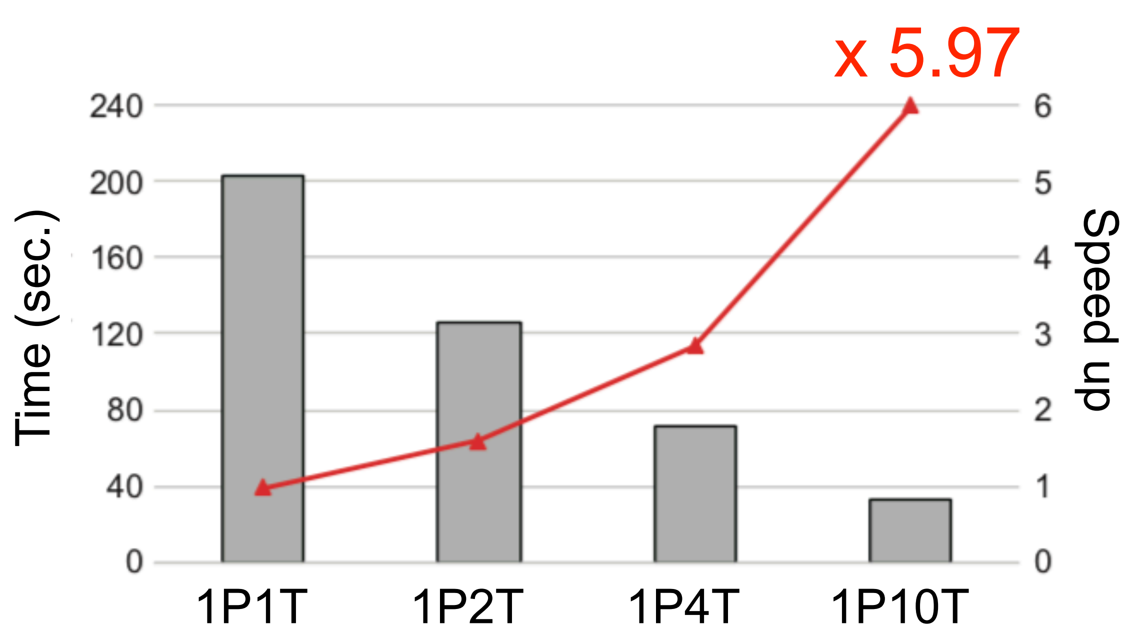
(n, d) = (72, 5) (n, d) = (256, 5) (n, d) = (256, 10)

- 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)

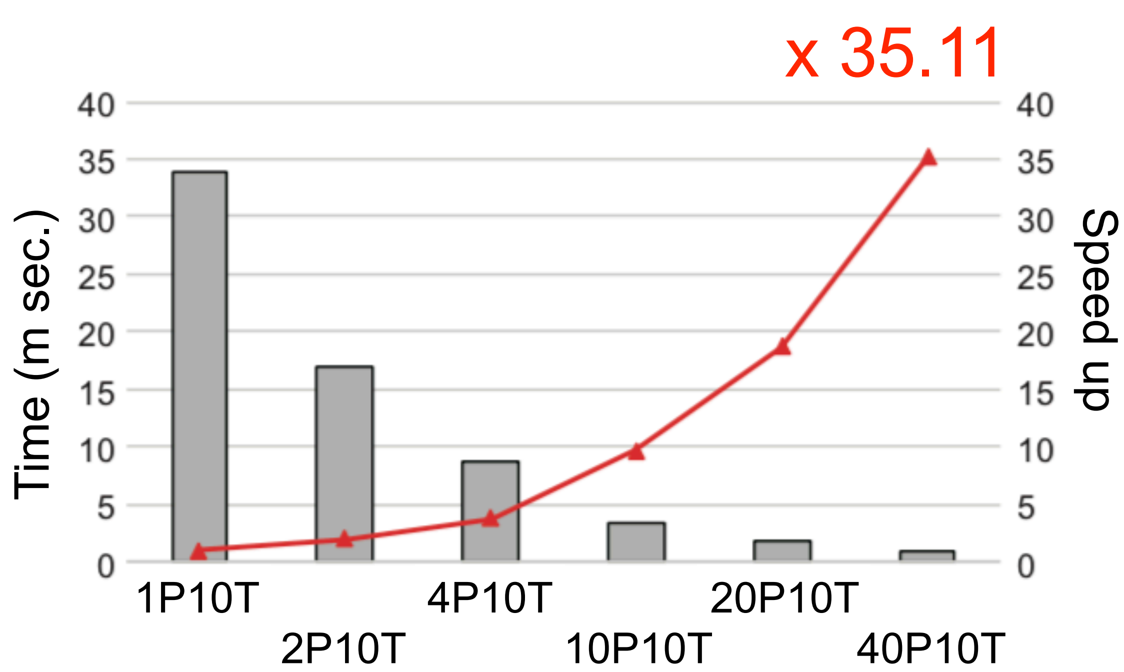
Performance results by Hybrid Parallelization



- Multiple BFS are simultaneously executed using MPI, and each BFS is executed in parallel using several OpenMP threads
- Number of Process is **P**, and Number of Threads is **T**
- The maximum value **P** is (n/g)
- In problem (n, d, g) = (400000, 32, 10000), the performance obtained with 40P10T is **209.80** (5.97 x 35.11) times better than that obtained with 1P1T



Thread parallelization with OpenMP



Hybrid parallelization with MPI and OpenMP

Results of Graph Golf 2018

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	🏆

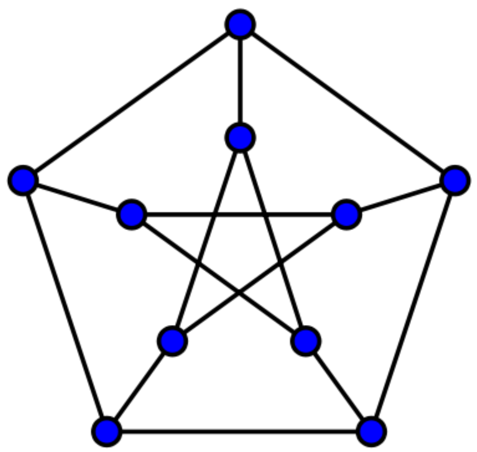
🏆 : Awarded

Proposed method won
8 problems in 14 problems

Related Work 2

	Rank	Author	Number of best solutions
🏆	1	Masahiro Nakao	8
	2	haruishi masato	6

Haruishi's algorithm uses **voltage graphs**



- Regular topology
- Merit
  - Relatively small diameter and ASPL
  - Calculation time for ASPL using regularity is small
- Demerit
  - Diameter and ASPL may not be small in some cases
  - Specific number of nodes

http://research.nii.ac.jp/graphgolf/2018/candar18/graphgolf2018-haruishi.pdf

Agenda

- Background
- Related works
- Explain our algorithm
- Evaluation of search and speed performances
- Summary

Conclusion

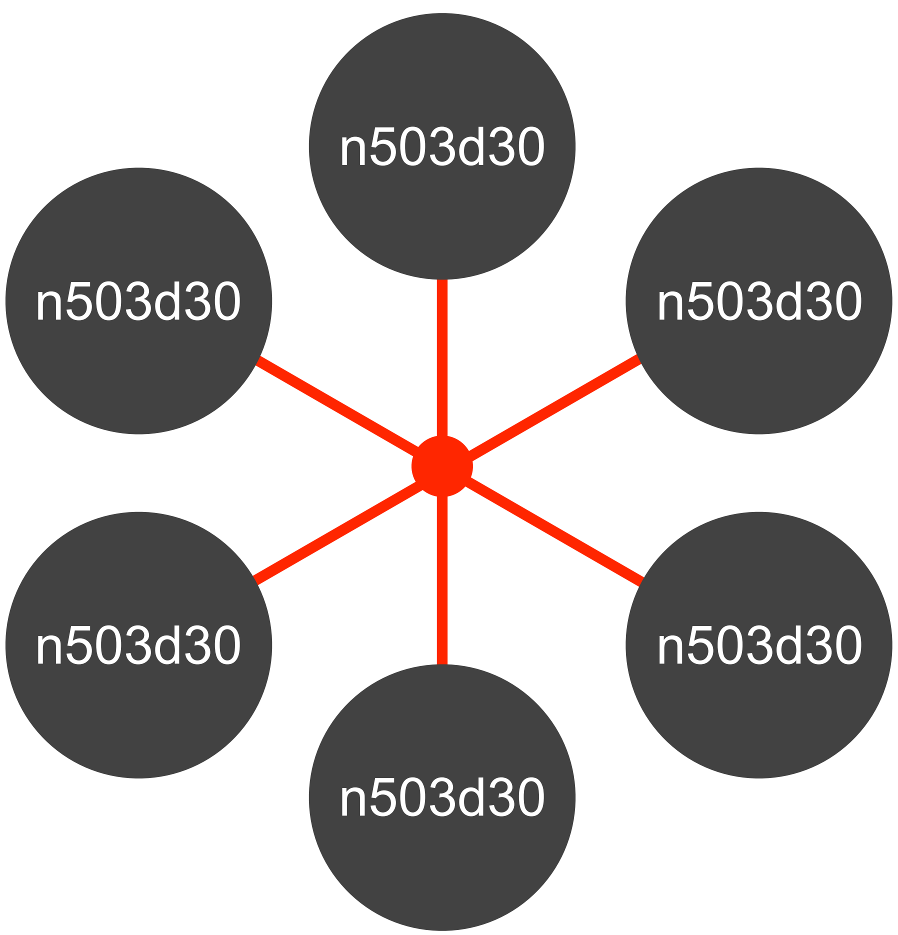
- In the proposed method, the topology is made **symmetrical**, making it possible to efficiently **find a good solution**
- Making the topology of the graph symmetrical reduced the calculation time required for the ASPL
  - Moreover, by utilizing hybrid parallelization with MPI and OpenMP, the calculation 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**

Future works

- Graph Symmetry is basic idea.
  - It can be combined with optimization algorithm other than SA
  - e.g. Deep Learning, Genetic Algorithms, etc.

When n is a prime number

- In Graph Golf 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



n503d30 x g6 + c1 = n3019d30

groups = 6 centers = 1

(n, d) = (503, 30)

503 x 6 + 1 = 3019

In addition, the following combinations are possible.

n301d30 x g10 + c9 = n3019d30
n200d30 x g15 + c19 = n3019d30
n100d30 x g30 + c19 = n3019d30

How are parameters of SA set？

- 最高温度：初期解（ランダムグラフ）に対して100回ランダムにエッジを交換して得られるエネルギーの差を50%で受理
- 最低温度：理論的な最小のエネルギー差（2/(n*(n-1))）を0.01%で受理
- クーリング率：1
- 総計算回数：100万回

詳細は予稿集の4.1「パラメータの設計指針」を参照ください