Efficient and Robust Parallel ILU Preconditioners for Quantum Eigenvalue Problems in ppOpen-HPC/ESSEX-II

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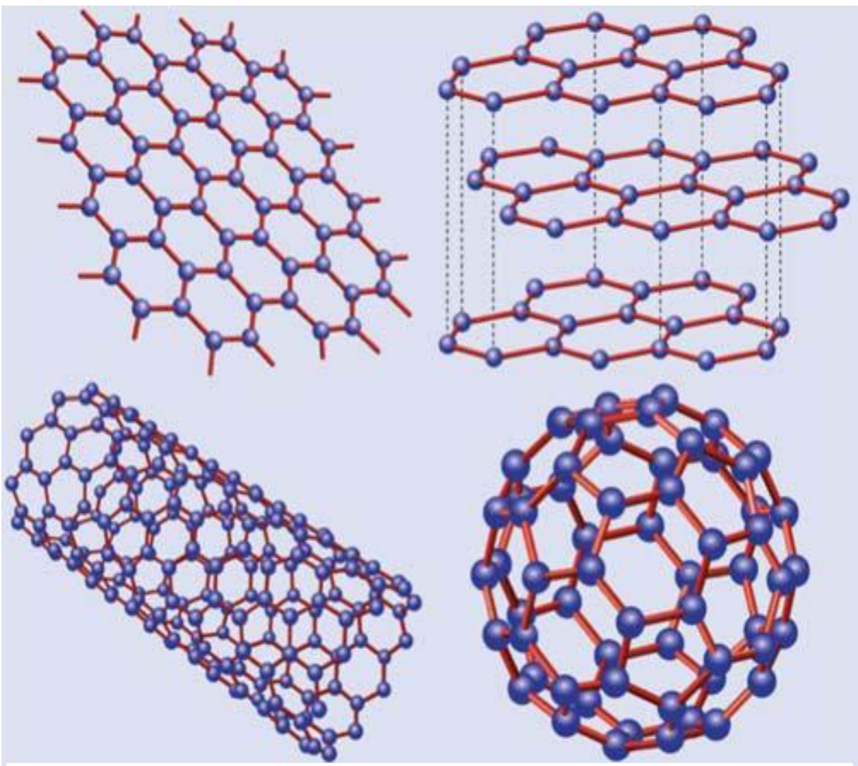
- Introduction
- Massively parallelized ILU preconditioner with robustness
- Parameter research of the ILU
- Conclusion

Motivation

Unraveling electrical properties of special materials by solving generalized eigenvalue problems

Graphene

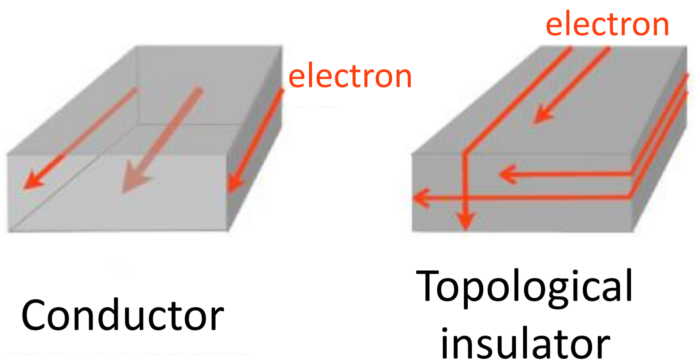
Several kinds of allotropes



Source : The electronic properties of graphene

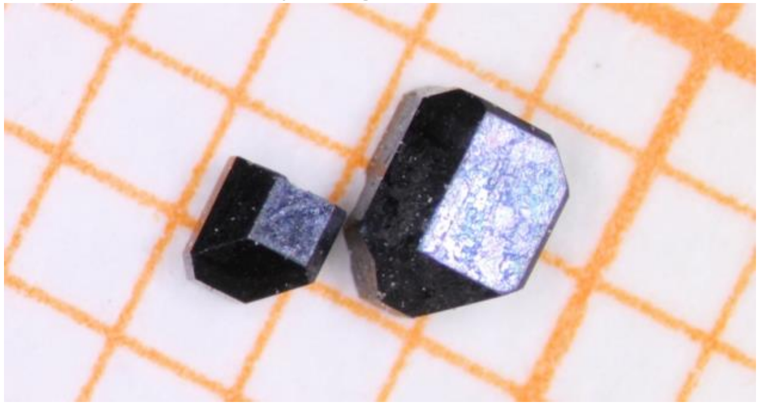
Topological insulator

A new material which has special properties
Inside : insulation Outside : conduction



Source:Telescope magazine

Sample of the topological insulator (SmB6)



Source:Nature

Solvers for generalized eigenvalue problems

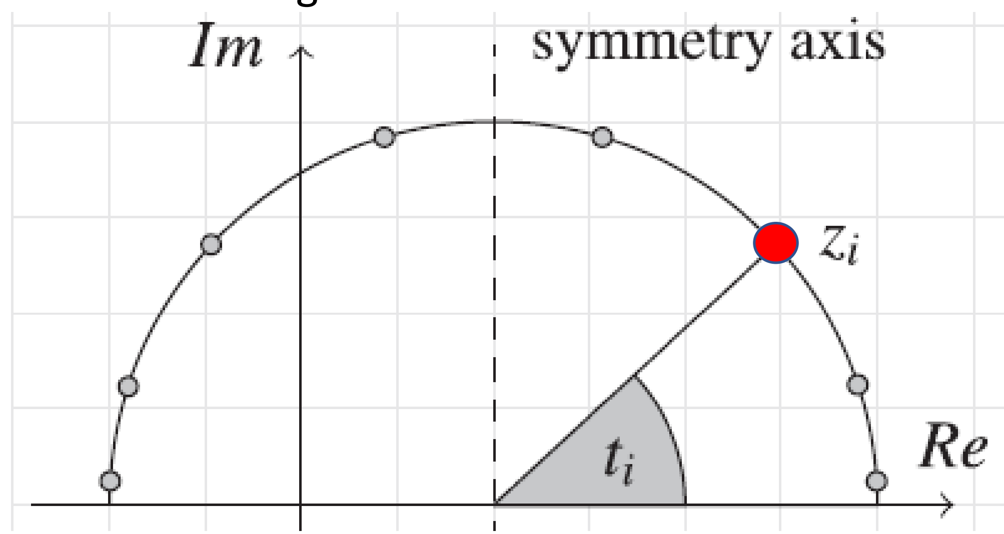
Focusing on *Sakurai-Sugiura*(*SS*) or *FEAST* method

→The *SS* and *FEAST* methods are obtaining eigenvalues in arbitrary area.

- SLEs are derived from each integral point in the *SS* or *FEAST* method.
  → Needed a solver for the SLEs ($A_z x = b$)

  - Properties of the matrix
    $A_z := z_i B - A \;:\; B = I$
    ✓ ill conditioned
    ✓ Large scale

Image of SS or FEAST method



- Requires of the solver
  - Robustness
    →Regularized ILU preconditioner
  - Massively parallelism
    →Hierarchical multi-coloring

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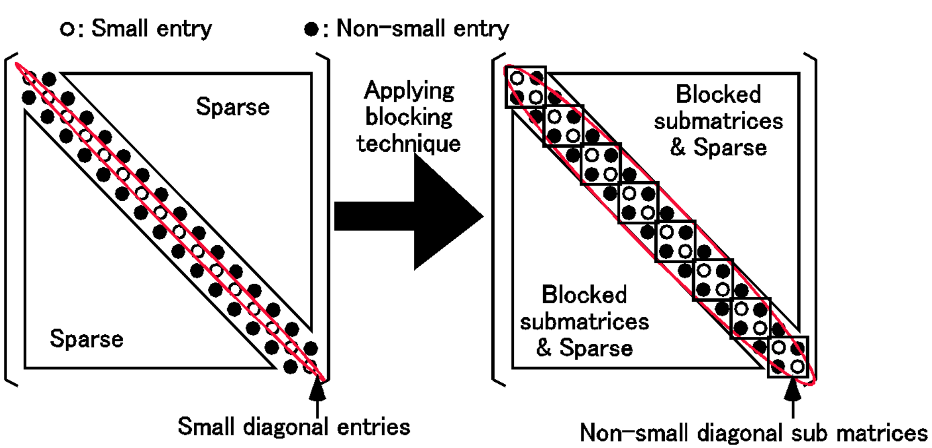
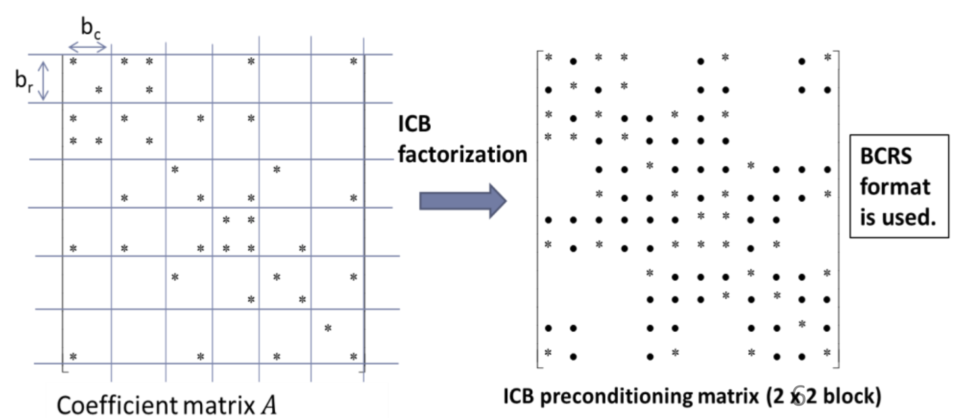
For robustness

Applying 2 regularization methods for ILU preconditioner
→For robustness and improving convergence

- **Blocking technique(Regularization①)**
  - Applying the incomplete decomposition to a block matrix
    1. More robustness because of including non-small off-diagonals
    2. Better convergence ratio because of allowing more fill-ins
- **Diagonal transformation(Regularization②)**
  - Adding constant value α to the diagonal elements
  - Directly method to make the diagonally dominant matrix





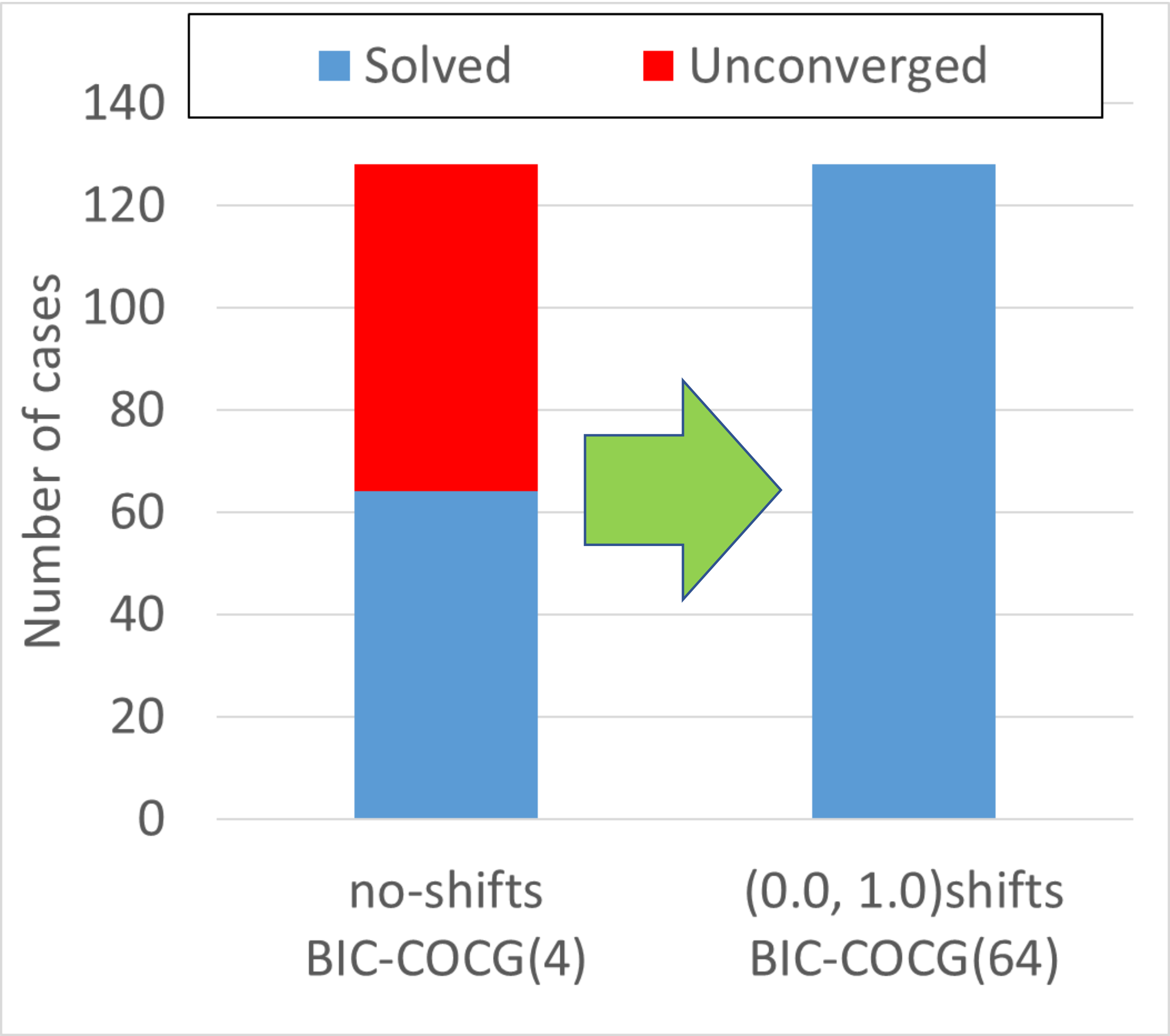
Conditions and target problems for numerical analysis

- Krylov subspace method: COCG
- $b = A_Z x \quad x^T = randam(min = 1, max = 10)$
- Iteration is stop if the number of iteration reach to DoF or relative residual fills the requirement $\left\|\frac{r^k}{r^0}\right\|_2 \leq 10^{-7}$
- Target problems
  - 128 data sets
    - ✓ Graphene model
      DoF = 1K, 130K, 1.3M, 13M
      16 shift values
      4 × 16 = 64 data sets
    - ✓ Topological insulator model
      DoF = 1K, 30K, 102K, 1M
      16 shift values
      4 × 16 = 64 data sets

Shift : Denotes shift values z of $zB - A = A_z$
Diagonal shifting : Denotes the regularization of preconditioning (proposed method)

Numerical evaluation

We solved all target problems by applying two regularization methods



- Diagonal shifting = (0.0, 1.0)
- The size of block is 64

For massively parallelization

Proposing parallelization method for multi-coloring algorithms

→Needed for solving the large scale SLEs on massively parallel systems

- Multi-color ordering is used for parallelize ILU preconditioner.
  - The effect of ILU preconditioner depend on a result of the multi-coloring
  - Multi-coloring algorithms are not parallelized.

Multi-coloring ← Still sequentially

Block IC decomposition

do itr = 1, DoF

dot_product

$q = \tilde{A}^{-1} r$(preconditioning)

Matrix Vector Multiplication

enddo

Parallelizing with multi-coloring

Parallelizing easily

Parallelization of multi-coloring algorithms

Proposing hierarchical parallelization for the multi-coloring algorithms

→For supporting any algorithms.

Existing reordering algorithms

■Level-set ordering

- Lexicographic
- Breadth First Search
- Cuthill-Mckee (CM)
- Reverse CM

■Independent set (Multi-color) ordering

- Greedy
- Algebraic Multi-coloring(AMC)
- Block AMC

1. The best algorithm depends on applications.
2. We need the robustness for the target problems.

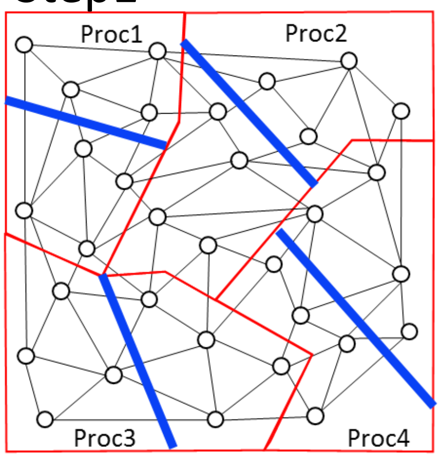
Need a versatile parallelization method which is not changing properties

Parallelization for multi-coloring algorithms

Proposing hierarchical parallelization for multi-coloring algorithms

→Versatile method

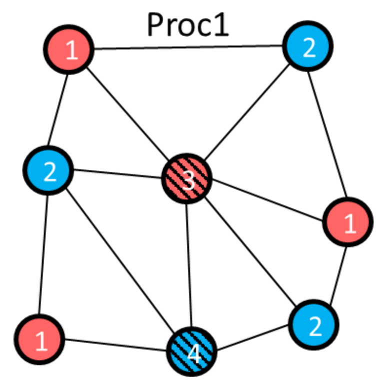
Step1



1, Each process separates elements to some parts.

2, The master process gathers the separates parts.

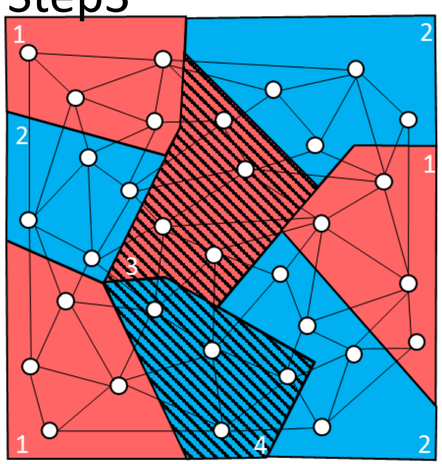
Step2



3, The master process creates a new graph.

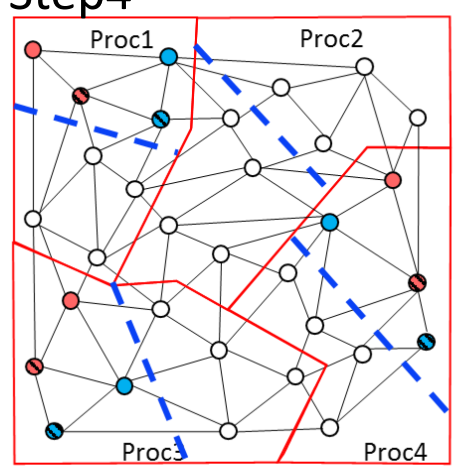
4, Master process colors the graph with any algorithms

Step3



5, The master process scattering the coloring results.
→ All process gets colored areas.

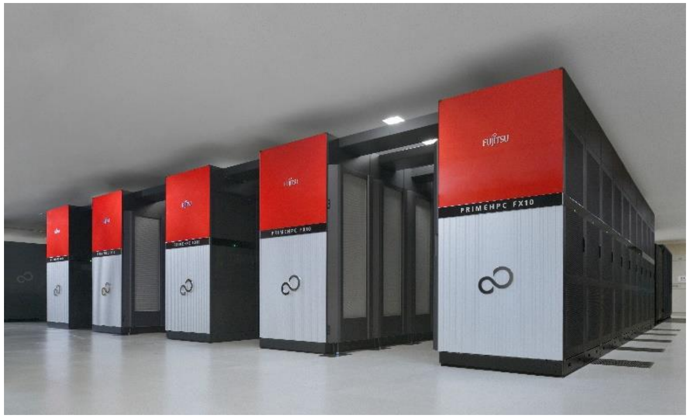
Step4



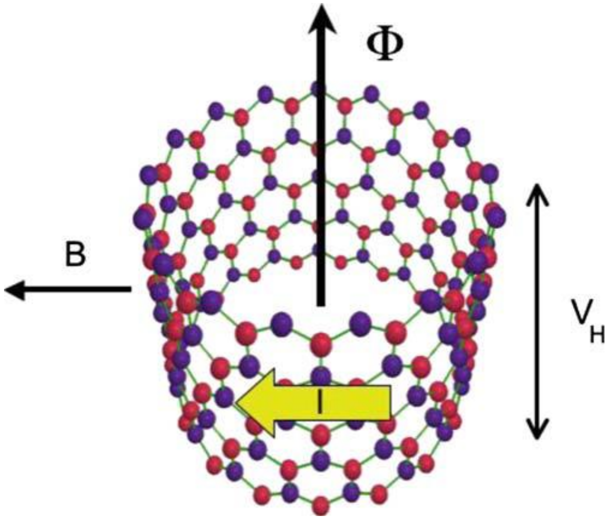
6, All process colors elements parallely based on the colored area.

Evaluations of the numerical analysis 2/2

- ■Oakleaf-FX 128～4800 nodes
  - Node specifications
    - ✓SPARC64™ IXfx 16cores
    - ✓32GiB
  - Network specifications
    - ✓Tofu



- ■The parameter of IC preconditioner
  - ✓ Block size = 4
  - ✓ Diagonal shifting = 100.0d0
- ■Coloring algorithm for test
  - Hierarchical parallelized AMC(10)
- ■Target problem
  - Graphen32,768x16,384 ≒ 500M DoF
    ≒ 7G Non-zero elements (Real values)

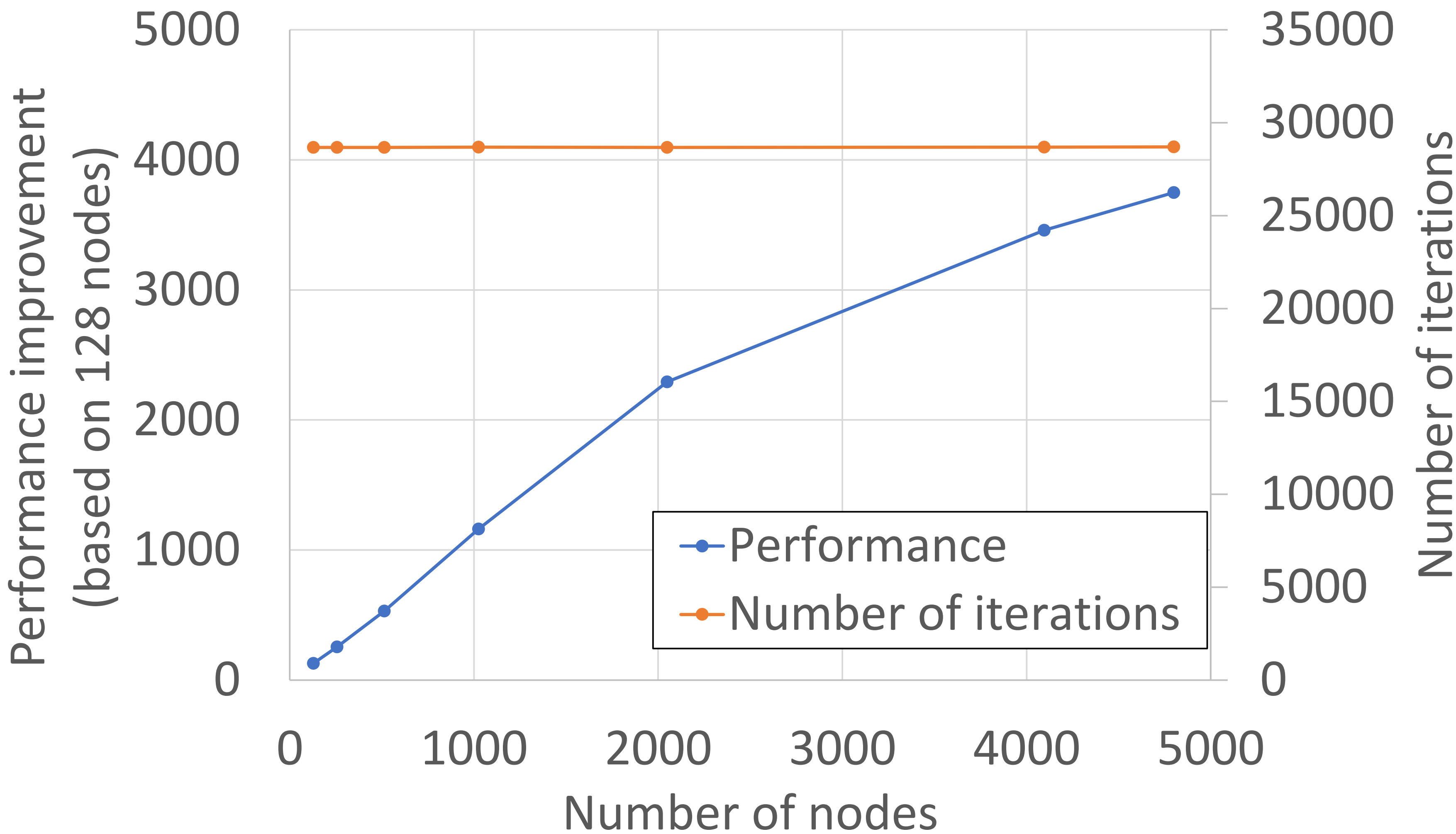


Source : The electronic properties of graphene

Needed more than 4.7 GiB memory for coloring!

Performance on graphene problem

Numbers of iterations is almost same.



Performance of the IC preconditioned CG is good.

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Best parameter of the Block ILU preconditioner

The size of block has the biggest impact in the performance of the ILU.

Parameter

- ✓ Value of diagonal shifting
- ✓ Size of block
- ✓ Number of parallelism

→

- Convergence
- Computational time per one iteration

Best parameter of the Block ILU preconditioner

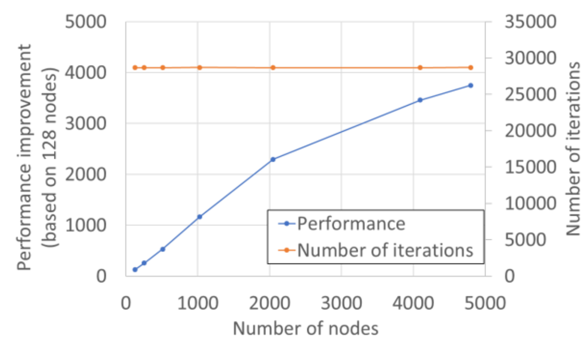
The size of block has the biggest impact in the performance of the ILU.

Parameter

- ✓ Value of diagonal shifting
- ✓ Size of block
- ✓ Number of parallelism

- Convergence
- Computational time per one iteration

	Convergence	Computational time per one itr
Diagonal shifting	✓	—
Size of block	✓	✓
Number of parallelism	—	✓



We have to find the best size of block for each problems.

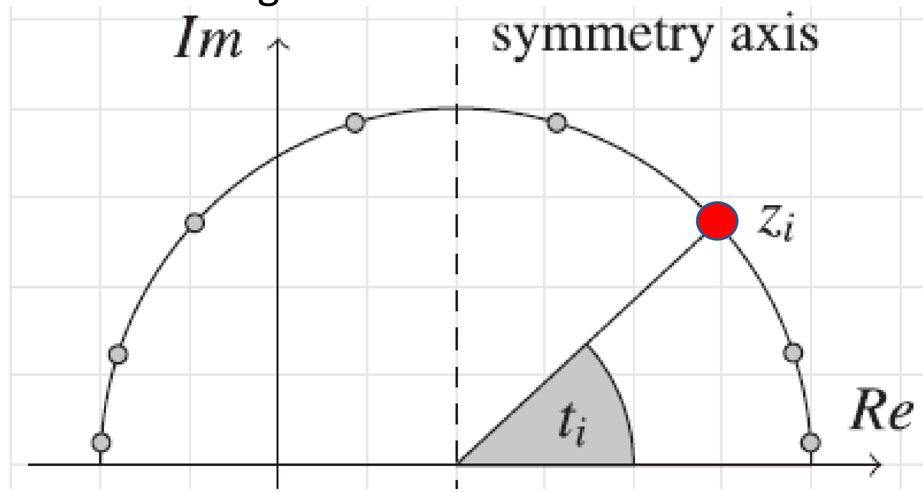
Strategy to find the best size

We try to find the best size of block in the few iterations.
← It is difficult to find it without any trials.

Brief implementation of the FEAST

```
Do 1, till converge eigenvalues….
    Do i = 1,  number of shifts
        Solve (z_i I − A)x = r
    Enddo
Enddo
```

Image of SS or FEAST method



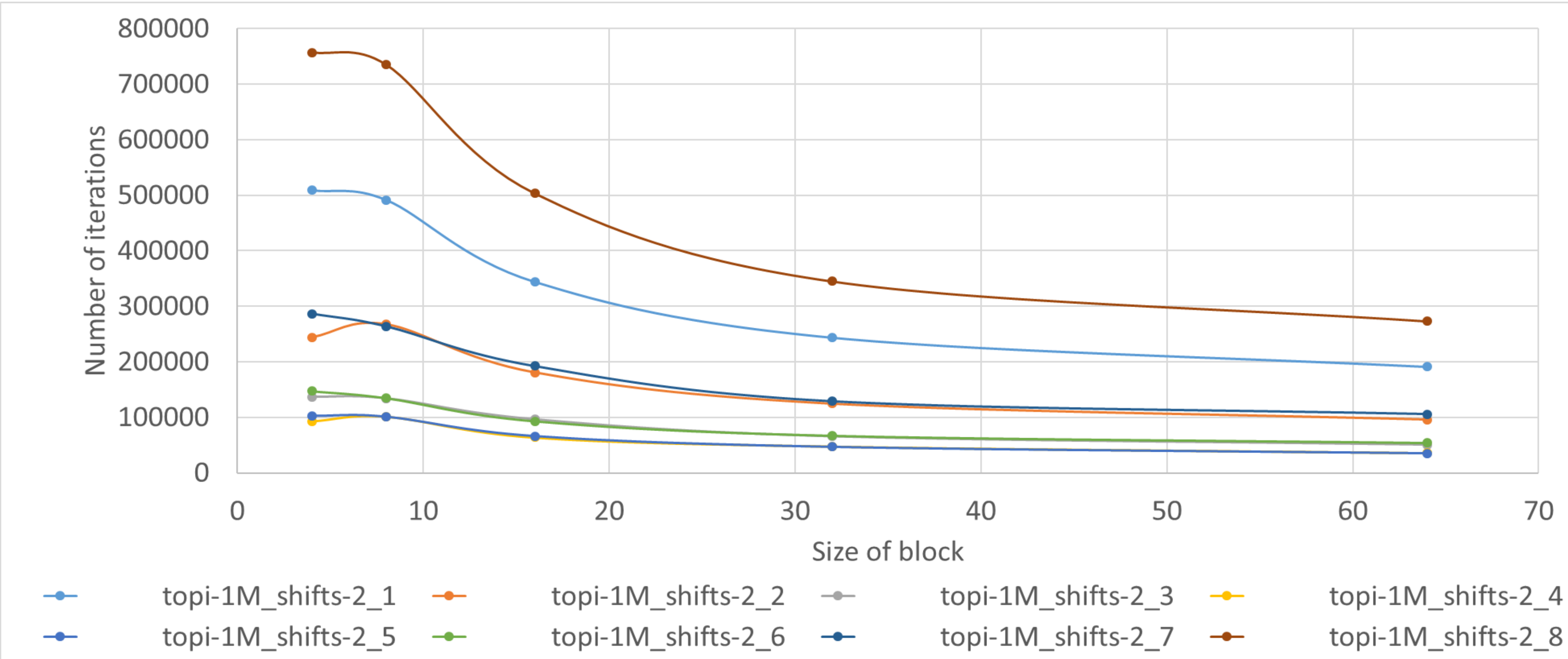
Number of solving equations
= "Number of shifts" * "Number iterations of outside"

- Measuring the computational time per iteration is easy
  There are no differences of non-zero patterns of the $(z_i I - A)$ among each shift.

- The convergence depends mainly on the z_i.
  1. Looking for the best size of block with each z_i is the easiest.
     → We need many iterations of outside loop.
  2. We try to find it with fewer iterations.

Relationships among convergence, block size and shift

Relationship between the block size and the convergence is similar for any z_i → Shifts values are close on imaginary plane.



On each line, the shift value is different.

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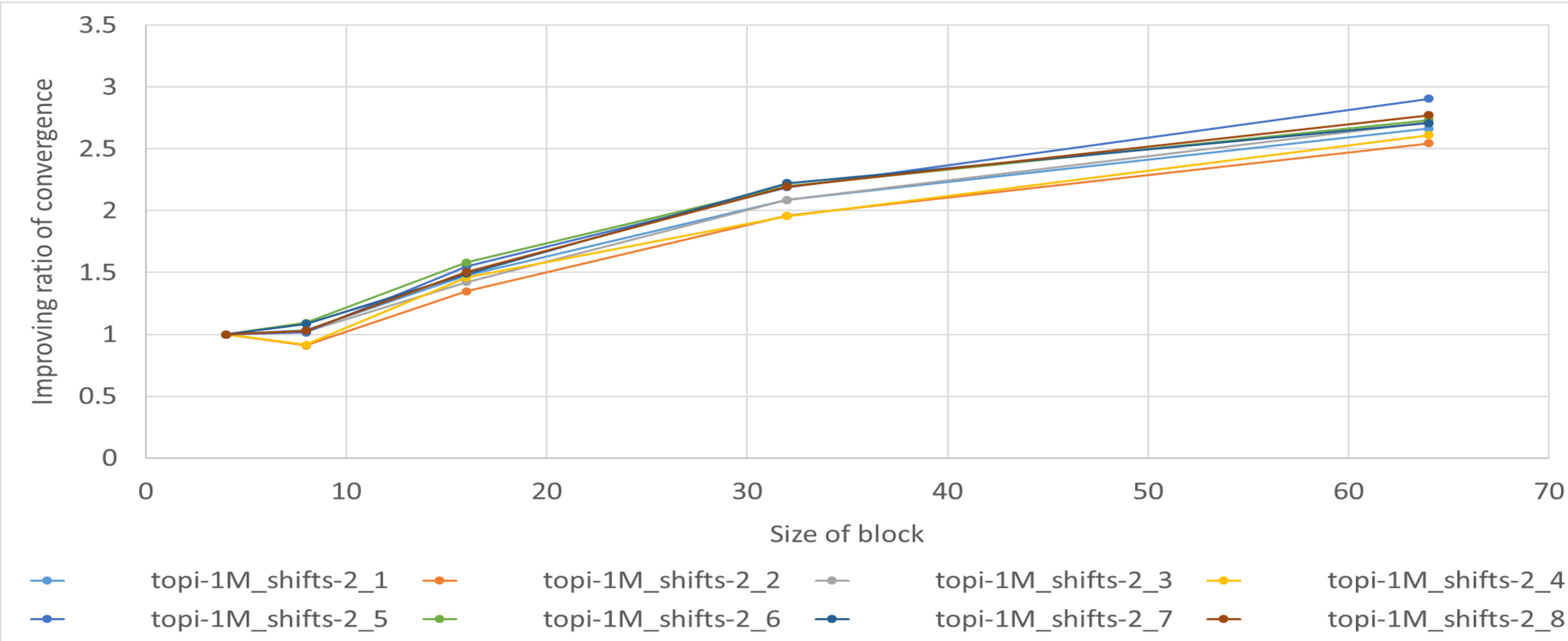


On each line, the shift value is different.
Y-Axis is calculated as “computational time with each block size / block size 4” on each shift.

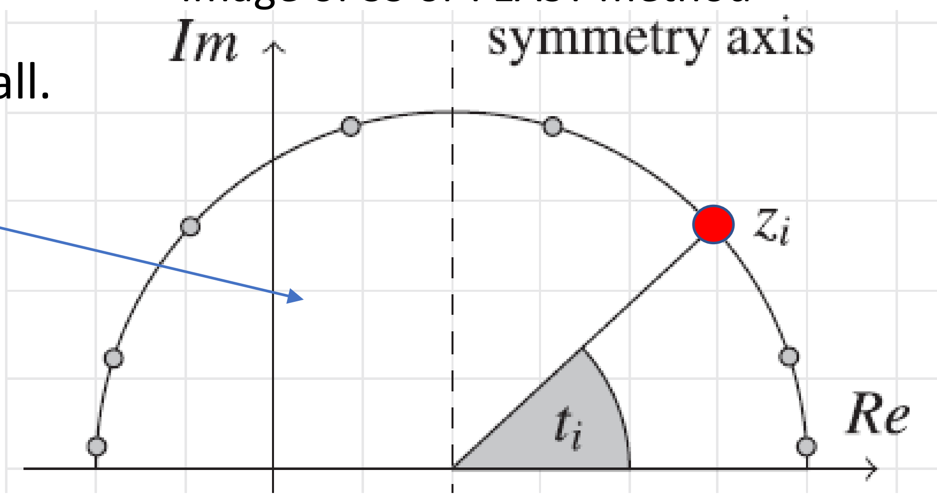
We can apply improvement ratios of the convergence to any $(z_i I - A)$.

→ The convergence ratio with block size 32 is twice as fast as block size 4 on shift data z_i, it is same on the other shifts

Method to find the best block size.

We can find the best size of block with "number of shift data" + "number of sampling points of block size" times trials.

Image of SS or FEAST method



The target range of the previous result is small.

$-5e^{-2}$ < Real part < $5e^{-2}$

$3e^{-3}$ < Imaginary part < $5e^{-2}$

We verified the same relationship on a larger target range and the other model.

To find the best size of block,

1. Solving the equations on all shifts with block size 4
   → Measuring the computational time per one iteration and convergence
2. Solving the equations with all block size (4, 8, 16, 32, 64) .

After above steps, we can use the suggested best size of the block on each iterations.

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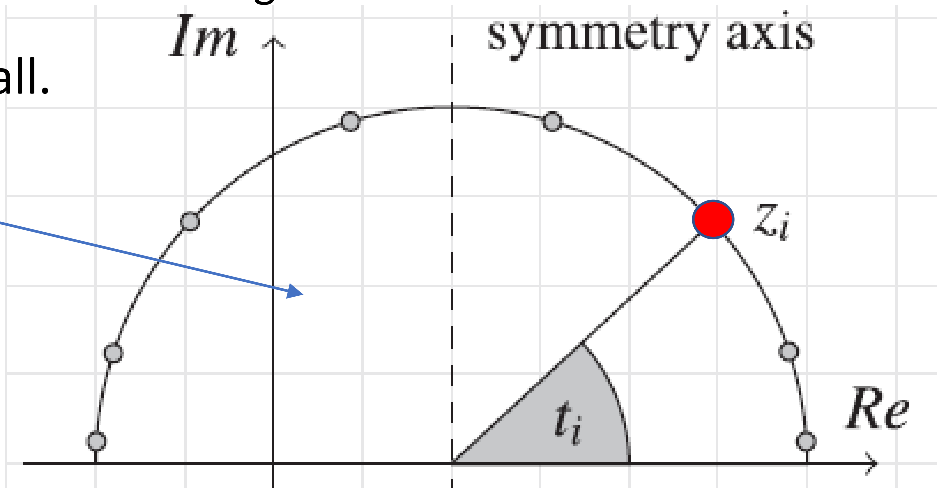

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To find the best size of block,

1. Solving the equations on all shifts with block size 4
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2. Solving the equations with all block size (4, 8, 16, 32, 64) .

After above steps, we can use the suggested best size of the block on each iterations.

I’m sorry, there is no evaluations…. This is a idea.

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Conclusion

- Introducing the parallel ILU preconditioner for eigenvalue problems of quantum systems
  - The regularizations for ILU preconditioner
  - The hierarchical parallelization for the multi-coloring

- We discussed to find the best size of block

Future works

- Numerical evaluations
- Checking the trends on more shifts and models
  - I checked on 2 models, 4 different DoF, 2 types of shifts
- The effect of matrix B and right hand vector r

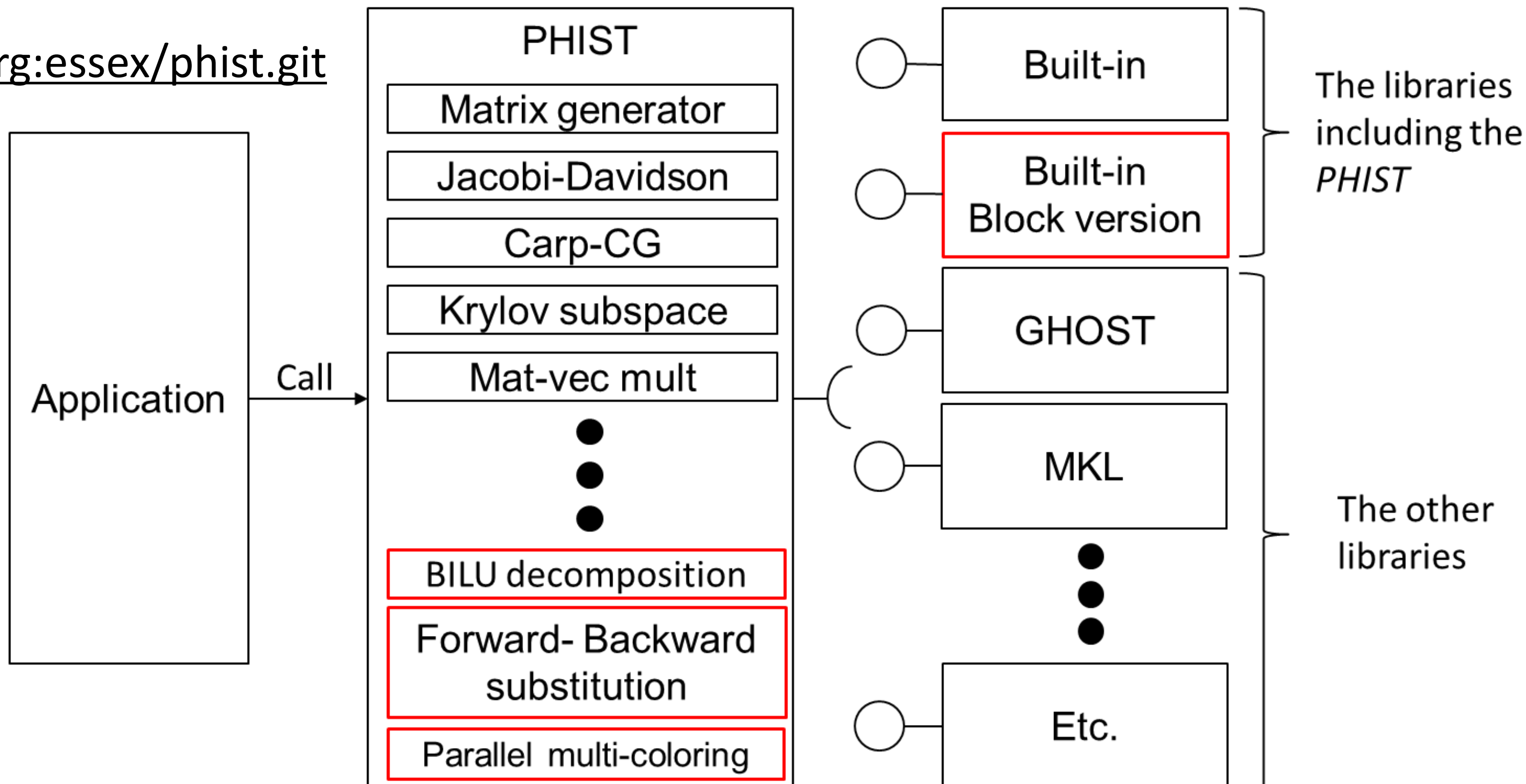
Publication of the parallelized ILU

We have implemented our ILU preconditioner in the PHIST.

PHIST is developed by ESSEX-II member of SPPEXA project.

- By using the PHIST, user can choose mathematical kernel libraries.
  - Implemented ILU preconditioner only supports symmetric real values.
    - Complex values will support in the near future.

git@bitbucket.org:essex/phist.git



For the Fortran user, we publish pk-Open-SOL on the ppOpen-HPC web page.

http://ppopenhpc.cc.u-tokyo.ac.jp/ppopenhpc/

Thank you for your kind attention

ESSEX-II

Evaluations of the numerical analysis 1/2

Evaluating differences between the sequential and the parallelized multi-coloring on the convergence and the performance

■Reedbush-u 32 nodes

Node specifications

✓Intel Xeon E5-2695v4 x 2socket (1.210 TF)

Broadwell-EP, 2.1GHz 18core

→36 Cores per node

✓256 GiB (153.6GB/sec)

Network specifications

✓InfiniBand EDR

■Hybrid parallelization

1process-18 threads (1process per socket)

■ Coloring algorithm for test

Greedy, AMC, CM-Greedy, CM-AMC

■ Iteration is stop if relative residual fills the requirement $\left\|\frac{r^k}{r^0}\right\|_2 \leq 10^{-7}$

■ Target problems

Parabolic_FEM, Thermal2, FLAN1565, Original Poisson model

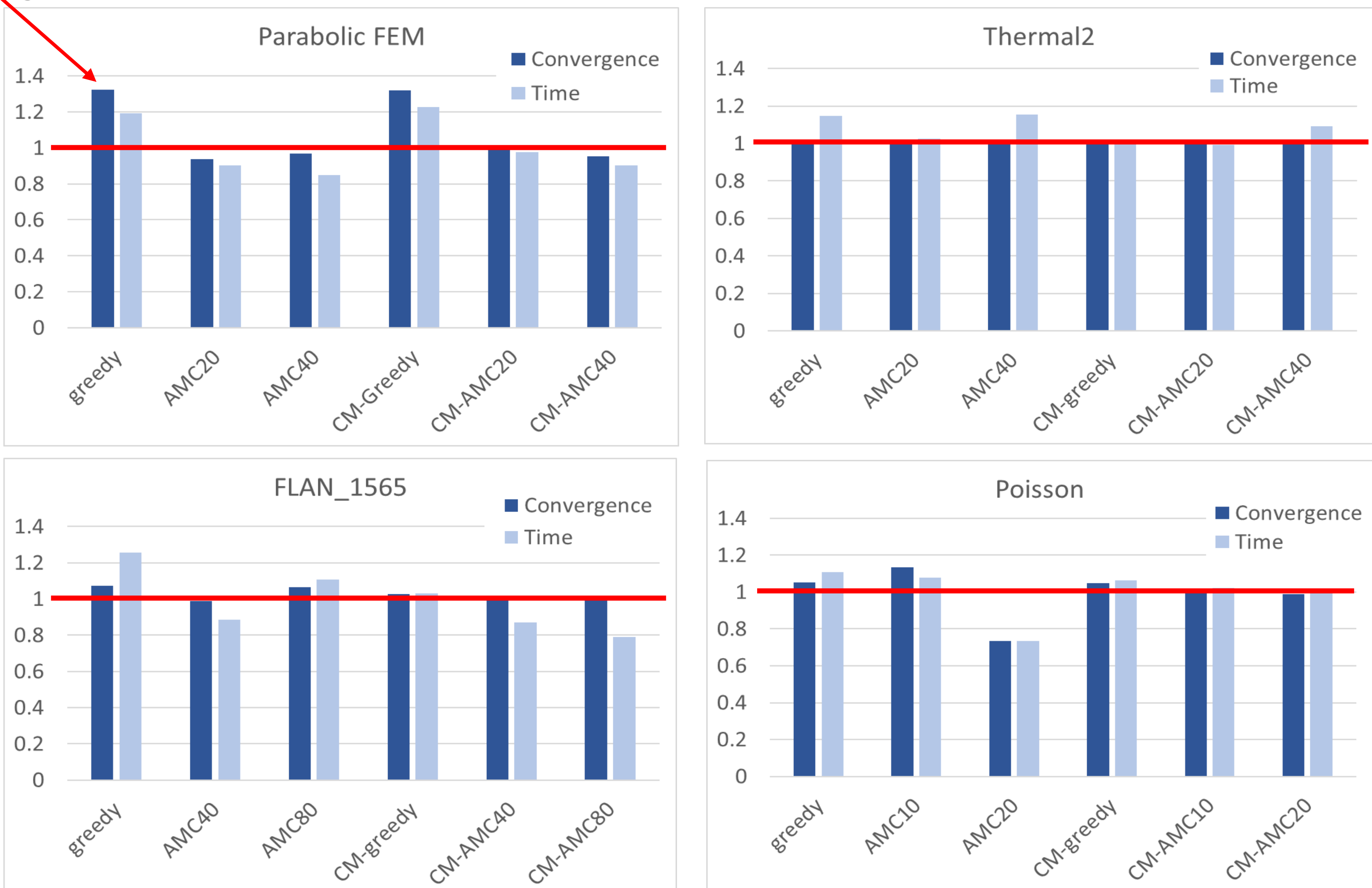
(Florida matrix collections)

Comparing the convergence and calculation time

Convergence and calculations are similar to sequential coloring.

1.32(largest)

Normalized result based on sequential coloring



Y-axis = sequential / parallel of computational time or convergence

Proposing hierarchical parallelization for the multi-coloring algorithms

→For supporting any algorithms.

Existing reordering algorithms

■Level-set ordering

- Lexicographic
- Breadth First Search
- Cuthill-Mckee (CM)
- Reverse CM

■Independent set (Multi-color) ordering

- Greedy
- Algebraic Multi-coloring(AMC)
- Block AMC

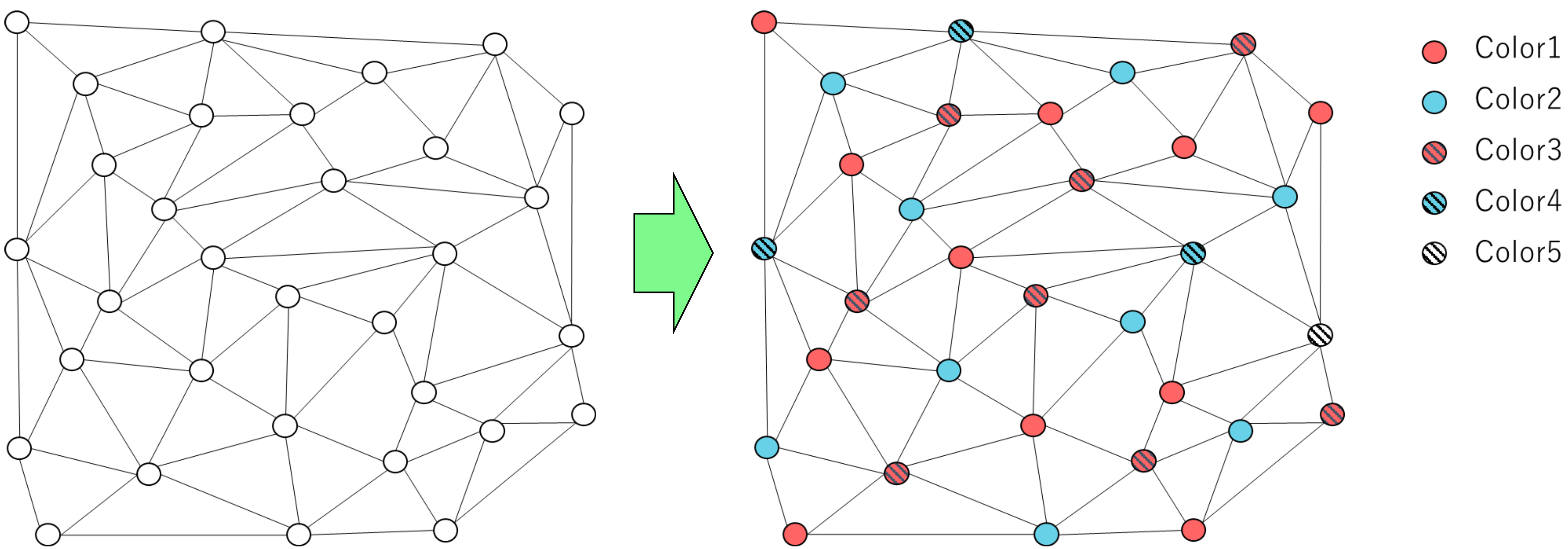
1. The best algorithm depends on applications.
2. We need the robustness for the target problems.

Need a versatile parallelization method which is not changing properties

Objective of multi-coloring

Coloring all nodes without neighboring same color

→ Parallelizing IC preconditioner based on coloring results

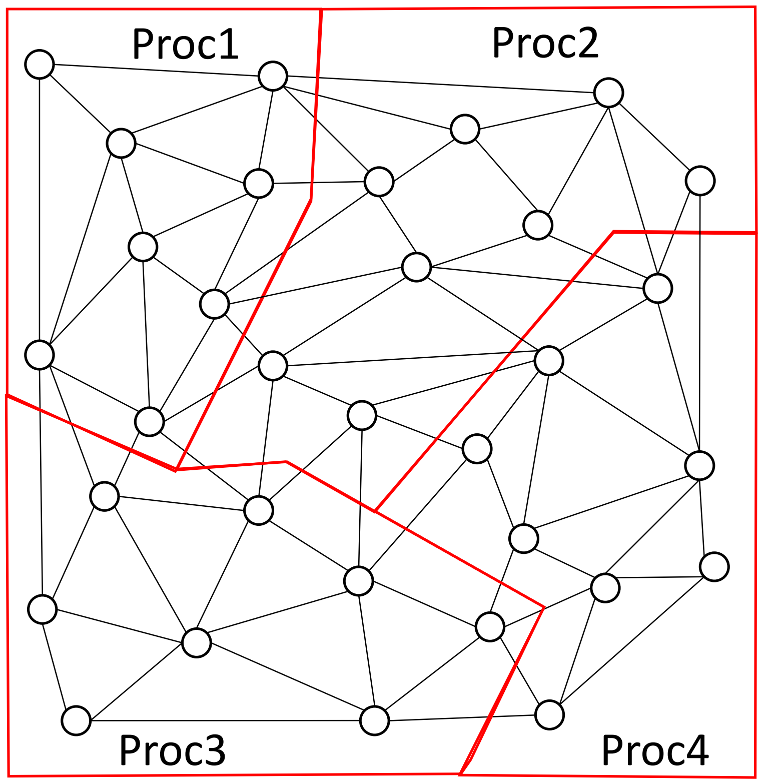


Parallelizing this process with hierarchical approach

Hierarchical parallelization (two-level) 1/9

Process of a two-level hierarchical parallelization

Initial conditions

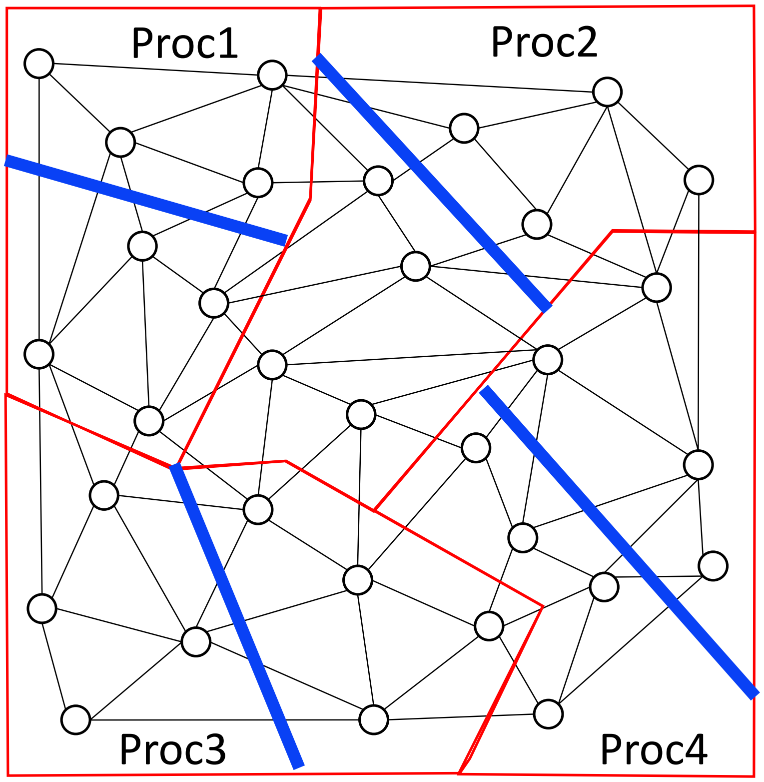


Hierarchical parallelization (two-level) 2/9

Process of the two-level hierarchical parallelization

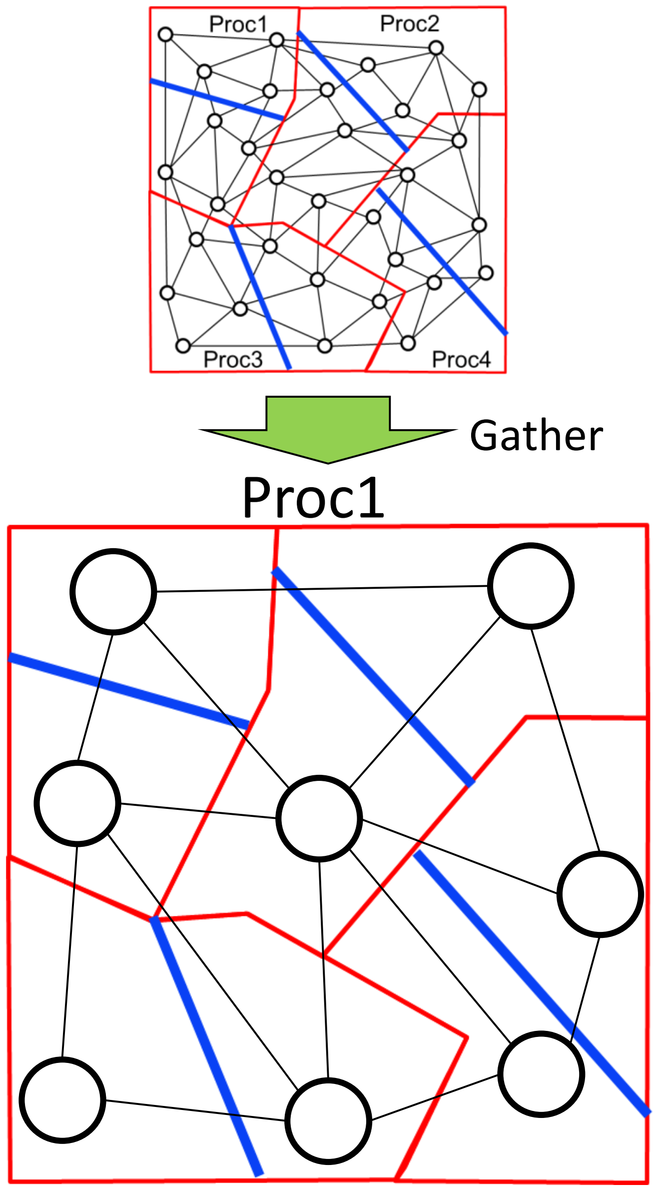
Initial conditions

1. Each process separates calculation area.



Hierarchical parallelization (two-level) 3/9

Process of the two-level hierarchical parallelization

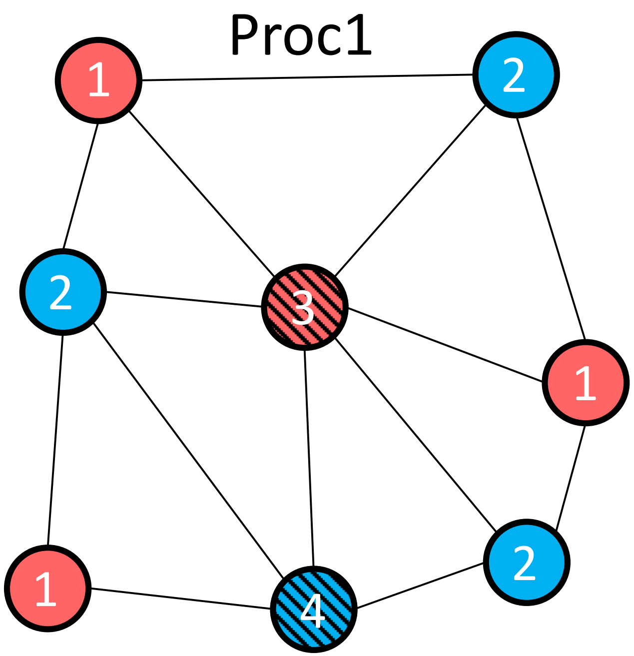


Initial conditions

1. Each process separates calculation area.
2. Gather the graph structures.

Hierarchical parallelization (two-level) 4/9

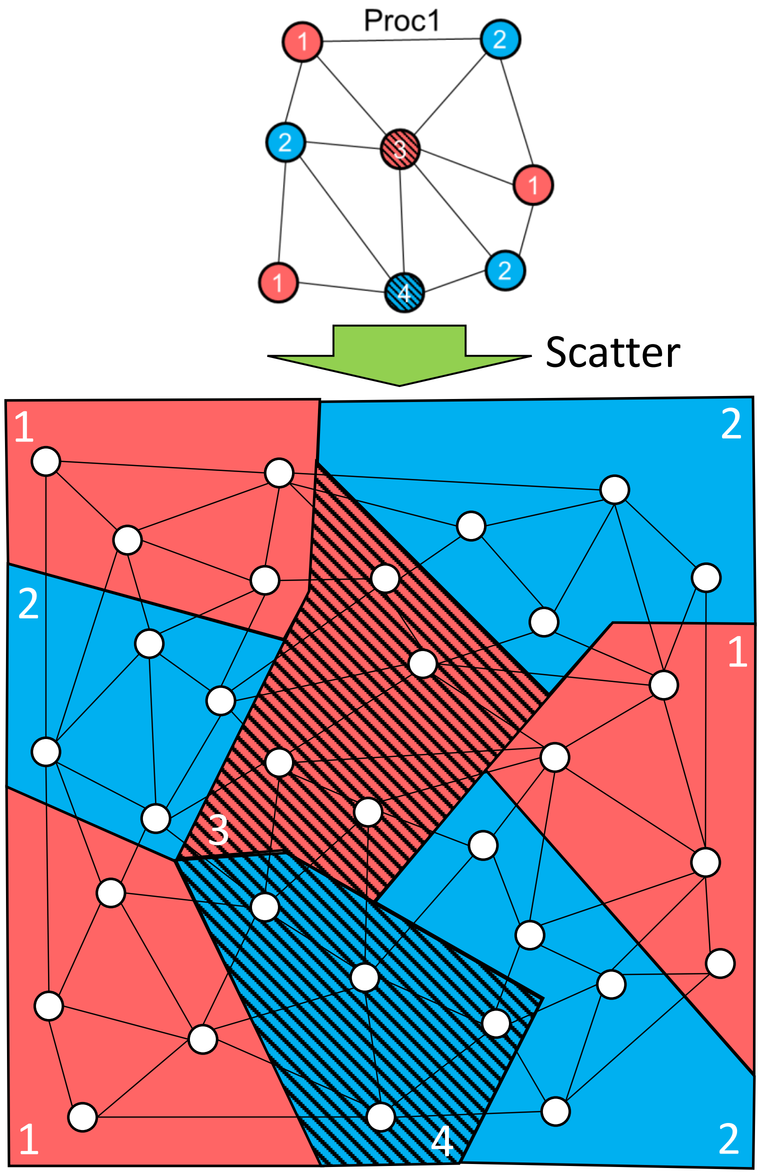
Process of the two-level hierarchical parallelization



Initial conditions

1. Each process separates calculation area.
2. Gather the graph structures.
3. Master process colors the nodes with any method.

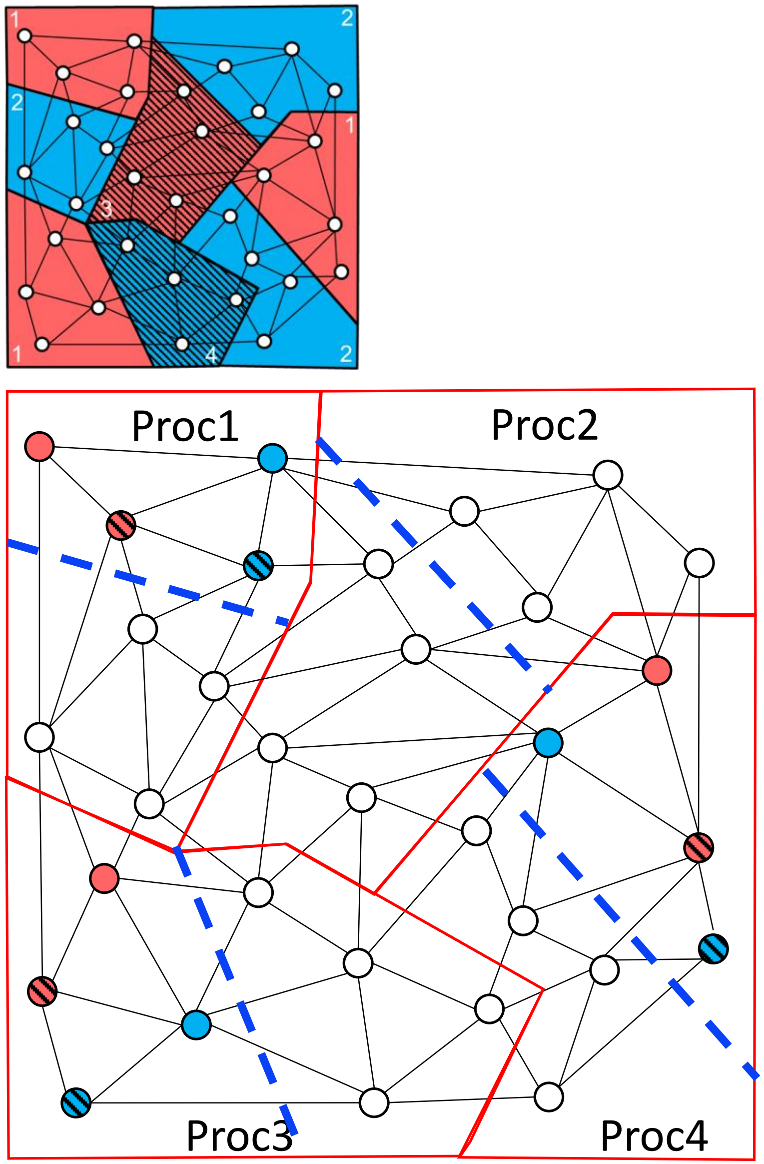
Process of the two-level hierarchical parallelization



Initial conditions

1. Each process separates calculation area.
2. Gather the graph structures.
3. Master process colors the nodes with any method.
4. Broadcast coloring result.

Process of the two-level hierarchical parallelization

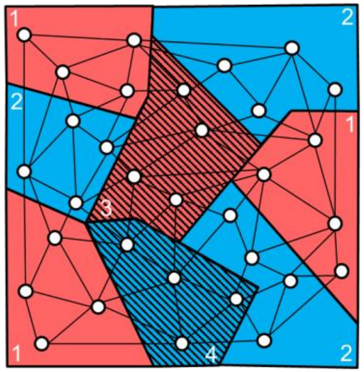


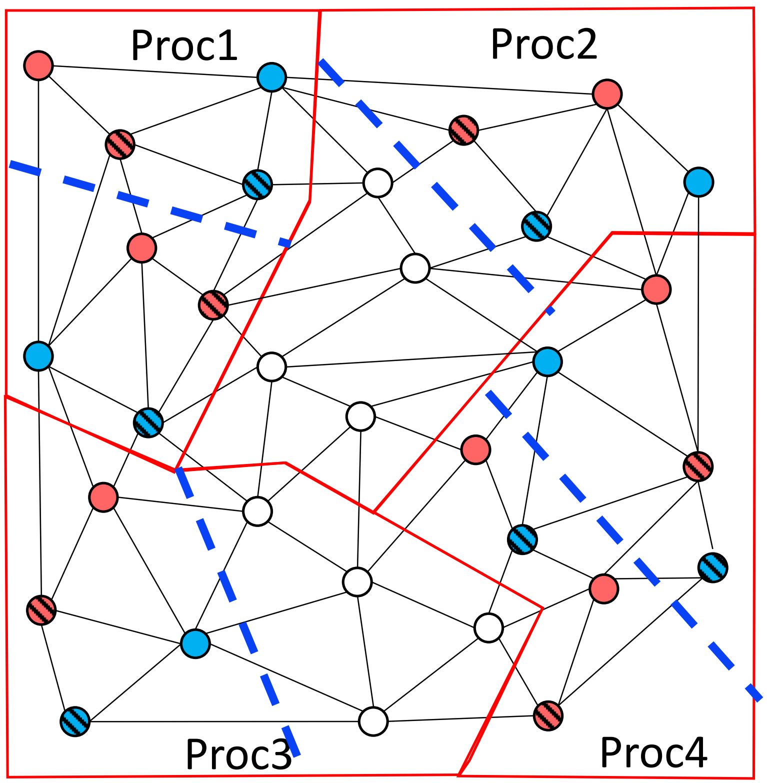
Initial conditions

1. Each process separates calculation area.
2. Gather the graph structures.
3. Master process colors the nodes with any method.
4. Broadcast coloring result.
5. Each process colors all nodes with any algorithm in parallel.

Hierarchical parallelization (two-level) 7/9

Process of the two-level hierarchical parallelization





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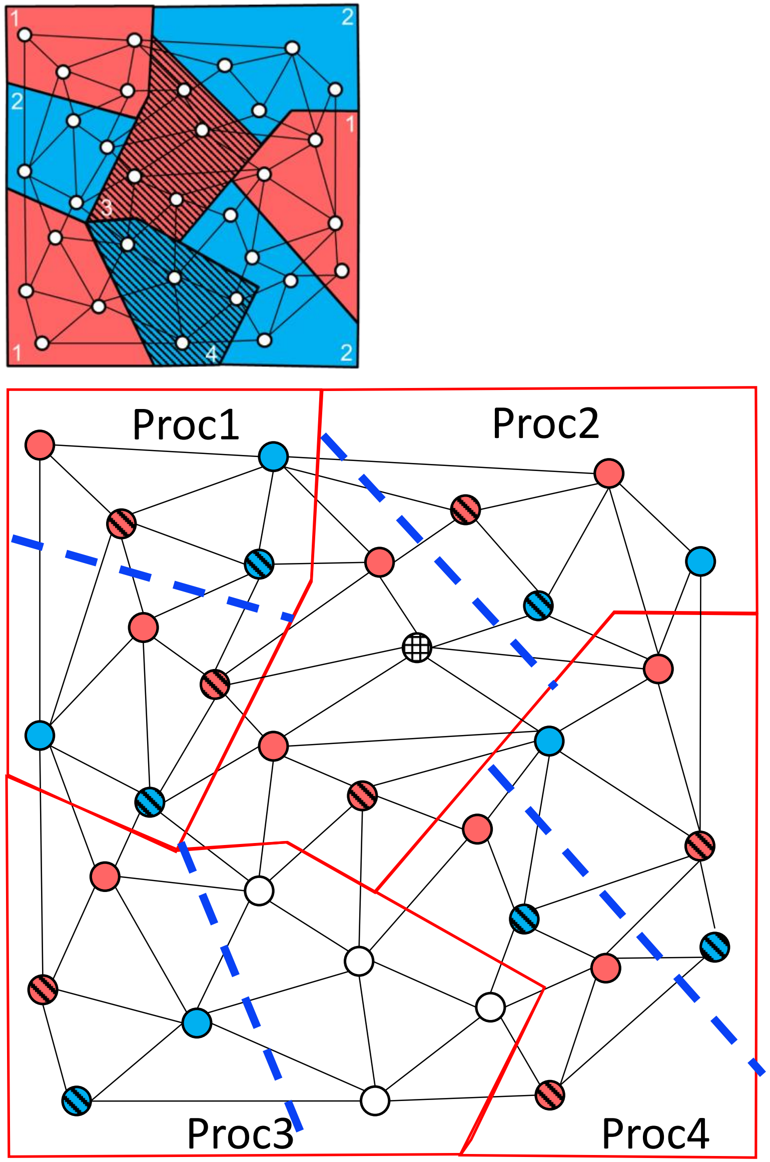

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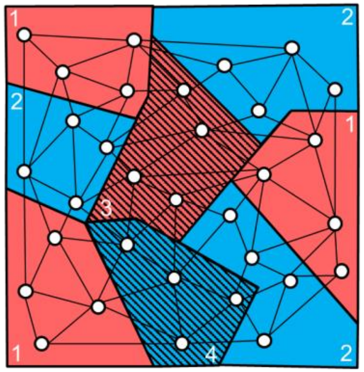

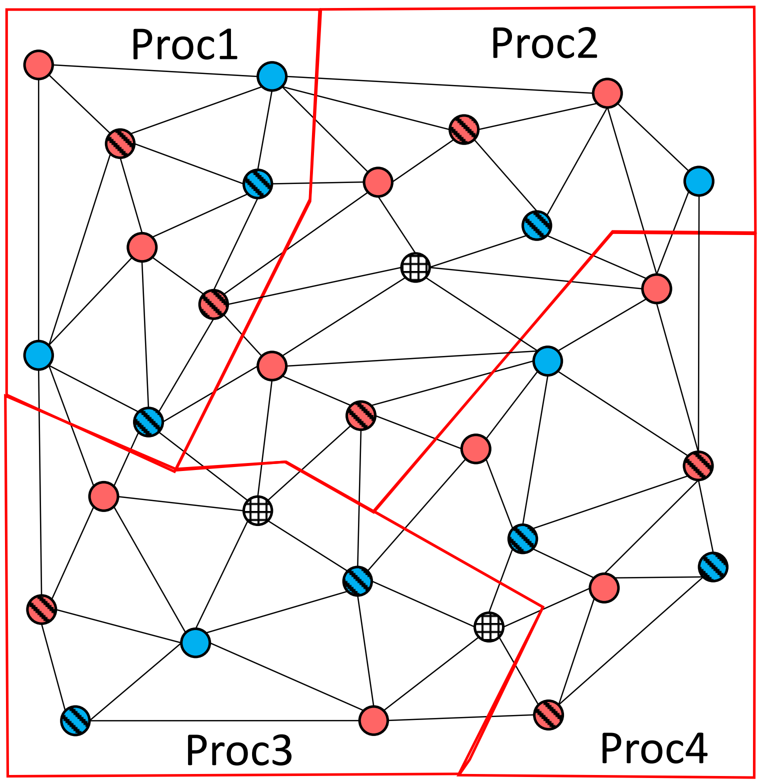

Initial conditions

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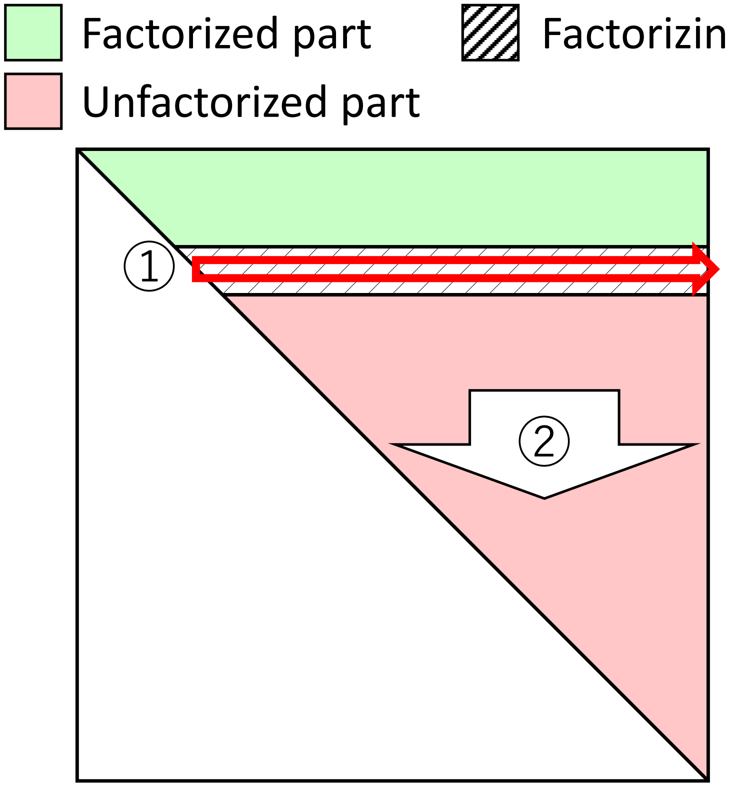
Finish

ILU preconditioner for the target problems

Needed a modification of the ILU preconditioner for more robustness

- IC preconditioning matrix is constructed through the incomplete version of a LU factorization.
- On ill-conditioned problem, ILU factorization increases numerical errors.

If the diagonal entries are much smaller than off-diagonal entries……



① In updating elements of a same row, off-diagonal(large) values divided by a diagonal(small) value have large numerical errors.

② Numerical errors are scattered in the process of updating unfactorized part.

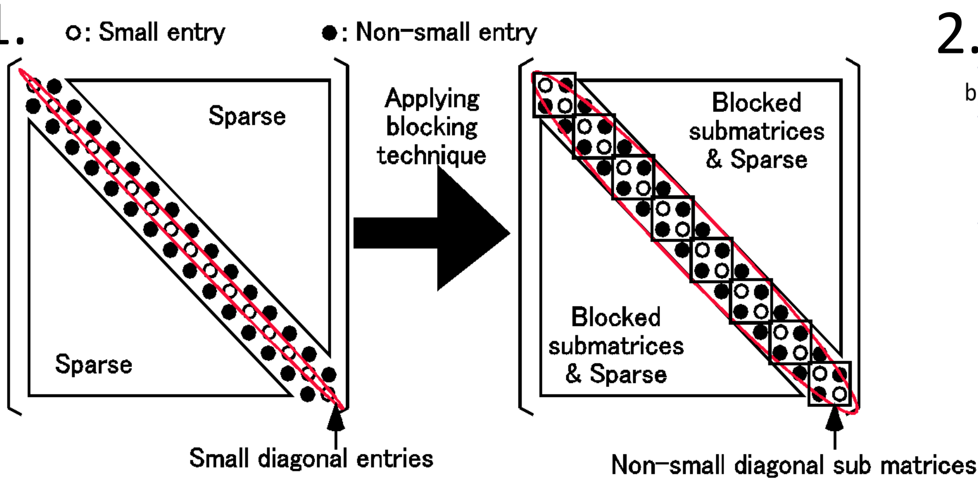
→On the worst case, a factorization fault occurs

Regularization ①

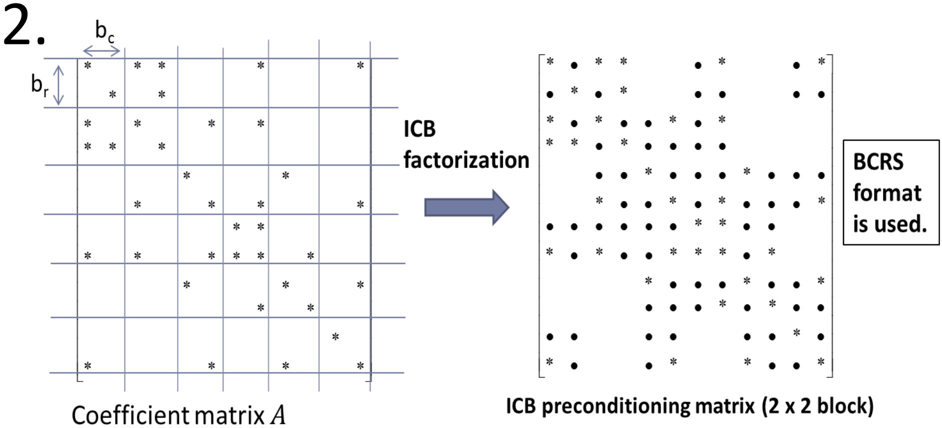
Applying 2 regularization methods for ILU preconditioner
→For robustness and improving convergence

- ■ Blocking technique (Regularization①)
  - Applying the incomplete decomposition to a block matrix
    1. More robustness because of including non-small off-diagonals
    2. Better convergence ratio because of allowing more fill-ins

1.



2.



Regularization ②

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- **Diagonal transformation (Regularization②)**
  - Adding constant value α to the diagonal elements
  - Directly method to make the diagonally dominant matrix

$$\widetilde{A_z} = A_z + \alpha I \quad I = \text{identity matrix}$$

Applying the ILU factorization to the matrix $\widetilde{A_z}$

Target problems

Total:128 data sets

- Graph
  - 4 data sets : 1k, 10k, 100k, 1M

	1k	10k	100k	1M
DoF	1,000	10,000	100,000	1,000,000
# non-zero	13,000	130,000	1,300,000	13,000,000

  - 2 shift data sets : shift-1, shift-2
  - 8 shift values in each data

- Topi
  - 4 data sets : 1k, 10k, 100k, 1M

	1k	10k	100k	1M
DoF	1,000	10,240	102,400	1,024,000
# non-zero	12,200	122,880	1,228,800	12,492,800

  - 2 shift data sets : shift-1, shift-2
  - 8 shift values in each data

Shift-2 of each problems make difficult conditions, comparatively

Multi-color ordering for parallelizing BIC preconditioner

Parallelization method of BIC preconditioner with multi-coloring

Example of 3-colored matrix

Forward and backward substitution has sequentiality.

By applying the Multi-color ordering,

Multi-color ordering for parallelizing BIC preconditioner

Parallelization method of BIC preconditioner with multi-coloring

Example of 3-colored matrix

Forward and backward substitution has sequentiality.

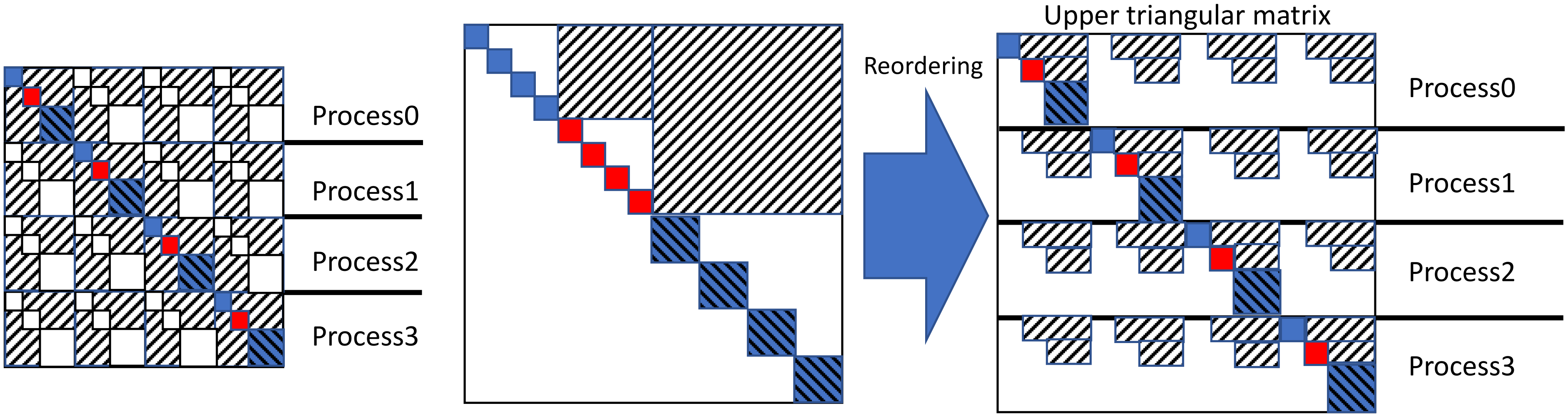
By applying the Multi-color ordering,

- No relationship between same color
- Calculating the elements with same color, parallelly

The convergence of the multi-colored ICCG is changed.

IC decomposition with multi-coloring

In the program, we calculate the upper triangular matrix directly from the colored base matrix.



Applying algebraic multi-coloring(AMC) method

Sample code of AMC

```
ncolor=some value ! Set number of used colors
color(1:n)=0 ! Initialize the array color
icolor=1
do i=1,n
    j=1
    do while(j <= lnz(i))
        if (color(lnzc(i, j))==icolor) then
            icolor=mod(icolor, ncolor)+1 !To next color
            j=0
        endif
        j=j+1
    enddo
    color(i)=icolor ! Assignment of color
    icolor=mod(icolor, ncolor)+1 !To next color
enddo
```

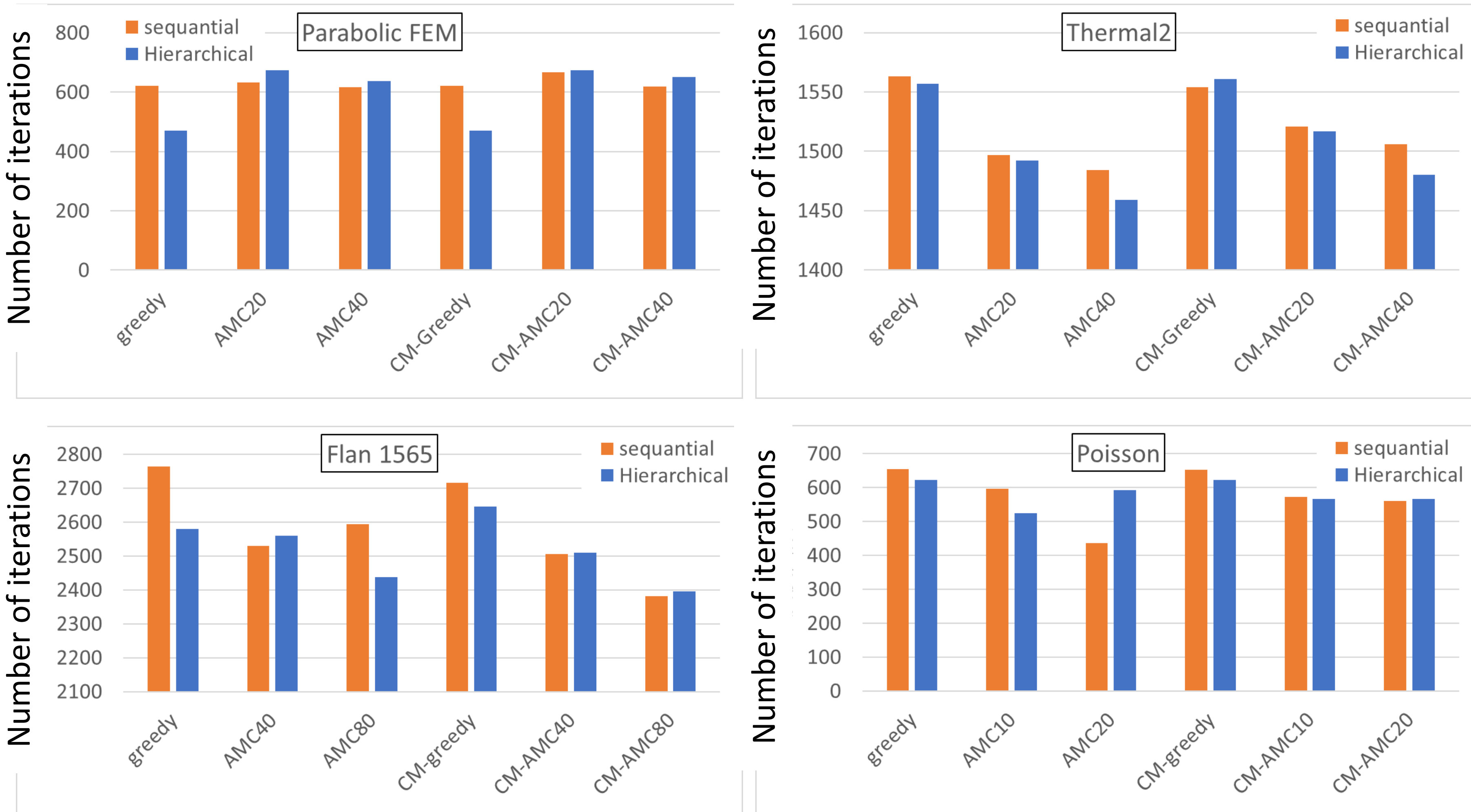
Ref: T. Iwashita. et al. “Algebraic Multi-Color Ordering Method for Parallelized ICCG Solver in Unstructured Finite Element Analyses”

- We can control the number of colors.
  → The convergence ratio and computation time have dependency on the number of colors.
- The number of unknowns are nearly even in each colors, relatively.
  → Load is evenly distributed.

Result of hierarchical coloring 1/3

Compared the convergence between the sequential method and the proposed(32 processes) method.

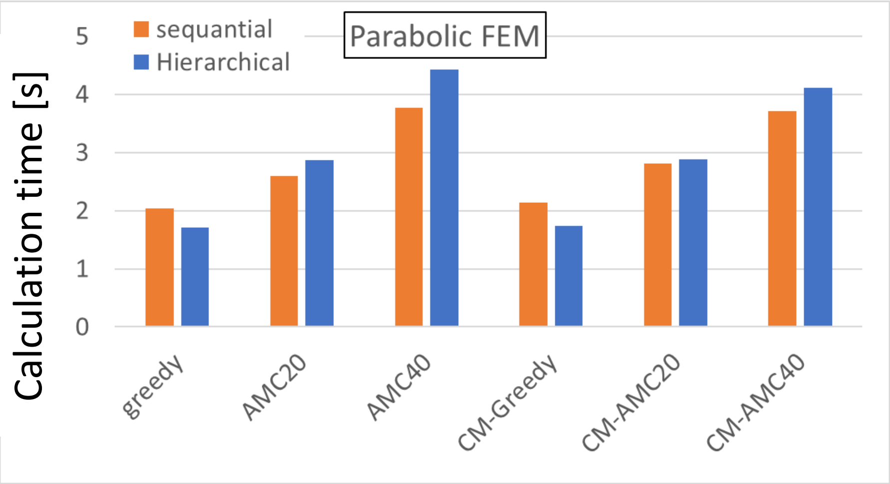
→Showed similar properties.

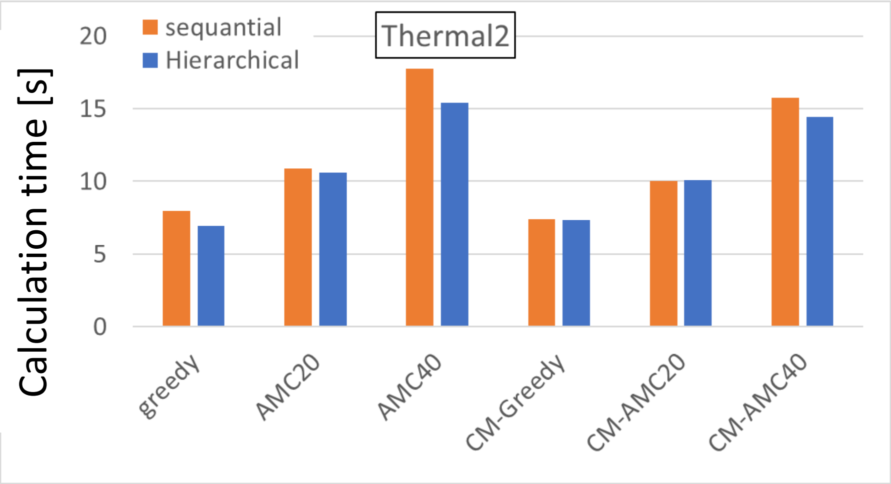


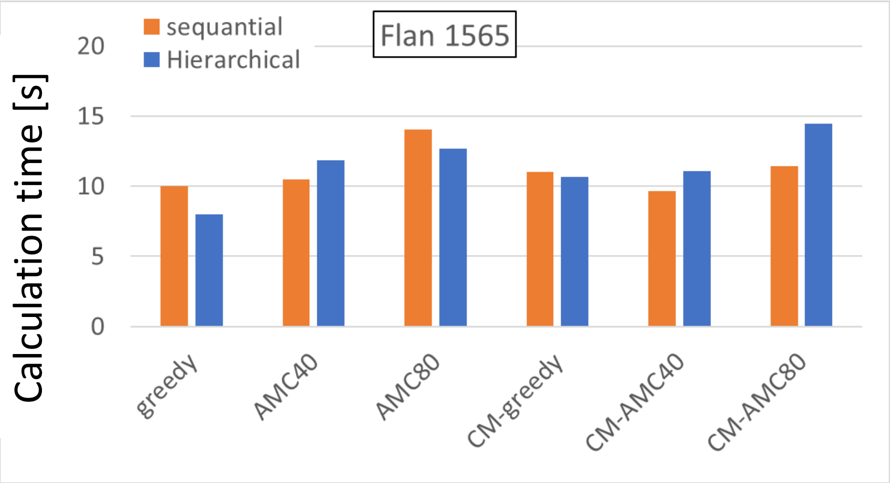
Result of hierarchical coloring 2/3

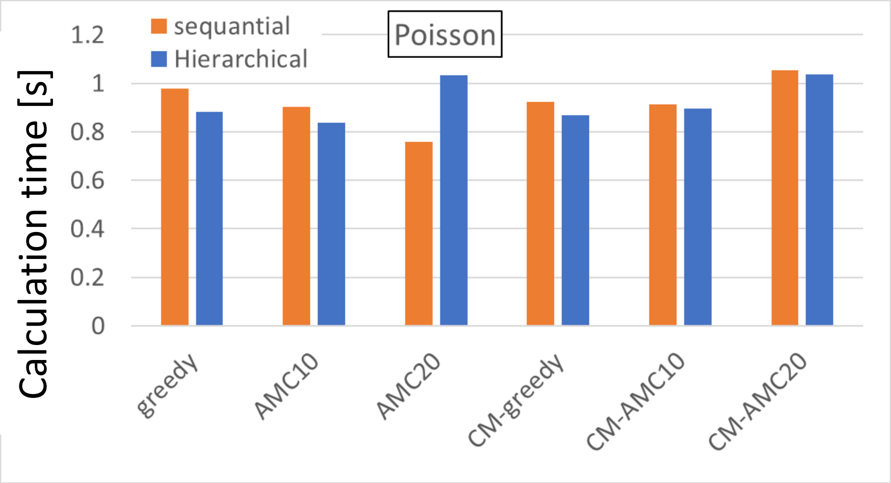
Unshowed large difference in the calculation times.

Graphs shows the computational time of iterations(32 processes).





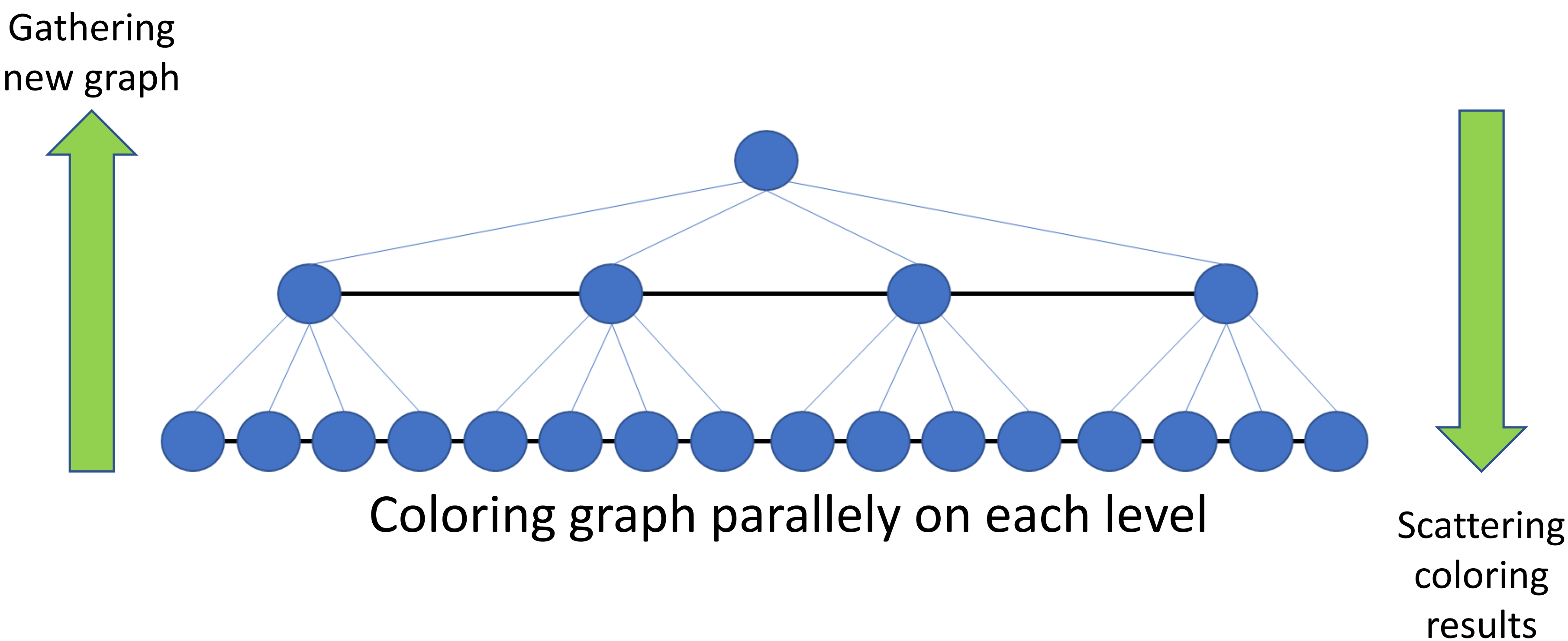




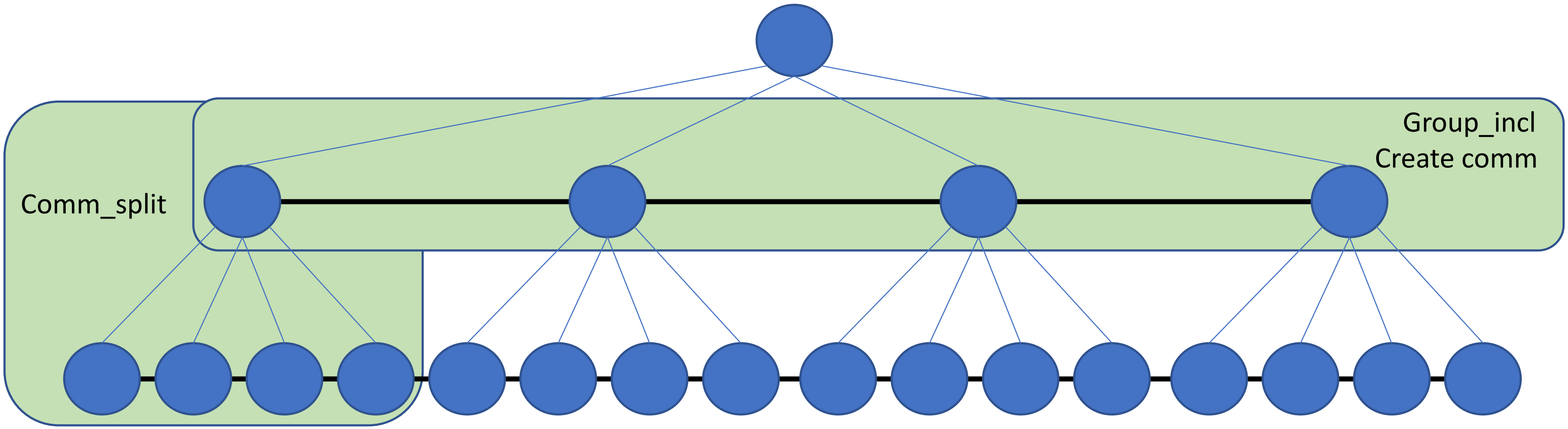
Hierarchical parallelization (Multi-level)

We applied the multi-level algorithm for massively parallelism.

→To reduce the time of the gathering, the scattering and the coloring on the master process



Implementation of hierarchical approach



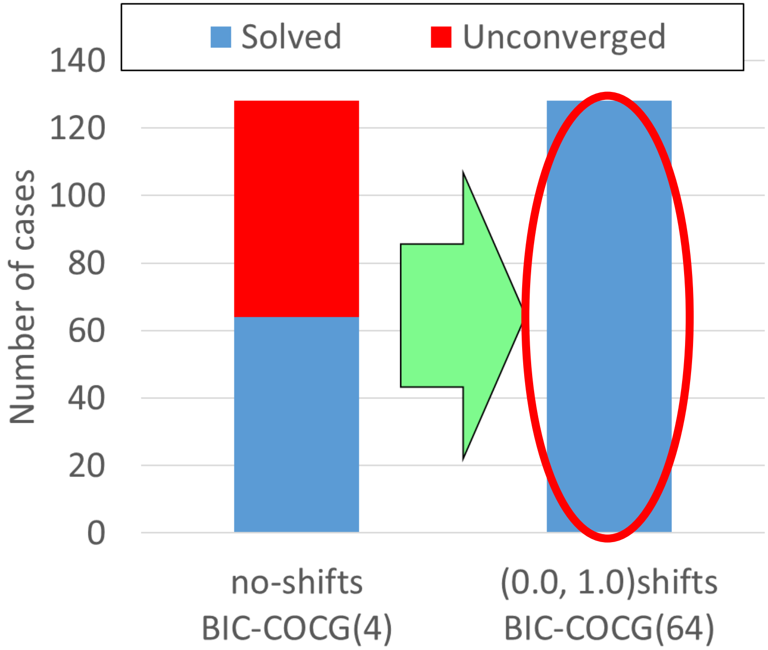
For robustness (Previous study)

IC preconditioned CG with regularization methods solve the targets

- Applied regularization methods
  - Blocking technique
  - Diagonal shifting

A simplified code of BIC-CG

```
Block IC decomposition
do itr = 1, DoF
        dot_product
        q = Ã^{-1} r (preconditioning)
        Matrix Vector Multiplication
enddo
```



For massively parallelization (Objective)

Proposing hierarchical parallelization for multi-color algorithms

→Needed for solving the large scale SLEs on massively parallel systems

```
Block IC decomposition
do itr = 1, DoF
        dot_product
        q = Ã^{-1} r (preconditioning)
        Matrix Vector Multiplication
enddo
```

For massively parallelization (Objective)

Proposing hierarchical parallelization for multi-coloring algorithms

→Needed for solving the large scale SLEs
on massively parallel systems

- Multi-color ordering is used for parallelize BIC-CG method.
  - Multi-coloring algorithms are not parallelized.

Multi-coloring ← Still sequentially

Block IC decomposition

do itr = 1, DoF

dot_product

$q = \tilde{A}^{-1} r$(preconditioning)

Matrix Vector Multiplication

enddo

Parallelizing with multi-coloring

Parallelizing easily

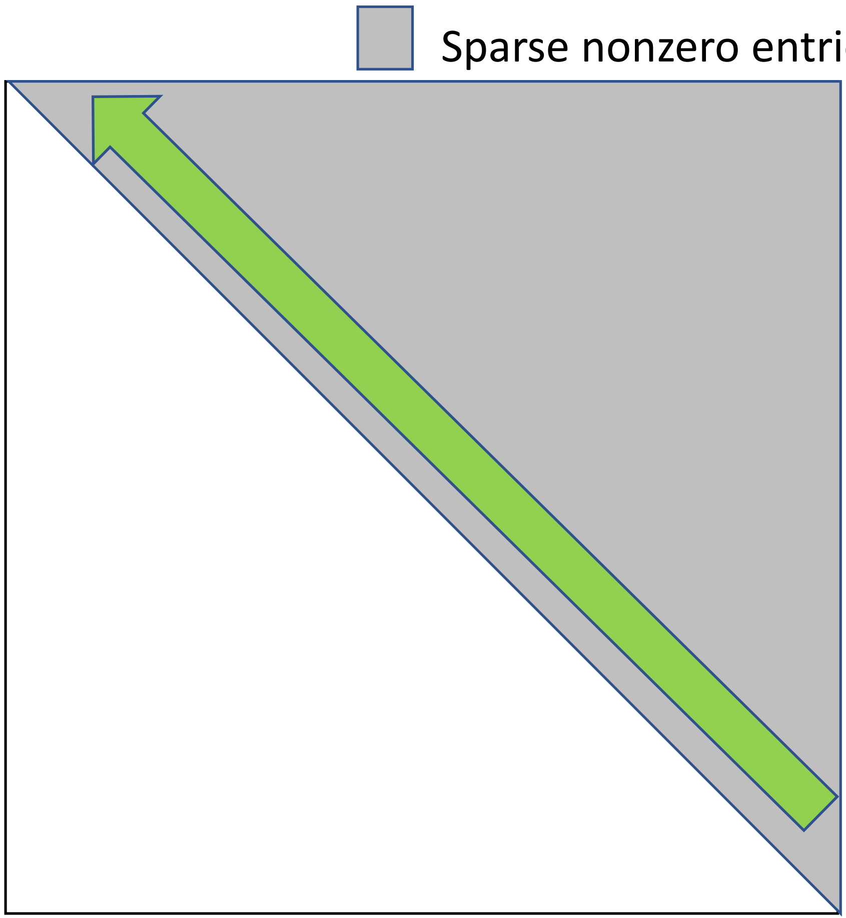
Index

- Introduction
- Parallelization of BIC-CG
- Hierarchical parallelization of multi-coloring algorithms
- Numerical experiments
- Conclusion

Multi-color ordering for parallelizing BIC preconditioner

Parallelizing the BIC preconditioner with multi-coloring

Example of IC decomposed matrix(Only upper)

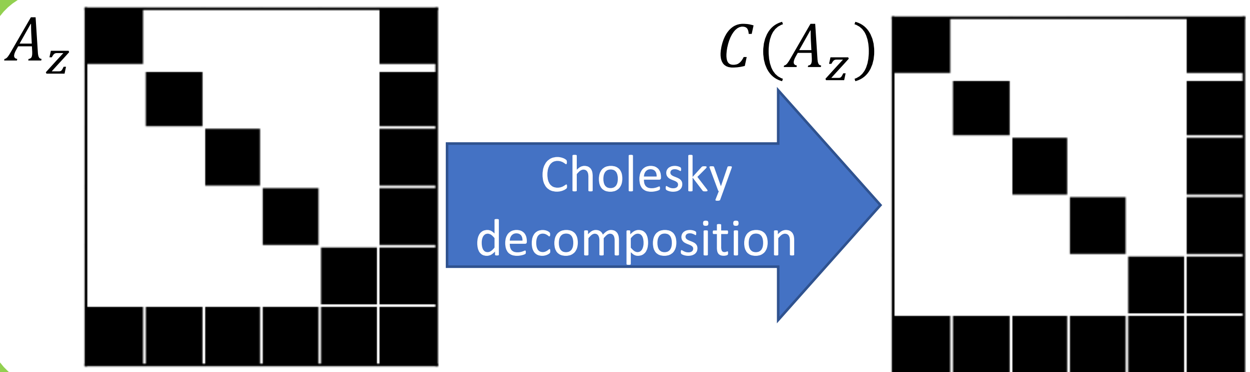


Forward and backward substitution has sequentiality.

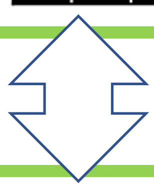
Effect of multi-coloring on convergence

The result of multi-coloring influences the convergence and performance.

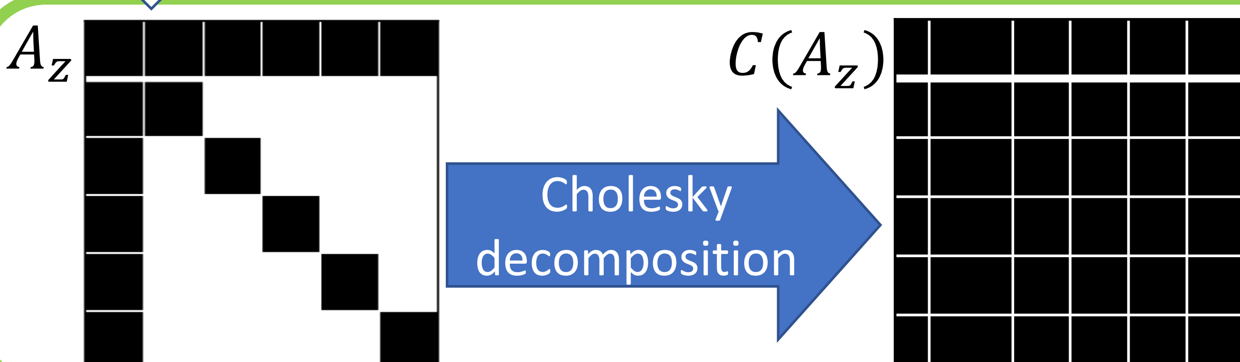
→ Multi-coloring changes the order of the matrices.
There are many multi-coloring algorithms.



Zero and Nonzero pattern is same completely.
$\rightarrow IC(A_z) = C(A_z)$



Same matrix



Decomposed matrix is dense
$\rightarrow IC(A_z) \approx C(A_z)$??

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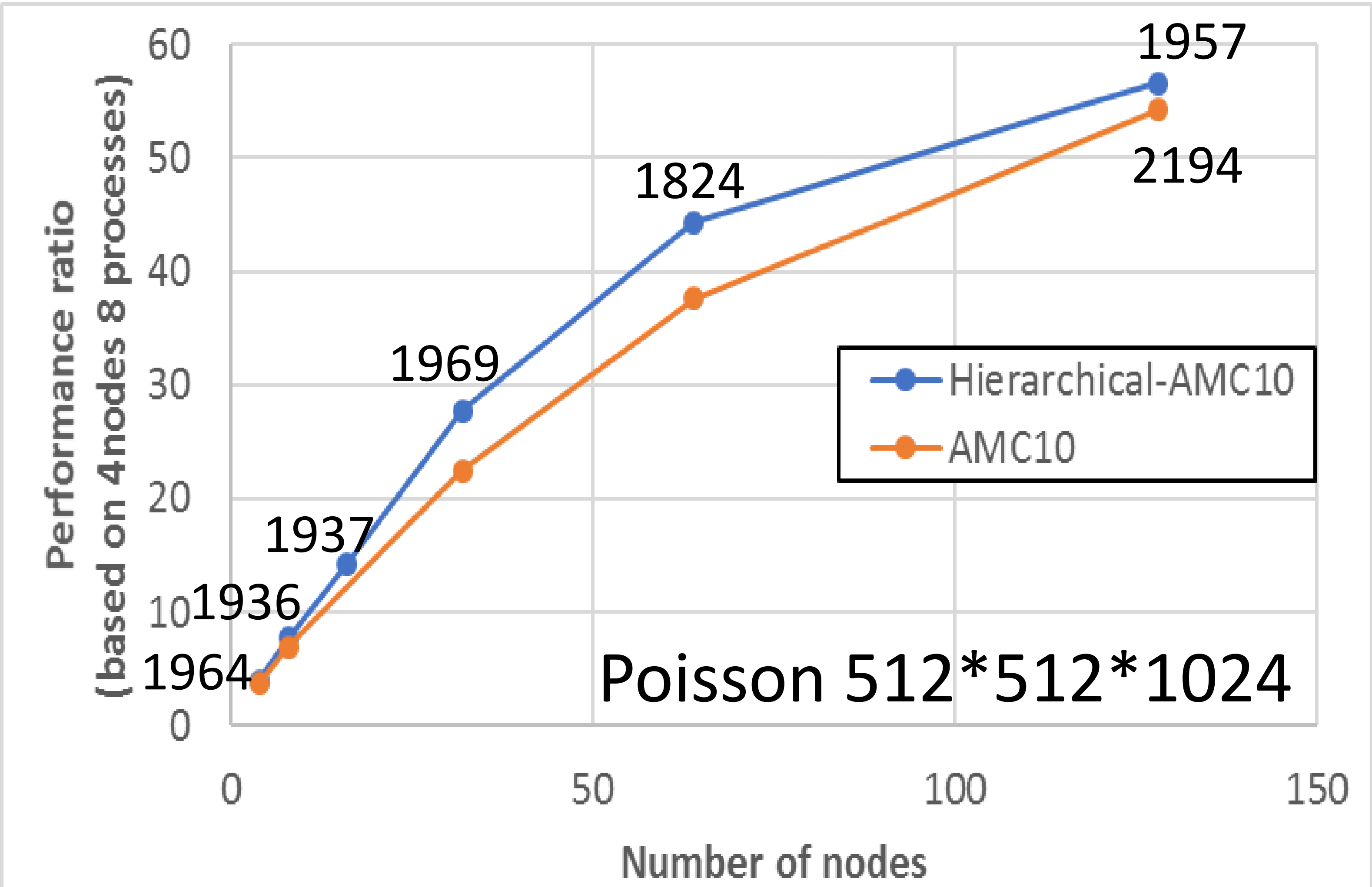
Result of computational time on larger problems.

Showed the similar convergence and performance on larger problems



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- Numerical experiments
- **Conclusion**

Conclusion

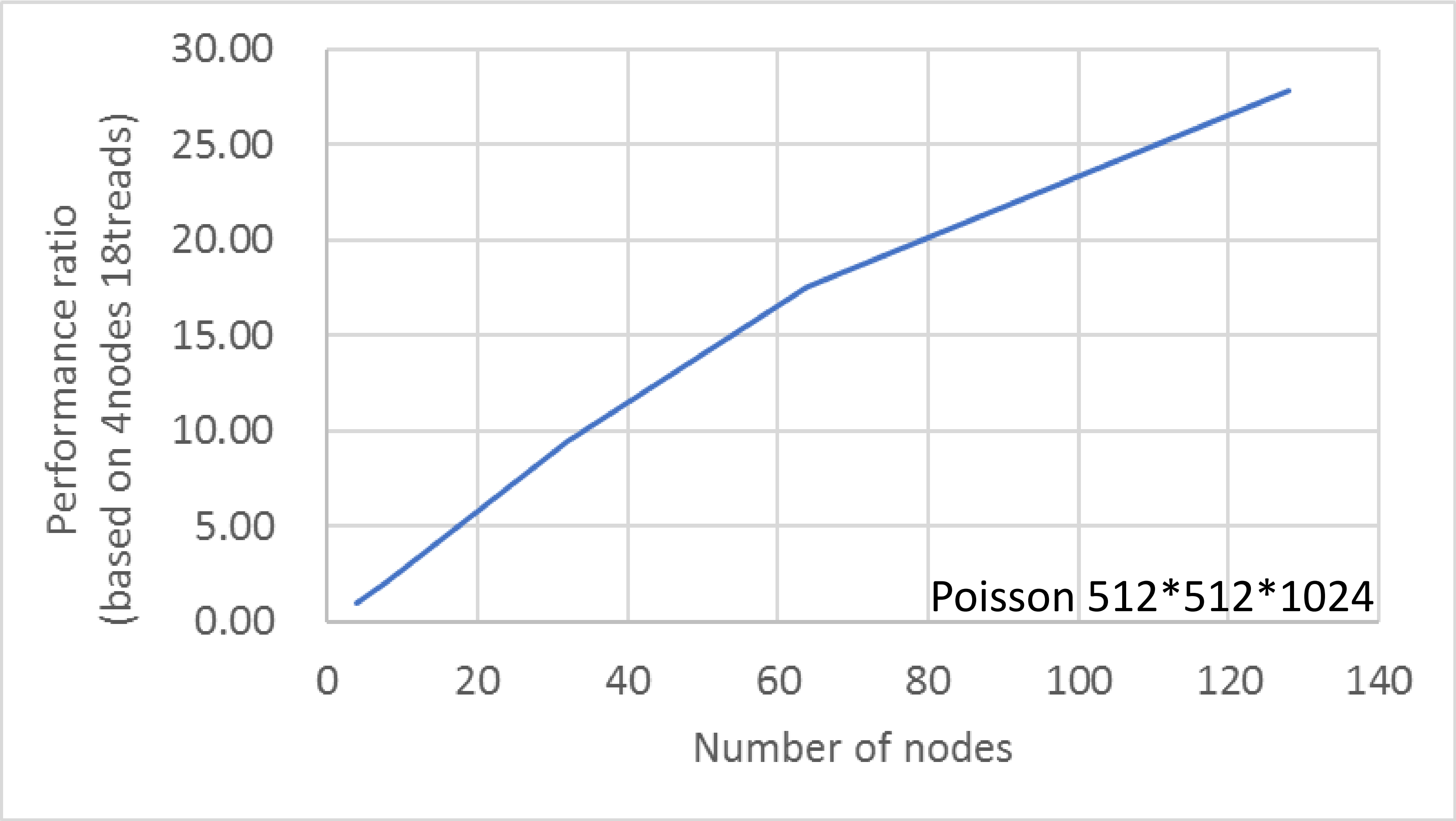
■Proposing the hierarchical parallelization for multi-coloring algorithms
- ●Versatile parallelization method

■Numerical experiments showed the results as we had expected.
- ●There are no large differences between the sequentially and the parallelized coloring.
  - → Properties of the existing coloring algorithms are not changed.
- ●We have solved the large scale problem.

Future works
- ●Needed more performance for massively parallel system
  - ✓ Communication hide by coloring
- ●Attacking to more large problems derived from quantum systems

Performance of the coloring

The performance of coloring routine is good.



The time of coloring is less than 2.5% in 128 nodes.

Evaluations of the numerical analysis 2/2

■Oakleaf-FX 4 ～ 1024 nodes

Node specifications

✓SPARC64™ IXfx 16cores

✓32GiB

Network specifications

✓Tofu

■Hybrid parallelization

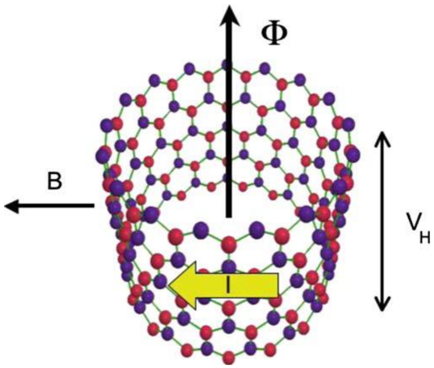
1process-16 threads (1process per node)

■ Coloring algorithm for test

Hierarchical parallelized AMC(10)

■ Target problem

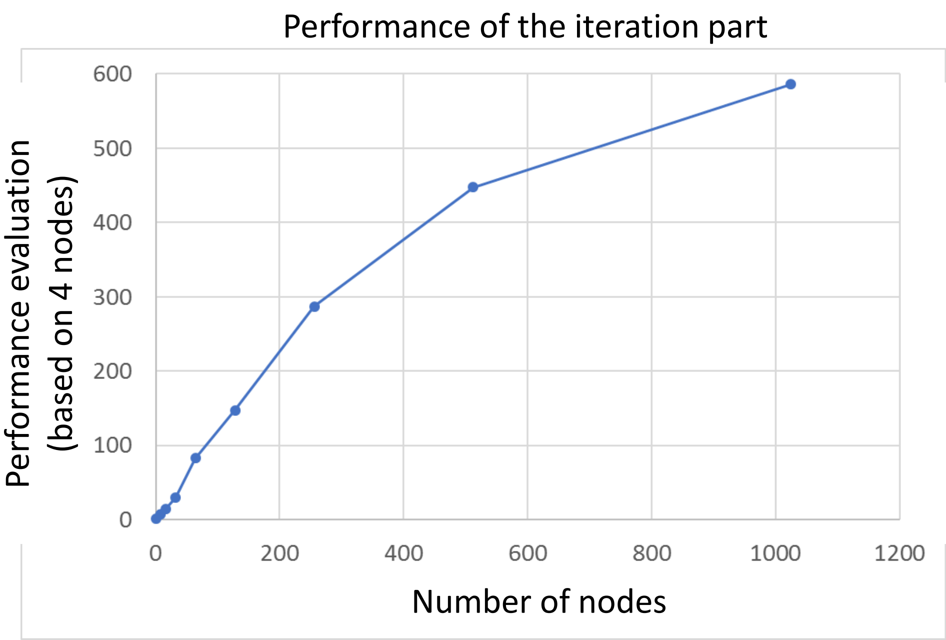
Graphen8194 × 4096 ≒ 33M DoF

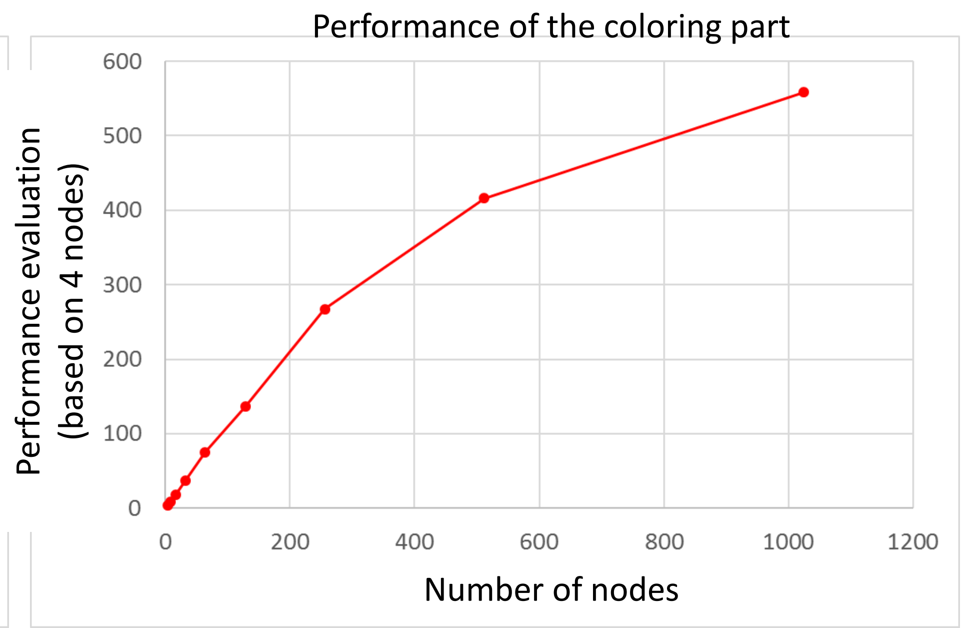


Source : The electronic properties of graphene

Performance on graphene problem

Showed good performance both iteration and coloring part





	Number of nodes								
	4	8	16	32	64	128	256	512	1024
# of iterations	27,812	27,823	27,812	27,823	27,801	27,823	27,823	27,801	27,823

Regularizations 1/2

Needed robust IC preconditioner to solve target SLEs
→Proposing to apply regularizations

Properties of the matrix A_z

- Complex symmetric
- Sparse
- Large DoF
- Small diagonal entries compared with off-diagonal
- Positive and negative diagonal entries
- ill-conditioned: high condition number

Needed robust IC preconditioner to solve target SLEs
→Proposing to apply regularizations

Properties of the matrix A_z

- Complex symmetric
- Sparse
- Large DoF
- Small diagonal entries compared with off-diagonals
- Positive and negative diagonal entries
- ill-conditioned: high condition number

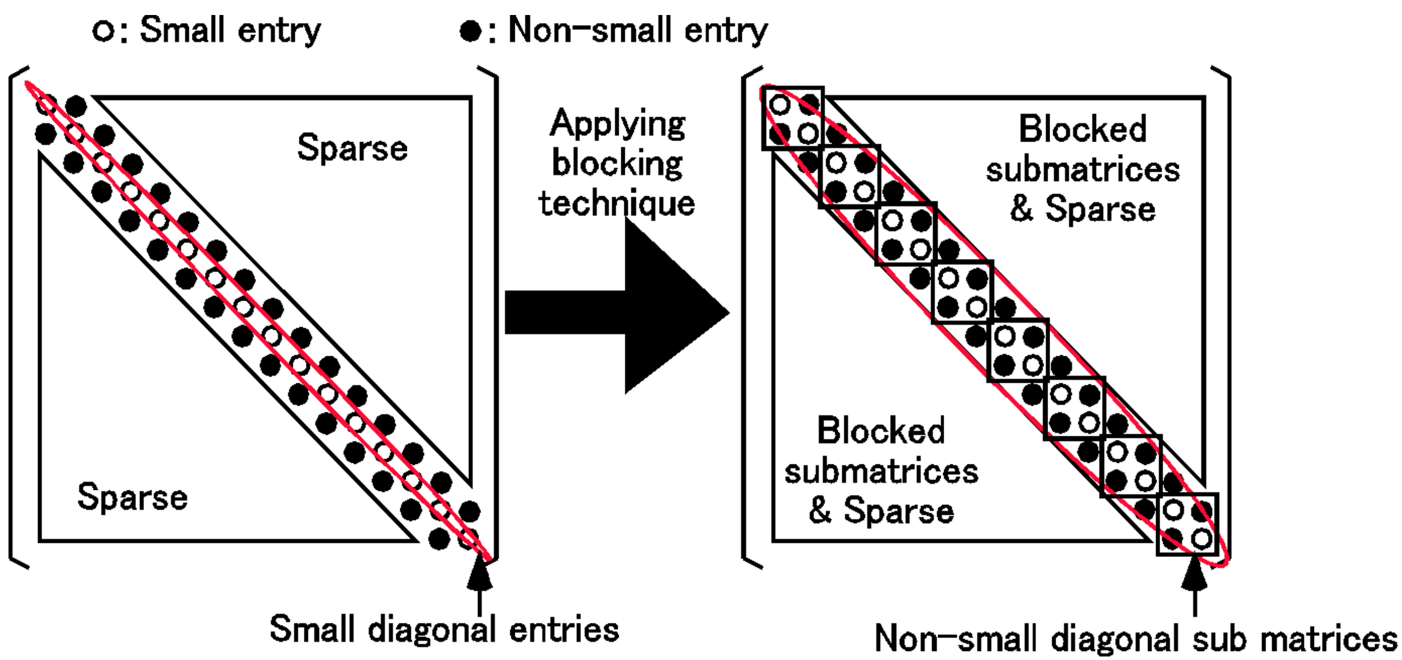
These properties is increasing computational errors in the IC factorization.
→① By applying regularizations, we try to approximating A_z by $\widetilde{A_z}$ which is a diagonal dominant matrix.
② Factorizing $\widetilde{A_z}$

Regularization① 1/2

Applying 2 regularization methods for IC preconditioner
→For robustness and improving convergence

- Blocking technique(Regularization①)
  - Applying the incomplete decomposition to a block matrix
    1. More robustness because of including non-small off-diagonals
    2. Better convergence ratio because of allowing more fill-ins

1.

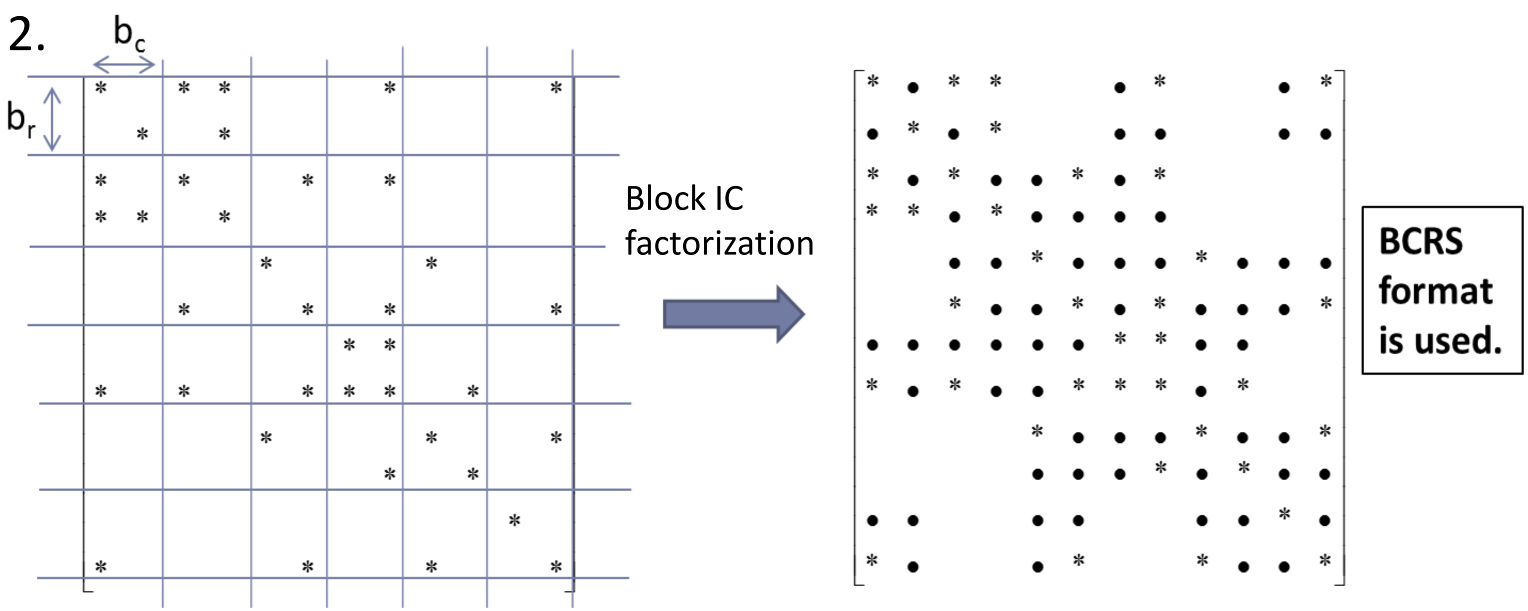


Regularization① 2/2

Applying 2 regularization methods for IC preconditioner
→For robustness and improving convergence

- Blocking technique(Regularization①)
  - Applying the incomplete decomposition to a block matrix
    1. More robustness because of including non-small off-diagonals
    2. Better convergence ratio because of allowing more fill-ins

2.



Coefficient matrix A

Block IC factorized matrix (block size is 2)

Regularization②

Applying 2 regularization methods for the IC preconditioner
→For robustness and improving convergence

- Blocking technique(Regularization①)
  - Applying the incomplete decomposition to a block matrix
    1. More robustness because of including non-small off-diagonals
    2. Better convergence ratio because of allowing more fill-ins

- Diagonal transformation(Regularization②)
  - Adding constant value α to the diagonal elements
  - Directly method to make the diagonally dominant matrix

$$\widetilde{A_z} = A_z + \alpha I \quad I = \text{identity matrix}$$

* $\widetilde{A_z}$ is a matrix for IC factorization.
Regularization② is only applied for the matrix.

Analysis conditions(previous report)

- Iteration method: COCG
  - The algorithm is similar to CG method
  - For the complex symmetric coefficient matrix

- Preconditioner : IC decomposition with
  - Blocking technique
  - Diagonal shifting

- $b = randam(min = 1, max = 10)$
  *both real and imaginary parts

- Iteration is stop if the number of iteration reach to DoF or relative residual fills the requirement $\left\|\frac{r^k}{r^0}\right\|_2 \leq 10^{-7}$

Target problems

Total:128 data sets

- Graphene (Real values)
  - 4 data sets : 1k, 10k, 100k, 1M

	1k	10k	100k	1M
DoF	1,000	10,000	100,000	1,000,000
# non-zero	13,000	130,000	1,300,000	13,000,000

  - 16 *z* data sets

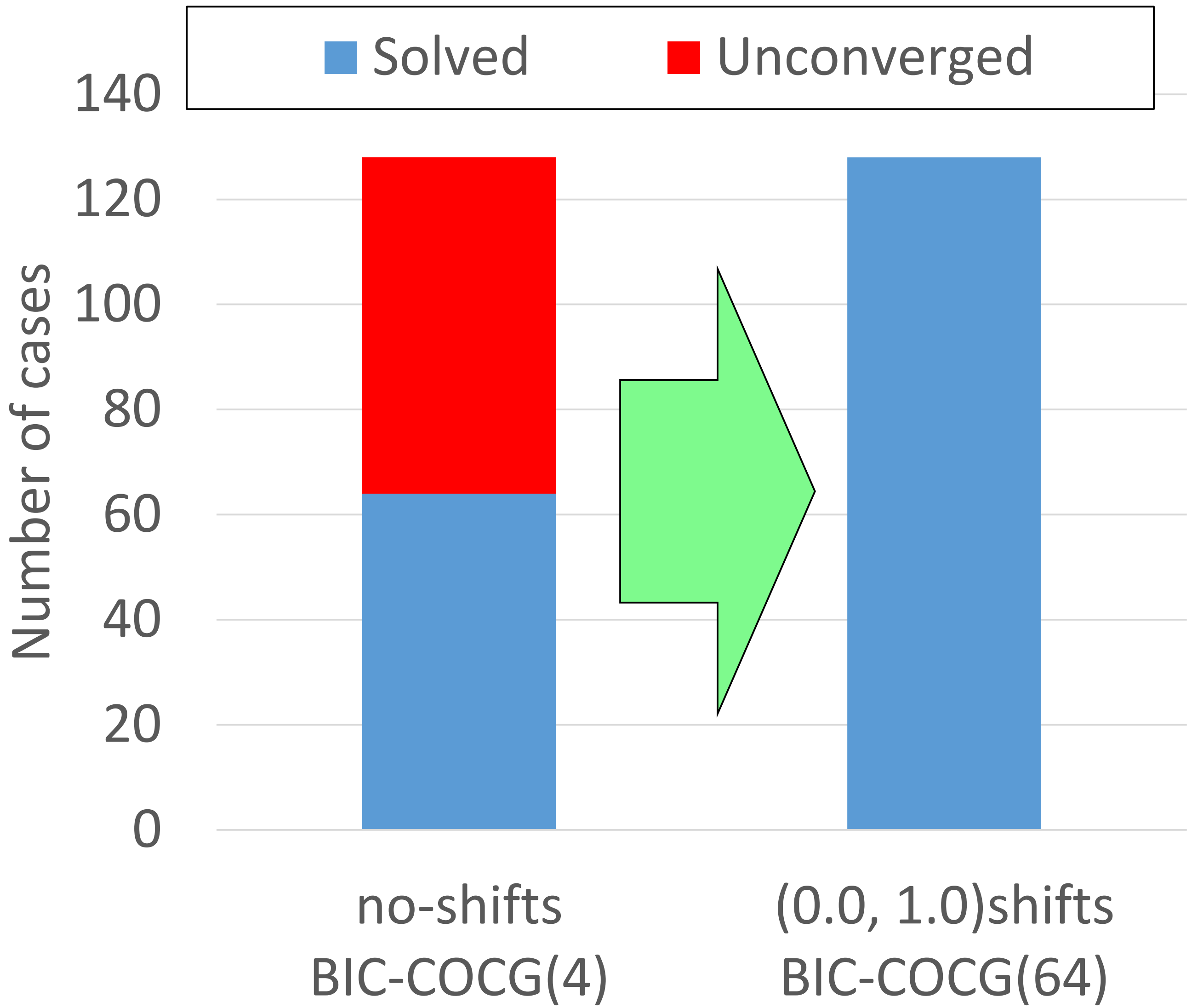
- Topological insulator (Complex values)
  - 4 data sets : 1k, 10k, 100k, 1M

	1k	10k	100k	1M
DoF	1,000	10,240	102,400	1,024,000
# non-zero	12,200	122,880	1,228,800	12,492,800

  - 16 *z* data sets

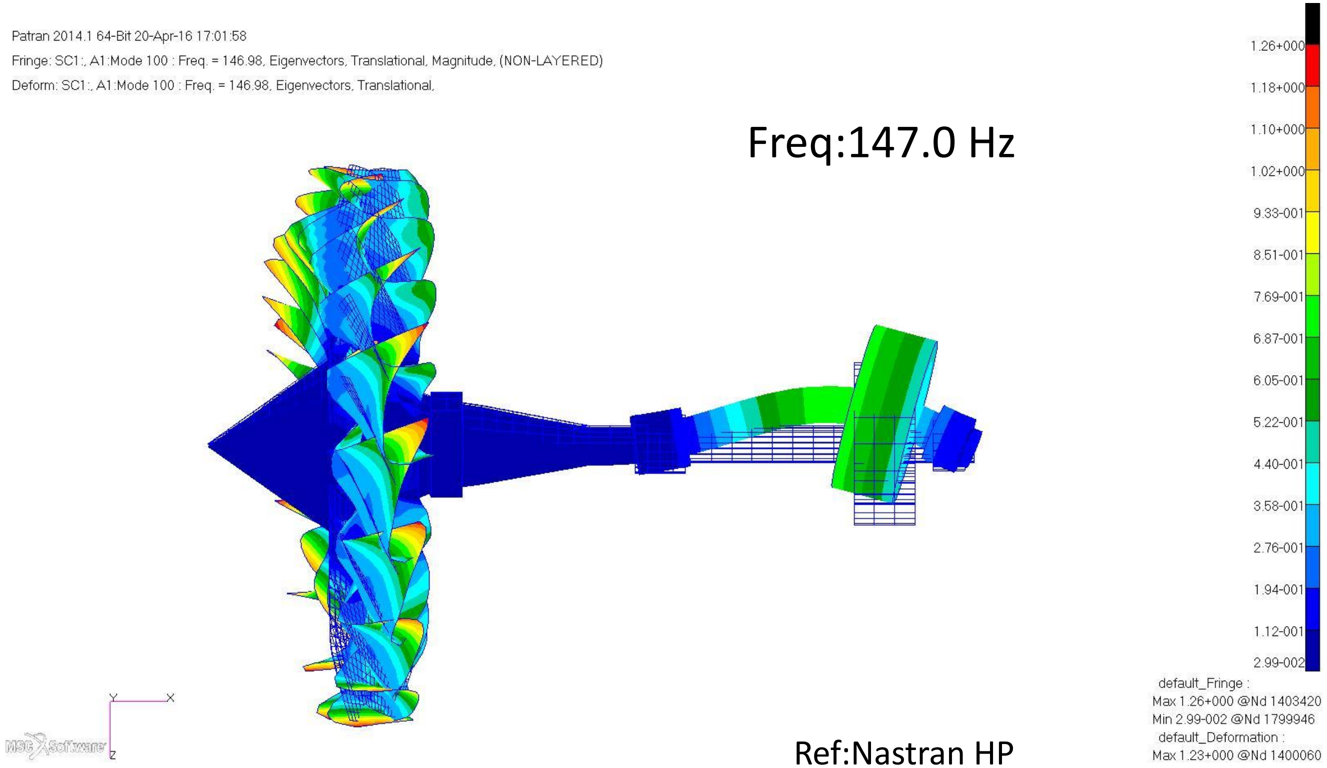
Result

Solved all data sets



(0.0,1.0)-BICCG(64) :Diagonal shifting is (0.0, 1.0) Block size is 64

Example of eigenvalue

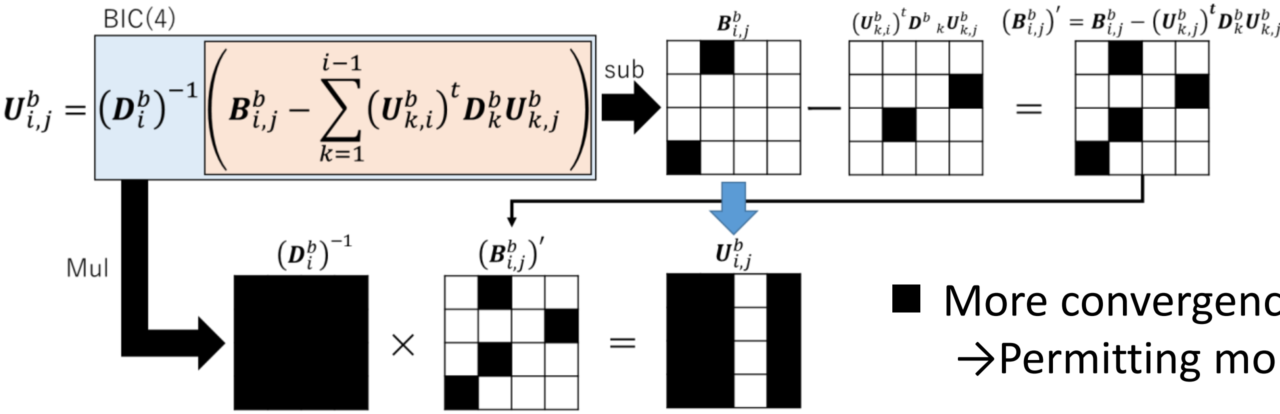


Freq:147.0 Hz

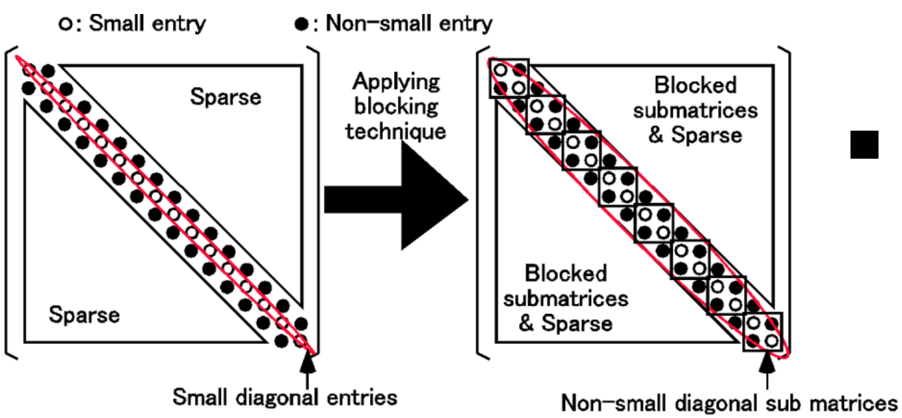
Ref:Nastran HP

Block ICCG preconditioner for CG method

The ICCG preconditioner with a blocking technique



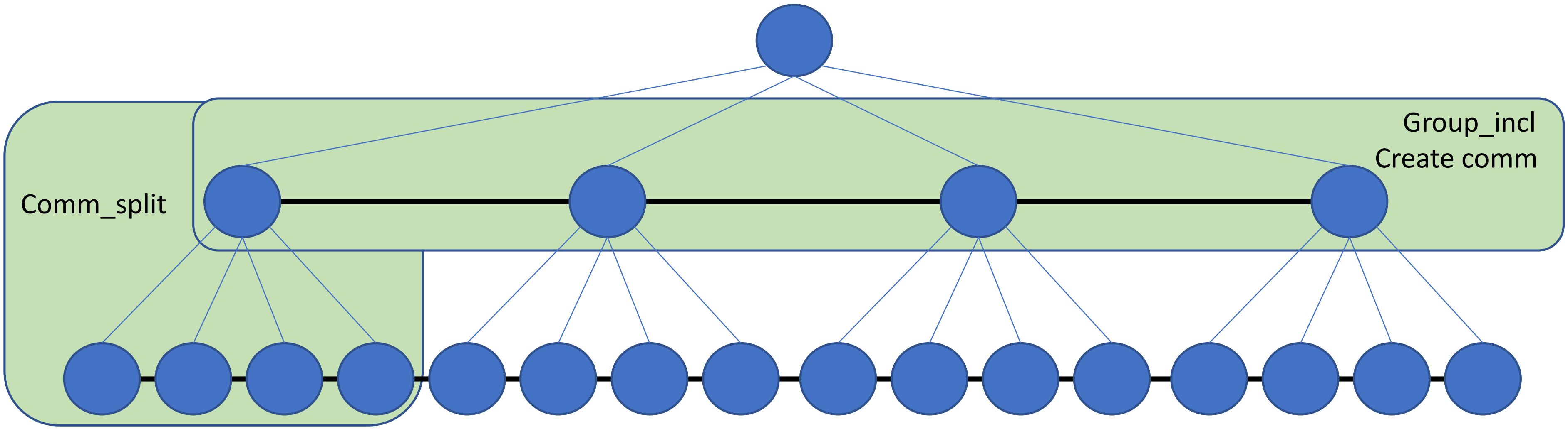
- More convergence than the general ICCG
  →Permitting more fill-ins



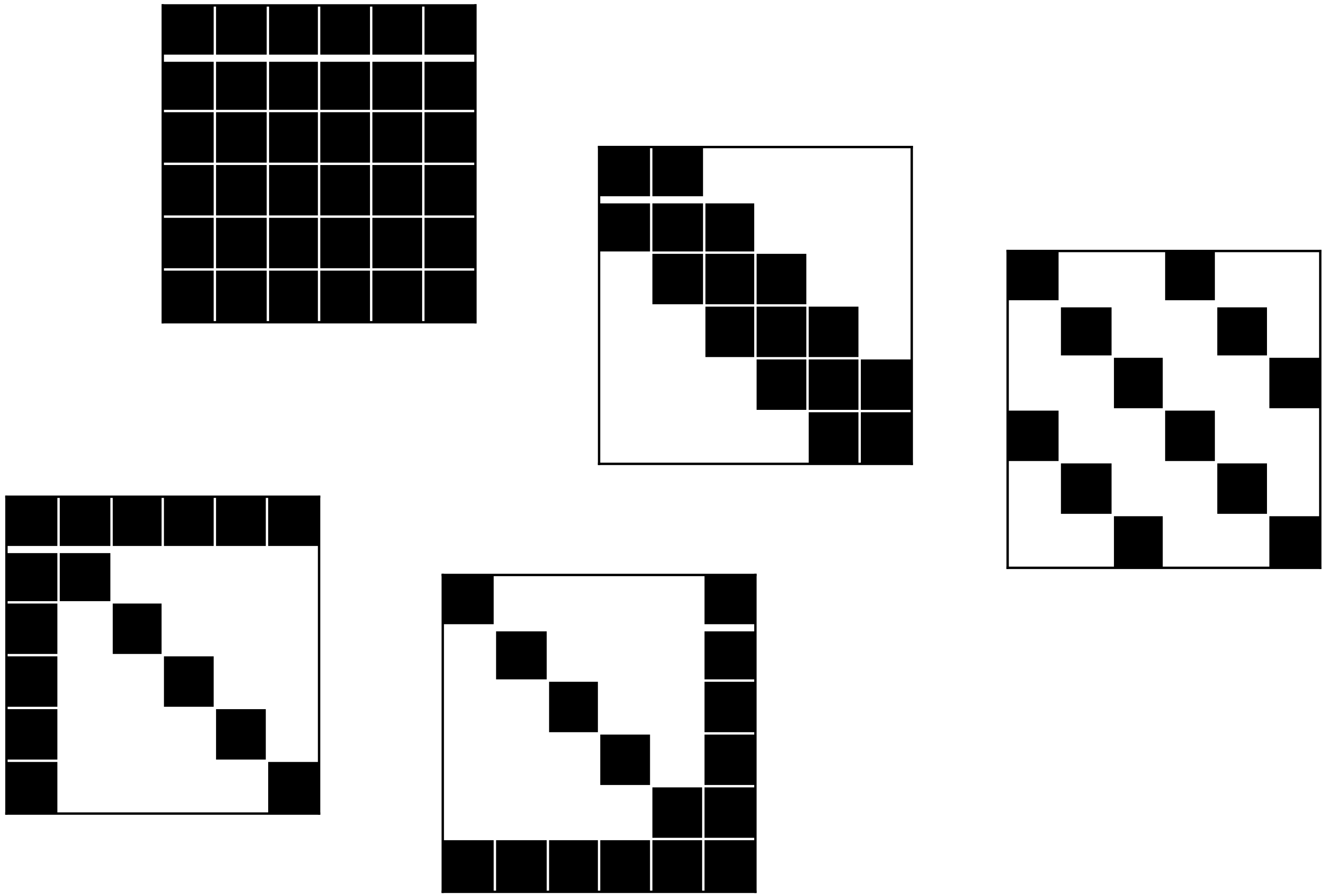
- More robustness
  →Diagonal matrix including off-diagonal elements

Hierarchical parallelization (Multi-level)

We applied the multi-level algorithm



e



Proposing hierarchical parallelization for the multi-coloring algorithms

General coloring algorithms are sequential.

Two approaches for parallelizing the multi-coloring algorithms

- ■ Proposing special parallelized multi-coloring algorithms.
  - ● Better for performance of coloring
  - ● Sometimes, not good for convergence and performance of BIC-CG
- ■ Proposing versatile parallelization method
  → Hierarchical approach
  - ● Parallelize any coloring algorithms
    - ✓ Can we parallelize coloring algorithms without changing properties?
      ←Investigating with numerical experiments