Introduction to Parallel Programming for Multicore/Manycore Clusters

Part B2: Reordering

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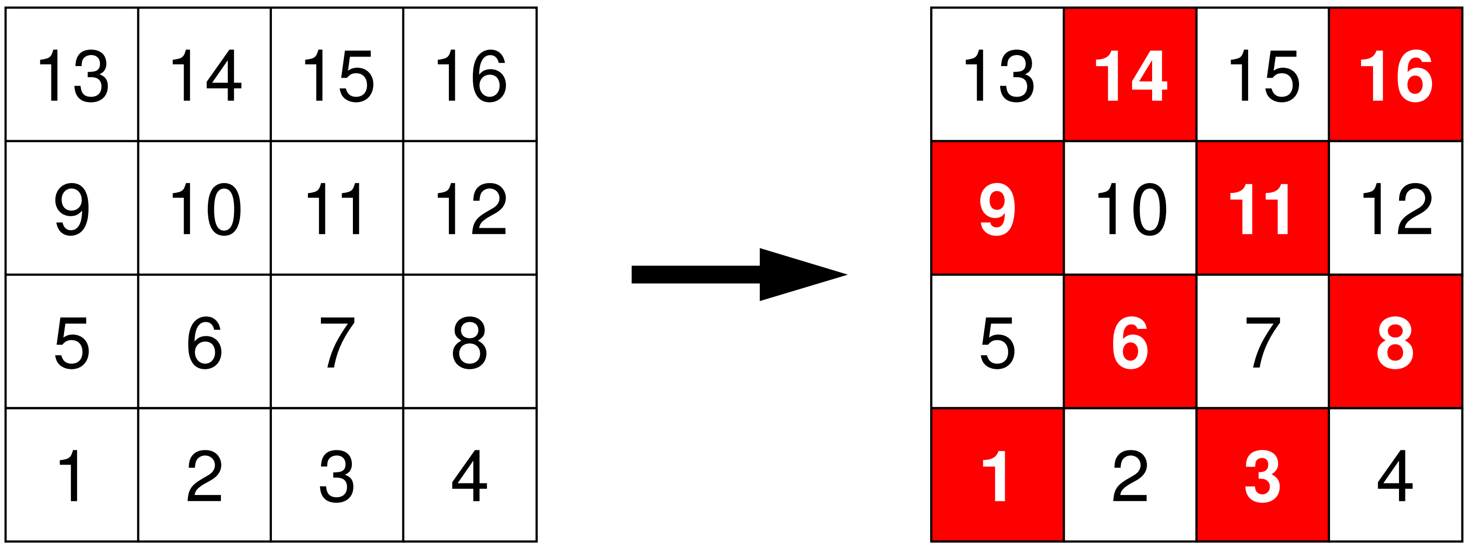
- Remedy for Data Dependency
- Ordering/Reordering
  - Red-Black, Multicoloring (MC)
  - Cuthill-McKee (CM), Reverse-CM (RCM)
  - Reordering and Convergence
- Implementation
- ICCG with Reordering

Parallelize ICCG Method

- Dot Product: OK
- DAXPY: OK
- Matrix-Vector Multiply: OK
- Preconditioning: Something special needed !
  - Just inserting OpenMP directive is not enough

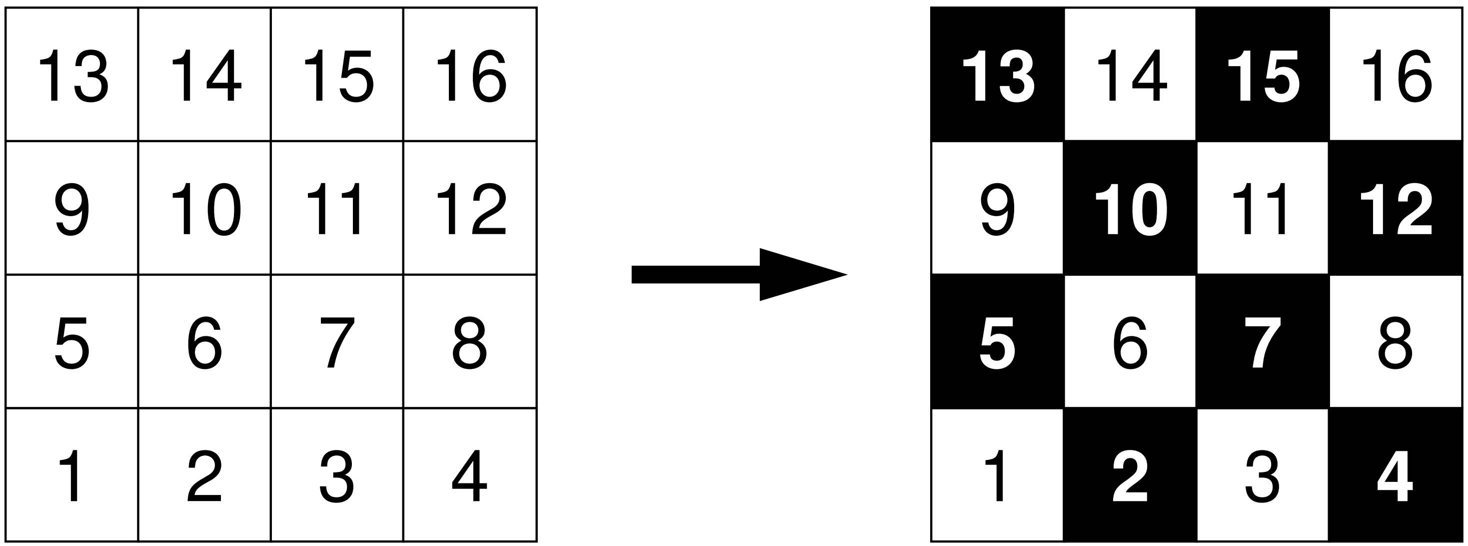
One Remedy for Data Dependency = Coloring

- Parallel (concurrent) processing is possible for independent meshes without dependency



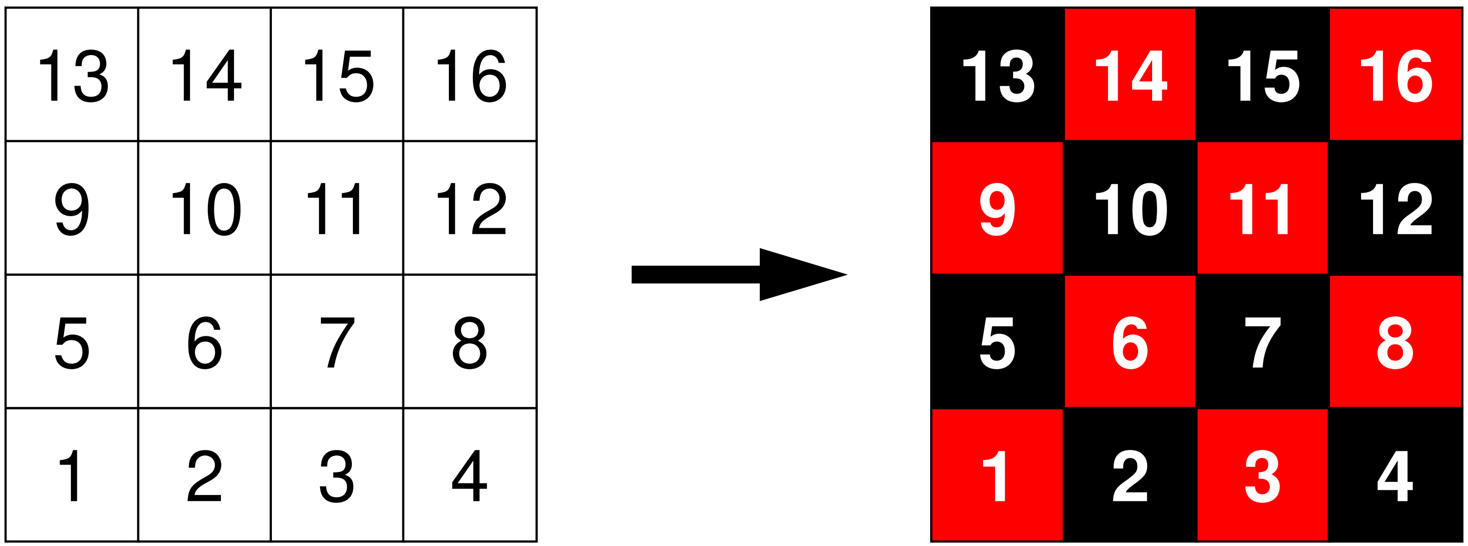
One Remedy for Data Dependency = Coloring

- Parallel (concurrent) processing is possible for independent meshes without dependency

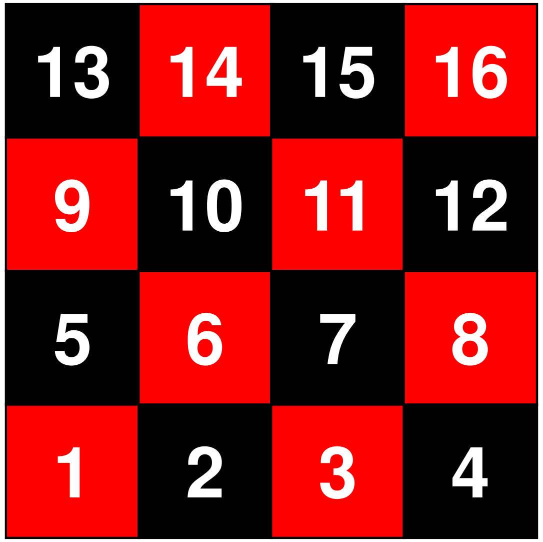


One Remedy for Data Dependency = Coloring

- Applying same "color" to independent meshes without dependency: Coloring
- Most simple case: Red-Black with 2 Colors



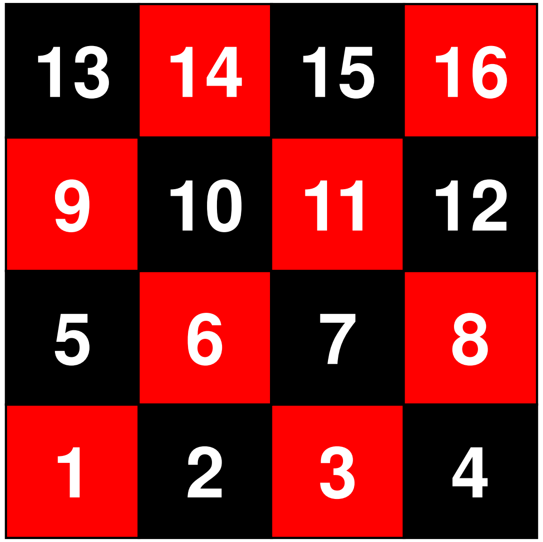
Red-Black (1/3)




```
!$omp parallel do private (ip,i,k,VAL)
  do ip= 1, 4
  do  i= INDEX(ip-1)+1, INDEX(ip)
    if (COLOR(i).eq.RED) then
      WVAL= W(i,Z)
      do k= indexL(i-1)+1, indexL(i)
        WVAL= WVAL -  AL(k) * W(itemL(k),Z)
      enddo
      W(i,Z)= WVAL * W(i,DD)
    endif
  enddo
  enddo
!$omp parallel enddo

!$omp parallel do private (ip,i,k,VAL)
  do ip= 1, 4
  do  i= INDEX(ip-1)+1, INDEX(ip)
    if (COLOR(i).eq.BLACK) then
      WVAL= W(i,Z)
      do k= indexL(i-1)+1, indexL(i)
        WVAL= WVAL -  AL(k) * W(itemL(k), Z)
      enddo
      W(i,Z)= WVAL * W(i,DD)
    endif
  enddo
  enddo
!$omp parallel enddo
```

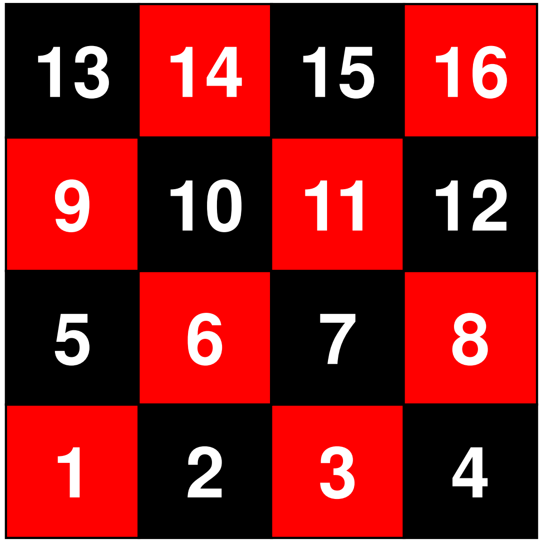
Red-Black (2/3)




```
!$omp parallel do private (ip,i,k,VAL)
  do ip= 1, 4
  do  i= INDEX(ip-1)+1, INDEX(ip)
    if (COLOR(i).eq.RED) then
      WVAL= W(i,Z)
      do k= indexL(i-1)+1, indexL(i)
        WVAL= WVAL -  AL(k) * W(itemL(k), Z)
      enddo
      W(i,Z)= WVAL * W(i,DD)
    endif
  enddo
  enddo
!$omp parallel enddo
```

- During operations on "red" meshes, only "black" meshes appear in RHS.
  - "red": writing, "black": reading
- During operations on "red" meshes, values on "black" meshes do not change.
- Data dependency is avoided.

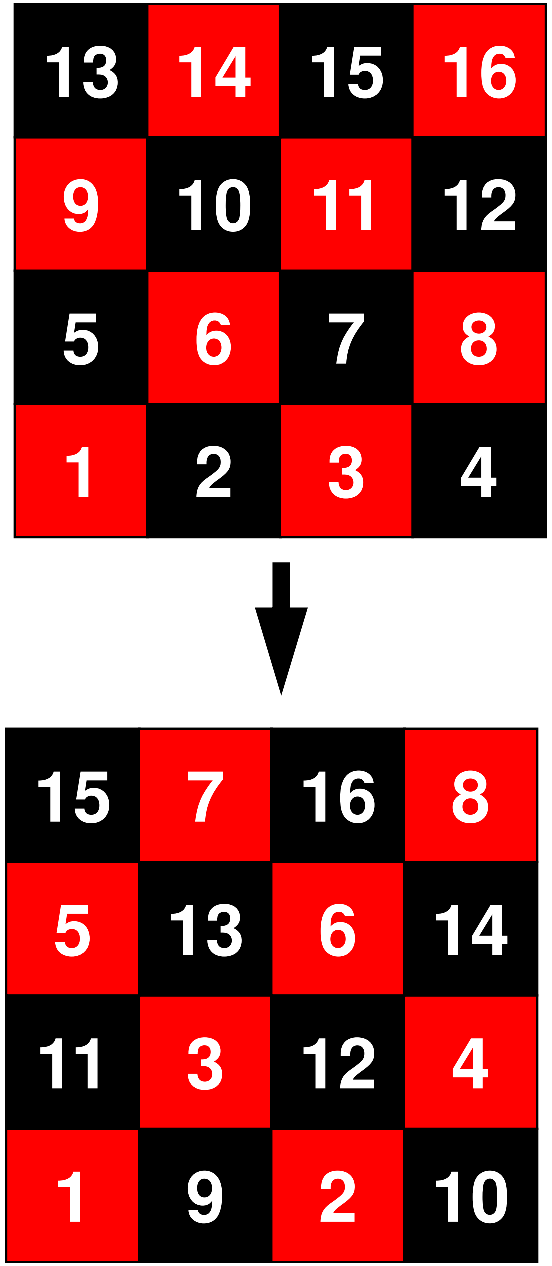
Red-Black (3/3)



- During operations on “black” meshes, only “red” meshes appear in RHS.
  - “black”: writing, “red”: reading
- During operations on “black” meshes, values on “red” meshes do not change.
- Data dependency is avoided.

```
!$omp parallel do private (ip,i,k,VAL)
  do ip= 1, 4
  do  i= INDEX(ip-1)+1, INDEX(ip)
    if (COLOR(i).eq.BLACK) then
      WVAL= W(i,Z)
      do k= indexL(i-1)+1, indexL(i)
        WVAL= WVAL -  AL(k) * W(itemL(k), Z)
      enddo
      W(i,Z)= WVAL * W(i,DD)
    endif
  enddo
  enddo
!$omp parallel enddo
```

Red-Black Ordering/Reordering




```
   do icol= 1, 2
!$omp parallel do private (ip,I,j,VAL)
     do ip= 1, 4
       do  i= INDEX(ip-1,icol)+1, INDEX(ip,icol)
         WVAL= W(i,Z)
         do k= indexL(i-1)+1, indexL(i)
           WVAL= WVAL -  AL(k) * W(itemL(k), Z)
         enddo
         W(i,Z)= WVAL * W(i,DD)
       enddo
     enddo
!$omp parallel enddo
   enddo
```

```
INDEX(0,1)= 0
INDEX(1,1)= 2
INDEX(2,1)= 4
INDEX(3,1)= 6
INDEX(4,1)= 8
```

```
INDEX(0,2)= 8
INDEX(1,2)=10
INDEX(2,2)=12
INDEX(3,2)=14
INDEX(4,2)=16
```

- Renumbering/reordering meshes from “red” to “black”
- Simpler, more efficient

- Remedy for Data Dependency
- **Ordering/Reordering**
  - **Red-Black, Multicoloring (MC)**
  - **Cuthill-McKee (CM), Reverse-CM (RCM)**
  - Reordering and Convergence
- Implementation
- ICCG with Reordering

Effect of Reordering

- **Extracting parallelism, removing dependency**
- Reducing
  - fill-in's, "bandwidth of matrix", "profile"
- Blocking

- Related to "four color problem", "travelling salesman problem" etc.
  - applied to numerical analysis

Ordering/Reordering Method for Parallel Computing

- Multicoloring (MC)
  - Parallelism
  - Red-Black with 2 colors
- CM (Cuthill-McKee), RCM (Reverse Cuthill-McKee)
  - Reducing fill-in’s, matrix bandwidth, profiles
  - Parallelism

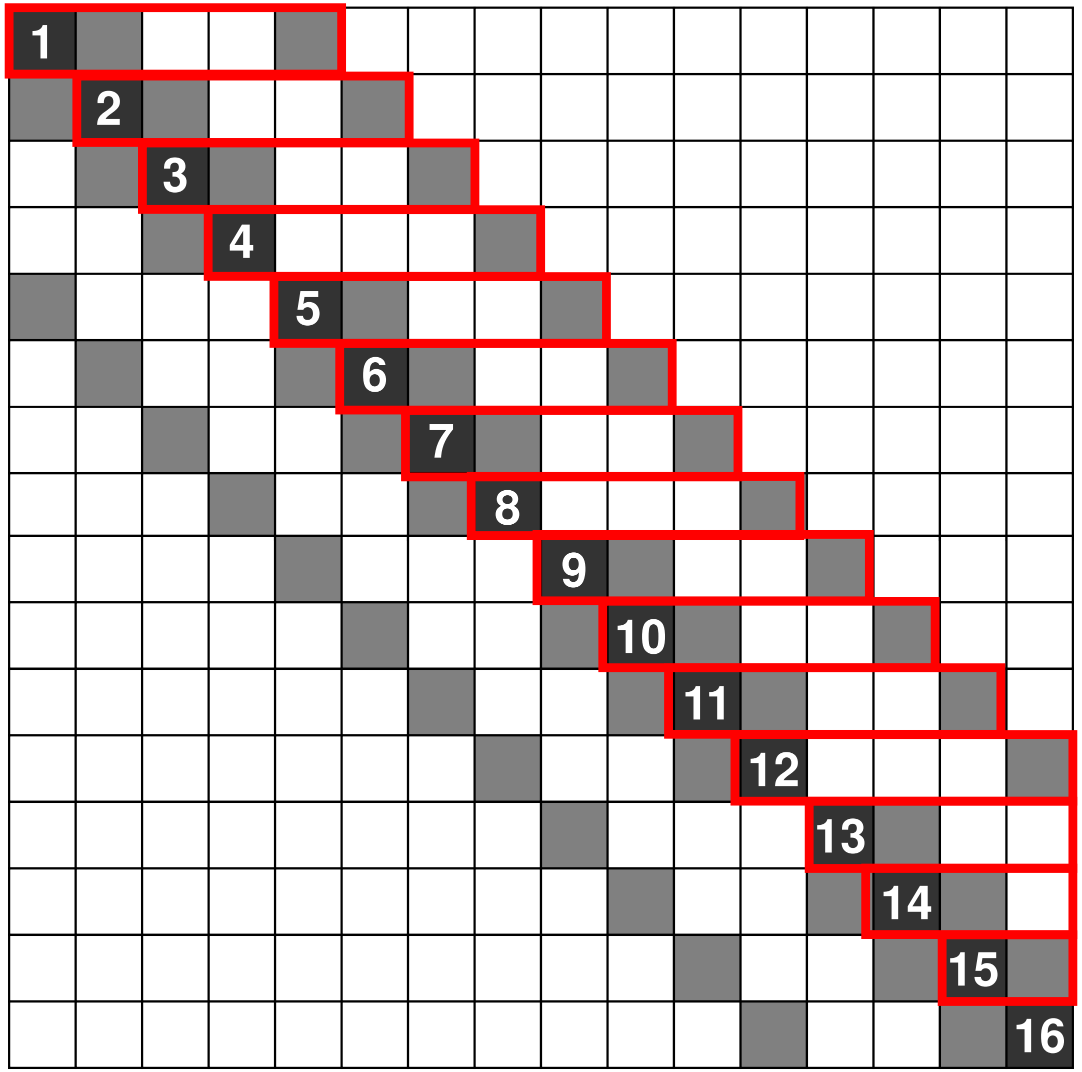
Technical Terms for Matrix

- β_i: $\beta_i = k - i$ where maximum ID number of non-zero column is k at i-th row of the target matrix
- Bandwidth: Maximum value of β_i
- Profile: Total sum of β_i

- Bandwidth, Profile, Fill-in
  - smaller is better
  - Both of “Bandwidth” and “Profile” of matrices affect convergence of preconditioned iterative sovers.

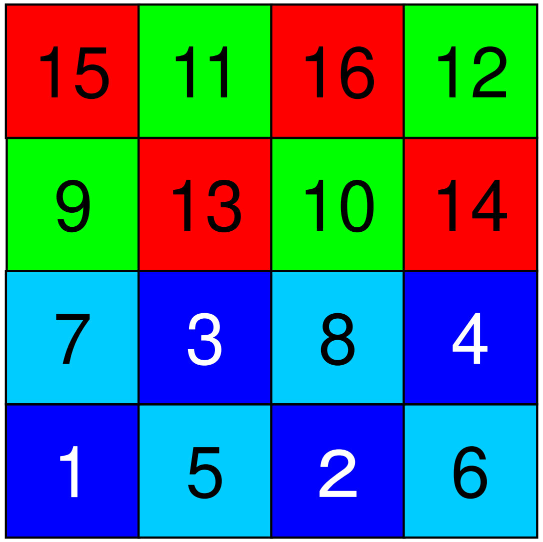
β_i

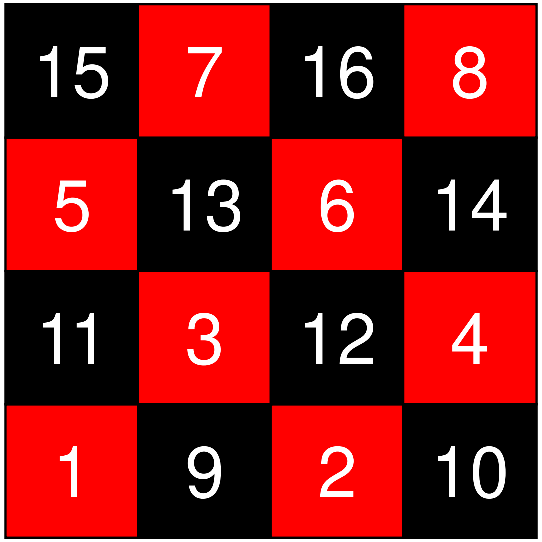
13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4



Non-zero off-diagonals

Multicoloring (MC), Multicolor Ordering





- Meshes in same color are independent, and renumbered according to the color ID.
  - Red-Black: MC with 2 colors
  - More colors needed for complicated geometries
- Parallel operations are possible for meshes in same color.
- A mesh and its neighboring meshes belong to different colors.

Fundamental Algorithm of MC Method

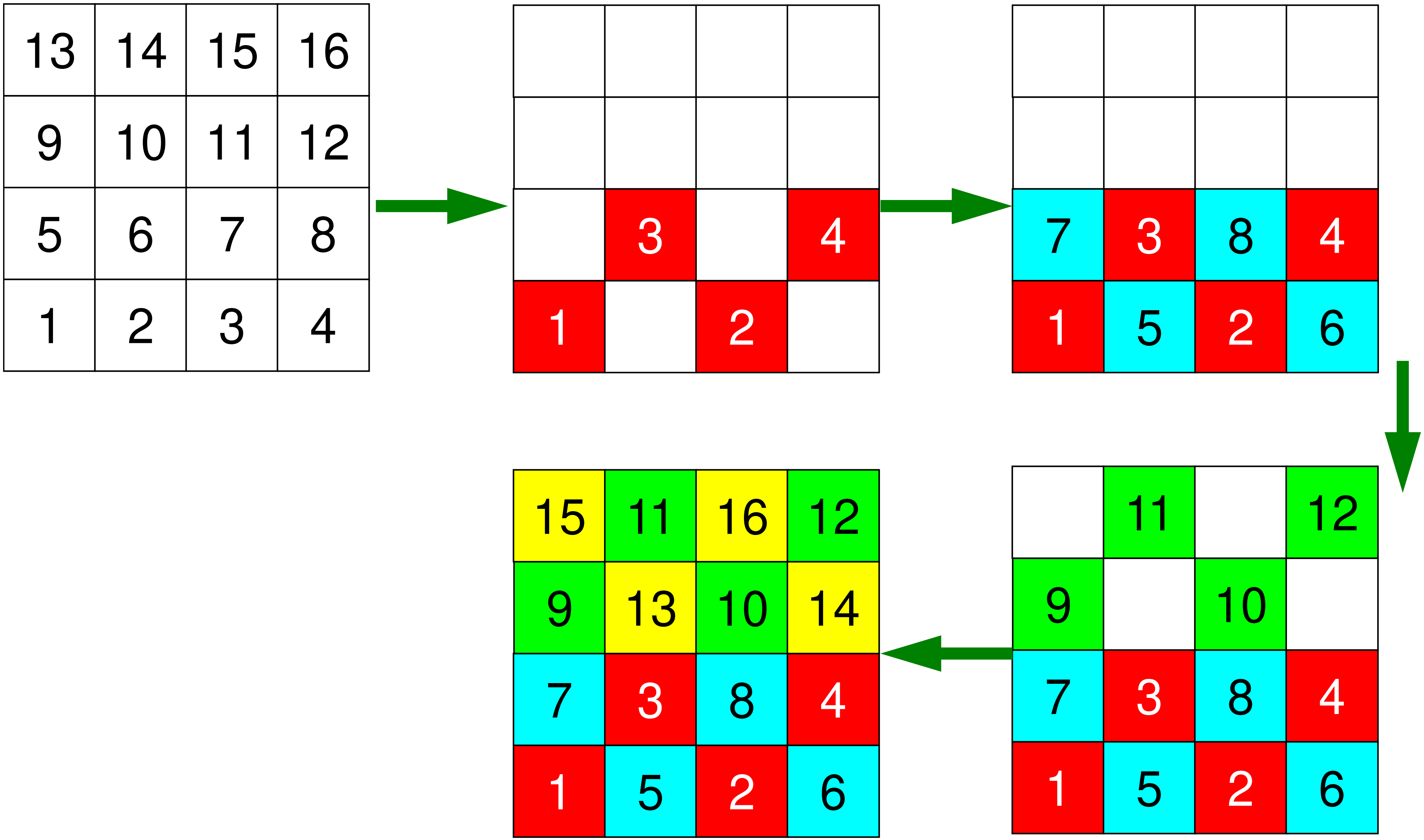
① m= mesh# / color#

② Color "m" independent meshes in ascending orders according to initial mesh ID, then proceed to the next "color"

③ Repeat ②, until every mesh is colored

④ Renumber meshes in ascending orders according to color ID. In each color, numbering is in ascending orders according to initial mesh ID.

MC with 4 Colors



Modified MC Method

① ONE mesh with minimum value of “degree” is set to “NEW mesh ID= 1”, “Color ID= 1”, and “counter for color number” is 1.

② Define “*ITEMcou= ICELTOT/NCOLORtot*”, where *ITEMcou* is maximum number of meshes in each color.

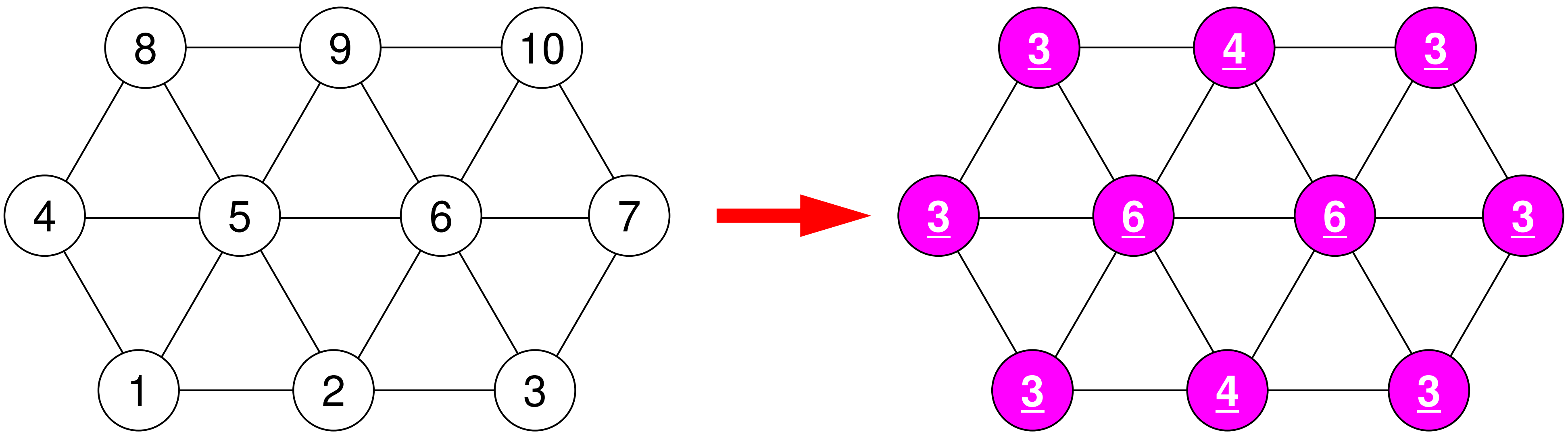
③ Color *ITEMcou* independent meshes in ascending order according to initial mesh ID.

④ If *ITEMcou* meshes are colored, or no more independent meshes do not exist, add “1” to the “counter for color number”, and proceed to the next color.

⑤ Repeat ③ and ④, until all meshes have been colored.

⑥ “Final counter for color” is *NCOLORtotF*. Renumber meshes in ascending orders according to color ID. In each color, numbering is in ascending orders according to initial mesh ID. In each color, new numbering of meshes is continuous.

“Degree”: Number of vertices adjacent to each vertex



Modified MC Method

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② Define "*ITEMcou= ICELTOT/NCOLORtot*", where *ITEMcou* is maximum number of meshes in each color.

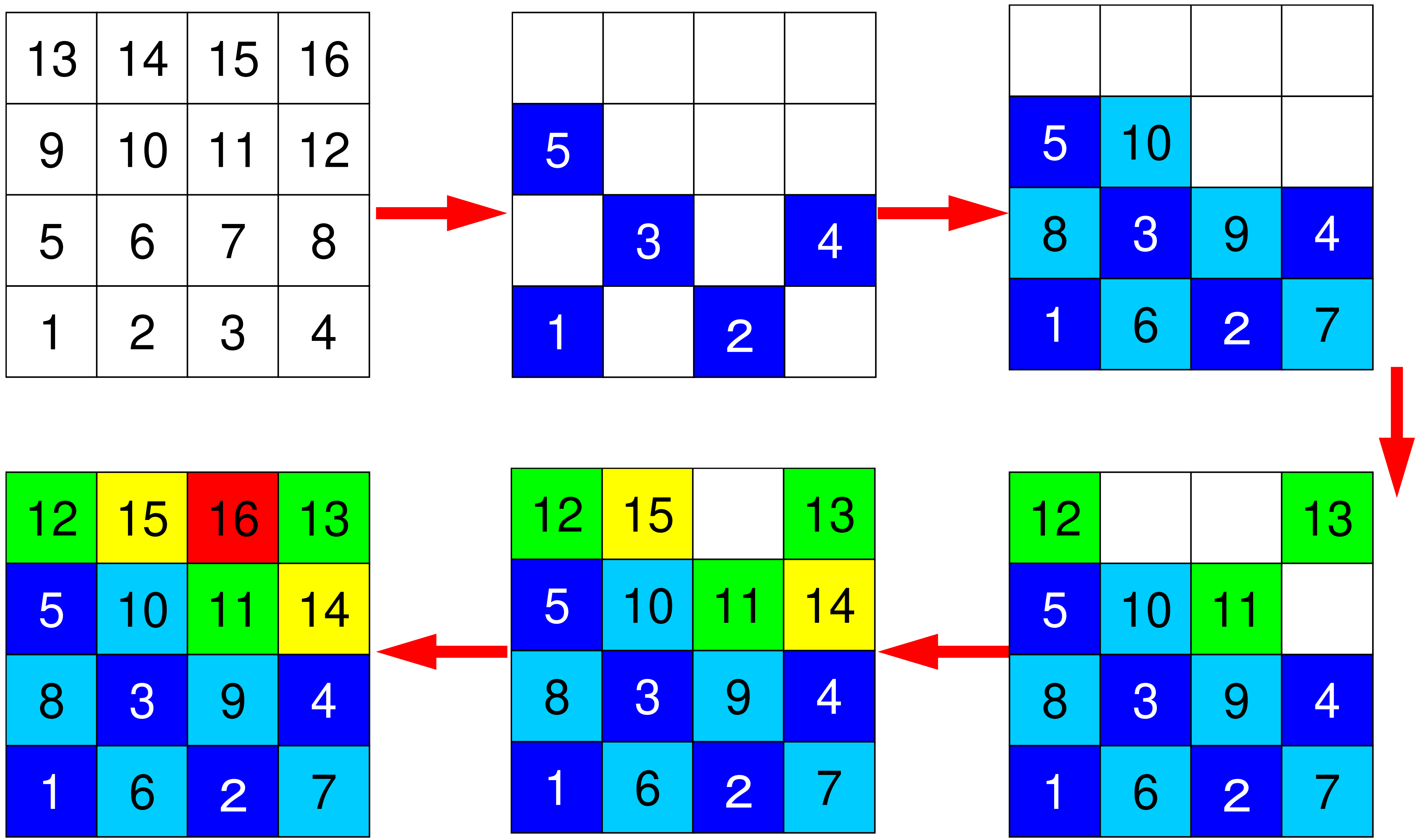
③ Color *ITEMcou* independent meshes in ascending order according to initial mesh ID.

④ If *ITEMcou* meshes are colored, or no more independent meshes do not exist, add "1" to the "counter for color number", and proceed to the next color.

⑤ Repeat ③ and ④, until all meshes have been colored.

⑥ "Final counter for color" is *NCOLORtotF*. Renumber meshes in ascending orders according to color ID. In each color, numbering is in ascending orders according to initial mesh ID. **In each color, new numbering of meshes is continuous.**

MC with 3 colors, finally 5 colors



Ordering/Reordering Method for Parallel Computing

- Multicoloring (MC)
  - Parallelism
  - Red-Black with 2 colors

- CM (Cuthill-McKee), RCM (Reverse Cuthill-McKee)
  - Reducing fill-in’s, matrix bandwidth, profiles
  - Parallelism

Fundamental Algorithm for CM Method (Cuthill-McKee)

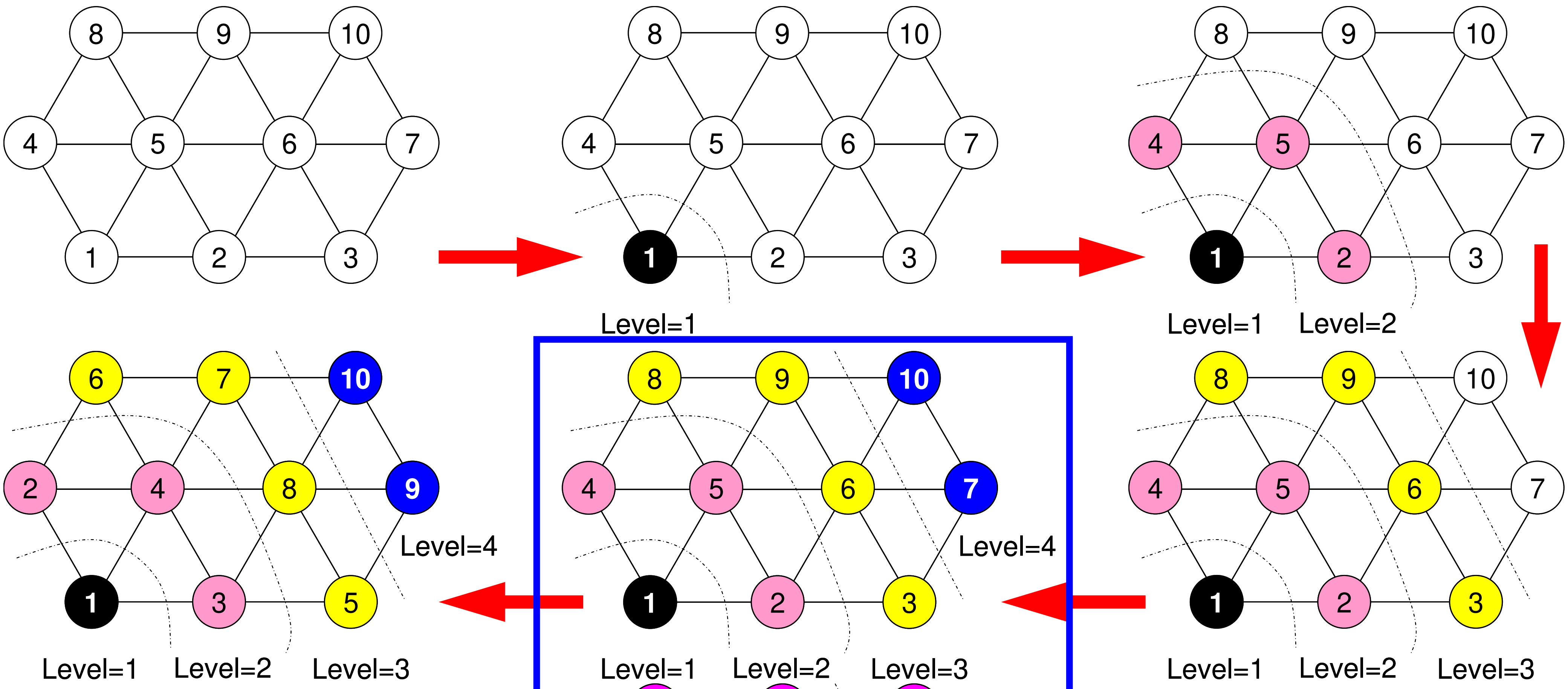
① ONE mesh with minimum value of “degree” is set to “Level=1”.

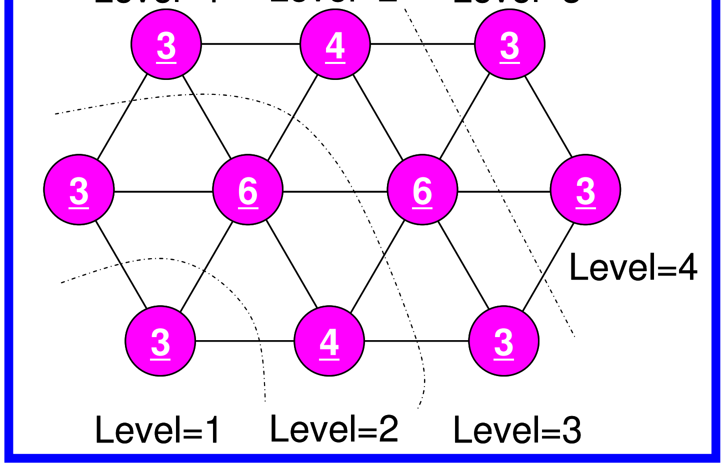
② Meshes adjacent to “Level=k-1” meshes are set to “Level=k”.

③ Repeat ②, until all meshes are flagged to “levels”

④ Renumber meshes in ascending orders according to “Level” ID. In each level, numbering is in ascending orders according to value of “degree” and initial mesh ID. In each level, new numbering of meshes is continuous.

Example of CM Method





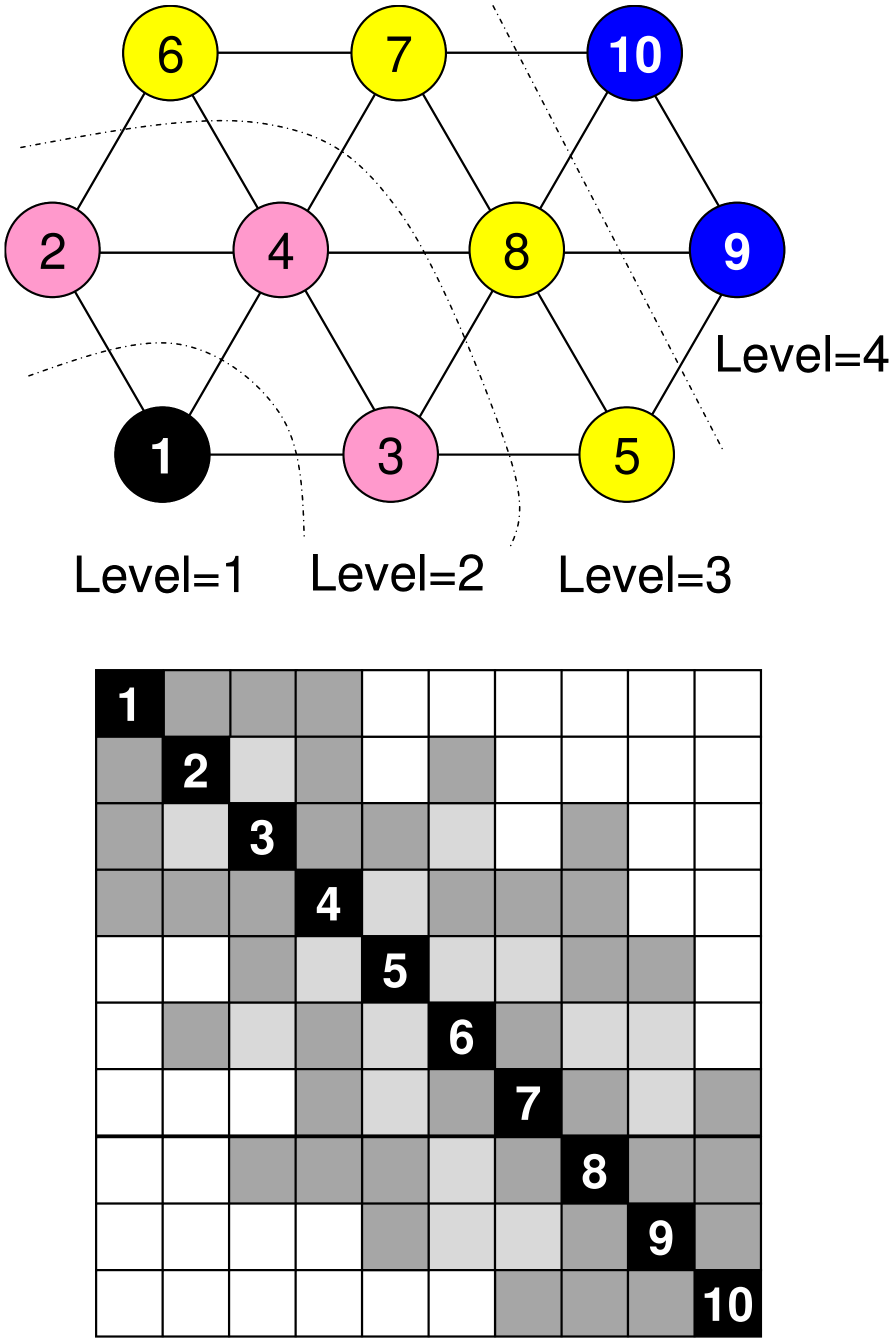
Renumber meshes in ascending orders according to "Level" ID. In each level, numbering is in ascending orders according to value of "degree" and initial mesh ID.

RCM: Reverse Cuthill-McKee

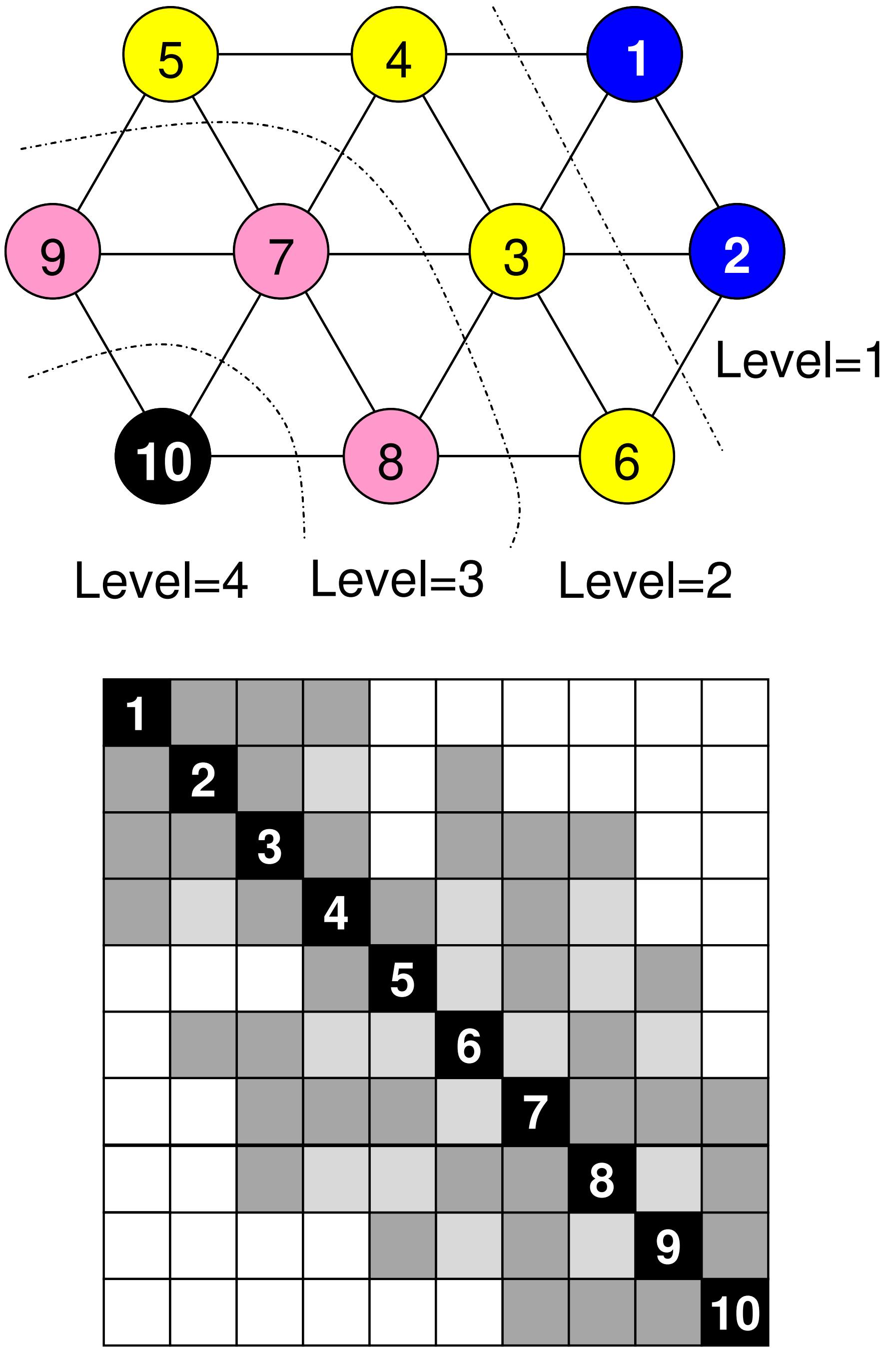
- Do operations for “CM” method
  - Calculate “degree” at each mesh
  - Flag “level k (1,2,...)” to meshes
  - Repeat processes, final renumbering

- Renumbering Again
  - Renumber meshes reordered by CM method in reverse order.
  - Fill-in’s (for full LU factorization) are fewer than CM

CM: 16 fill-in's



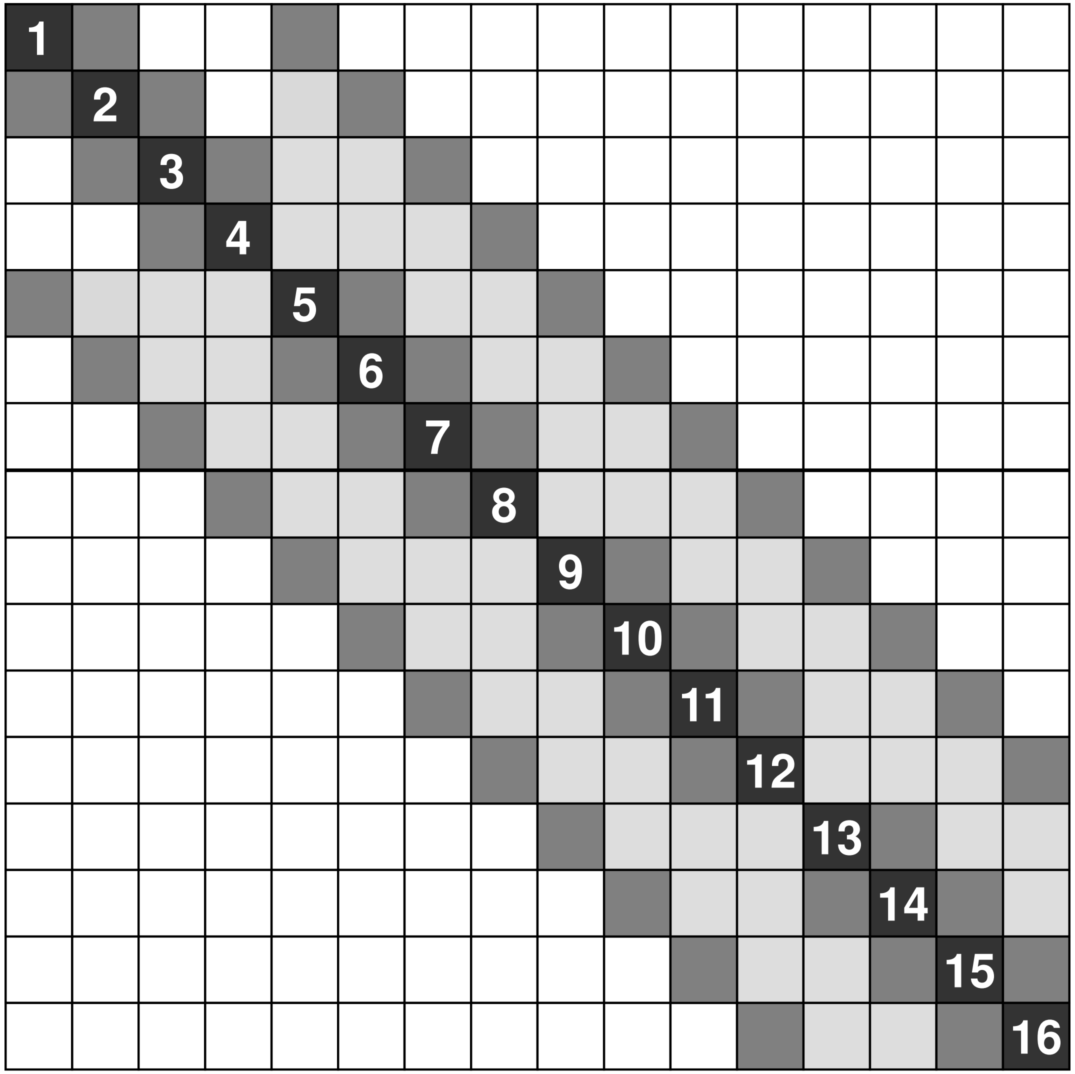
RCM: 14 fill-in's



Initial Matrix

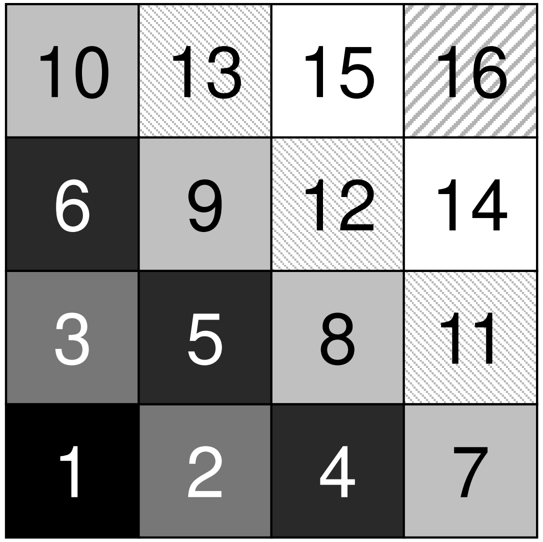
13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

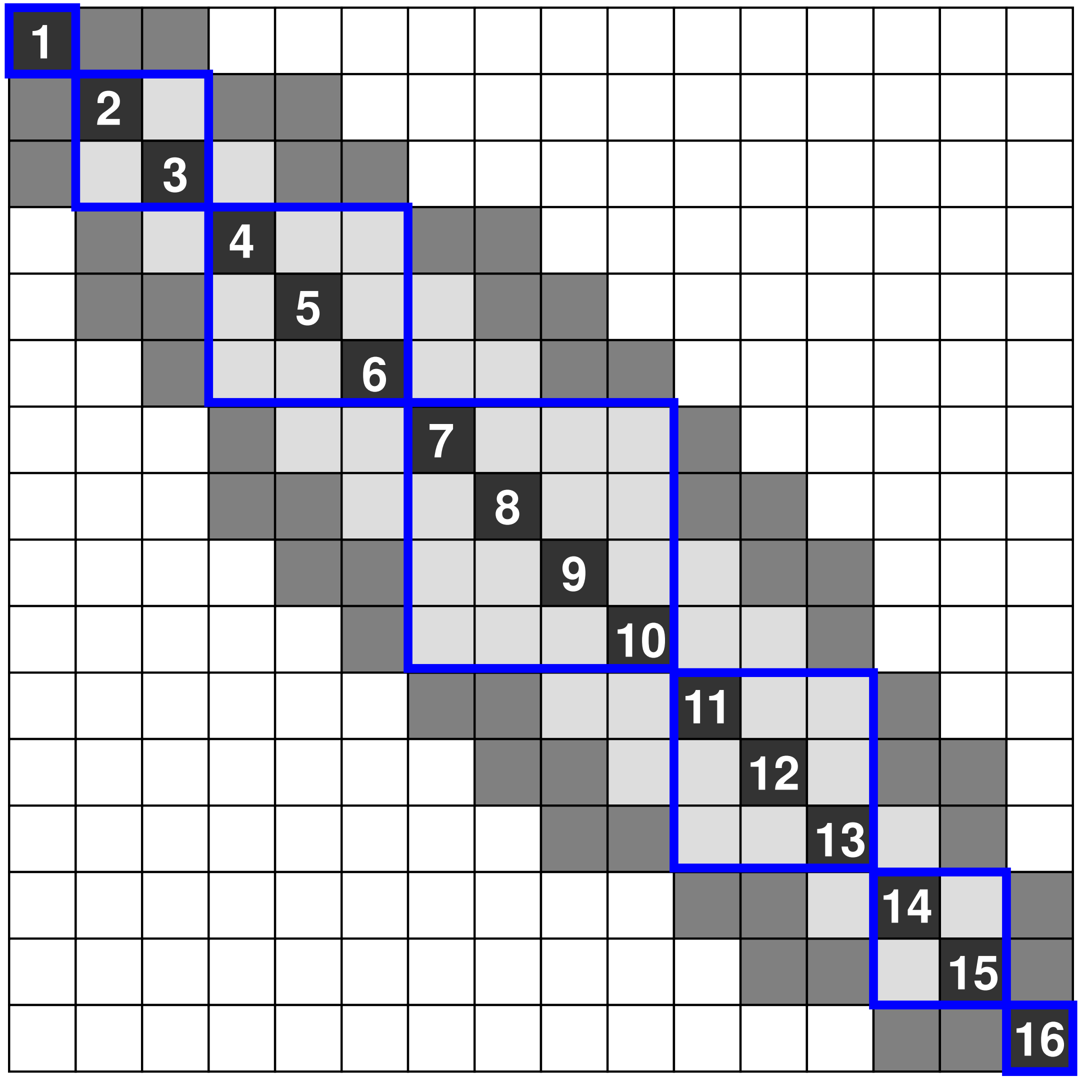
Bandwidth 4
Profile 51
Fill-in 54



Non-zero, Fill-in

CM

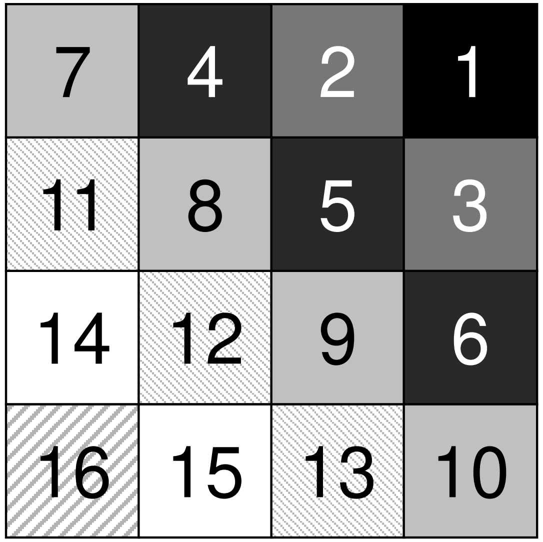




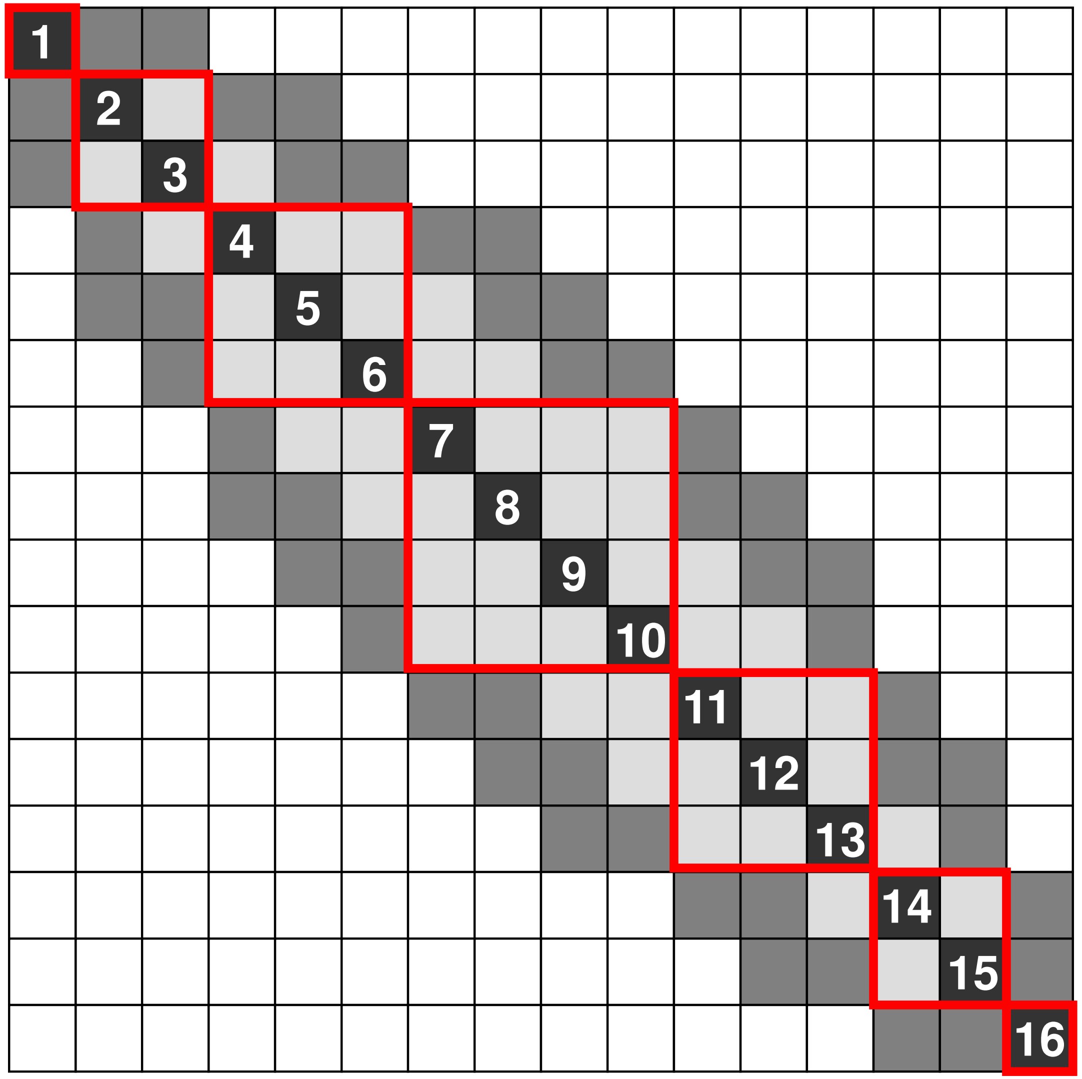
Bandwidth 4
Profile 46
Fill-in 44

Non-zero, Fill-in

RCM

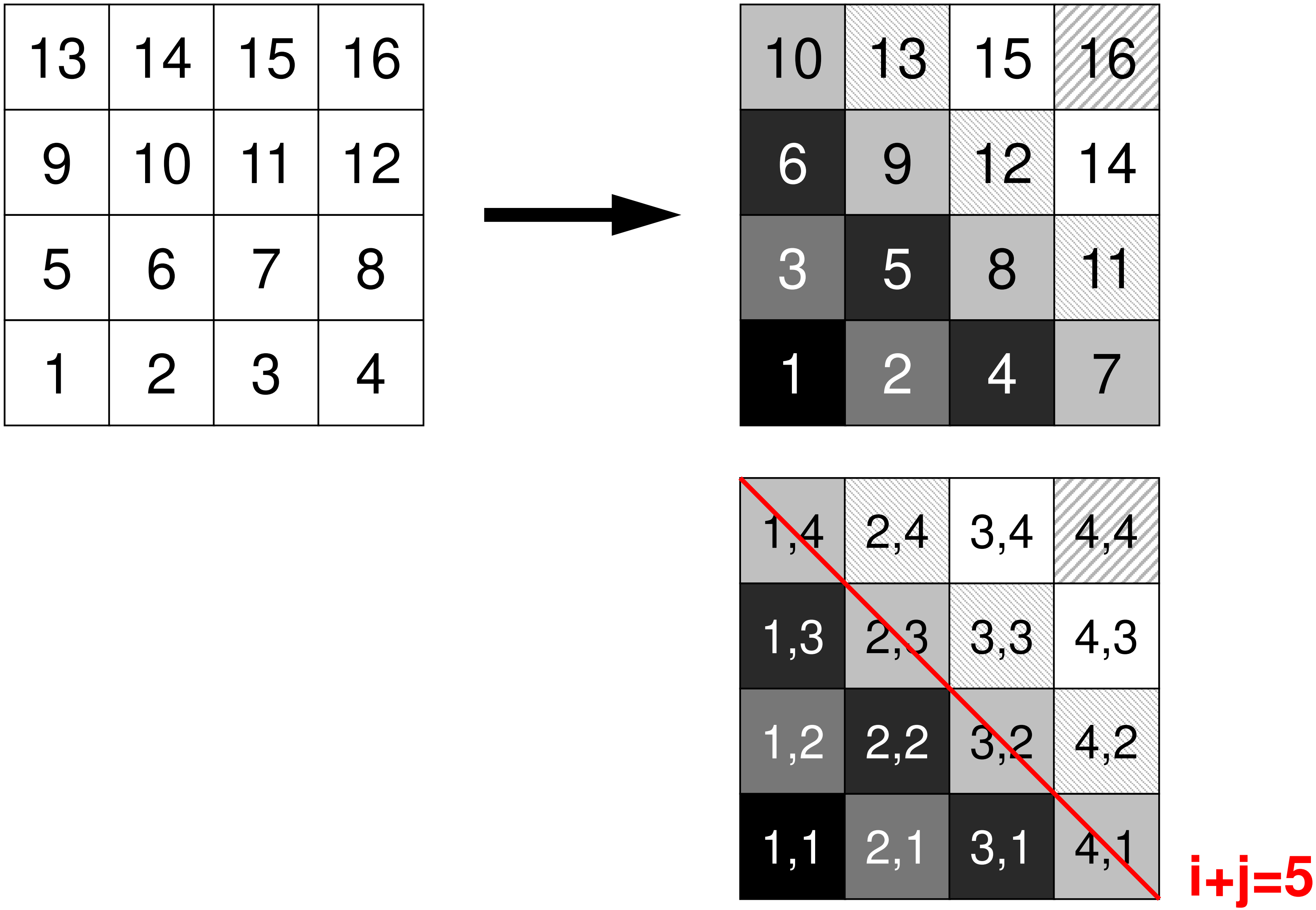


Bandwidth 4
Profile 46
Fill-in 44



Non-zero, Fill-in

CM, RCM: Hyperline (i+j=const.) 3D: Hyperplane (i+j+k=cons.)



Modified CM Method for Parallel Computing

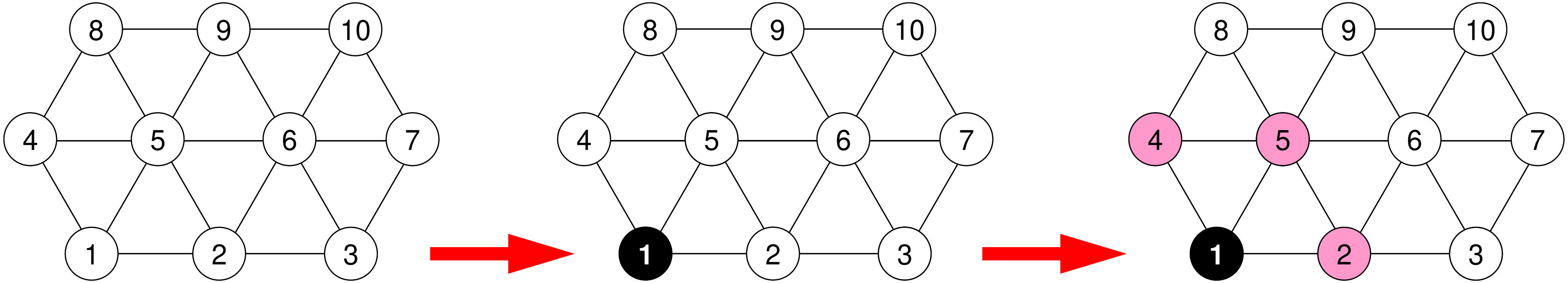
① ONE mesh with minimum value of “degree” is set to “Level=1”.

② Meshes adjacent to “Level=k-1” meshes are set to “Level=k”. In each level, meshes must be independent (not directly connected). If a dependent pair is found in same color, one mesh is removed (In current implementation, a mesh found later is removed).

③ Repeat ②, until all meshes are flagged to “levels”

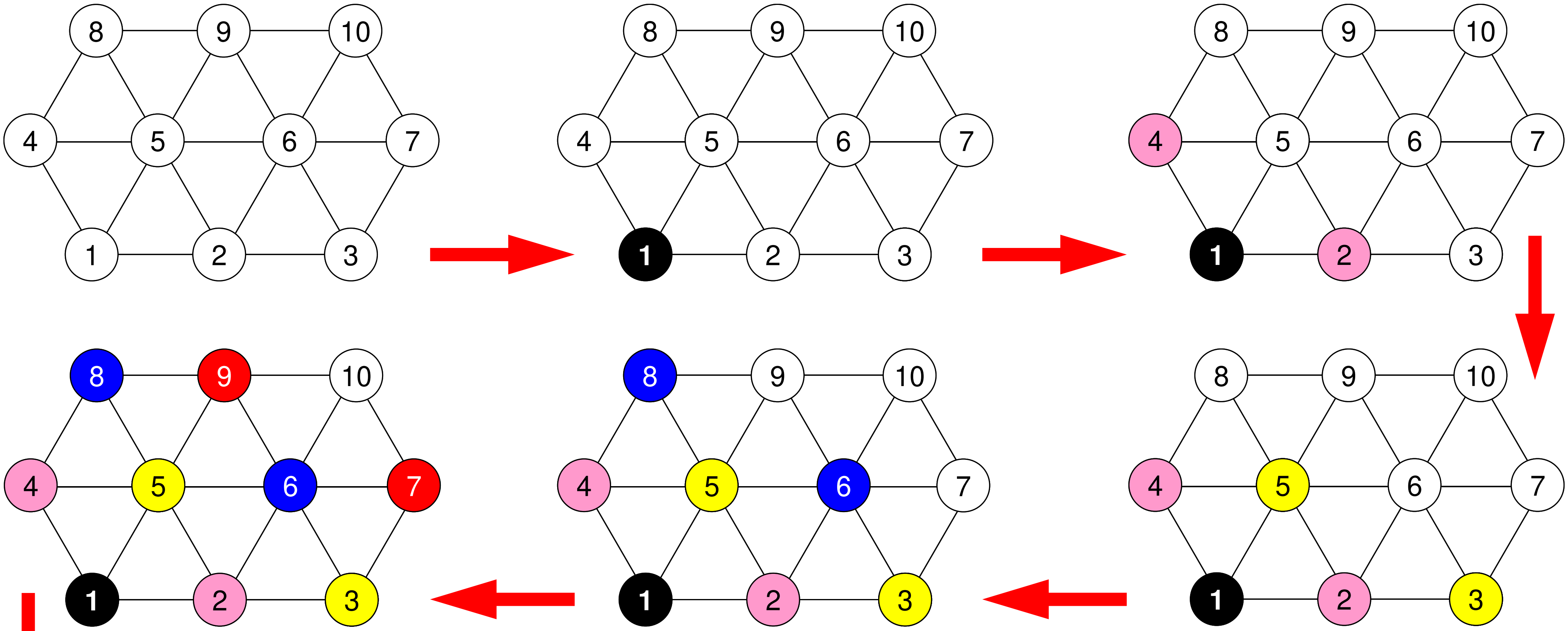
④ Renumber meshes in ascending orders according to “Level” ID. In each level, numbering is in ascending orders according to initial mesh ID. In each level, new numbering of meshes is continuous.

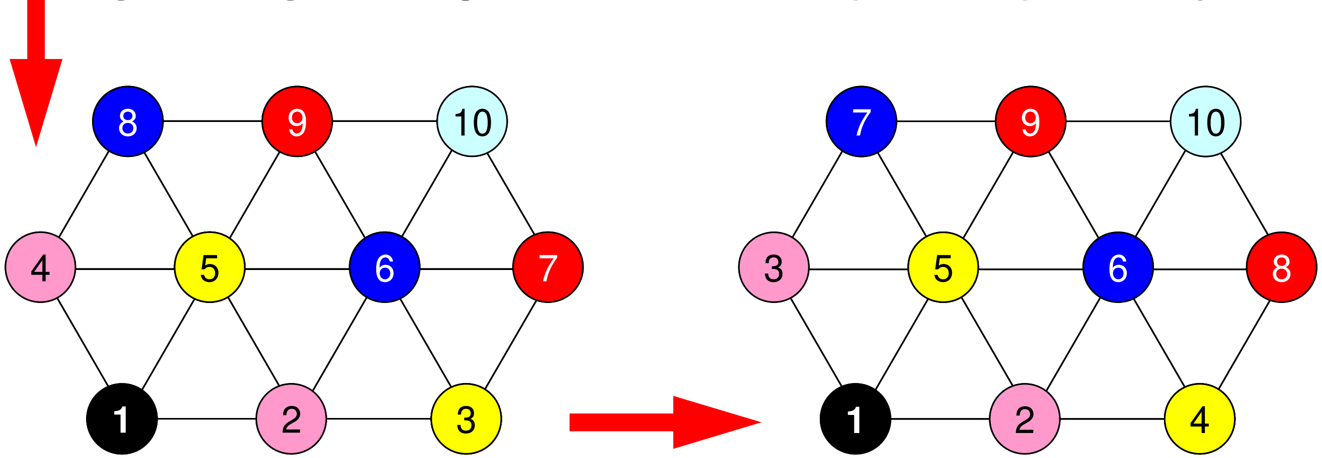
Modified CM Method



In each level, meshes are independent

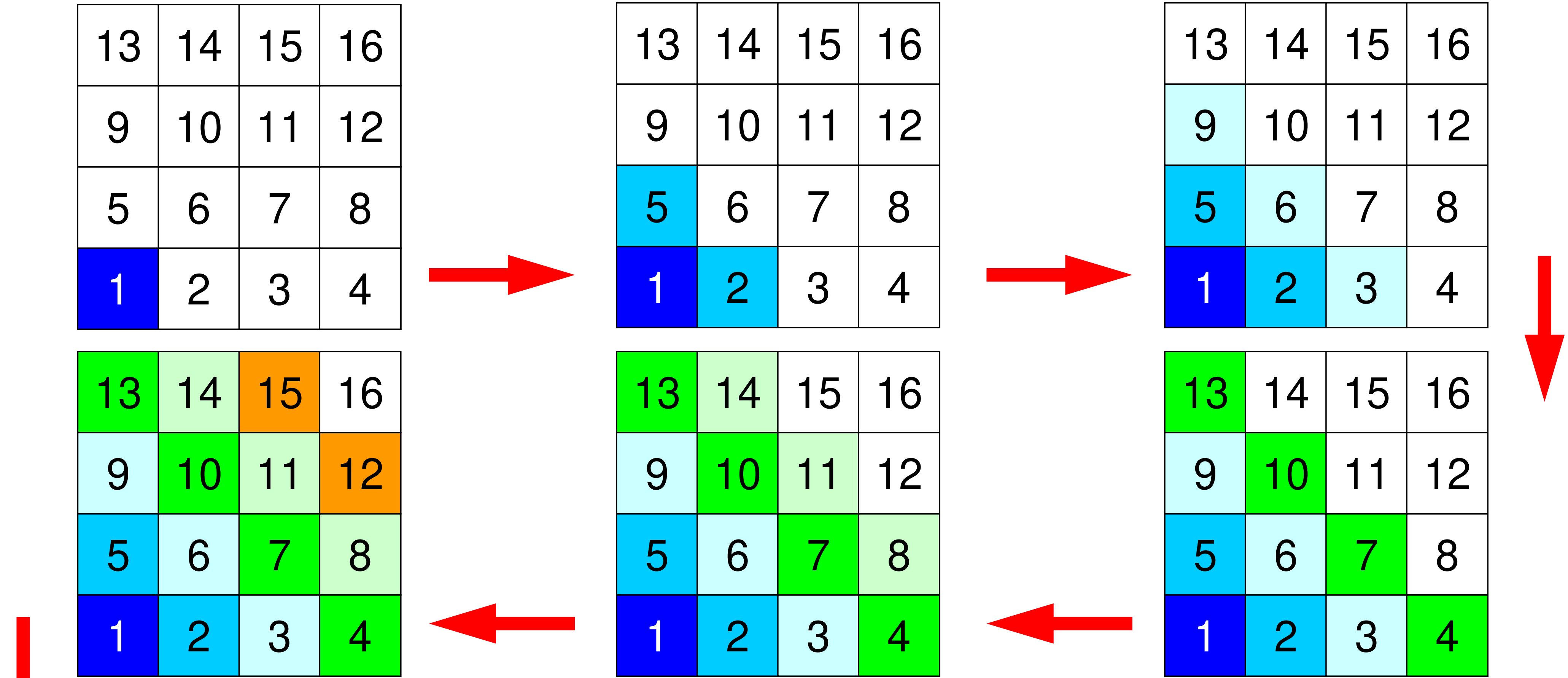
Modified CM Method

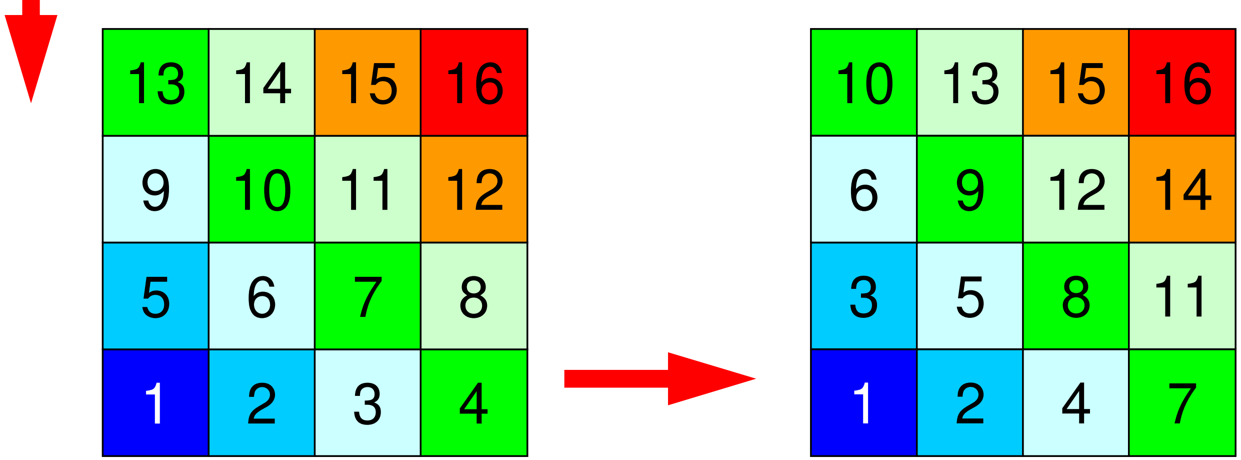




Renumber meshes in ascending orders according to "Level" ID. In each level, numbering is in ascending orders according to initial mesh ID.

Modified CM Method

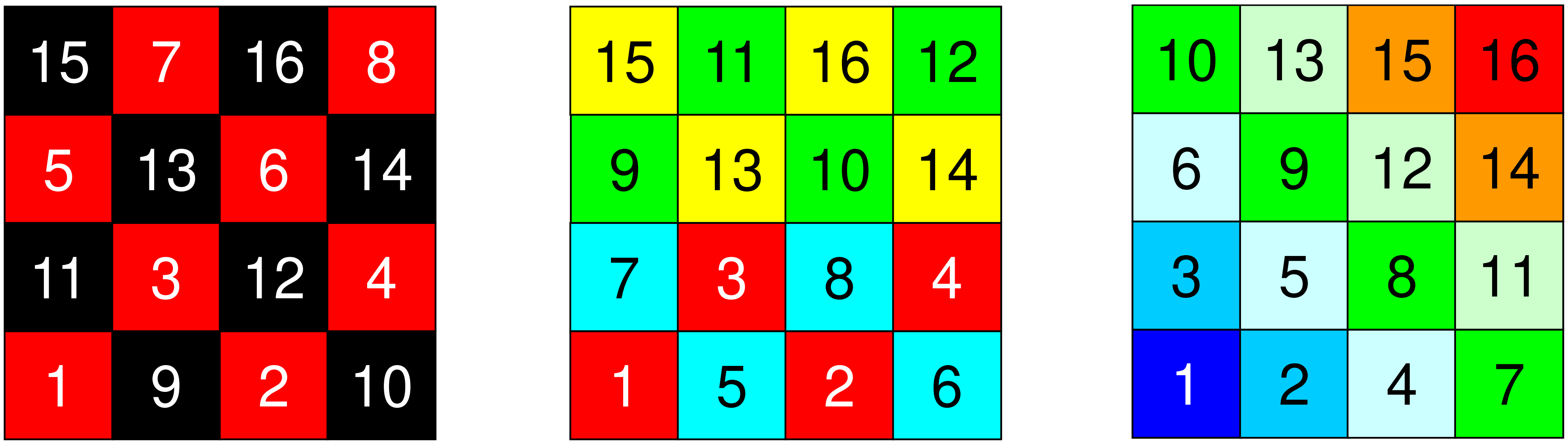




Renumber meshes in ascending orders according to “Level” ID. In each level, numbering is in ascending orders according to initial mesh ID.

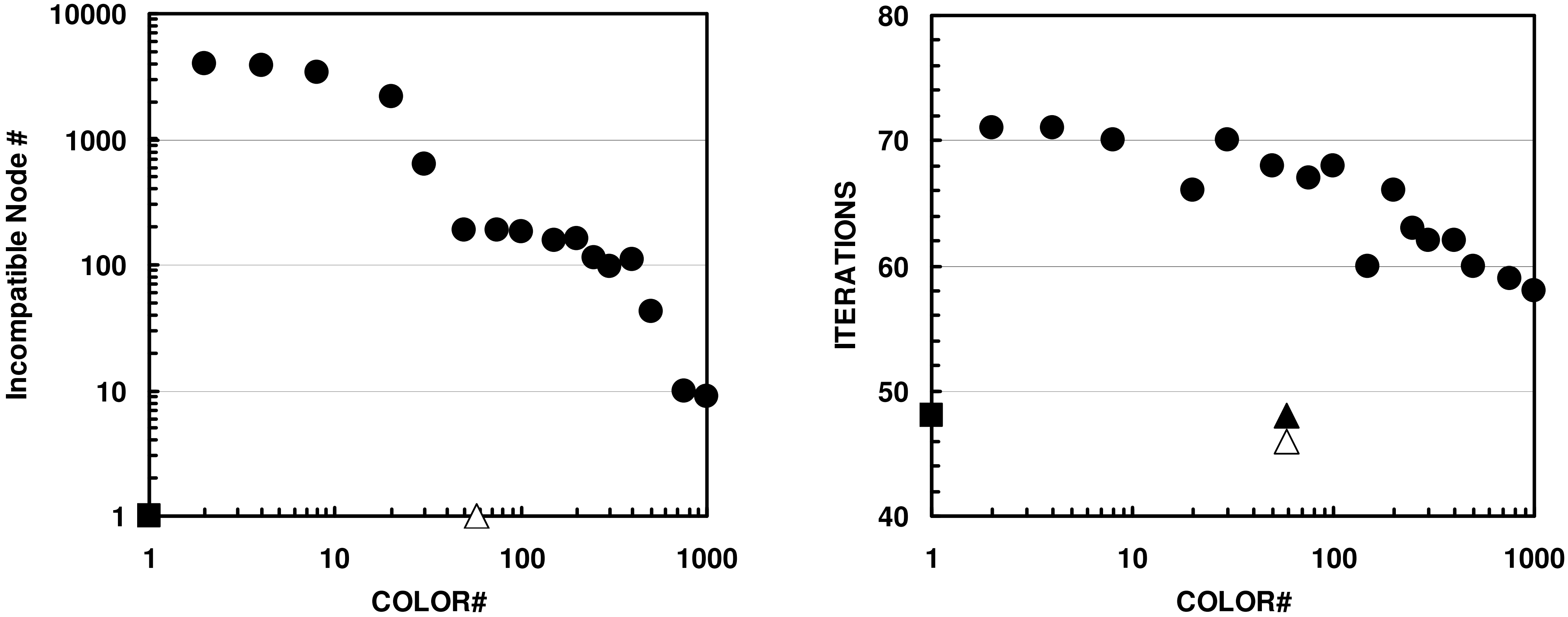
MC and CM/RCM

- In CM/RCM, sequence of computations, and dependency between levels (color) are also considered.



- Remedy for Data Dependency
- **Ordering/Reordering**
  - Red-Black, Multicoloring (MC)
  - Cuthill-McKee (CM), Reverse-CM (RCM)
  - **Reordering and Convergence**
- Implementation
- ICCG with Reordering

Effect of Color Number on Convergence of ICCG



(20^3=8,000 meshe, EPSICCG=10^{-8})

(■ : ICCG(L1), ● : ICCG-MC, ▲ : ICCG-CM, △ : ICCG-RCM)

Effect of Color Number on Convergence of ICCG

- Number of Elements: 20^3
- Red-Black ~ 4-Colors < Initial Numbering ~ CM, RCM

Initial Numbering	
Bandwidth	4
Profile	51
Fill-in	54

Red-Black	
Bandwidth	10
Profile	77
Fill-in	44

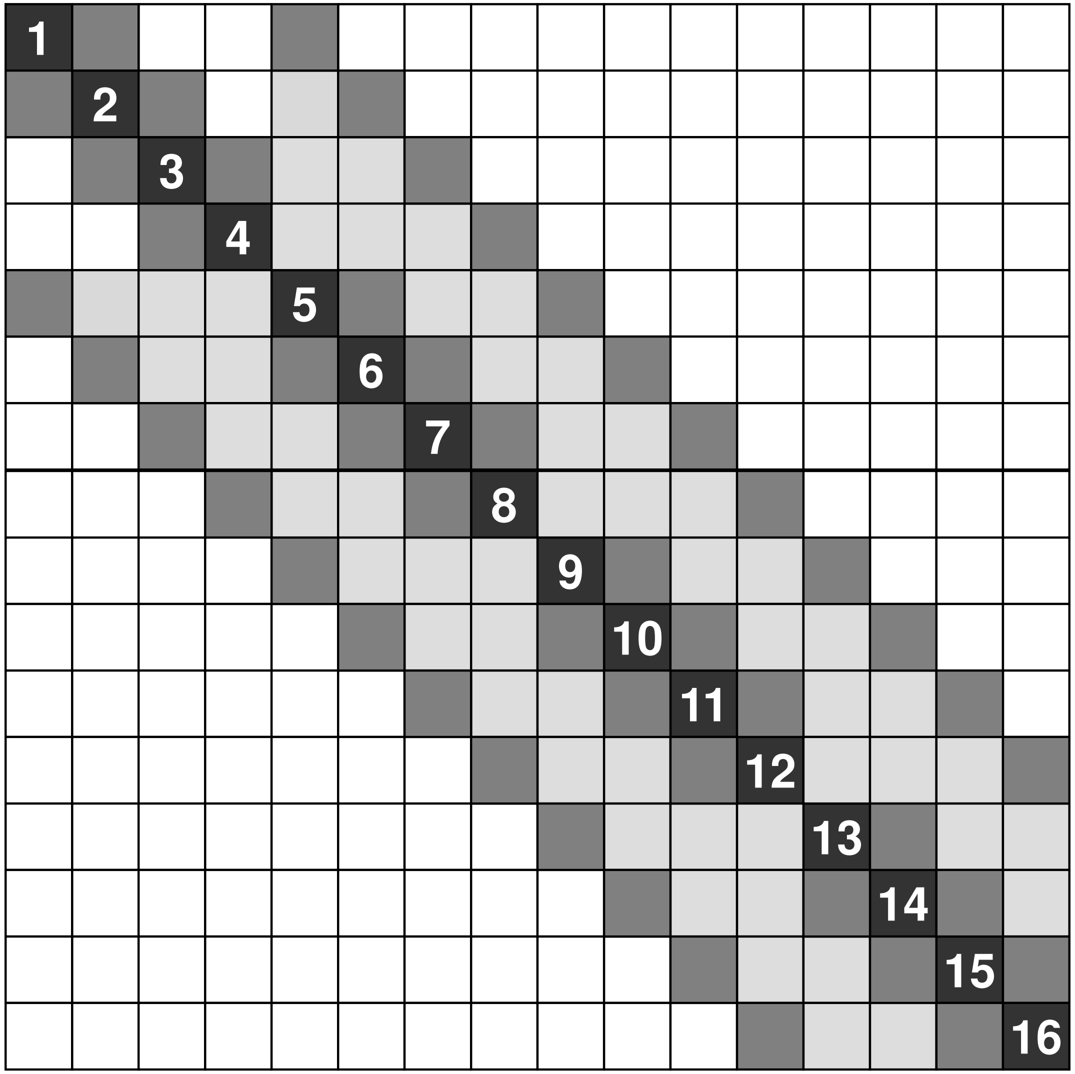
4-Colors	
Bandwidth	10
Profile	57
Fill-in	46

CM, RCM	
Bandwidth	4
Profile	46
Fill-in	44

Initial Matrix

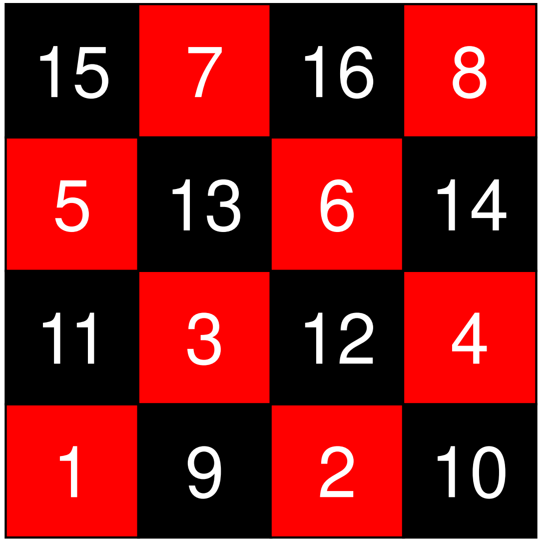
13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

Bandwidth	4
Profile	51
Fill-in	54

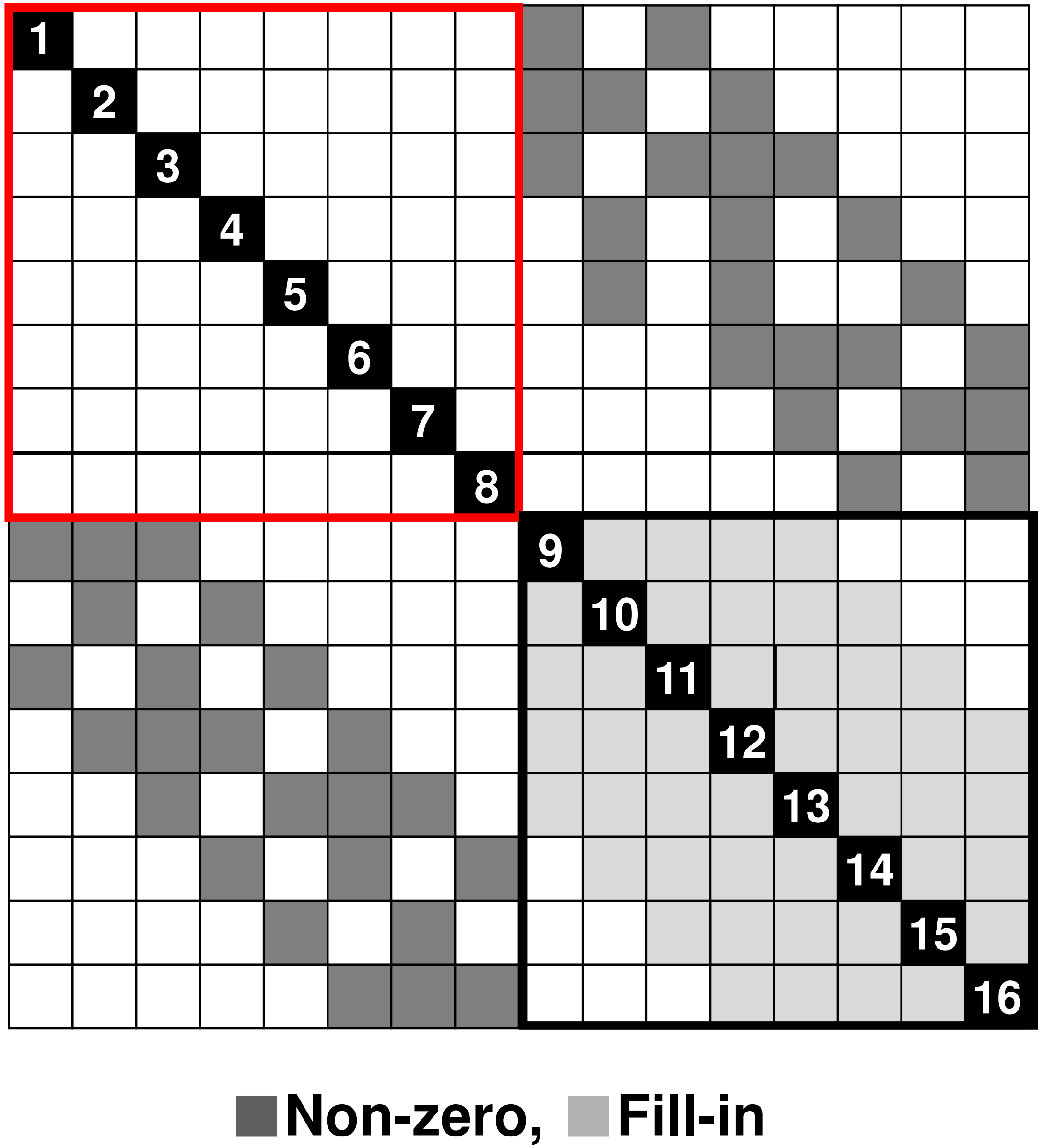


Non-zero, Fill-in

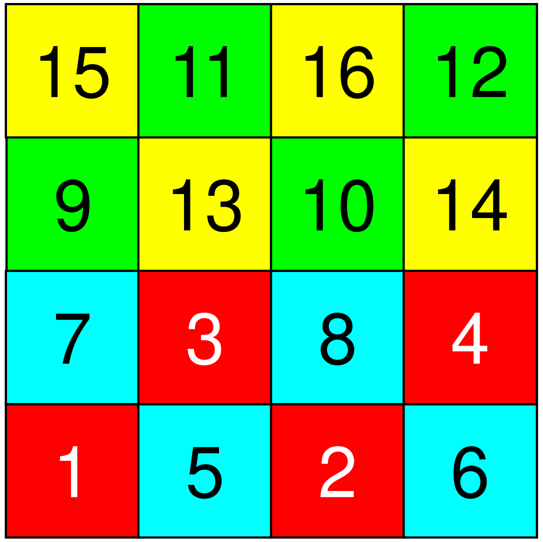
Red-Black (2-Colors)



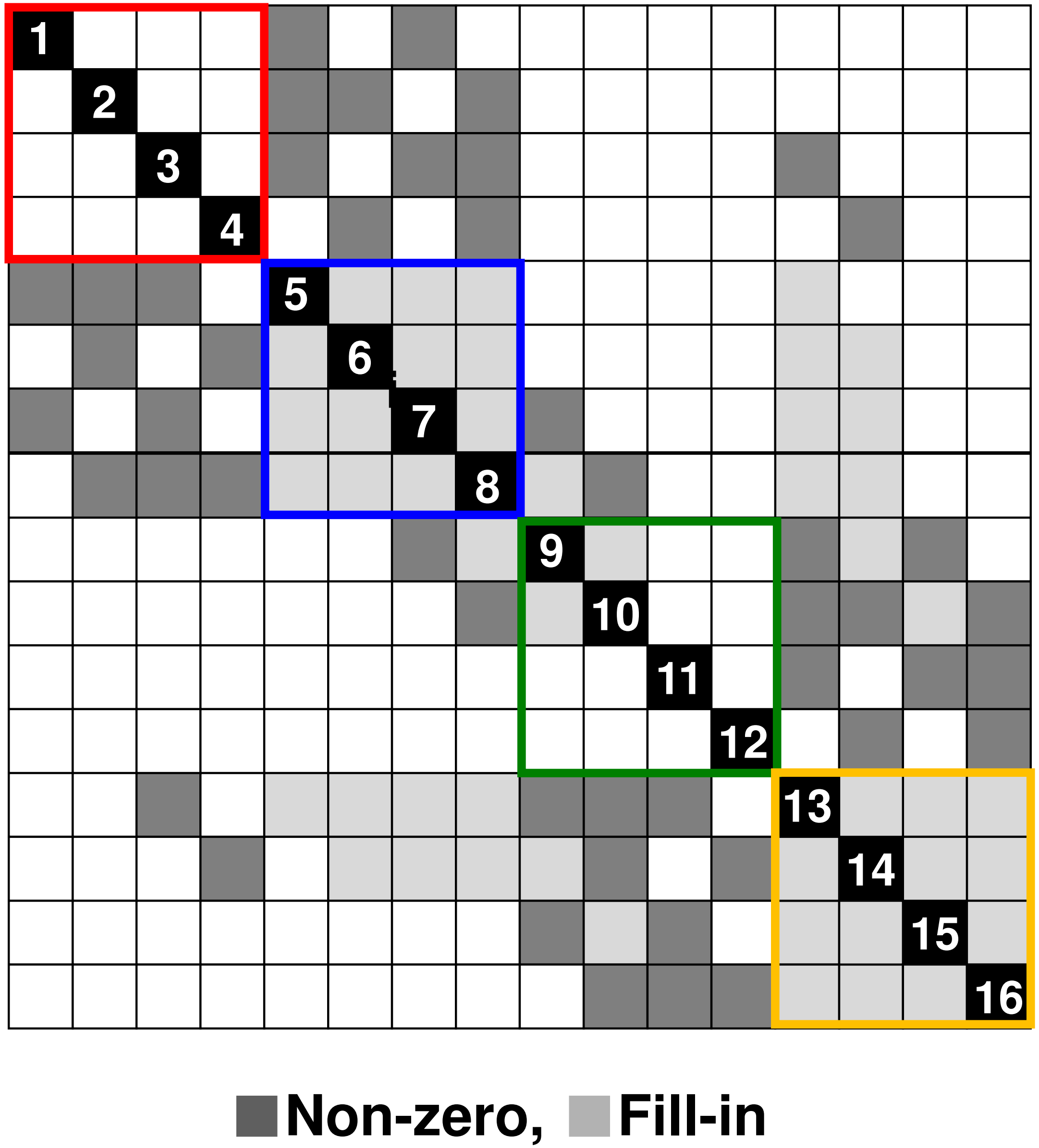
Bandwidth 10
Profile 77
Fill-in 44



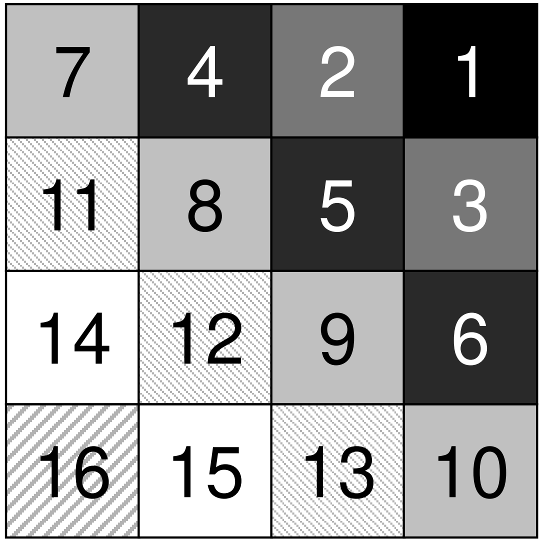
MC (4-Colors)



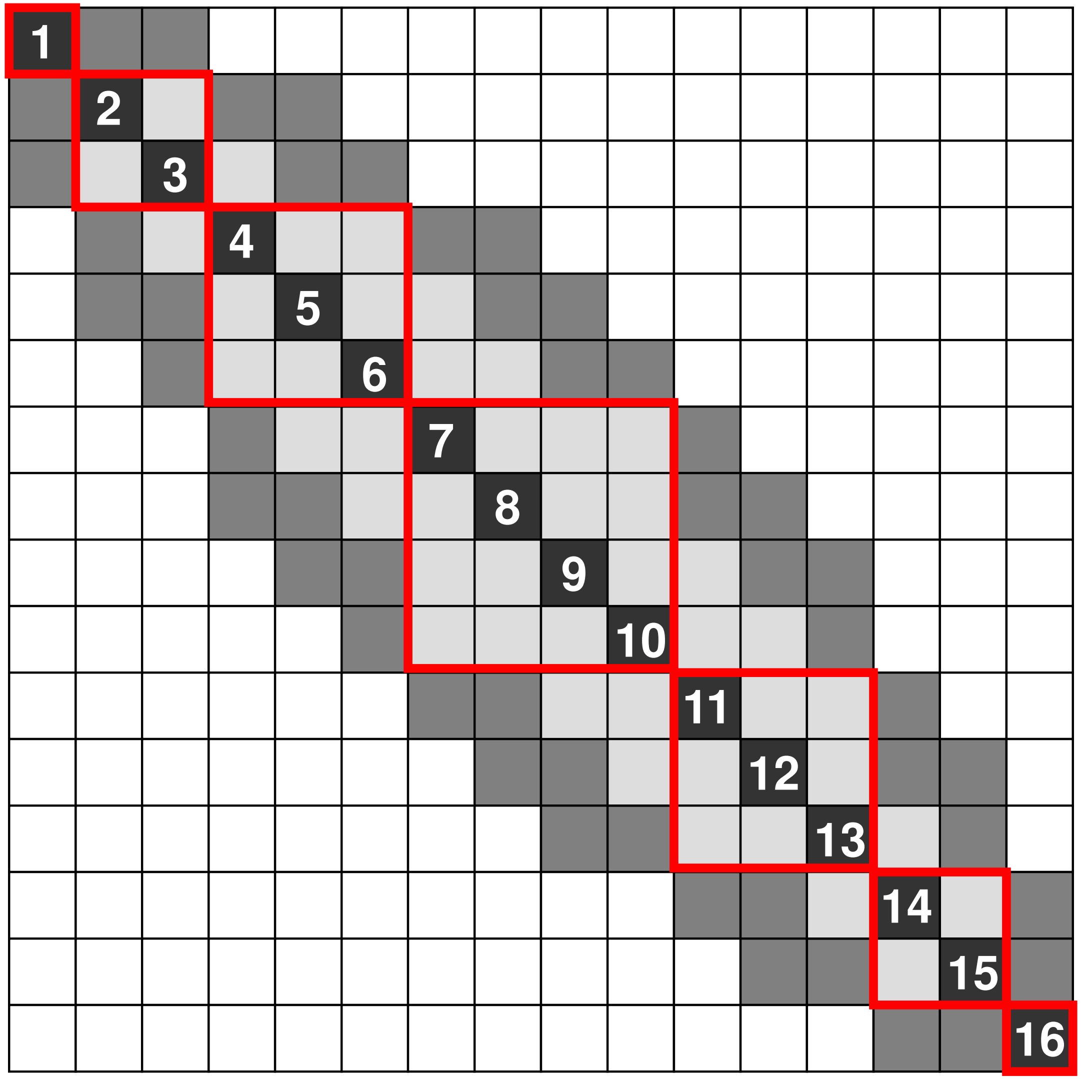
Bandwidth 10
Profile 57
Fill-in 46



RCM



Bandwidth 4
Profile 46
Fill-in 44

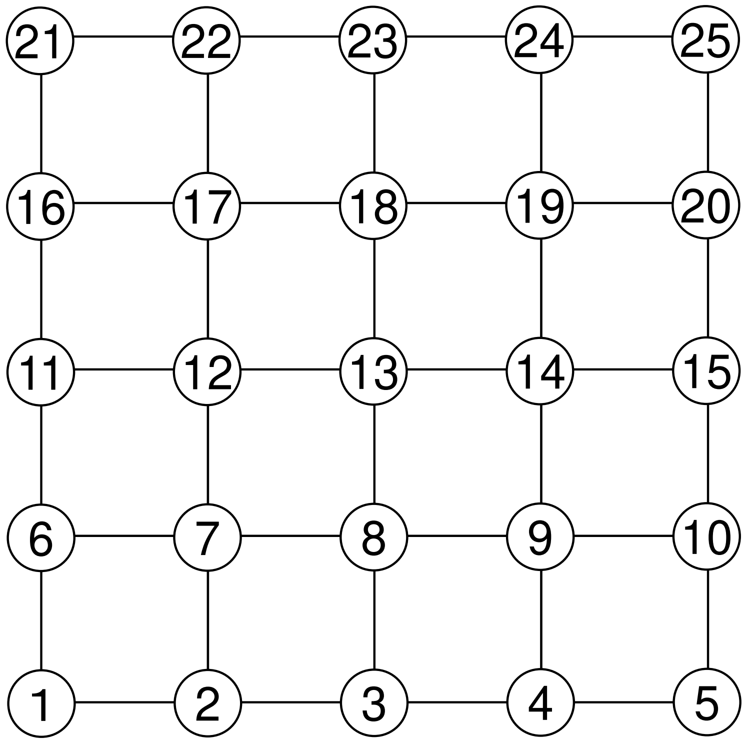


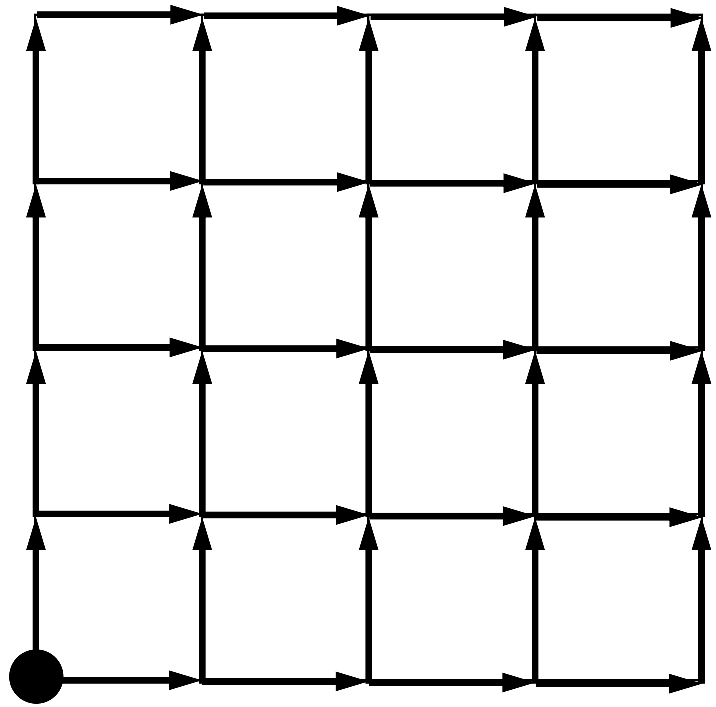
Non-zero, Fill-in

Color Number and Convergence Incompatible Nodes

Doi, S. (NEC) et al.

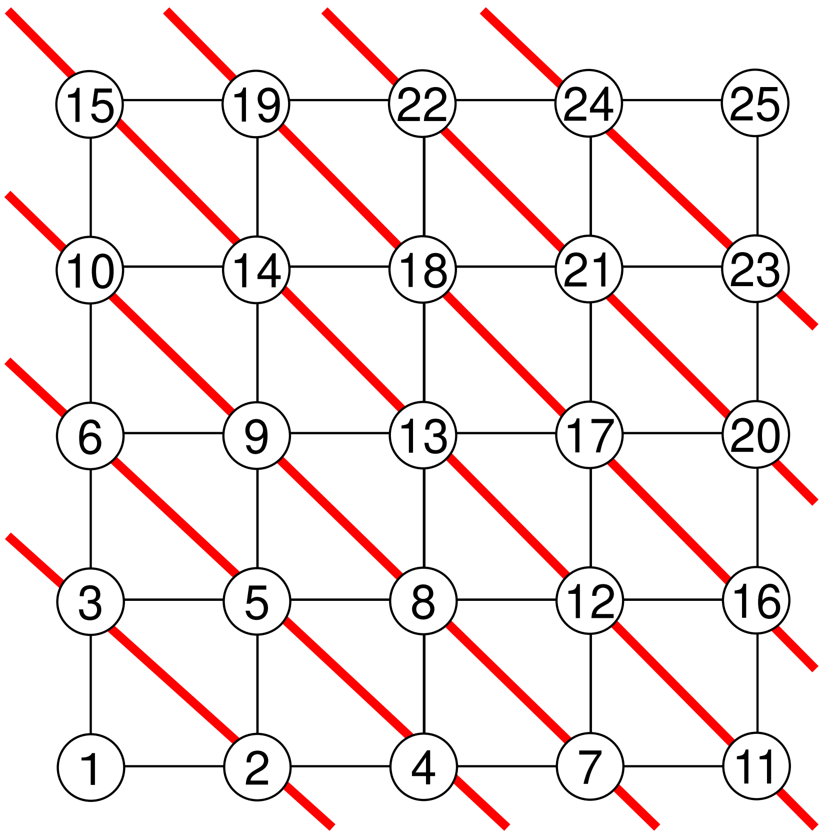
Propagation of effects in Forward Substitution

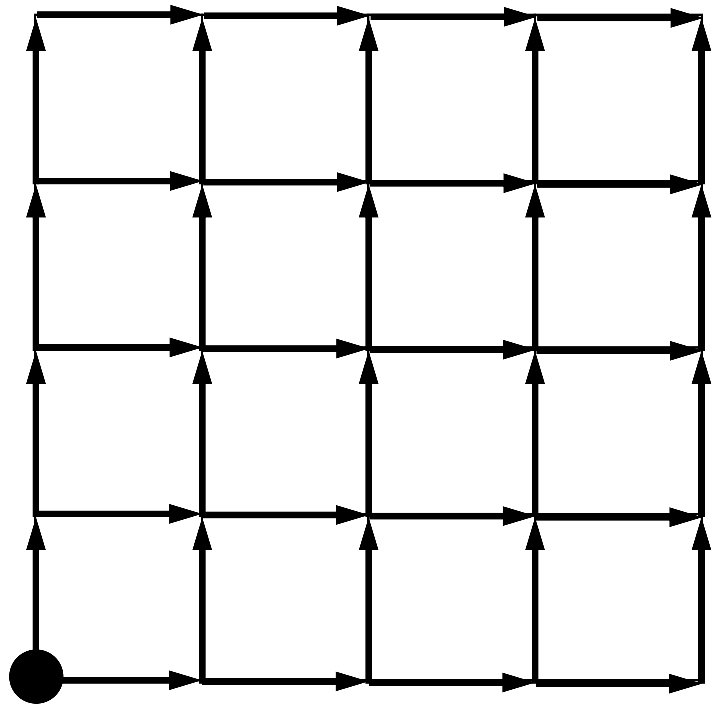




“Incompatible Nodes” not affected by other nodes. ID of such node is smaller than those of adjacent nodes. If we have smaller number of “incompatible nodes”, convergence is faster.

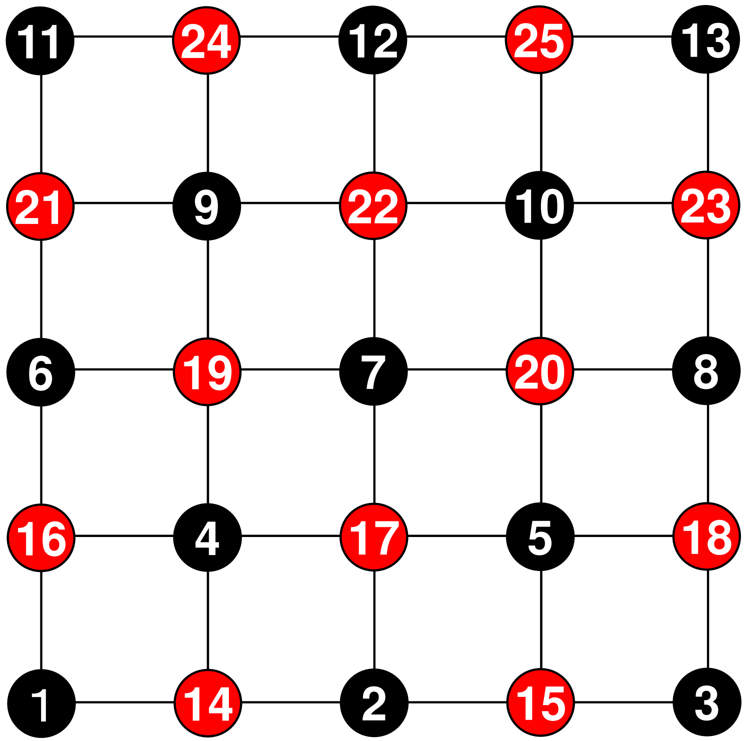
CM (Cuthill-McKee)

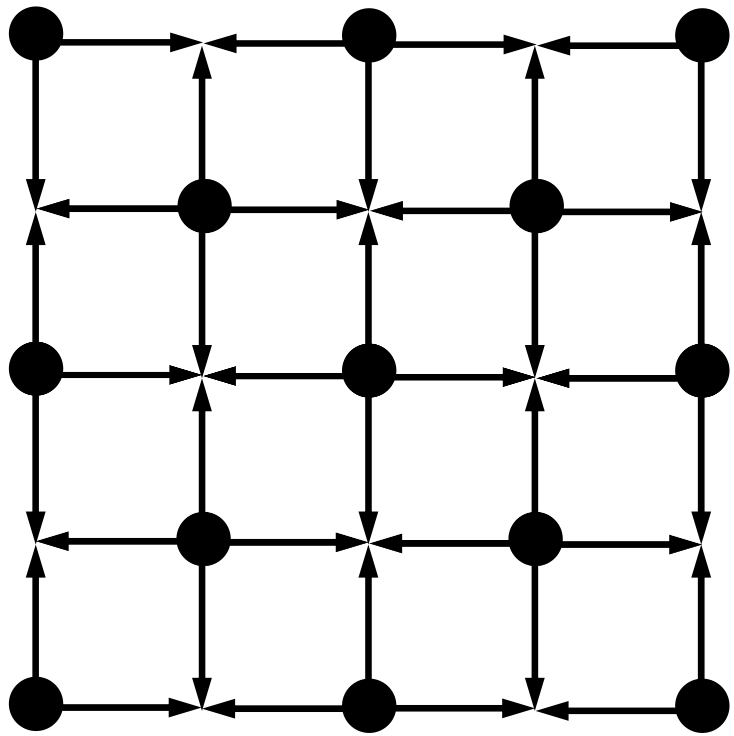




Red-Black

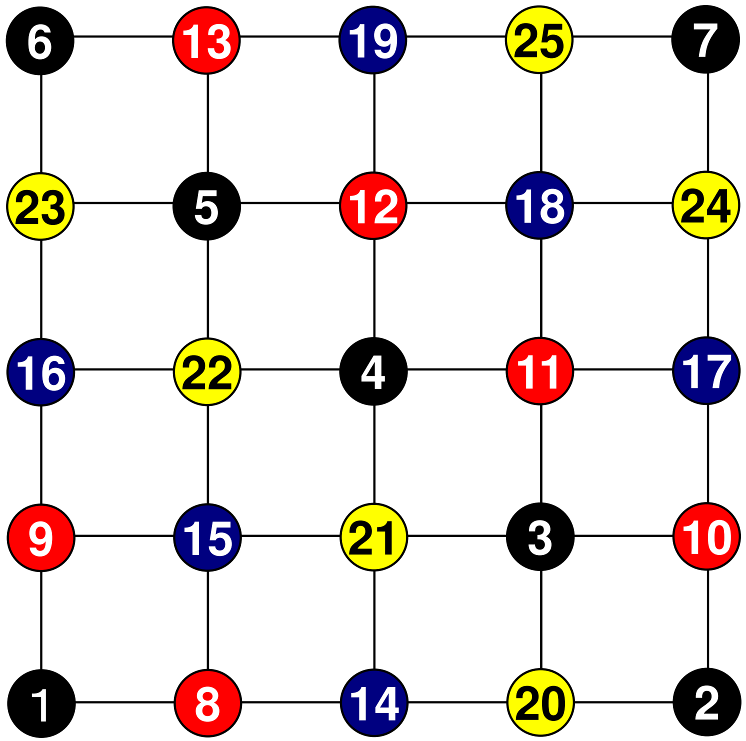
Higher parallelism, but many “incompatible nodes”
Slower convergence in ICCG, Gauss-Seidel etc.

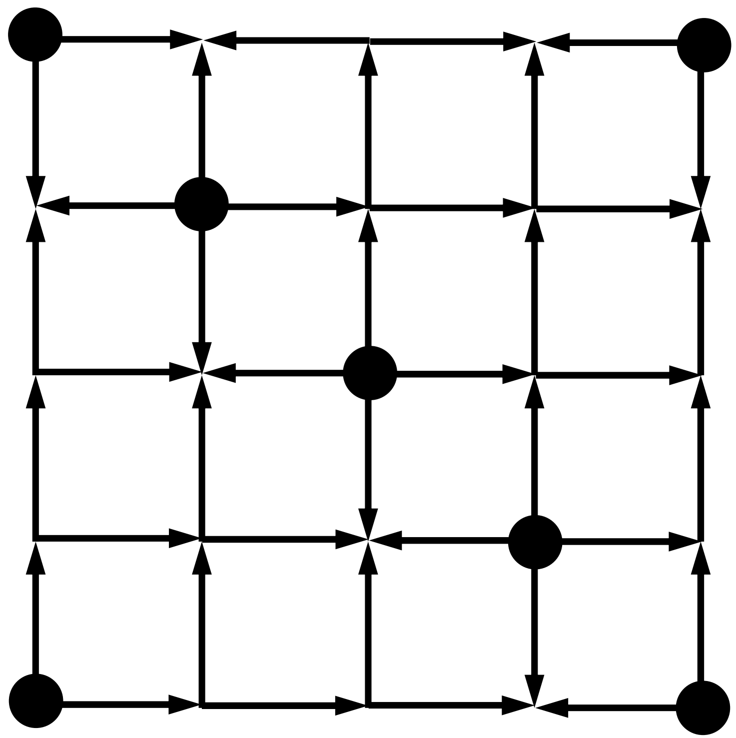




4-Colors

Still many “incompatible nodes”
Slower convergence in ICCG, Gauss-Seidel etc.





Generally speaking, convergence of ICCG is better for configurations with …

- More Colors

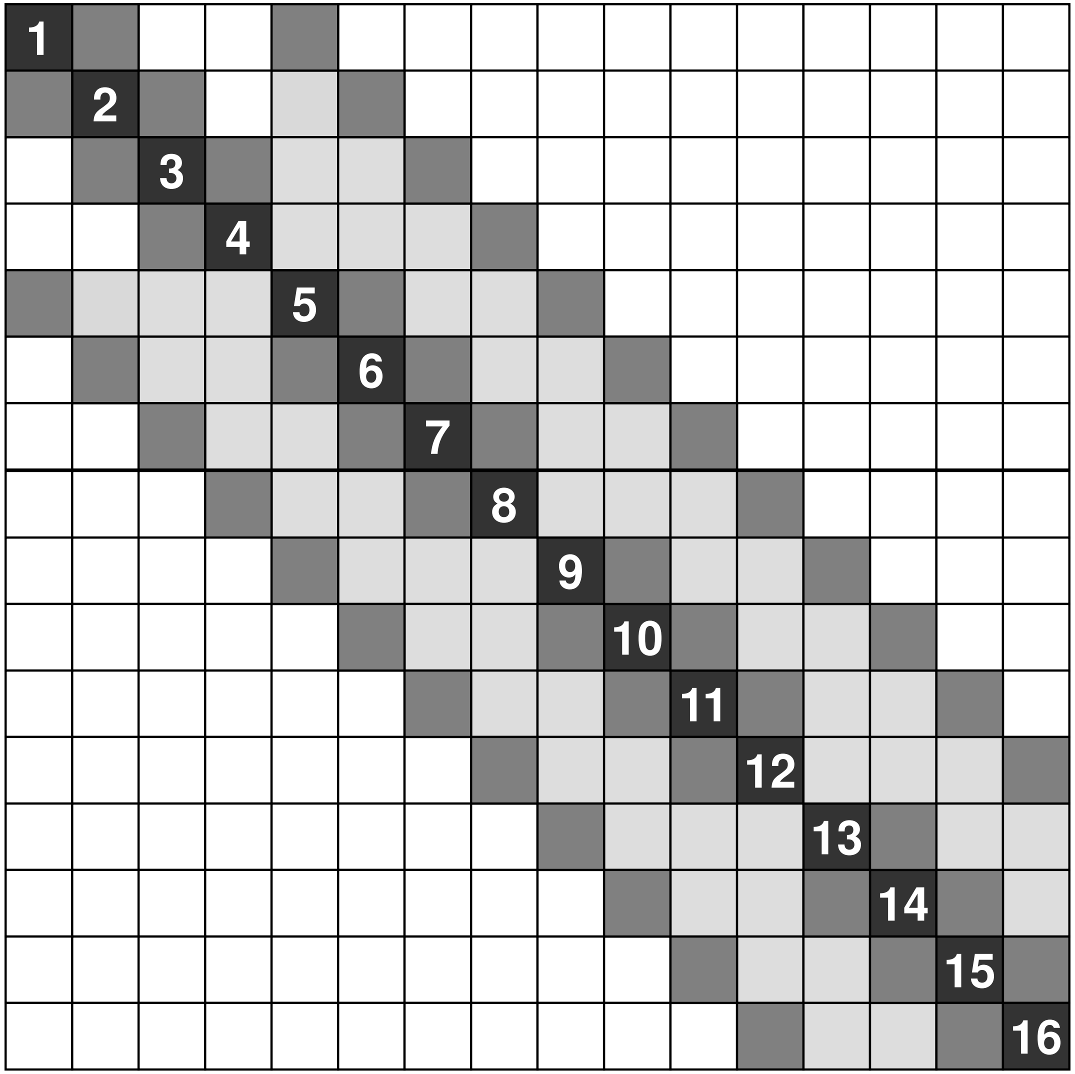
- Smaller Bandwidth
- Smaller Profile
- Fewer Fill-in’s
- Fewer Incompatible Nodes

Generally speaking, convergence of ICCG is better for configurations with <u>fewer fill-in's</u>

- ICCG (IC(0)-CG) ignores fill-in's
- **More fill-in's are ignored for configurations (e.g. coloring) with more fill-in's**
  - **IC(0) for configurations with more fill-in's may be weaker than that with fewer fill-in's**
- **Distribution of fill-in's may affect the convergence**
  - **Initial Matrix**
  - **Red-Black (MC with 2-Colors)**

Initial Matrix

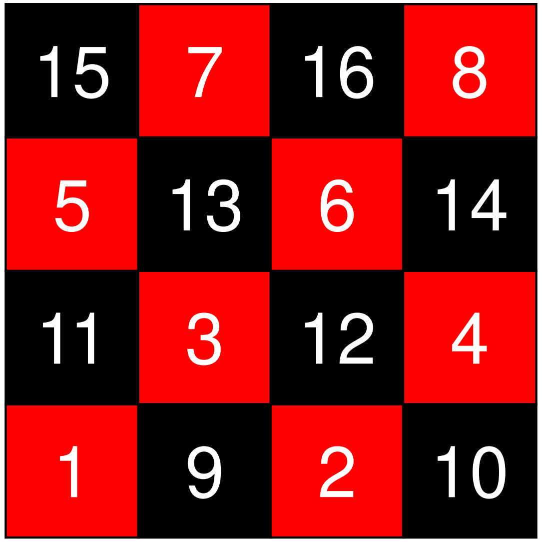
13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4



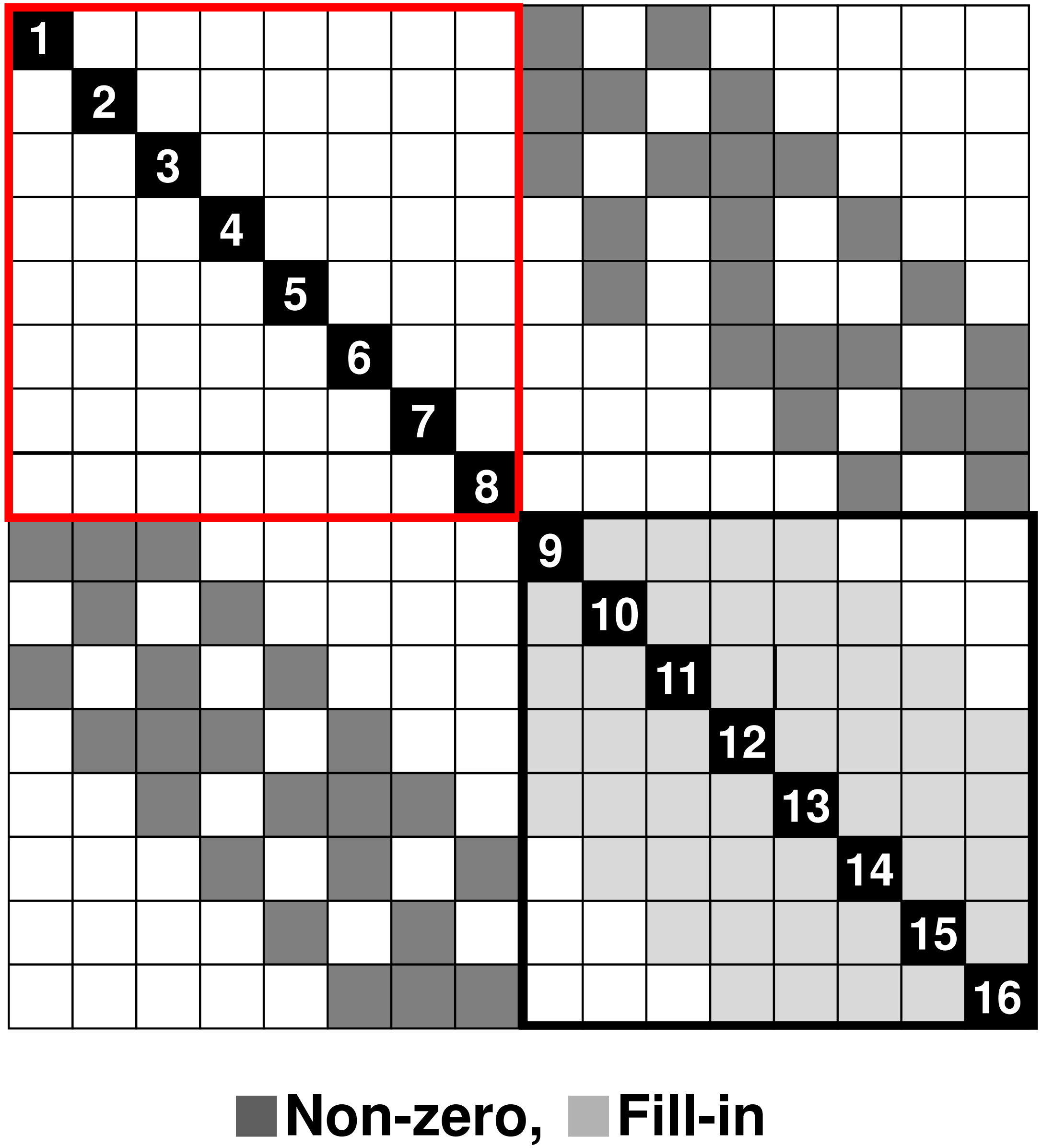
Bandwidth 4
Profile 51
Fill-in 54

Non-zero, Fill-in

Red-Black (2-Colors)



Bandwidth 10
Profile 77
Fill-in 44



Effect of Reordering/Color # on Convergence

- Other effects (e.g. B.C.) should be considered.
- It is difficult to provide very general remarks.
- e.g. RCM provides slightly faster convergence than CM, although parameters (Bandwidth, profile, fill-in's) are same.

Effect of Reordering

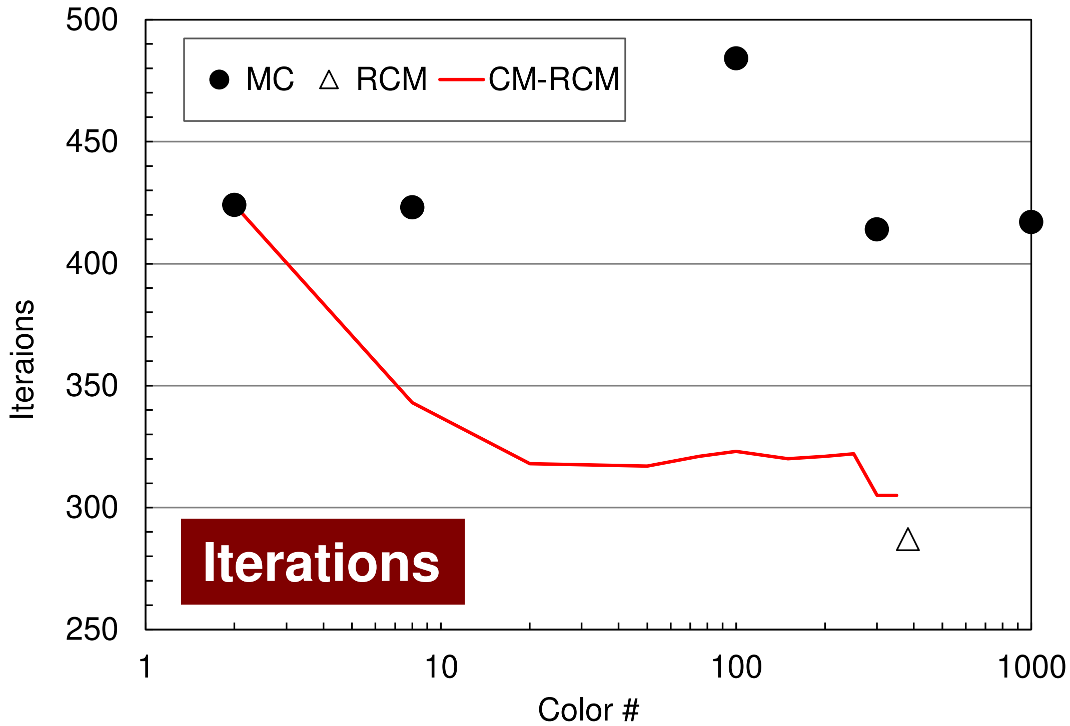
- Reordering changes sequence of matrix operations, and sometimes improves convergence.
  - Parallelism, Faster Convergence
- We need some kind of reordering for parallel ICCG on such simple meshes described in examples.

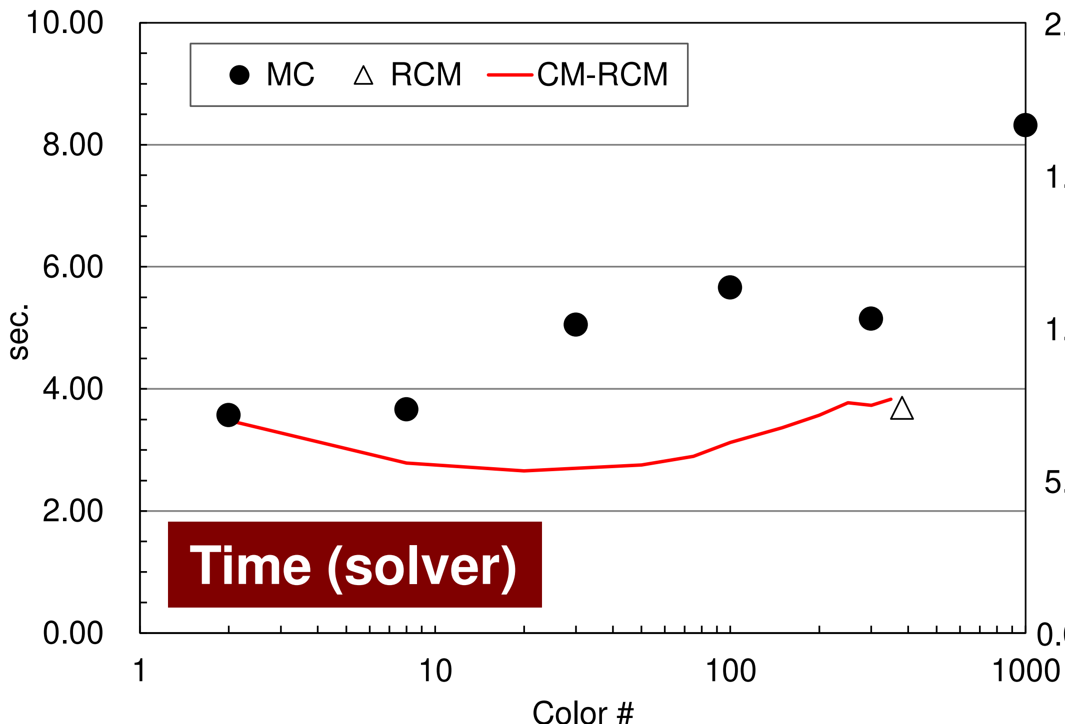
- Notice
  - Reordering may change results.
  - We need deep insight and understanding on background physics and mathematics.

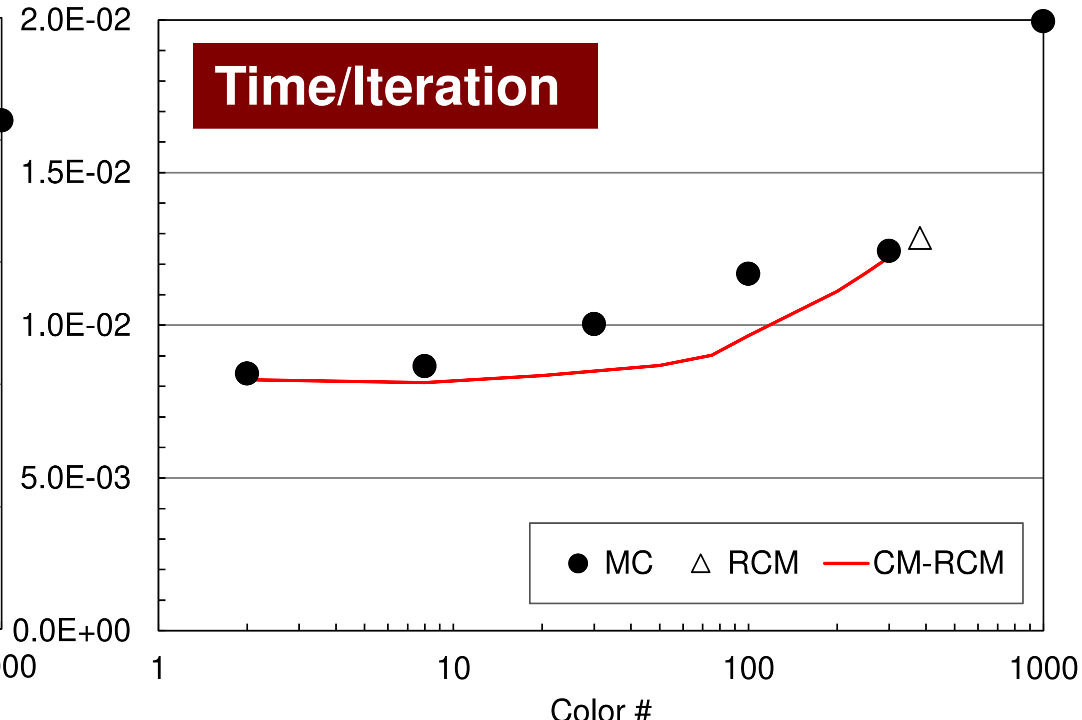
Odyssey

1-CMG/12-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)

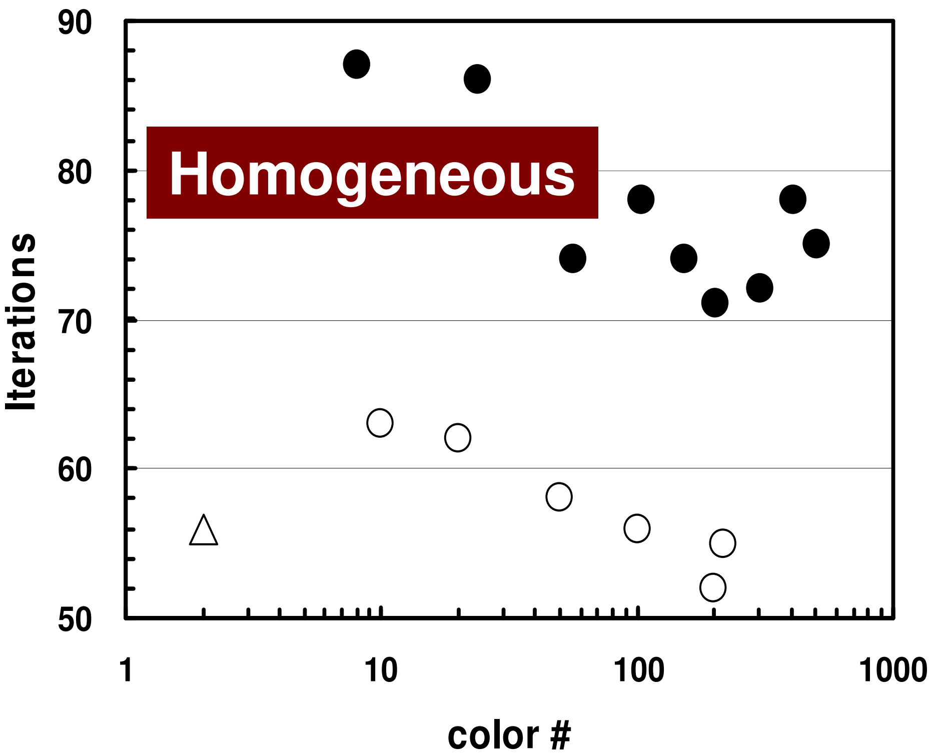


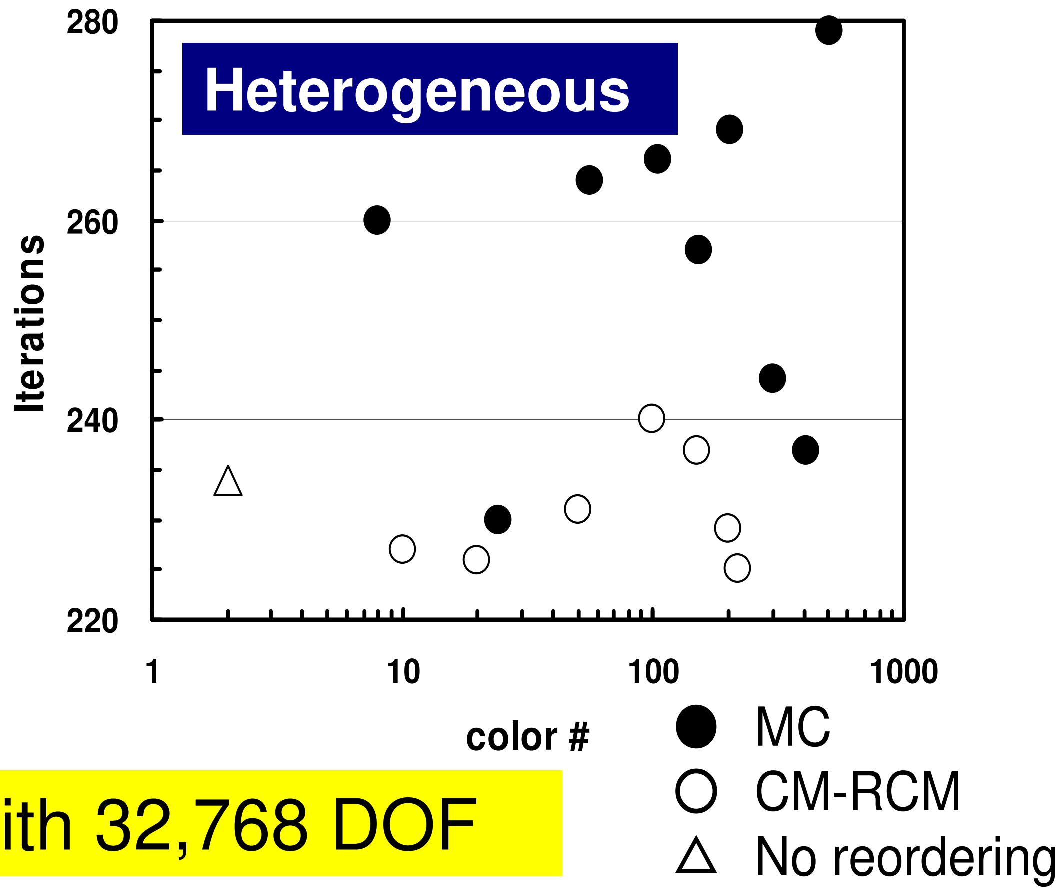




Comparison of Reordering Methods
3D Linear Elastic Problems

- MC: Slow convergence, unstable for heterogeneous cases (ill-conditioned problems).
- Cyclic-Mulricoloring + RCM (CM-RCM) is effective





3D Linear-Elastic Problems with 32,768 DOF

- Remedy for Data Dependency
- Ordering/Reordering
  - Red-Black, Multicoloring (MC)
  - Cuthill-McKee (CM), Reverse-CM (RCM)
  - Reordering and Convergence
- **Implementation**
- ICCG with Reordering

Implementation: L2-color (1/2)

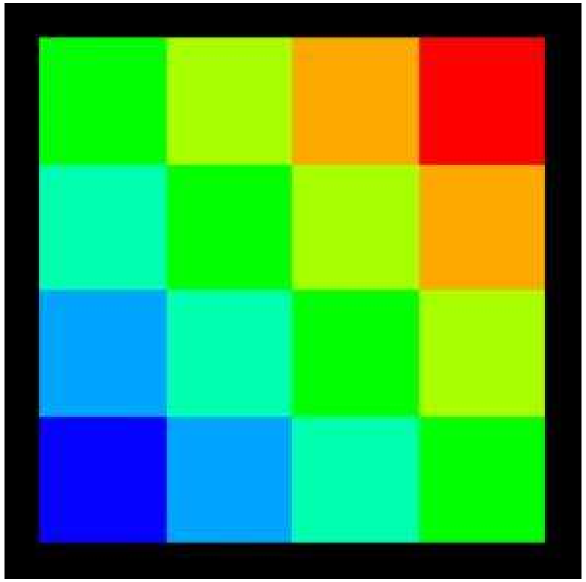
- Program for Coloring
  - MC, CM, RCM, and CM-RCM

```
$ cd multicore-f/L2/coloring/src
$ make
$ cd ../run
$ ./L2-color
  NX/NY/NZ ?

4    4    1         2D geometry with 16 meshes
You have       16 elements.
How many colors do you need ?
  #COLOR must be more than 2 and
  #COLOR must not be more than      16
   CM if #COLOR .eq. 0
  RCM if #COLOR .eq.-1
CMRCM if #COLOR .le.-2
=>
```

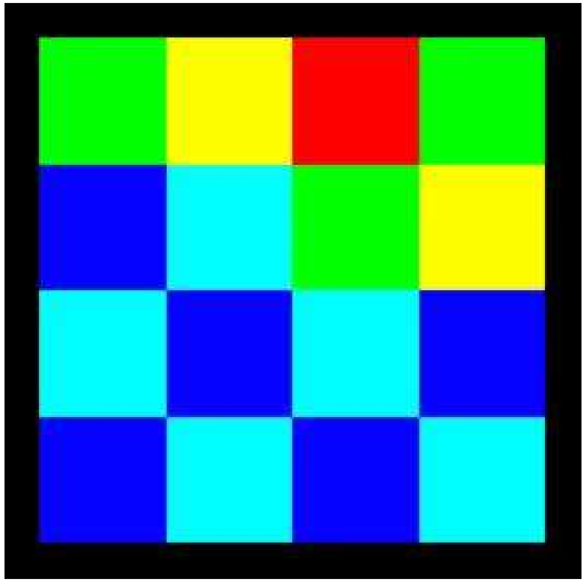
13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

Results: L2-color

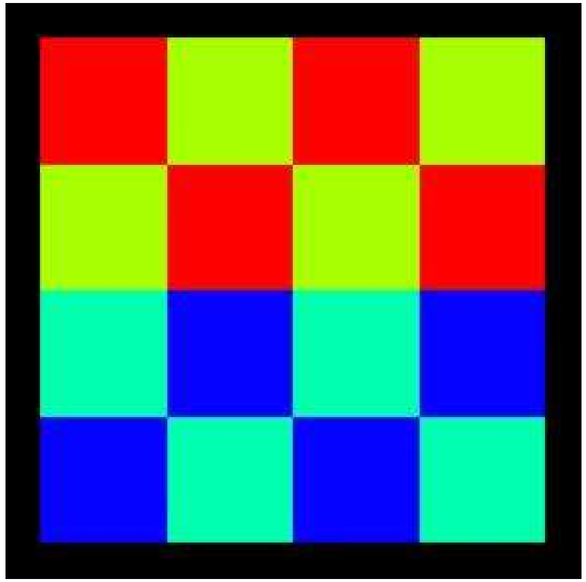
- 2 files are created
  - color.log Table of OLD-to-NEW mesh ID
    Information of the matrix
  - color.inp Colors/levels of meshes (ParaView)



INPUT: 0
(CM, 7 levels)

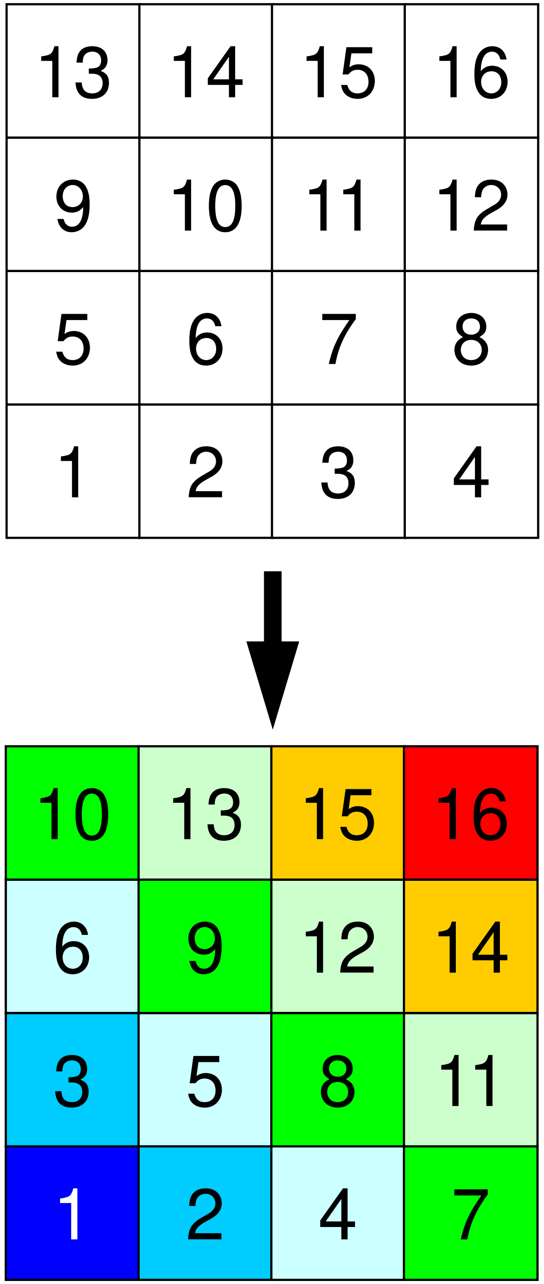


INPUT: 3
(MC, 5 colors)

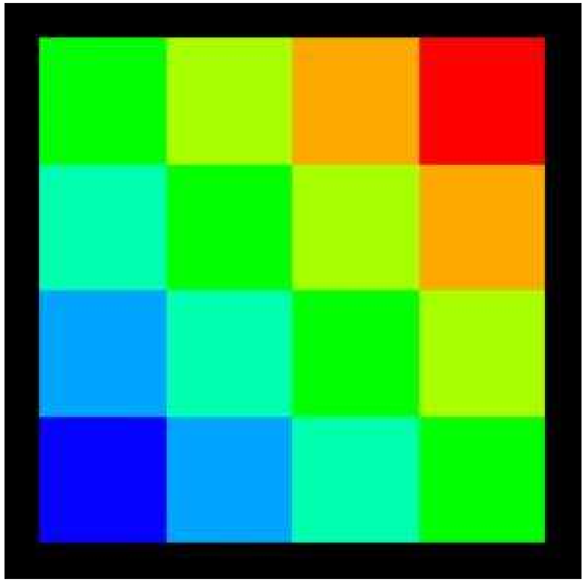


INPUT: 4
(MC, 4 colors)

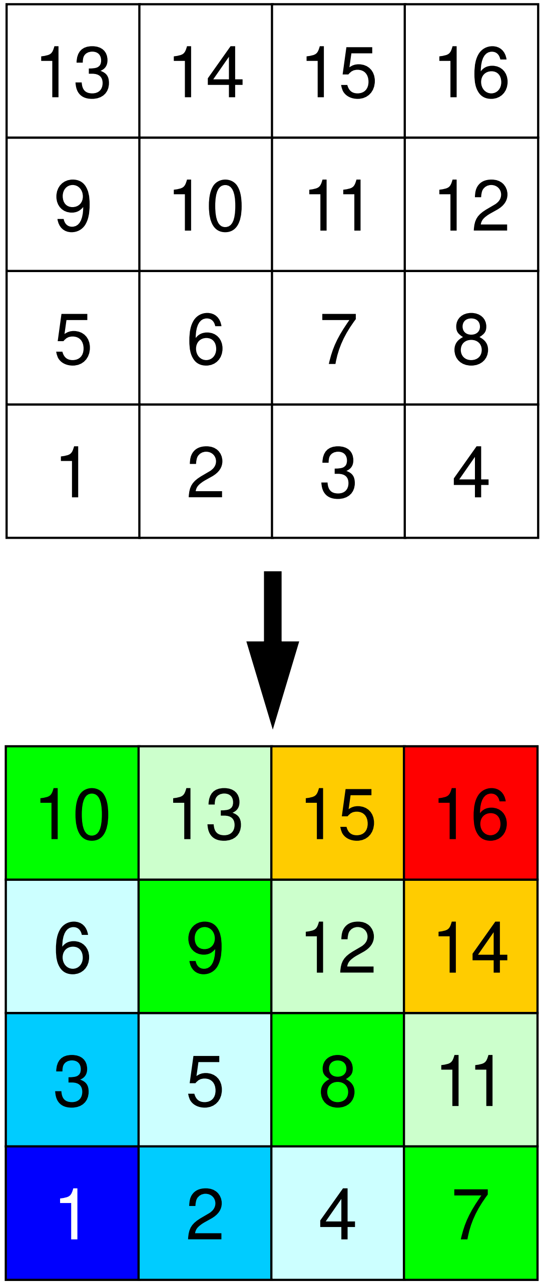
INPUT=0: CM, 7-Levels



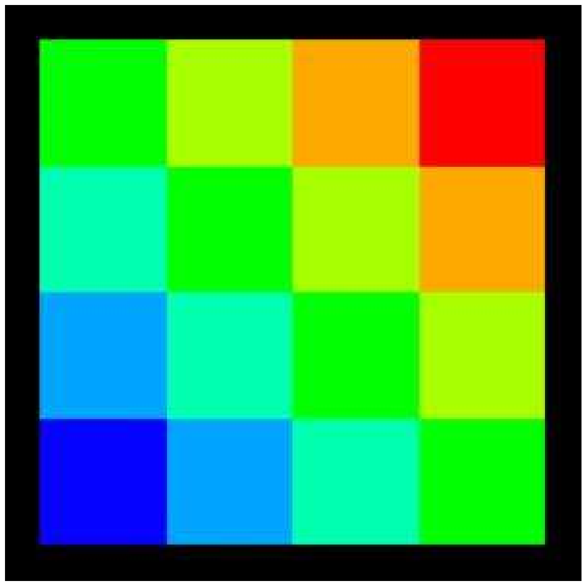
#new	1	#old	1	color	1
#new	2	#old	2	color	2
#new	3	#old	5	color	2
#new	4	#old	3	color	3
#new	5	#old	6	color	3
#new	6	#old	9	color	3
#new	7	#old	4	color	4
#new	8	#old	7	color	4
#new	9	#old	10	color	4
#new	10	#old	13	color	4
#new	11	#old	8	color	5
#new	12	#old	11	color	5
#new	13	#old	14	color	5
#new	14	#old	12	color	6
#new	15	#old	15	color	6
#new	16	#old	16	color	7



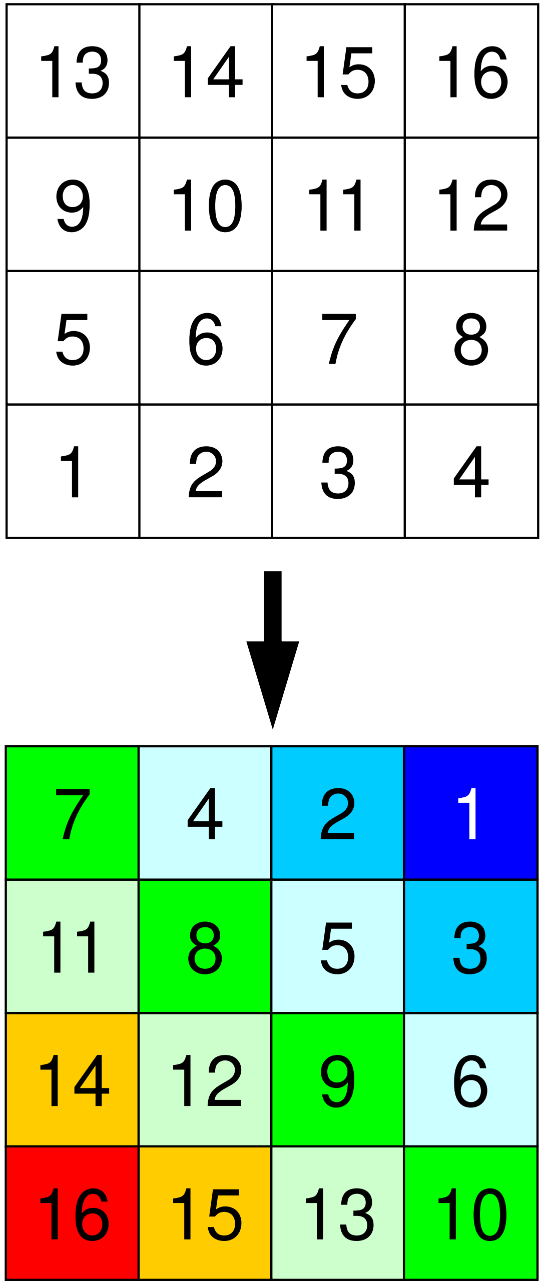
INPUT=0: CM, 7-Levels



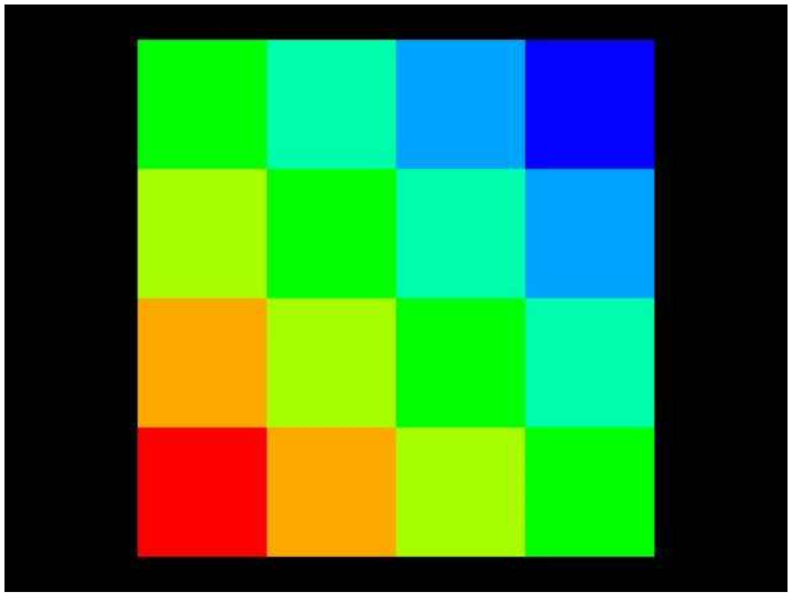
#new	1	#old	1	color	1
#new	2	#old	2	color	2
#new	3	#old	5	color	2
#new	4	#old	3	color	3
#new	5	#old	6	color	3
#new	6	#old	9	color	3
#new	7	#old	4	color	4
#new	8	#old	7	color	4
#new	9	#old	10	color	4
#new	10	#old	13	color	4
#new	11	#old	8	color	5
#new	12	#old	11	color	5
#new	13	#old	14	color	5
#new	14	#old	12	color	6
#new	15	#old	15	color	6
#new	16	#old	16	color	7



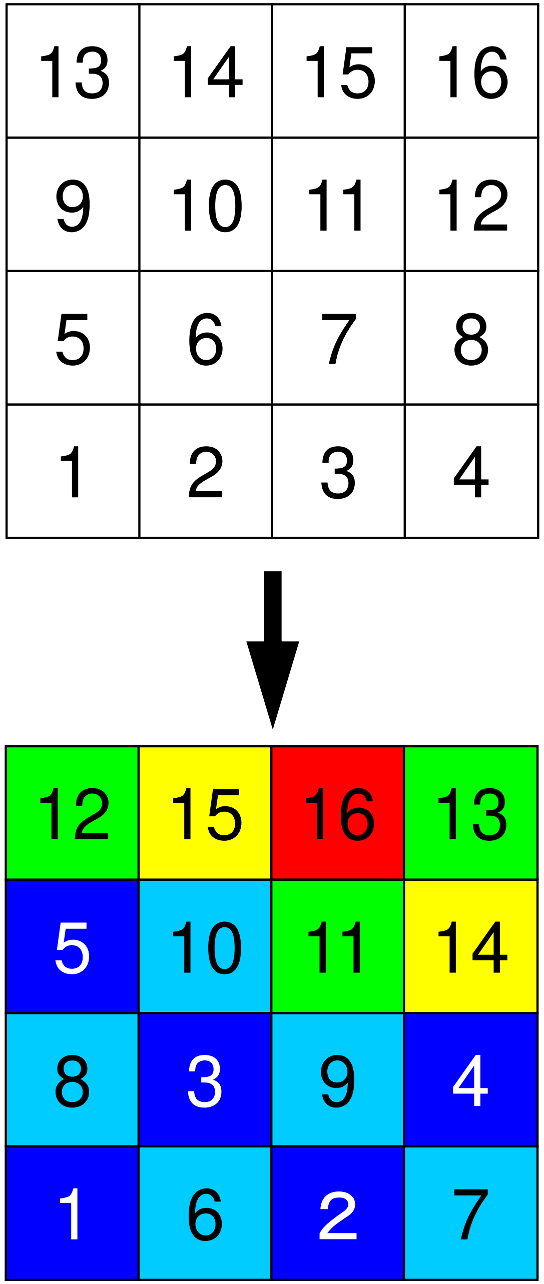
INPUT=-1: RCM, 7-Levels



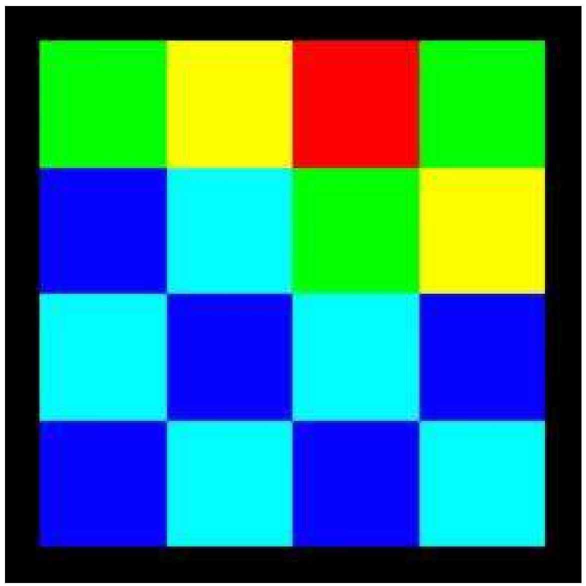

```
#new      1   #old   16   color    1
#new      2   #old   15   color    2
#new      3   #old   12   color    2
#new      4   #old   14   color    3
#new      5   #old   11   color    3
#new      6   #old    8   color    3
#new      7   #old   13   color    4
#new      8   #old   10   color    4
#new      9   #old    7   color    4
#new     10   #old    4   color    4
#new     11   #old    9   color    5
#new     12   #old    6   color    5
#new     13   #old    3   color    5
#new     14   #old    5   color    6
#new     15   #old    2   color    6
#new     16   #old    1   color    7
```



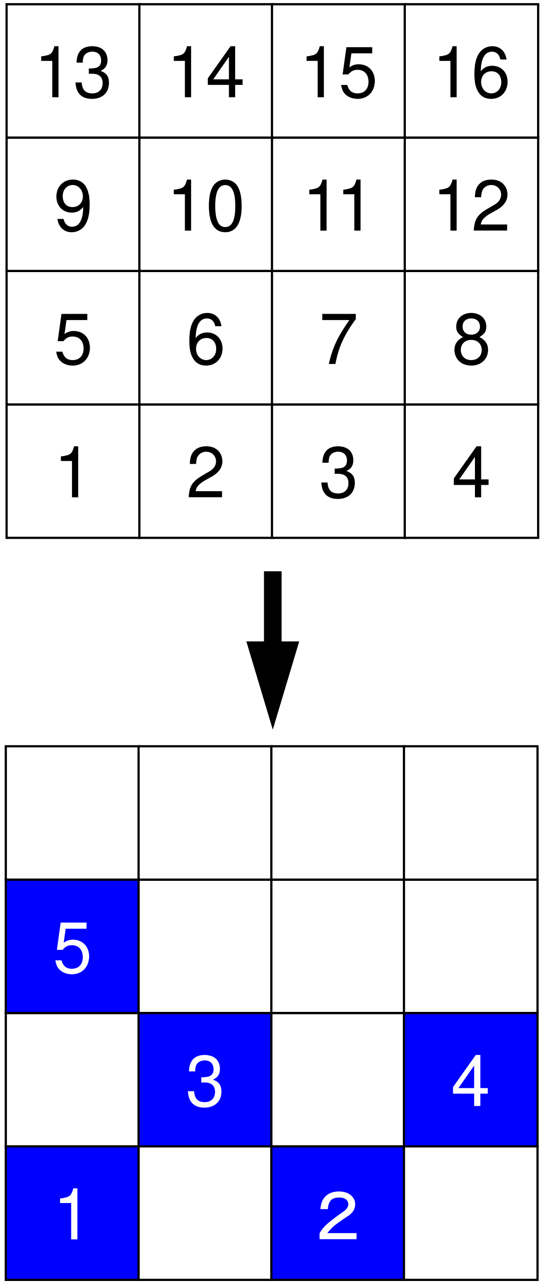
INPUT=3: MC, 5-Colors



#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5



INPUT=3: MC, 5-Colors

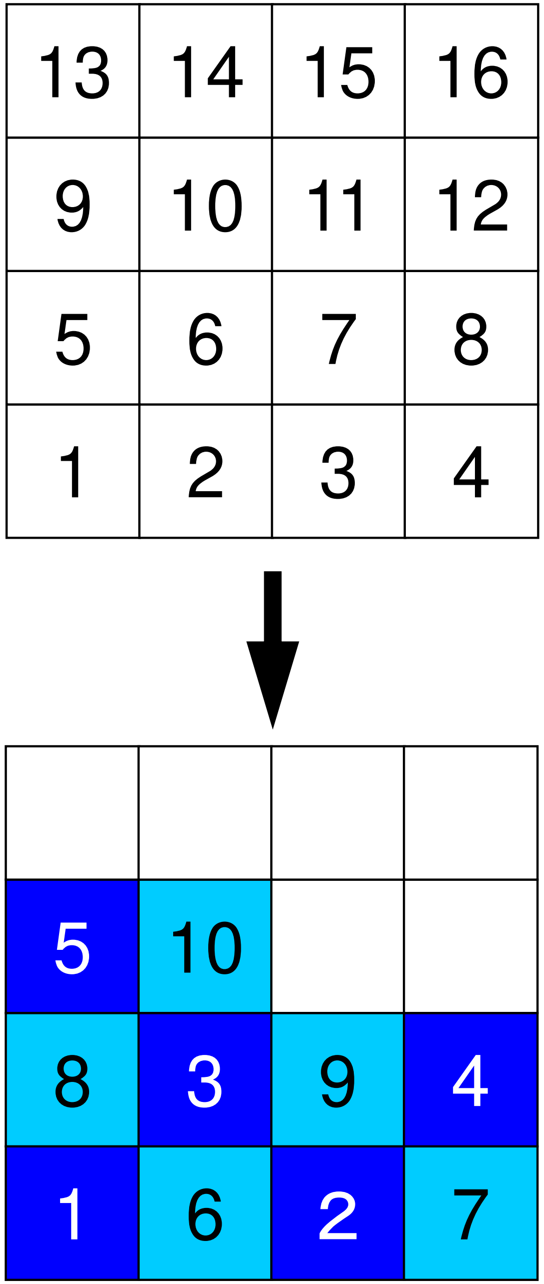


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

5 independent meshes

INPUT=3: MC, 5-Colors

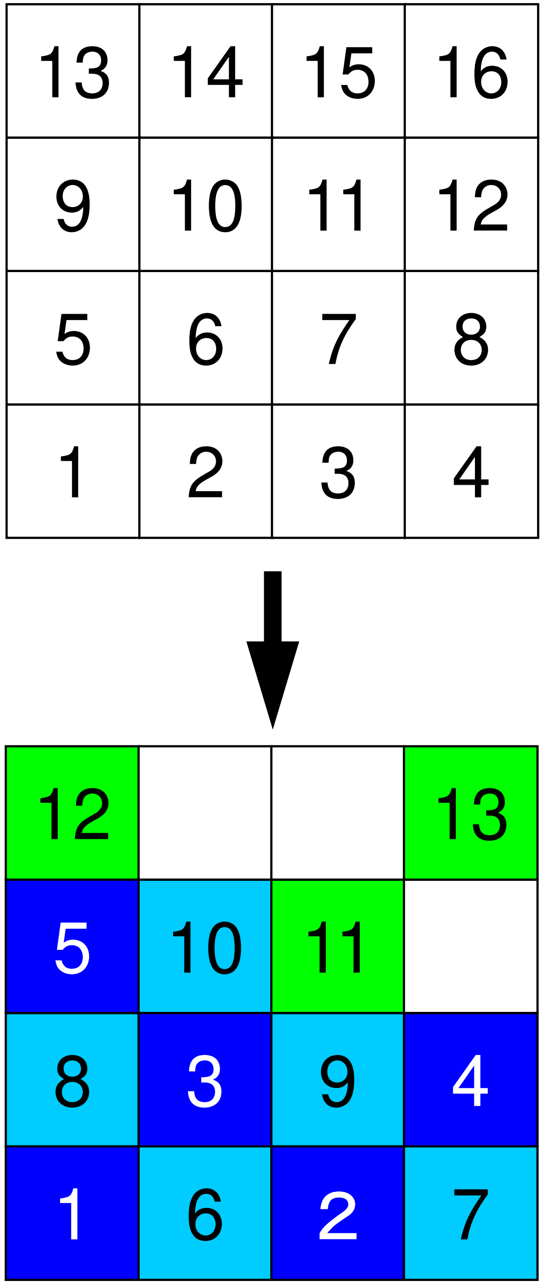


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

5 independent meshes

INPUT=3: MC, 5-Colors

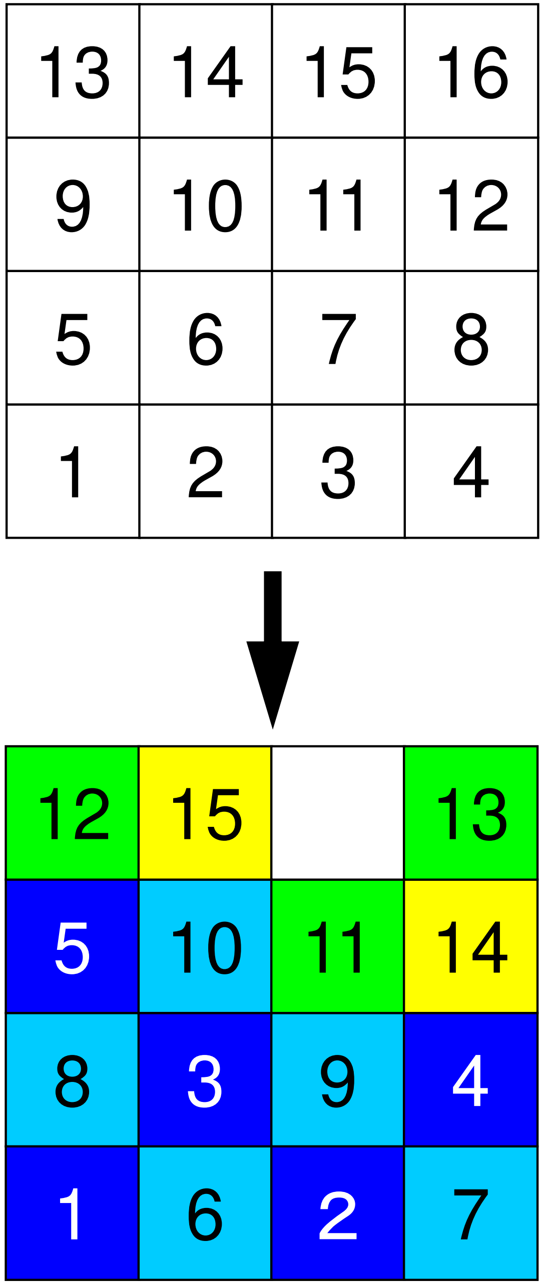


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

Proceed to the next color, if no more independent meshes.

INPUT=3: MC, 5-Colors

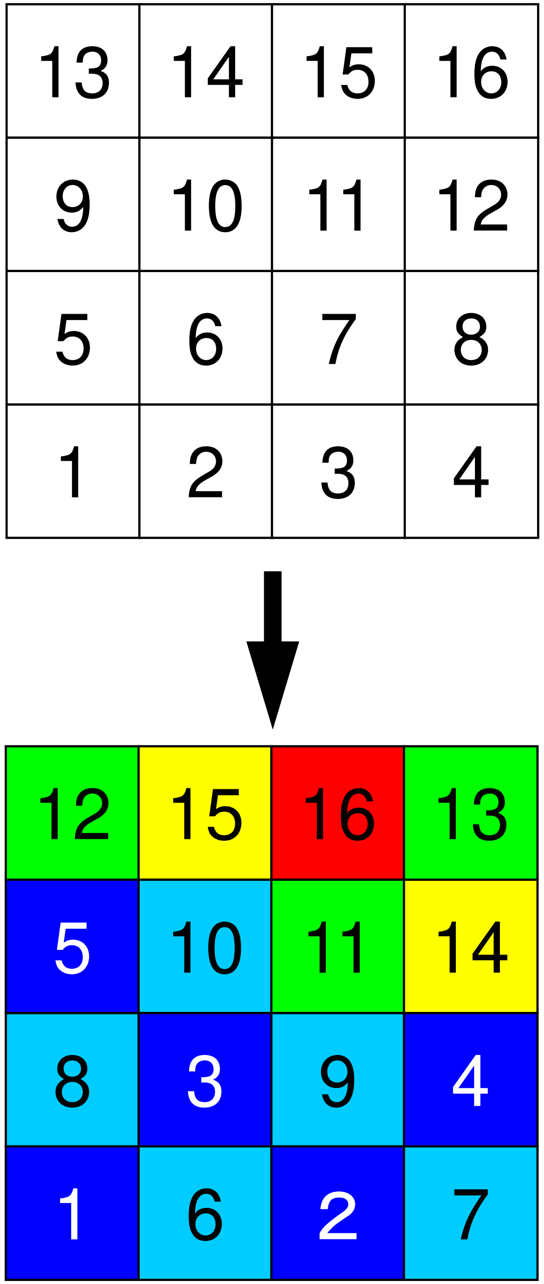


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

Proceed to the next color, if no more independent meshes.

INPUT=3: MC, 5-Colors

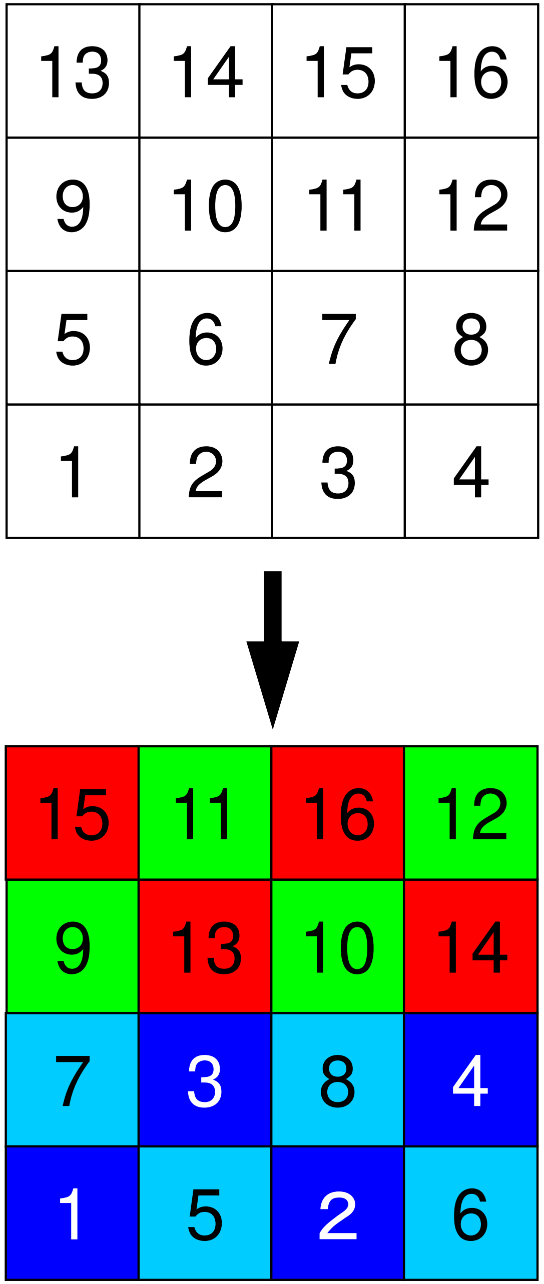



```
#new      1   #old     1   color     1
#new      2   #old     3   color     1
#new      3   #old     6   color     1
#new      4   #old     8   color     1
#new      5   #old     9   color     1
#new      6   #old     2   color     2
#new      7   #old     4   color     2
#new      8   #old     5   color     2
#new      9   #old     7   color     2
#new     10   #old    10   color     2
#new     11   #old    11   color     3
#new     12   #old    13   color     3
#new     13   #old    16   color     3
#new     14   #old    12   color     4
#new     15   #old    14   color     4
#new     16   #old    15   color     5
```

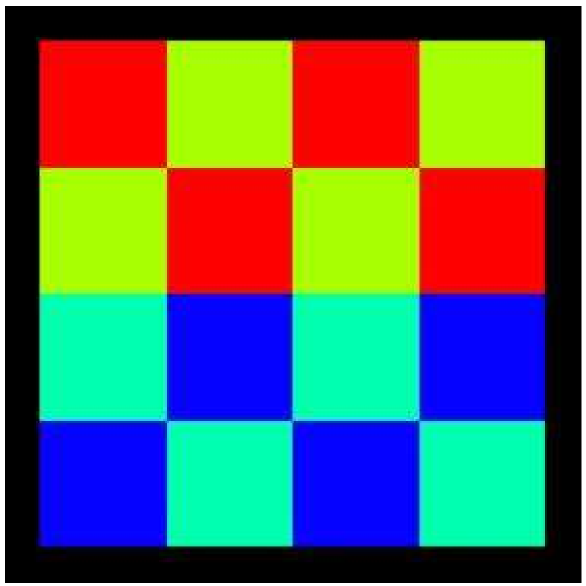
16/3=5= **ITEMcou**

Finally, 5 colors are needed.

INPUT=4: MC, 4-Colors



#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	2	color	2
#new	6	#old	4	color	2
#new	7	#old	5	color	2
#new	8	#old	7	color	2
#new	9	#old	9	color	3
#new	10	#old	11	color	3
#new	11	#old	14	color	3
#new	12	#old	16	color	3
#new	13	#old	10	color	4
#new	14	#old	12	color	4
#new	15	#old	13	color	4
#new	16	#old	15	color	4



INPUT=3: MC, 5-Colors

color.log: matrix info.

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

↓

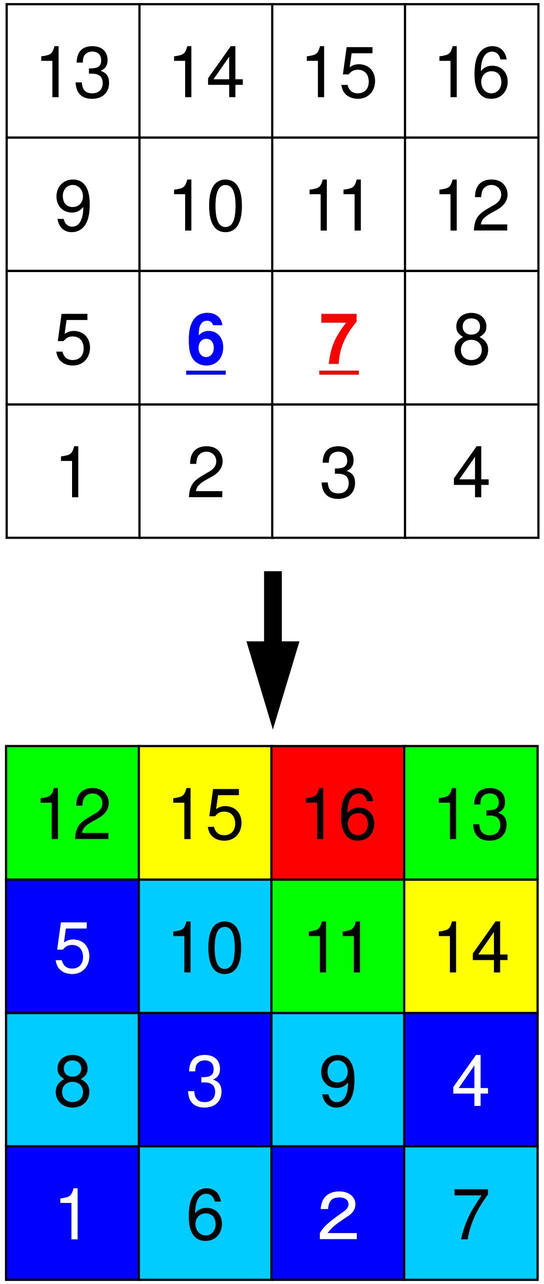
12	15	16	13
5	10	11	14
8	3	9	4
1	6	2	7

```
### INITIAL connectivity
I=     1       INL(i)=     0       INU(i)=     2
   IAL:
   IAU:      2     5
I=     2       INL(i)=     1       INU(i)=     2
   IAL:      1
   IAU:      3     6
I=     3       INL(i)=     1       INU(i)=     2
   IAL:      2
   IAU:      4     7
I=     4       INL(i)=     1       INU(i)=     1
   IAL:      3
   IAU:      8
I=     5       INL(i)=     1       INU(i)=     2
   IAL:      1
   IAU:      6     9
I=     6       INL(i)=     2       INU(i)=     2
   IAL:      2     5
   IAU:      7    10
I=     7       INL(i)=     2       INU(i)=     2
   IAL:      3     6
   IAU:      8    11
I=     8       INL(i)=     2       INU(i)=     1
   IAL:      4     7
   IAU:     12
I=     9       INL(i)=     1       INU(i)=     2
   IAL:      5
   IAU:     10    13
I=    10       INL(i)=     2       INU(i)=     2
   IAL:      6     9
   IAU:     11    14
I=    11       INL(i)=     2       INU(i)=     2
   IAL:      7    10
   IAU:     12    15
I=    12       INL(i)=     2       INU(i)=     1
   IAL:      8    11
   IAU:     16
I=    13       INL(i)=     1       INU(i)=     1
   IAL:      9
   IAU:     14
```

```
I=    14       INL(i)=   2       INU(i)=   1
   IAL:     10    13
   IAU:     15
I=    15       INL(i)=   2       INU(i)=   1
   IAL:     11    14
   IAU:     16
I=    16       INL(i)=   2       INU(i)=   0
   IAL:     12    15
   IAU:


COLOR number          5

  #new       1    #old       1   color       1
  #new       2    #old       3   color       1
  #new       3    #old       6   color       1
  #new       4    #old       8   color       1
  #new       5    #old       9   color       1
  #new       6    #old       2   color       2
  #new       7    #old       4   color       2
  #new       8    #old       5   color       2
  #new       9    #old       7   color       2
  #new      10    #old      10   color       2
  #new      11    #old      11   color       3
  #new      12    #old      13   color       3
  #new      13    #old      16   color       3
  #new      14    #old      12   color       4
  #new      15    #old      14   color       4
  #new      16    #old      15   color       5
```

INPUT=3: MC, 5-Colors

color.log: matrix info.




```
### FINAL connectivity
I=     1       INL(i)=     0       INU(i)=     2
   IAL:
   IAU:     6     8
I=     2       INL(i)=     0       INU(i)=     3
   IAL:
   IAU:     6     7     9
I=     3       INL(i)=     0       INU(i)=     4
   IAL:
   IAU:     6     8     9    10
I=     4       INL(i)=     0       INU(i)=     3
   IAL:
   IAU:     7     9    14
I=     5       INL(i)=     0       INU(i)=     3
   IAL:
   IAU:     8    10    12
I=     6       INL(i)=     3       INU(i)=     0
   IAL:     1     2     3
   IAU:
I=     7       INL(i)=     2       INU(i)=     0
   IAL:     2     4
   IAU:
I=     8       INL(i)=     3       INU(i)=     0
   IAL:     1     3     5
   IAU:
I=     9       INL(i)=     3       INU(i)=     1
   IAL:     2     3     4
   IAU:    11
I=    10       INL(i)=     2       INU(i)=     2
   IAL:     3     5
   IAU:    11    15
I=    11       INL(i)=     2       INU(i)=     2
   IAL:     9    10
   IAU:    14    16
I=    12       INL(i)=     1       INU(i)=     1
   IAL:     5
   IAU:    15
I=    13       INL(i)=     0       INU(i)=     2
   IAL:
   IAU:    14    16
```

```
I=    14       INL(i)=   3       INU(i)=   0
   IAL:     4    11    13
   IAU:
I=    15       INL(i)=   2       INU(i)=   1
   IAL:    10    12
   IAU:    16
I=    16       INL(i)=   3       INU(i)=   0
   IAL:    11    15    13
   IAU:
```

Source Files: L2-color

```
$ cd multicore-f/L2/coloring/src
$ ls
```

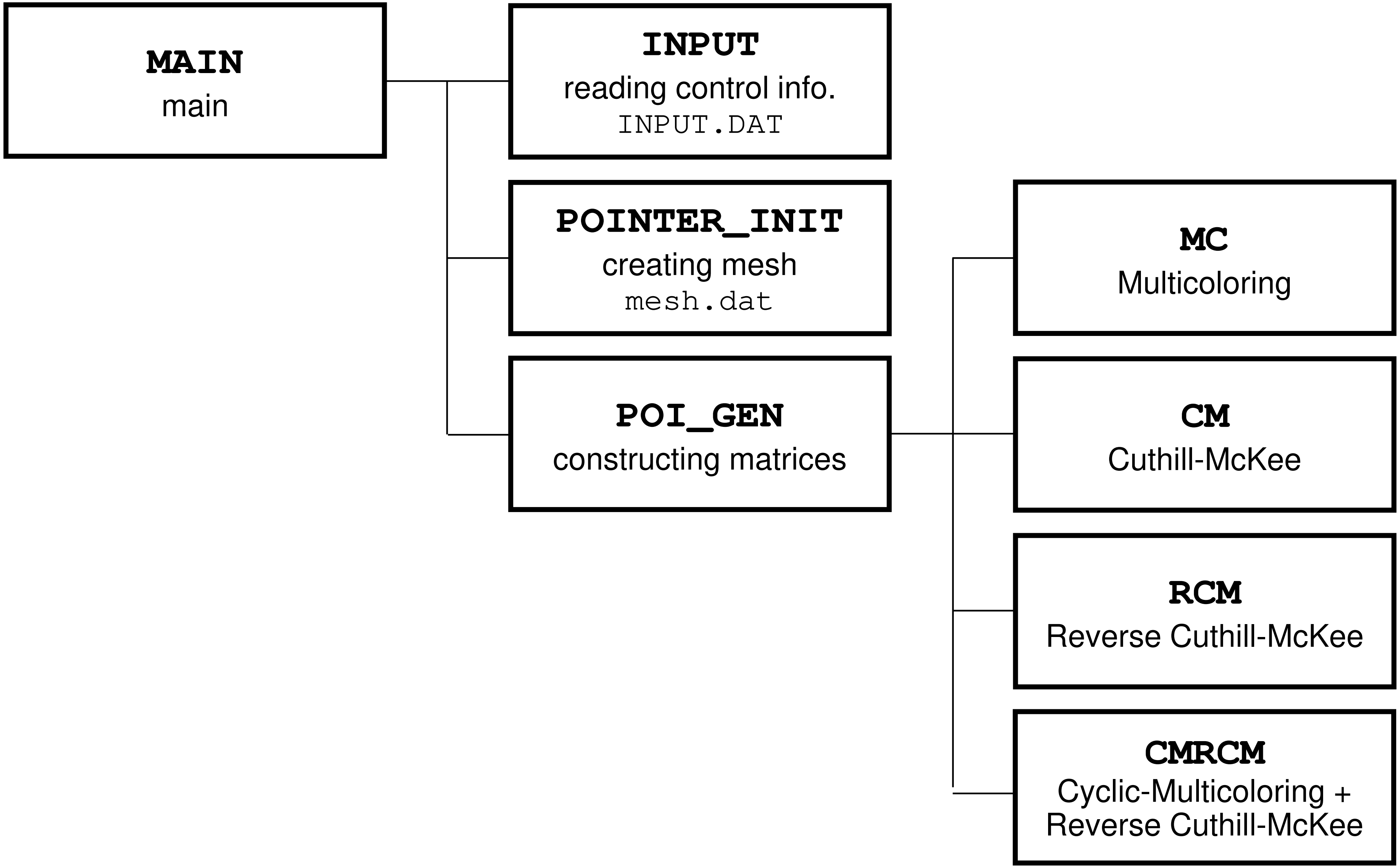
13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

Target geometry to be colored

Main Program

```
      program MAIN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

      call POINTER_INIT
      call POI_GEN

      call OUTUCD

      open (21, file='color.log', status='unknown')
        write (21,'(//,a,i8,/)') 'COLOR number', NCOLORtot
        do ic= 1, NCOLORtot
          do i= COLORindex(ic-1)+1, COLORindex(ic)
            write (21,'(3(a,i8))') '  #new', i, '   #old', NEWtoOLD(i), &
     &                             '  color', ic
          enddo
        enddo
      close (21)

      stop
      end
```

Structure of L2-color



Main Program

```
      program MAIN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

      call POINTER_INIT
      call POI_GEN

      call OUTUCD

      open (21, file='color.log', status='unknown')
        write (21,'(//,a,i8,/)') 'COLOR number', NCOLORtot
        do ic= 1, NCOLORtot
          do i= COLORindex(ic-1)+1, COLORindex(ic)
            write (21,'(3(a,i8))') '   #new', i, '    #old', NEWtoOLD(i), &
     &                             '   color', ic
          enddo
        enddo
      close (21)

      stop
      end
```

module STRUCT

```
      module STRUCT

      include 'precision.inc'

!C
!C-- METRICs & FLUX
      integer (kind=kint) :: ICELTOT, ICELTOTp, N
      integer (kind=kint) :: NX, NY, NZ, NXP1, NYP1, NZP1, IBNODTOT
      integer (kind=kint) :: NXc, NYc, NZc

      real (kind=kreal) ::                                          &
     &      DX, DY, DZ, XAREA, YAREA, ZAREA, RDX, RDY, RDZ,         &
     &      RDX2, RDY2, RDZ2, R2DX, R2DY, R2DZ

      real (kind=kreal), dimension(:), allocatable ::               &
     &     VOLCEL, VOLNOD, RVC, RVN

      integer (kind=kint), dimension(:,:), allocatable ::           &
     &         XYZ, NEIBcell

!C
!C-- BOUNDARYs
      integer (kind=kint) :: ZmaxCELtot
      integer (kind=kint), dimension(:), allocatable :: BC_INDEX, BC_NOD
      integer (kind=kint), dimension(:), allocatable :: ZmaxCEL

!C
!C-- WORK
      integer (kind=kint), dimension(:,:), allocatable :: IWKX
      real(kind=kreal),    dimension(:,:), allocatable :: FCV

      end module STRUCT
```

ICELTOT:
Number of meshes (NX x NY x NZ)

N:
Number of modes

NX,NY,NZ:
Number of meshes in x/y/z directions

NXP1,NYP1,NZP1:
Number of nodes in x/y/z directions

IBNODTOT:
= NXP1 x NYP1

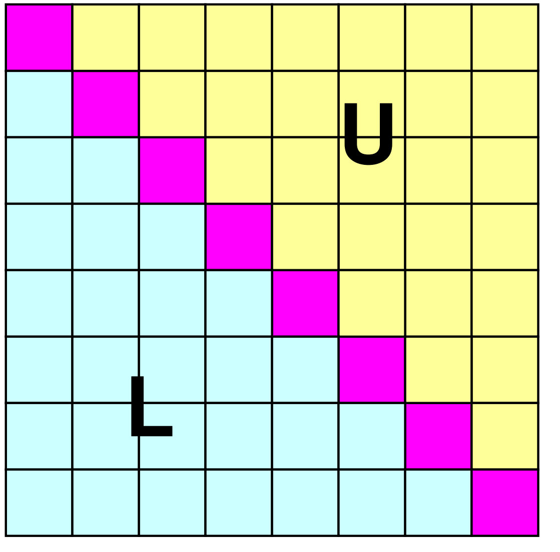
XYZ(ICELTOT,3):
Location of meshes

NEIBcell(ICELTOT,6):
Neighboring meshes

module PCG

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL

real(kind=8) :: EPSICCG

real(kind=8), dimension(:  ), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:,:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

end module PCG
```

- Sparse Matrix
- Only non-zero off-diagonal components (CRS)
- Diagonal/Lower/Upper components are stored separately



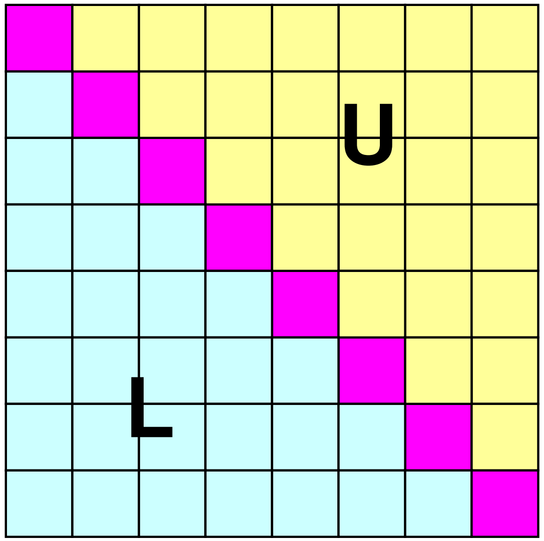
module PCG

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL

real(kind=8) :: EPSICCG

real(kind=8), dimension(:  ), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:,:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

end module PCG
```

Lower Part (Column ID)
`IAL(icou,i) < i`

Upper Part (Column ID)
`IAU(icou,i) > i`

`INL(ICELTOT)`	# Non-zero off-diag. components (lower)
`IAL(NL,ICELTOT)`	**Col. ID: non-zero off-diag. comp. (lower)**
`INU(ICELTOT)`	# Non-zero off-diag. components (upper)
`IAU(NU,ICELTOT)`	**Col. ID: non-zero off-diag. comp. (upper)**
`NU,NL`	Max # of L/U non-zero off-diag. comp.s (=6)
`NCOLORtot`	Total number of colors/levels
`COLORindex` `(0:NCOLORtot)`	Index of number of meshes in each color/level `(COLORindex(icol)- COLORindex(icol-1))`
`OLDtoNEW, NEWtoOLD`	Reference table before/after renumbering



module PCG

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL

real(kind=8) :: EPSICCG

real(kind=8), dimension(:  ), allocatable :: D, PHI, BFORCE
real(kind=8), dimension(:,:), allocatable :: AL, AU

integer, dimension(:), allocatable :: INL, INU, COLORindex
integer, dimension(:), allocatable :: OLDtoNEW, NEWtoOLD

integer, dimension(:,:), allocatable :: IAL, IAU

end module PCG
```

Lower Part (Column ID)

`IAL(icou,i) < i`

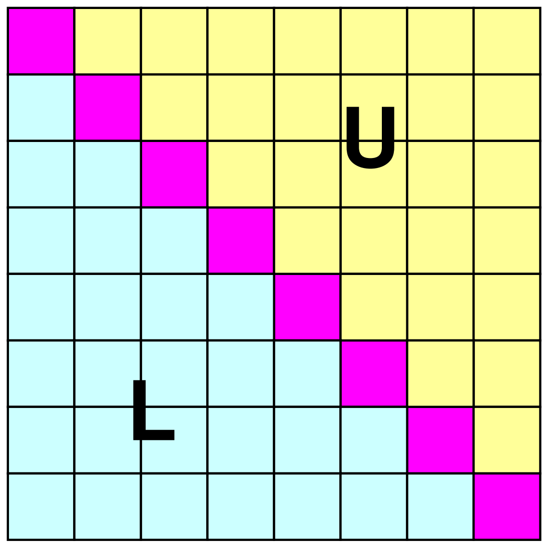
`INL(i)` : Number@each row

Upper Part (Column ID)

`IAU(icou,i) > i`

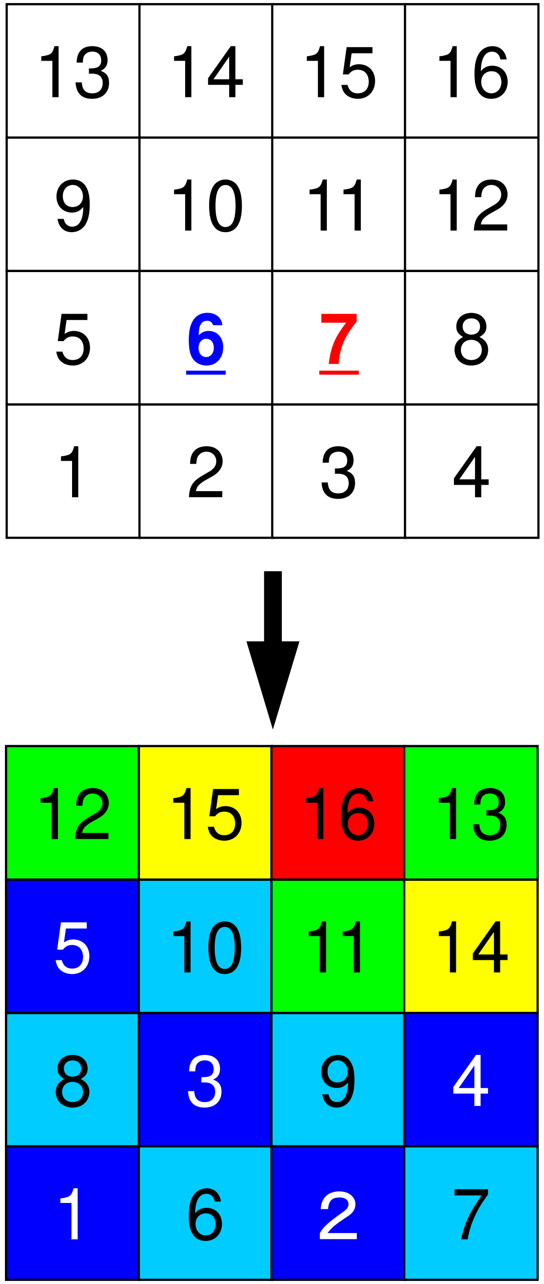
`INU(i)` : Number@each row

`INL(ICELTOT)`	**# Non-zero off-diag. components (lower)**
`IAL(NL,ICELTOT)`	Col. ID: non-zero off-diag. comp. (lower)
`INU(ICELTOT)`	**# Non-zero off-diag. components (upper)**
`IAU(NU,ICELTOT)`	Col. ID: non-zero off-diag. comp. (upper)
`NU,NL`	Max # of L/U non-zero off-diag. comp.s (=6)
`NCOLORtot`	Total number of colors/levels
`COLORindex` `(0:NCOLORtot)`	Index of number of meshes in each color/level `(COLORindex(icol)- COLORindex(icol-1))`
`OLDtoNEW, NEWtoOLD`	Reference table before/after renumbering



INPUT=3: MC, 5-Colors

color.log: matrix info.

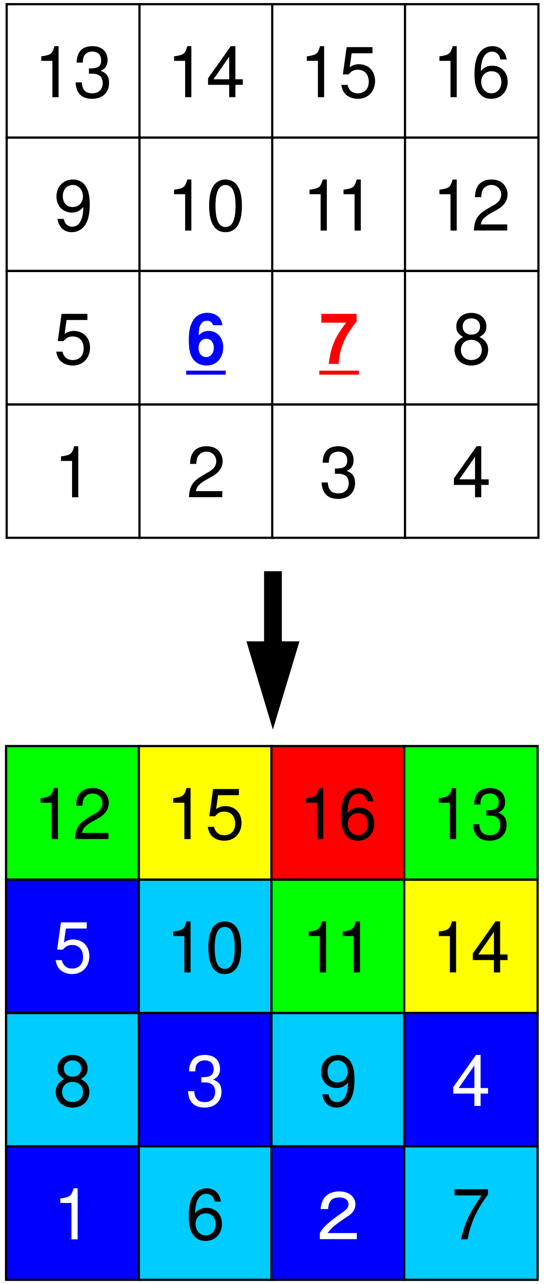



```
### INITIAL connectivity
I=     1       INL(i)=     0       INU(i)=     2
   IAL:
   IAU:      2     5
I=     2       INL(i)=     1       INU(i)=     2
   IAL:      1
   IAU:      3     6
I=     3       INL(i)=     1       INU(i)=     2
   IAL:      2
   IAU:      4     7
I=     4       INL(i)=     1       INU(i)=     1
   IAL:      3
   IAU:      8
I=     5       INL(i)=     1       INU(i)=     2
   IAL:      1
   IAU:      6     9
I=     6       INL(i)=     2       INU(i)=     2
   IAL:      2     5
   IAU:      7    10
I=     7       INL(i)=     2       INU(i)=     2
   IAL:      3     6
   IAU:      8    11
I=     8       INL(i)=     2       INU(i)=     1
   IAL:      4     7
   IAU:     12
I=     9       INL(i)=     1       INU(i)=     2
   IAL:      5
   IAU:     10    13
I=    10       INL(i)=     2       INU(i)=     2
   IAL:      6     9
   IAU:     11    14
I=    11       INL(i)=     2       INU(i)=     2
   IAL:      7    10
   IAU:     12    15
I=    12       INL(i)=     2       INU(i)=     1
   IAL:      8    11
   IAU:     16
I=    13       INL(i)=     1       INU(i)=     1
   IAL:      9
   IAU:     14
```

```
I=    14       INL(i)=  2       INU(i)=  1
   IAL:    10    13
   IAU:    15
I=    15       INL(i)=  2       INU(i)=  1
   IAL:    11    14
   IAU:    16
I=    16       INL(i)=  2       INU(i)=  0
   IAL:    12    15
   IAU:


COLOR number          5

  #new       1    #old       1   color     1
  #new       2    #old       3   color     1
  #new       3    #old       6   color     1
  #new       4    #old       8   color     1
  #new       5    #old       9   color     1
  #new       6    #old       2   color     2
  #new       7    #old       4   color     2
  #new       8    #old       5   color     2
  #new       9    #old       7   color     2
  #new      10    #old      10   color     2
  #new      11    #old      11   color     3
  #new      12    #old      13   color     3
  #new      13    #old      16   color     3
  #new      14    #old      12   color     4
  #new      15    #old      14   color     4
  #new      16    #old      15   color     5
```

INPUT=3: MC, 5-Colors

color.log: matrix info.




```
### FINAL connectivity
I=     1      INL(i)=     0      INU(i)=     2
   IAL:
   IAU:     6     8
I=     2      INL(i)=     0      INU(i)=     3
   IAL:
   IAU:     6     7     9
I=     3      INL(i)=     0      INU(i)=     4
   IAL:
   IAU:     6     8     9    10
I=     4      INL(i)=     0      INU(i)=     3
   IAL:
   IAU:     7     9    14
I=     5      INL(i)=     0      INU(i)=     3
   IAL:
   IAU:     8    10    12
I=     6      INL(i)=     3      INU(i)=     0
   IAL:     1     2     3
   IAU:
I=     7      INL(i)=     2      INU(i)=     0
   IAL:     2     4
   IAU:
I=     8      INL(i)=     3      INU(i)=     0
   IAL:     1     3     5
   IAU:
I=     9      INL(i)=     3      INU(i)=     1
   IAL:     2     3     4
   IAU:    11
I=    10      INL(i)=     2      INU(i)=     2
   IAL:     3     5
   IAU:    11    15
I=    11      INL(i)=     2      INU(i)=     2
   IAL:     9    10
   IAU:    14    16
I=    12      INL(i)=     1      INU(i)=     1
   IAL:     5
   IAU:    15
I=    13      INL(i)=     0      INU(i)=     2
   IAL:
   IAU:    14    16
```

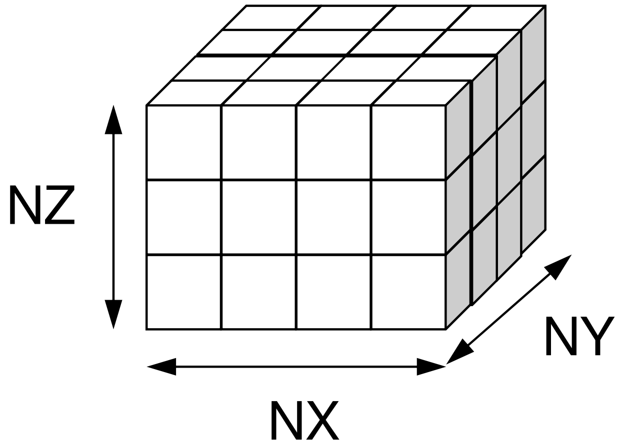
```
I=    14      INL(i)=   3      INU(i)=   0
   IAL:     4    11    13
   IAU:
I=    15      INL(i)=   2      INU(i)=   1
   IAL:    10    12
   IAU:    16
I=    16      INL(i)=   3      INU(i)=   0
   IAL:    11    15    13
   IAU:
```

Main Program

```
      program MAIN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

      call POINTER_INIT
      call POI_GEN

      call OUTUCD

      open (21, file='color.log', status='unknown')
        write (21,'(//,a,i8,/)') 'COLOR number', NCOLORtot
        do ic= 1, NCOLORtot
          do i= COLORindex(ic-1)+1, COLORindex(ic)
            write (21,'(3(a,i8))') '  #new', i, '   #old', NEWtoOLD(i), &
     &                             '  color', ic
          enddo
        enddo
      close (21)

      stop
      end
```

pointer_init (1/3)

```
!C
!C***
!C*** POINTER_INIT
!C***
!C
      subroutine POINTER_INIT
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)
!C
!C +-----------------------+
!C | Generating MESH info. |
!C +-----------------------+
!C===
      write (*,*) 'NX/NY/NZ ?'
      read  (*,*)  NX, NY, NZ

      ICELTOT= NX  * NY  * NZ

      NXP1= NX + 1
      NYP1= NY + 1
      NZP1= NZ + 1

      allocate (NEIBcell(ICELTOT,6), XYZ(ICELTOT,3))
      NEIBcell= 0
```



NX,NY,NZ:
Number of meshes in x/y/z directions

NXP1,NYP1,NZP1:
Number of nodes in x/y/z directions (for visualization)

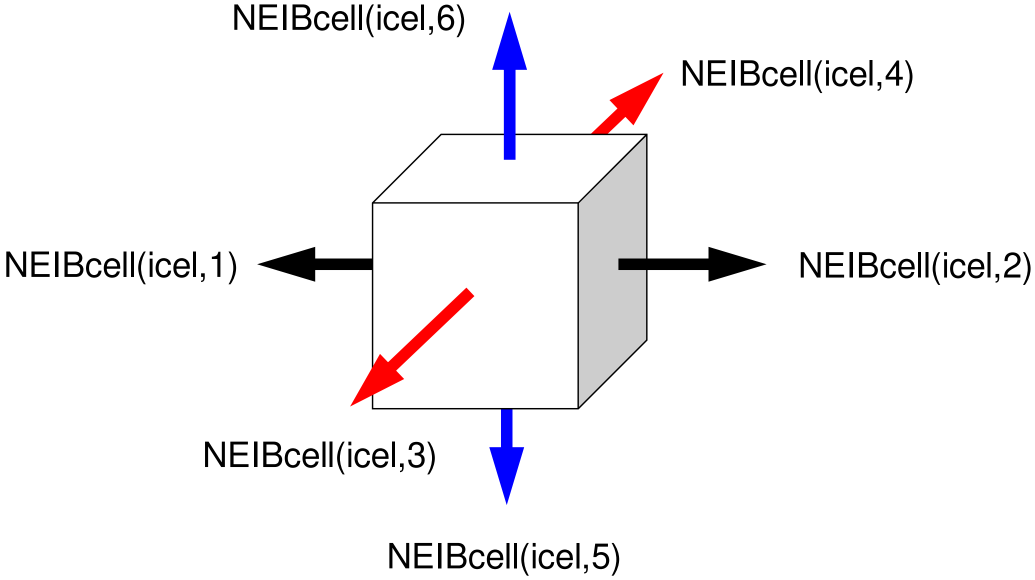
ICELTOT:
Number of meshes (NX x NY x NZ)

XYZ(ICELTOT,3):
Location of meshes

NEIBcell(ICELTOT,6):
Neighboring meshesc

pointer_init (2/3)

```
      do k= 1, NZ
        do j= 1, NY
          do i= 1, NX
            icel= (k-1)*NX*NY + (j-1)*NX + i
            NEIBcell(icel,1)= icel - 1
            NEIBcell(icel,2)= icel + 1
            NEIBcell(icel,3)= icel - NX
            NEIBcell(icel,4)= icel + NX
            NEIBcell(icel,5)= icel - NX*NY
            NEIBcell(icel,6)= icel + NX*NY
            if (i.eq. 1) NEIBcell(icel,1)= 0
            if (i.eq.NX) NEIBcell(icel,2)= 0
            if (j.eq. 1) NEIBcell(icel,3)= 0
            if (j.eq.NY) NEIBcell(icel,4)= 0
            if (k.eq. 1) NEIBcell(icel,5)= 0
            if (k.eq.NZ) NEIBcell(icel,6)= 0

            XYZ(icel,1)= i
            XYZ(icel,2)= j
            XYZ(icel,3)= k

          enddo
        enddo
      enddo
!C===
```



i= XYZ(icel,1)
j= XYZ(icel,2), k= XYZ(icel,3)
icel= (k-1)*NX*NY + (j-1)*NX + i

NEIBcell(icel,1)= icel – 1
NEIBcell(icel,2)= icel + 1
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,6)= icel + NX*NY

pointer_init (3/3)

```
!C
!C +------------+
!C | Parameters |
!C +------------+
!C===
      if (DX.le.0.0e0) then
        DX= 1.d0 / dfloat(NX)
        DY= 1.d0 / dfloat(NY)
        DZ= 1.d0 / dfloat(NZ)
      endif

      NXP1= NX + 1
      NYP1= NY + 1
      NZP1= NZ + 1

      IBNODTOT= NXP1 * NYP1
      N       = NXP1 * NYP1 * NZP1
!C===
      return
      end
```

Main Program

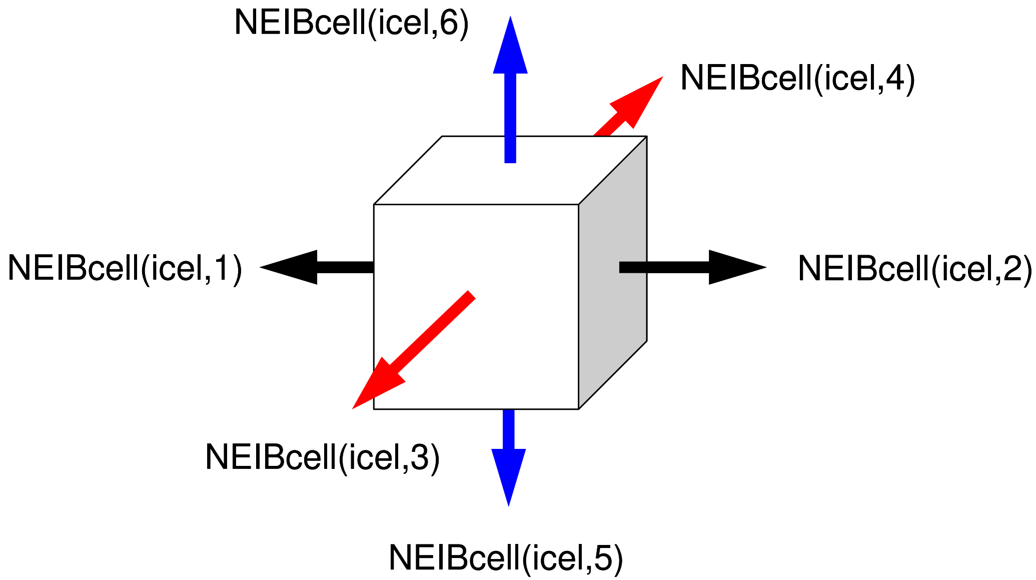
```
      program MAIN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

      call POINTER_INIT
      call POI_GEN

      call OUTUCD

      open (21, file='color.log', status='unknown')
        write (21,'(//,a,i8,/)') 'COLOR number', NCOLORtot
        do ic= 1, NCOLORtot
          do i= COLORindex(ic-1)+1, COLORindex(ic)
            write (21,'(3(a,i8))') '   #new', i, '   #old', NEWtoOLD(i), &
     &                             '   color', ic
          enddo
        enddo
      close (21)

      stop
      end
```

poi_gen (1/4)

```
      subroutine POI_GEN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

!C
!C-- INIT.
      nn = ICELTOT

      NU= 6
      NL= 6

      allocate (INL(nn), INU(nn), IAL(NL,nn), IAU(NU,nn))

      INL= 0
      INU= 0
      IAL= 0
      IAU= 0
```

poi_gen (2/4)

```
!C
!C +--------------+
!C | CONNECTIVITY |
!C +--------------+
!C===
      do icel= 1, ICELTOT
        icN1= NEIBcell(icel,1)
        icN2= NEIBcell(icel,2)
        icN3= NEIBcell(icel,3)
        icN4= NEIBcell(icel,4)
        icN5= NEIBcell(icel,5)
        icN6= NEIBcell(icel,6)

        icouG= 0
        if (icN5.ne.0.and.icN5.le.ICELTOT) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN5
          INL(     icel)= icou
        endif

        if (icN3.ne.0.and.icN3.le.ICELTOT) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN3
          INL(     icel)= icou
        endif

        if (icN1.ne.0.and.icN1.le.ICELTOT) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN1
          INL(     icel)= icou
        endif
```



Lower Triangular Part

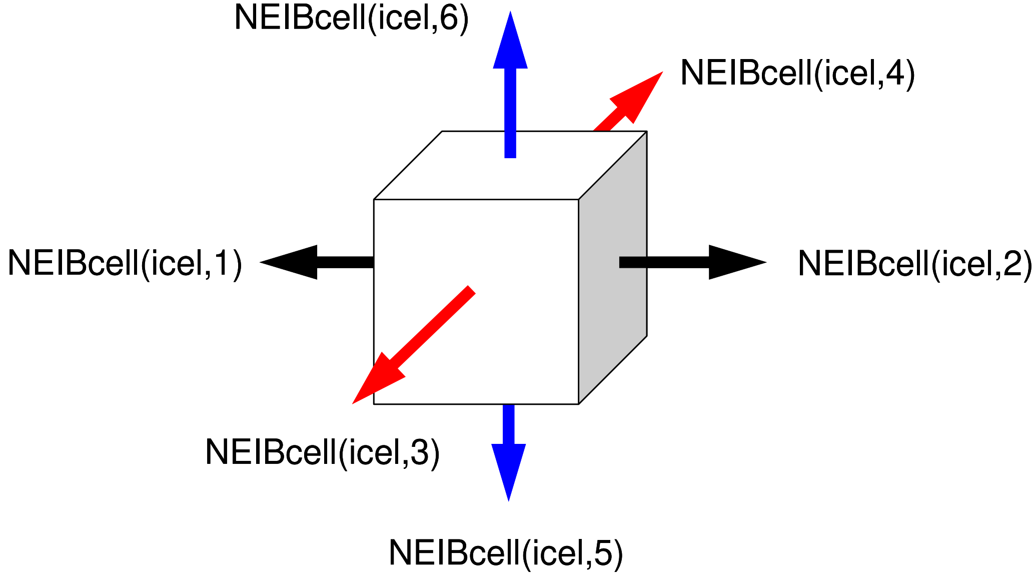
NEIBcell(icel,5)= icel – NX*NY

NEIBcell(icel,3)= icel – NX

NEIBcell(icel,1)= icel – 1

poi_gen (3/4)

```
!C
!C +--------------+
!C | CONNECTIVITY |
!C +--------------+
!C===
      do icel= 1, ICELTOT
        icN1= NEIBcell(icel,1)
        icN2= NEIBcell(icel,2)
        icN3= NEIBcell(icel,3)
        icN4= NEIBcell(icel,4)
        icN5= NEIBcell(icel,5)
        icN6= NEIBcell(icel,6)

…

        if (icN2.ne.0.and.icN2.le.ICELTOT) then
          icou= INU(icel) + 1
          IAU(icou,icel)= icN2
          INU(     icel)= icou
        endif

        if (icN4.ne.0.and.icN4.le.ICELTOT) then
          icou= INU(icel) + 1
          IAU(icou,icel)= icN4
          INU(     icel)= icou
        endif

        if (icN6.ne.0.and.icN6.le.ICELTOT) then
          icou= INU(icel) + 1
          IAU(icou,icel)= icN6
          INU(     icel)= icou
        endif
      enddo
!C===
```



Uppr Triangular Part

NEIBcell(icel,2)= icel + 1
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,6)= icel + NX*NY

poi_gen (4/4)

```
!C
!C +---------------+
!C | MULTICOLORING |
!C +---------------+
!C===
 111  continue
      write (*,'(//a,i8,a)') 'You have', ICELTOT, ' elements.'
      write (*,'(  a     )') 'How many colors do you need ?'
      write (*,'(  a     )') '  #COLOR must be more than 2 and'
      write (*,'(  a,i8  )') '  #COLOR must not be more than', ICELTOT
      write (*,'(  a     )') '  if #COLOR=0 :  CM ordering'
      write (*,'(  a     )') '  if #COLOR<0 : RCM ordering'
      write (*,'(  a     )') '=>'
      read  (*,*)            NCOLORtot
      if (NCOLORtot.eq.1.or.NCOLORtot.gt.ICELTOT) goto 111

      allocate (OLDtoNEW(ICELTOT), NEWtoOLD(ICELTOT))
      allocate (COLORindex(0:ICELTOT))

      if (NCOLORtot.gt.0) then
        call MC (ICELTOT, NL, NU, INL, IAL, INU, IAU,                    &
     &           NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.eq.0) then
        call  CM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.lt.0) then
        call RCM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
!C===

      write (*,'(/a, i8)') '# TOTAL COLOR number', NCOLORtot
```

Reading “initial” color number

poi_gen (4/4)

```
!C
!C +---------------+
!C | MULTICOLORING |
!C +---------------+
!C===
 111  continue
      write (*,'(//a,i8,a)') 'You have', ICELTOT, ' elements.'
      write (*,'(  a     )') 'How many colors do you need ?'
      write (*,'(  a     )') '  #COLOR must be more than 2 and'
      write (*,'(  a,i8  )') '  #COLOR must not be more than', ICELTOT
      write (*,'(  a     )') '   if #COLOR=0 :  CM ordering'
      write (*,'(  a     )') '   if #COLOR<0 : RCM ordering'
      write (*,'(  a     )') '=>'
      read  (*,*)              NCOLORtot
      if (NCOLORtot.eq.1.or.NCOLORtot.gt.ICELTOT) goto 111

      allocate (OLDtoNEW(ICELTOT), NEWtoOLD(ICELTOT))
      allocate (COLORindex(0:ICELTOT))

      if (NCOLORtot.gt.0) then
        call MC (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &           NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.eq.0) then
        call  CM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                  &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.lt.0) then
        call RCM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                  &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
!C===

      write (*,'(/a, i8)') '# TOTAL COLOR number', NCOLORtot
```

Allocate matrices

poi_gen (4/4)

```
!C
!C +---------------+
!C | MULTICOLORING |
!C +---------------+
!C===

...
      if (NCOLORtot.gt.0) then
        call MC (ICELTOT, NL, NU, INL, IAL, INU, IAU,                    &
     &           NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.eq.0) then
        call  CM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.lt.0) then
        call RCM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
!C===

      write (*,'(/a, i8)') '# TOTAL COLOR number', NCOLORtot
```

INL, INU, IAL, IAU	Info. after renumbering
OLDtoNEW, NEWtoOLD	Reference table before/after renumbring
NCOLORtot	Final number of colors (g.e. initial number)
COLORindex(0:NCOLORtot)	Meshes from **COLORindex(ic-1)+1** to **COLORindex(ic)** are in ic-th color. Meshes in same color are independent: Parallel processing can be applied.

COLORindex

`COLORindex(0:NCOLORtot)`	Meshes from **`COLORindex(ic-1)+1`** to **`COLORindex(ic)`** are in ic-th color. Meshes in same color are independent: Parallel processing can be applied.

```
do ic= 1, NCOLORtot
  do i= COLORindex(ic-1)+1, COLORindex(ic)
    write (21,*) i, NEWtoOLD(i), ic
  enddo
enddo
```

```
COLOR number       5
  #new        1    #old         1   color         1
  #new        2    #old         3   color         1
  #new        3    #old         6   color         1
  #new        4    #old         8   color         1
  #new        5    #old         9   color         1
  #new        6    #old         2   color         2
  #new        7    #old         4   color         2
  #new        8    #old         5   color         2
  #new        9    #old         7   color         2
  #new       10    #old        10   color         2
  #new       11    #old        11   color         3
  #new       12    #old        13   color         3
  #new       13    #old        16   color         3
  #new       14    #old        12   color         4
  #new       15    #old        14   color         4
  #new       16    #old        15   color         5
```

Modified MC Method

① ONE mesh with minimum value of "degree" is set to "NEW mesh ID= 1", "Color ID= 1", and "counter for color number" is 1.

② Define "*ITEMcou= ICELTOT/NCOLORtot*", where *ITEMcou* is maximum number of meshes in each color.

③ Color *ITEMcou* independent meshes in ascending order according to initial mesh ID.

④ If *ITEMcou* meshes are colored, or no more independent meshes do not exist, add "1" to the "counter for color number", and proceed to the next color.

⑤ Repeat ③ and ④, until all meshes have been colored.

⑥ "Final counter for color" is *NCOLORtotF*. Renumber meshes in ascending orders according to color ID. In each color, numbering is in ascending orders according to initial mesh ID. In each color, new numbering of meshes is continuous.

mc (1/8)

```
!C
!C***
!C*** MC
!C***
!C
!C    Multicolor Ordering Method
!C

      subroutine MC (N, NL, NU, INL, IAL, INU, IAU,              &
     &               NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)

      implicit REAL*8(A-H,O-Z)

      integer, dimension(N)   :: INL, INU, NEWtoOLD, OLDtoNEW
      integer, dimension(0:N) :: COLORindex
      integer, dimension(NL,N):: IAL
      integer, dimension(NU,N):: IAU

      integer, dimension(:)  , allocatable :: IW, INLw, INUw
      integer, dimension(:,:), allocatable :: IALw, IAUw
```

mc (2/8)

```
!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (IW(N))
      IW= 0

      NCOLORk  = NCOLORtot

      do i= 1, N
        NEWtoOLD  (i)= i
        OLDtoNEW  (i)= i
      enddo

       INmin= N
      NODmin= 0
      do i= 1, N
        icon= INL(i) + INU(i)
        if (icon.lt.INmin) then
           INmin= icon
          NODmin= i
        endif
      enddo

      OLDtoNEW(NODmin)= 1
      NEWtoOLD(     1)= NODmin
      IW         = 0
      IW(NODmin)= 1

      ITEMcou= N/NCOLORk
!C===
```

IW:
Work array
"Color ID" of each mesh
IW=0 at initial stage

NODmin:
ID of the mesh with minimum value of "degree"

mc (2/8)

```
!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (IW(N))
      IW= 0

      NCOLORk  = NCOLORtot

      do i= 1, N
        NEWtoOLD  (i)= i
        OLDtoNEW  (i)= i
      enddo

       INmin= N
      NODmin= 0
      do i= 1, N
        icon= INL(i) + INU(i)
        if (icon.lt.INmin) then
           INmin= icon
          NODmin= i
        endif
      enddo

      OLDtoNEW(NODmin)= 1
      NEWtoOLD(     1)= NODmin
      IW         = 0
      IW(NODmin)= 1

      ITEMcou= N/NCOLORk
!C===
```

New mesh ID of **NODmin** is set to 1
Color ID of **NODmin** is set to 1

OLDtoNEW(NODmin)= 1
NEWtoOLD(1)= NODmin

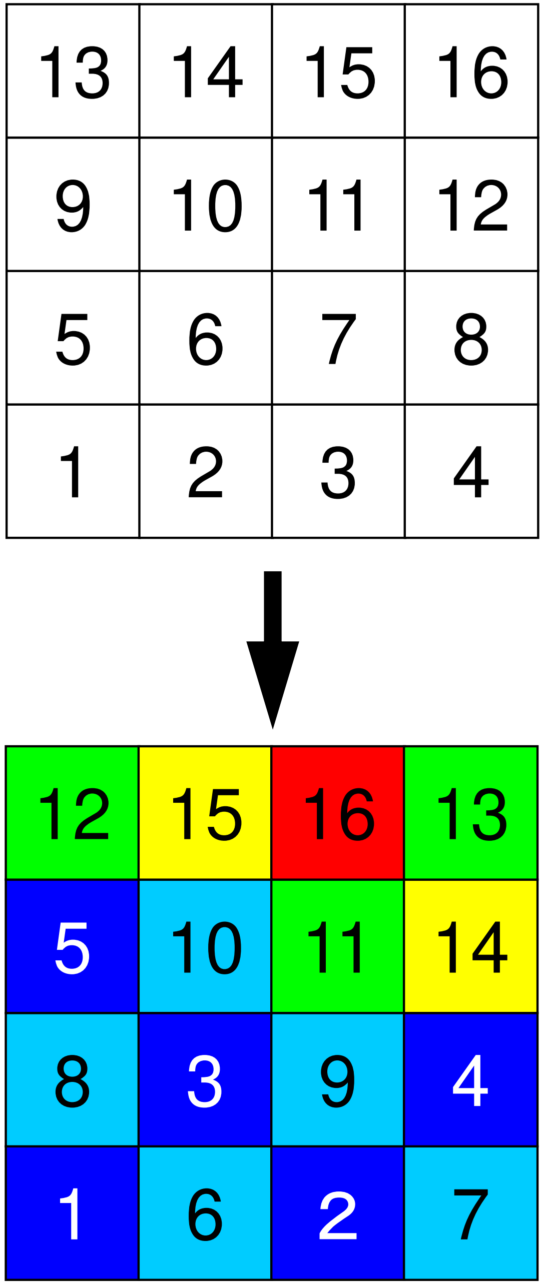
IW(NODmin)=1: Color ID

mc (2/8)

```
!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (IW(N))
      IW= 0

      NCOLORk  = NCOLORtot

      do i= 1, N
        NEWtoOLD  (i)= i
        OLDtoNEW  (i)= i
      enddo

       INmin= N
      NODmin= 0
      do i= 1, N
        icon= INL(i) + INU(i)
        if (icon.lt.INmin) then
           INmin= icon
          NODmin= i
        endif
      enddo

      OLDtoNEW(NODmin)= 1
      NEWtoOLD(     1)= NODmin
      IW        = 0
      IW(NODmin)= 1

      ITEMcou= N/NCOLORk
!C===
```

ITEMcou= N/NCOLORk:
(Maximum) number of meshes in each color

INPUT=3: MC, 5-Colors



#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

Finally, 5 colors are needed.
Affected by revaluation/devaluation

mc (3/8)

```
!C
!C +----------------+
!C | MULTIcoloring |
!C +----------------+
!C===
      icou = 1
      icouK= 1

      do icol= 1, N
        NCOLORk= icol
        do i= 1, N
          if (IW(i).le.0) IW(i)= 0
        enddo

        do i= 1, N
!C
!C-- already COLORED
          if (IW(i).eq.icol) then
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
!C
!C-- not COLORED
          if (IW(i).eq.0) then
            icou = icou  + 1
            icouK= icouK + 1
            IW(i)= icol
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
```

Initialization of Counters

icou : Global Counter

icouK: Intra-Color Counter

mc (3/8)

Loop on Colors

```
!C
!C +---------------+
!C | MULTIcoloring |
!C +---------------+
!C===
      icou = 1
      icouK= 1

      do icol= 1, N
        NCOLORk= icol
        do i= 1, N
          if (IW(i).le.0) IW(i)= 0
        enddo

        do i= 1, N
!C
!C-- already COLORED
          if (IW(i).eq.icol) then
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
!C
!C-- not COLORED
          if (IW(i).eq.0) then
            icou = icou  + 1
            icouK= icouK + 1
            IW(i)= icol
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
```

mc (3/8)

```
!C
!C +----------------+
!C | MULTIcoloring |
!C +----------------+
!C===
      icou = 1
      icouK= 1

      do icol= 1, N
        NCOLORk= icol
        do i= 1, N
          if (IW(i).le.0) IW(i)= 0
        enddo

        do i= 1, N
!C
!C-- already COLORED
          if (IW(i).eq.icol) then
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
!C
!C-- not COLORED
          if (IW(i).eq.0) then
            icou = icou  + 1
            icouK= icouK + 1
            IW(i)= icol
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
```

NCOLORk:
Current number of colors

IW(i)=0:
If i-th mesh (original numbering) is not colored.

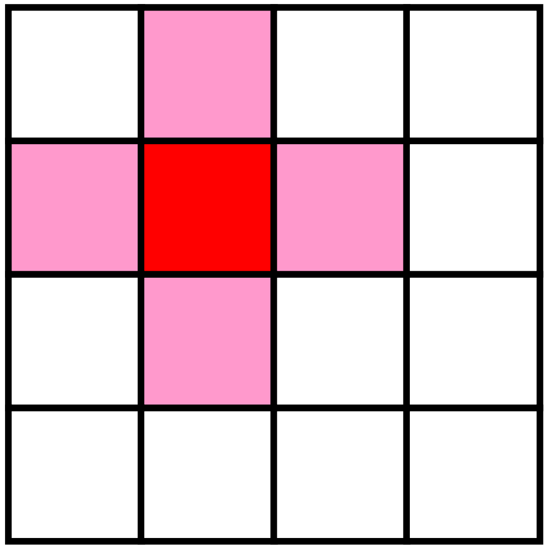
mc (3/8)

```
!C
!C +----------------+
!C | MULTIcoloring |
!C +----------------+
!C===
      icou = 1
      icouK= 1

      do icol= 1, N
        NCOLORk= icol
        do i= 1, N
          if (IW(i).le.0) IW(i)= 0
        enddo

        do i= 1, N
!C
!C-- already COLORED
          if (IW(i).eq.icol) then
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
!C
!C-- not COLORED
          if (IW(i).eq.0) then
            icou = icou  + 1
            icouK= icouK + 1
            IW(i)= icol
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
```

Loop on Colors

If mesh is already assigned to the "current color", components of **IW** array for adjacent meshes are set to "-1".

Remove meshes connected to meshes assigned to the "current color", because they cannot be into the "current color".



mc (3/8)

```
!C
!C +---------------+
!C | MULTIcoloring |
!C +---------------+
!C===
      icou = 1
      icouK= 1

      do icol= 1, N
        NCOLORk= icol
        do i= 1, N
          if (IW(i).le.0) IW(i)= 0
        enddo

        do i= 1, N
!C
!C-- already COLORED
          if (IW(i).eq.icol) then
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
!C
!C-- not COLORED
          if (IW(i).eq.0) then
            icou = icou  + 1
            icouK= icouK + 1
            IW(i)= icol
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
```

if **IW(i)=0:**

- **icou =icou+1**
- **icouK=icouK+1**
- **IW(i)=icol:** Color ID

- **IW(ik)=-1** where ***ik-th*** mesh is adjacent to ***i-th*** mesh

mc (3/8)

```
      do icol= 1, N
        NCOLORk= icol
        do i= 1, N
          if (IW(i).le.0) IW(i)= 0
        enddo

        do i= 1, N
!C
!C-- already COLORED
          if (IW(i).eq.icol) then
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
!C
!C-- not COLORED
          if (IW(i).eq.0) then
            icou = icou  + 1
            icouK= icouK + 1
            IW(i)= icol
            do k= 1, INL(i)
              ik= IAL(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
            do k= 1, INU(i)
              ik= IAU(k,i)
              if (IW(ik).le.0) IW(ik)= -1
            enddo
          endif
          if (icou .eq.N)       goto 200
          if (icouK.eq.ITEMcou) goto 100
        enddo
 100    continue
        icouK= 0
      enddo
 200  continue
```

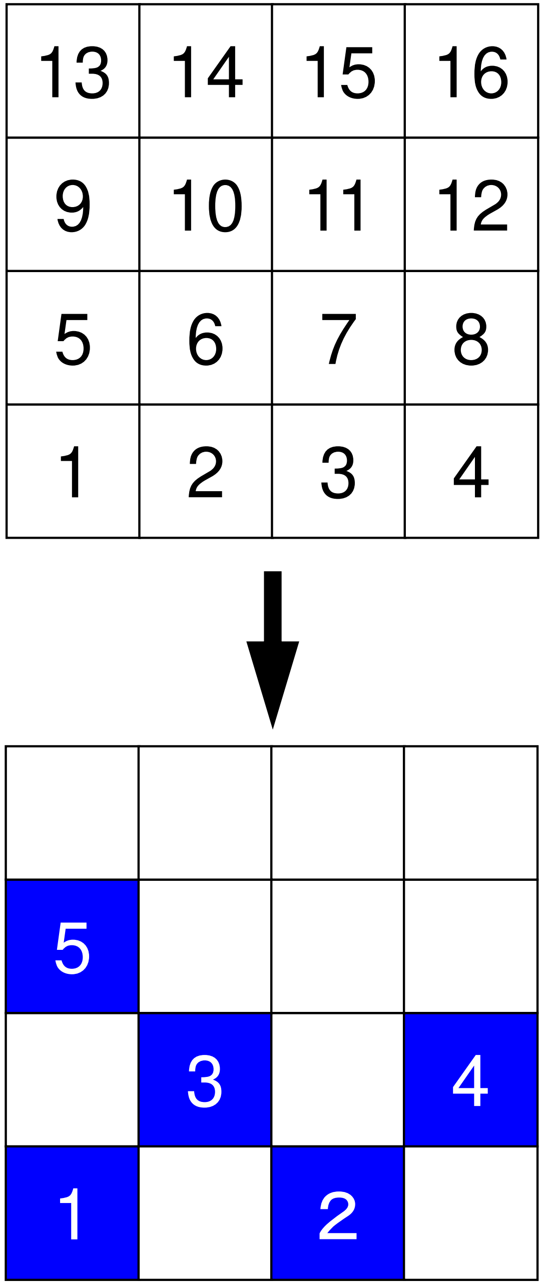
icou : Global Counter
icouK: Intra-Color Counter

if **icou=N (ICELTOT)**:
- All meshes are colored (completed).

if **icouK=ITEMcou**:
- **icouK=0**
- Proceed to the next color.

if **icouK<ITEMcou.and.i=N**:
- No more independent meshes.
- Proceed to the next color.

INPUT=3: MC, 5-Colors

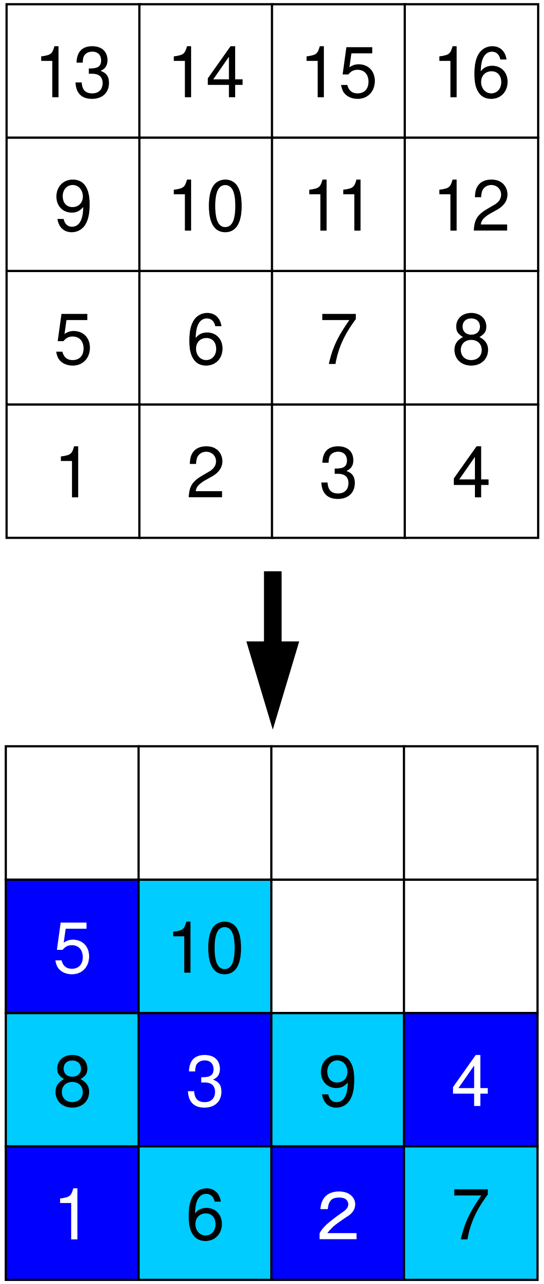


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

5 independent meshes

INPUT=3: MC, 5-Colors

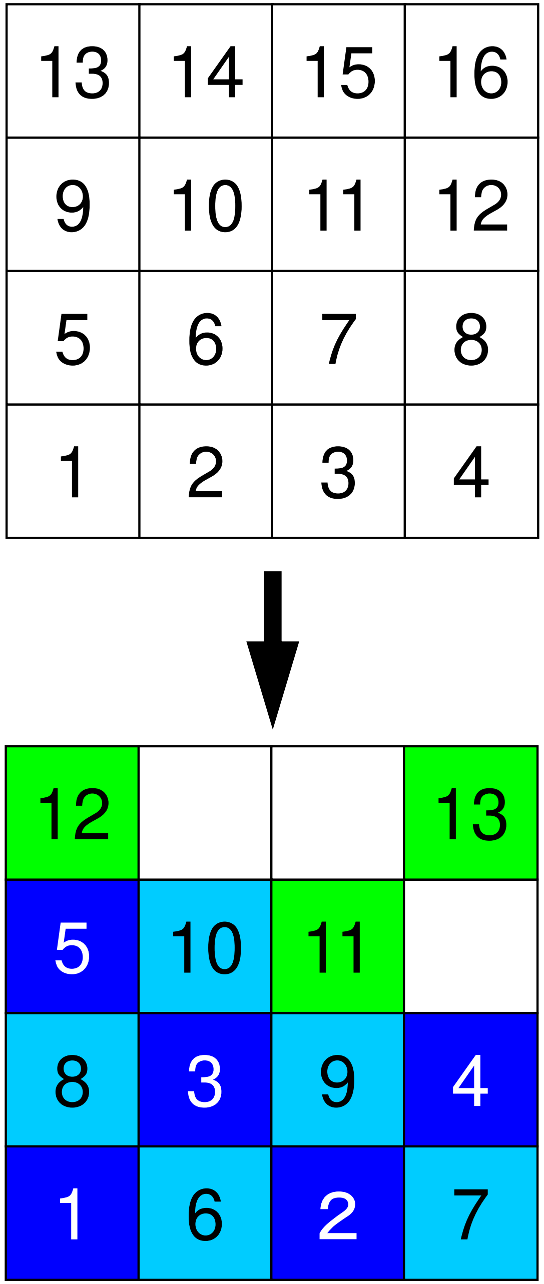


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

5 independent meshes

INPUT=3: MC, 5-Colors

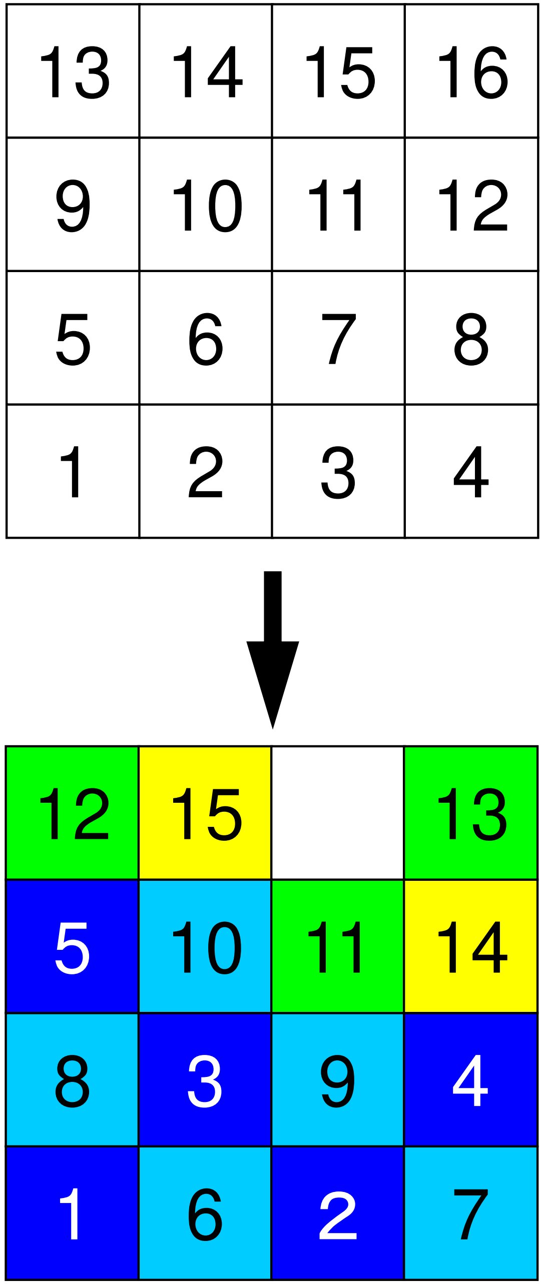


#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= <u>**ITEMcou**</u>

Proceed to the next color, if no more independent meshes.

INPUT=3: MC, 5-Colors



#new	1	#old	1	color	1
#new	2	#old	3	color	1
#new	3	#old	6	color	1
#new	4	#old	8	color	1
#new	5	#old	9	color	1
#new	6	#old	2	color	2
#new	7	#old	4	color	2
#new	8	#old	5	color	2
#new	9	#old	7	color	2
#new	10	#old	10	color	2
#new	11	#old	11	color	3
#new	12	#old	13	color	3
#new	13	#old	16	color	3
#new	14	#old	12	color	4
#new	15	#old	14	color	4
#new	16	#old	15	color	5

16/3=5= **ITEMcou**

Proceed to the next color, if no more independent meshes.

mc (5/8)

```
!C
!C +----------------+
!C | FINAL COLORING |
!C +----------------+
!C===
      NCOLORtot= NCOLORk
      COLORindex= 0
      icoug= 0
      do ic= 1, NCOLORtot
        icou= 0
        do i= 1, N
          if (IW(i).eq.ic) then
            icou = icou + 1
            icoug= icoug + 1
            NEWtoOLD(icoug)= i
            OLDtoNEW(i    )= icoug
          endif
        enddo
        COLORindex(ic)= icou
      enddo

      do ic= 1, NCOLORtot
        COLORindex(ic)= COLORindex(ic-1) + COLORindex(ic)
      enddo
!C===
```

NCOLORtot= NCOLORk:
Final number of colors.

NCOLORtot g.e. (Initial number of colors provided by user)

mc (5/8)

```
!C
!C +----------------+
!C | FINAL COLORING |
!C +----------------+
!C===
      NCOLORtot= NCOLORk
      COLORindex= 0
      icoug= 0
      do ic= 1, NCOLORtot
        icou= 0
        do i= 1, N
          if (IW(i).eq.ic) then
            icou = icou + 1
            icoug= icoug + 1
            NEWtoOLD(icoug)= i
            OLDtoNEW(i    )= icoug
          endif
        enddo
        COLORindex(ic)= icou
      enddo

      do ic= 1, NCOLORtot
        COLORindex(ic)= COLORindex(ic-1) + COLORindex(ic)
      enddo
!C===
```

Renumber meshes in ascending orders according to color ID.

OLDtoNEW(OldID)= NewID
NEWtoOLD(NewID)= OldID

COLODindex(ic):
At this stage, number of meshes in each color (ic) is stored.

mc (6/8)

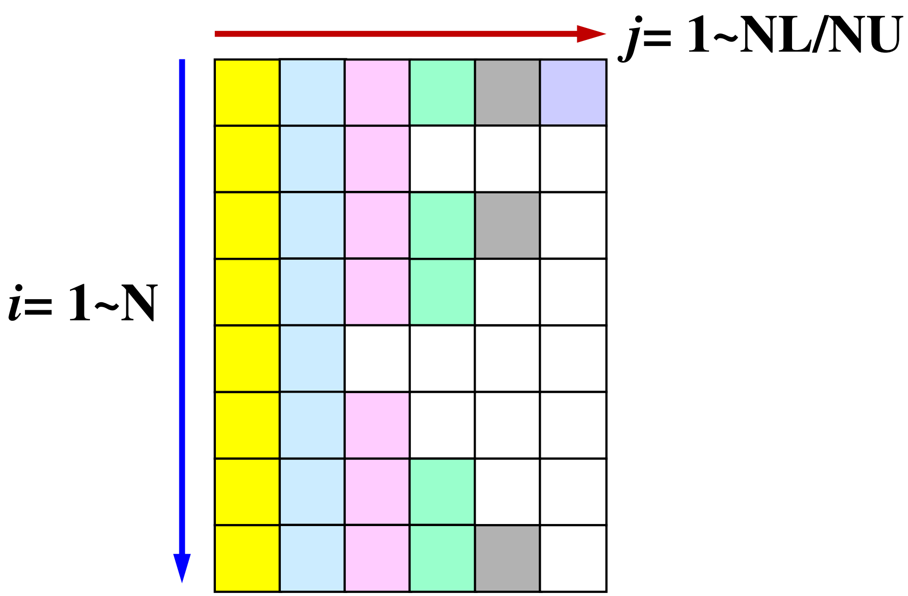
```
!C
!C +----------------+
!C | FINAL COLORING |
!C +----------------+
!C===
      NCOLORtot= NCOLORk
      COLORindex= 0
      icoug= 0
      do ic= 1, NCOLORtot
        icou= 0
        do i= 1, N
          if (IW(i).eq.ic) then
            icou = icou + 1
            icoug= icoug + 1
            NEWtoOLD(icoug)= i
            OLDtoNEW(i    )= icoug
          endif
        enddo
        COLORindex(ic)= icou
      enddo

      do ic= 1, NCOLORtot
        COLORindex(ic)= COLORindex(ic-1) + COLORindex(ic)
      enddo
!C===
```

COLODindex(ic):

Now it is 1D index.

mc (6/8)

```
!C
!C +------------------+
!C | MATRIX transfer |
!C +------------------+
!C===
      allocate (INLw(N), INUw(N), IALw(NL,N), IAUw(NU,N))

      do j= 1, NL
        do i= 1, N
          IW(i) = IAL(j,NEWtoOLD(i))
        enddo
        do i= 1, N
          IAL(j,i) = IW(i)
        enddo
      enddo

      do j= 1, NU
        do i= 1, N
          IW(i) = IAU(j,NEWtoOLD(i))
        enddo
        do i= 1, N
          IAU(j,i) = IW(i)
        enddo
      enddo
```



Arrays for Work

- **INLw(N)**
- **INUw(N)**
- **IALw(NL,N)**
- **IAUw(NU,N)**

Lower/upper components (column ID) are reordered according to new numbering.

ID's of column ID are by old numbering.

mc (7/8)

```
do i= 1, N
  IW(i) = INL(NEWtoOLD(i))
enddo

do i= 1, N
  INLw(i) = IW(i)
enddo

do i= 1, N
  IW(i) = INU(NEWtoOLD(i))
enddo

do i= 1, N
  INUw(i) = IW(i)
enddo

do j= 1, NL
  do i= 1, N
    if (IAL(j,i).eq.0) then
      IALw(j,i) = 0
     else
      IALw(j,i) = OLDtoNEW(IAL(j,i))
    endif
  enddo
enddo

do j= 1, NU
  do i= 1, N
    if ( IAU(j,i).eq.0) then
      IAUw(j,i) = 0
     else
      IAUw(j,i) = OLDtoNEW(IAU(j,i))
    endif
  enddo
enddo
```

Information for number of lower/upper components based on new numbering is stored into:

- **INL -> INLw**
- **INU -> INUw**

mc (7/8)

```
do i= 1, N
  IW(i) = INL(NEWtoOLD(i))
enddo

do i= 1, N
  INLw(i) = IW(i)
enddo

do i= 1, N
  IW(i) = INU(NEWtoOLD(i))
enddo

do i= 1, N
  INUw(i) = IW(i)
enddo

do j= 1, NL
 do i= 1, N
   if (IAL(j,i).eq.0) then
     IALw(j,i) = 0
    else
     IALw(j,i) = OLDtoNEW(IAL(j,i))
   endif
 enddo
enddo

do j= 1, NU
 do i= 1, N
   if ( IAU(j,i).eq.0) then
     IAUw(j,i) = 0
    else
     IAUw(j,i) = OLDtoNEW(IAU(j,i))
   endif
 enddo
enddo
```

"Renumbered" lower/upper components (column ID) are stored into:

- **IAL -> IALw**
- **IAU -> IAUw**

mc (8/8)

```
      INL= 0
      INU= 0
      IAL= 0
      IAU= 0

      do i= 1, N
        jL= 0
        jU= 0
        do j= 1, INLw(i)
          if (IALw(j,i).gt.i) then
            jU= jU + 1
            IAU(jU,i)= IALw(j,i)
           else
            jL= jL + 1
            IAL(jL,i)= IALw(j,i)
          endif
         enddo

        do j= 1, INUw(i)
          if (IAUw(j.i).gt.i) then
            jU= jU + 1
            IAU(jU,i)= IAUw(j,i)
           else
            jL= jL + 1
            IAL(jL,i)= IAUw(j,i)
          endif
         enddo

         INL(i)= jL
         INU(i)= jU
      enddo
!C===
      deallocate (IW, INLw, INUw, IALw, IAUw)

      return
      end
```

Operation for lower triangular components (column ID) in the original matrix. "Renumbered" components (column ID) are stored into:

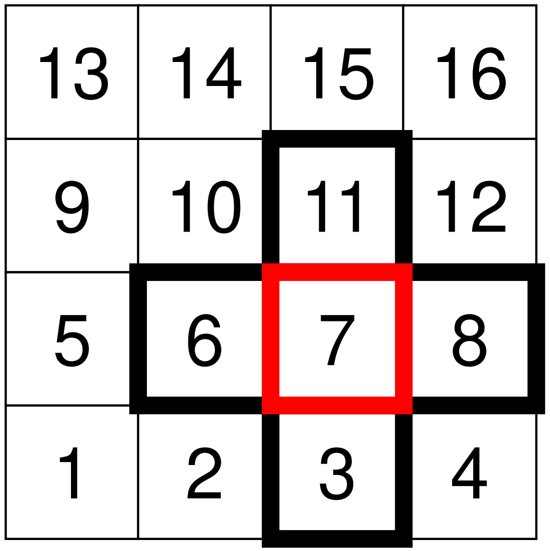
- **IALw -> IAL, IAU**

```
do i= 1, N
  jL= 0
  jU= 0
  do j= 1, INLw(i)
    if (IALw(j,i).gt.i) then
      jU= jU + 1
     IAU(jU,i)= IALw(j,i)
    else
      jL= jL + 1
     IAL(jL,i)= IALw(j,i)
    endif
  enddo
enddo
```

Because **IALw(j,i)** could be larger than **i** according to new numbering.

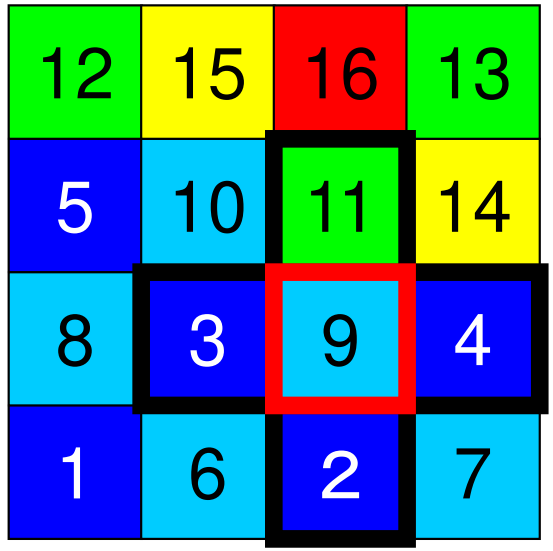
Why do we need these operations ?

Original




```
INL(  7)= 2
IAL(1,7)= 3,  IAL(2,7)= 6

INU(  7)= 2
IAU(1,7)= 8,  IAU(2,7)=11
```

5 Color




```
INL(  9)= 3
IAL(1,9)= 2,  IAL(2,9)= 3
IAL(3,9)= 4

INU(  9)= 1
IAU(1,9)=11
```

Magnitude correlation with adjacent meshes could change after renumbering.

mc (8/8)

```
      INL= 0
      INU= 0
      IAL= 0
      IAU= 0

      do i= 1, N
        jL= 0
        jU= 0
        do j= 1, INLw(i)
          if (IALw(j,i).gt.i) then
            jU= jU + 1
            IAU(jU,i)= IALw(j,i)
           else
            jL= jL + 1
            IAL(jL,i)= IALw(j,i)
          endif
         enddo

        do j= 1, INUw(i)
          if (IAUw(j.i).gt.i) then
            jU= jU + 1
            IAU(jU,i)= IAUw(j,i)
           else
            jL= jL + 1
            IAL(jL,i)= IAUw(j,i)
          endif
         enddo

         INL(i)= jL
         INU(i)= jU
      enddo
!C===
      deallocate (IW, INLw, INUw, IALw, IAUw)

      return
      end
```

Operation for upper triangular components (column ID) in the original matrix. “Renumbered” components (column ID) are stored into:

- **IAUw -> IAL,IAU**

mc (8/8)

```
      INL= 0
      INU= 0
      IAL= 0
      IAU= 0

      do i= 1, N
        jL= 0
        jU= 0
        do j= 1, INLw(i)
          if (IALw(j,i).gt.i) then
            jU= jU + 1
            IAU(jU,i)= IALw(j,i)
           else
            jL= jL + 1
            IAL(jL,i)= IALw(j,i)
          endif
         enddo

        do j= 1, INUw(i)
          if (IAUw(j.i).gt.i) then
            jU= jU + 1
            IAU(jU,i)= IAUw(j,i)
           else
            jL= jL + 1
            IAL(jL,i)= IAUw(j,i)
          endif
         enddo

         INL(i)= jL
         INU(i)= jU
      enddo
!C===
      deallocate (IW, INLw, INUw, IALw, IAUw)

      return
      end
```

“Final” number of upper/lower components (column ID) in the renumbered new matrix.

- **INL**
- **INU**

Modified CM Method for Parallel Computing

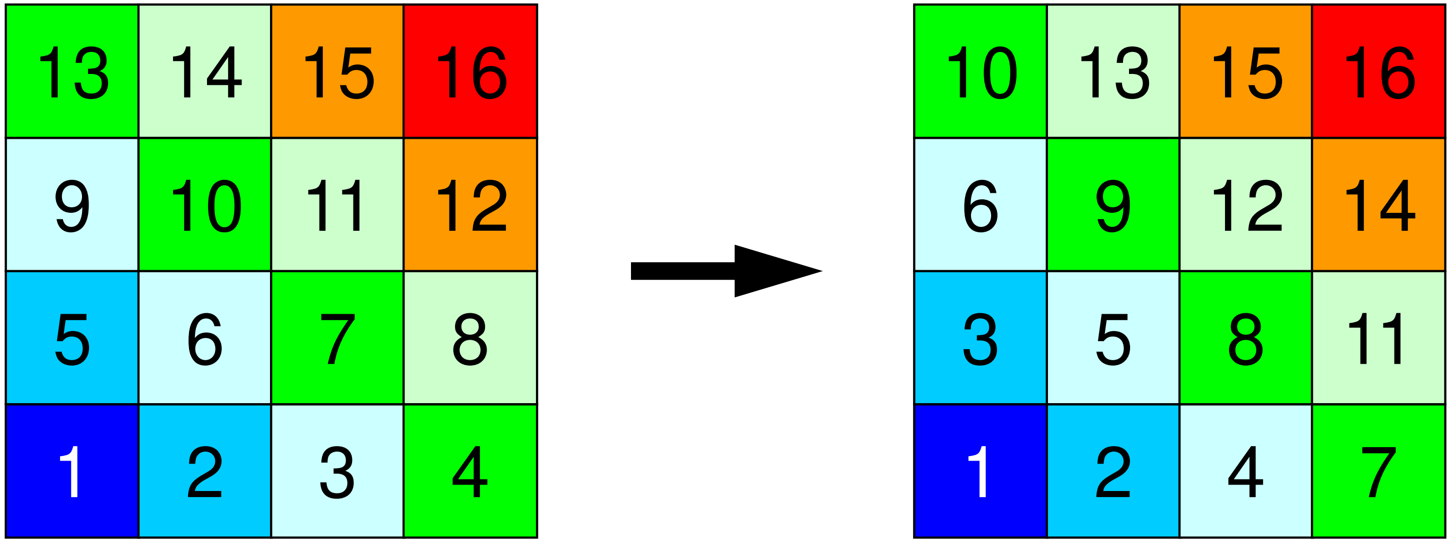
① ONE mesh with minimum value of "degree" is set to "Level=1".

② Meshes adjacent to "Level=k-1" meshes are set to "Level=k". In each level, meshes must be independent (not directly connected). If a dependent pair is found in same color, one mesh is removed (In current implementation, a mesh found later is removed).

③ Repeat ②, until all meshes are flagged to "levels"

④ Renumber meshes in ascending orders according to "Level" ID. In each level, numbering is in ascending orders according to initial mesh ID. In each level, new numbering of meshes is continuous.

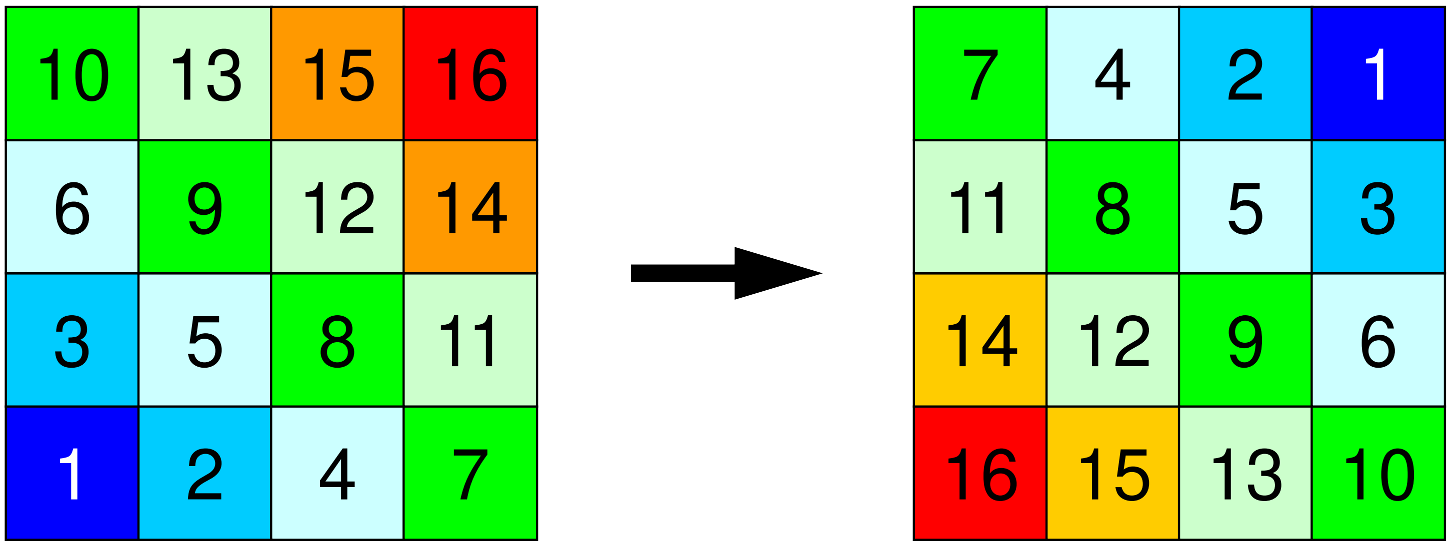
Procedure of CM Method



- Meshes adjacent to "Level=k-1" meshes are set to "Level=k" (Repeat until all meshes are flagged into "levels")
  - In each level, meshes must be independent (not directly connected). If a dependent pair is found in same color, one mesh is removed (In current implementation, a mesh found later is removed).
- Renumber meshes in ascending orders according to "Level" ID.

RCM: Reverse Cuthill-McKee

- Do operations for "CM" method
  - Calculate "degree" at each mesh
  - Flag "level k (1,2,...)" to meshes
  - Repeat processes, final renumbering
- Renumbering Again
  - Renumber meshes reordered by CM method in reverse order.
  - Fill-in's are fewer than CM



cm (1/5)

```
!C
!C***
!C*** CM
!C***
!C
      subroutine CM  (N, NL, NU, INL, IAL, INU, IAU,
     &                NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)

      implicit REAL*8(A-H,O-Z)
      integer, dimension(N)   :: INL, INU, NEWtoOLD, OLDtoNEW
      integer, dimension(0:N) :: COLORindex
      integer, dimension(NL,N):: IAL
      integer, dimension(NU,N):: IAU

      integer, dimension(:,:), allocatable :: IW
      integer, dimension(:)  , allocatable :: INLw, INUw
      integer, dimension(:,:), allocatable :: IALw, IAUw
```

cm (2/5)

```
!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (IW(N,2))

      IW = 0

       INmin= N
      NODmin= 0

      do i= 1, N
        icon= 0
        do k= 1, INL(i)
          icon= icon + 1
        enddo
        do k= 1, INU(i)
          icon= icon + 1
        enddo

        if (icon.lt.INmin) then
          INmin = icon
          NODmin= i
        endif
      enddo
 200  continue


      if (NODmin.eq.0) NODmin= 1

      IW(NODmin,2)= 1

      NEWtoOLD(1     )= NODmin
      OLDtoNEW(NODmin)= 1

      icol= 1
!C===
```

IW(i,1):
Work array

IW(i,2):
"Level ID" of each mesh

cm (2/5)

```
!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (IW(N,2))

      IW = 0

       INmin= N
      NODmin= 0

      do i= 1, N
        icon= 0
        do k= 1, INL(i)
          icon= icon + 1
        enddo
        do k= 1, INU(i)
          icon= icon + 1
        enddo

        if (icon.lt.INmin) then
          INmin = icon
          NODmin= i
        endif
      enddo
 200  continue


      if (NODmin.eq.0) NODmin= 1

      IW(NODmin,2)= 1

      NEWtoOLD(1     )= NODmin
      OLDtoNEW(NODmin)= 1

      icol= 1
!C===
```

NODmin:
ID of the mesh with minimum value of “degree”

cm (2/5)

```
!C
!C +--------+
!C | INIT.  |
!C +--------+
!C===
      allocate (IW(N,2))

      IW = 0

       INmin= N
      NODmin= 0

      do i= 1, N
        icon= 0
        do k= 1, INL(i)
          icon= icon + 1
        enddo
        do k= 1, INU(i)
          icon= icon + 1
        enddo

        if (icon.lt.INmin) then
          INmin = icon
          NODmin= i
        endif
      enddo
 200  continue


      if (NODmin.eq.0) NODmin= 1

      IW(NODmin,2)= 1

      NEWtoOLD(1     )= NODmin
      OLDtoNEW(NODmin)= 1

      icol= 1
!C===
```

New mesh ID of **NODmin** is set to 1
Level ID of **NODmin** is set to 1

OLDtoNEW(NODmin)= 1
NEWtoOLD(1)= NODmin

IW(NODmin,2)=1: Level ID

cm (3/5)

```
!C
!C +-----------+
!C | COLORING |
!C +-----------+
!C===
      icouG= 1
      do icol= 2, N
        icou = 0
        do i= 1, N
          if (IW(i,2).eq.icol-1) then
            do k= 1, INL(i)
              in= IAL(k,i)
              if (IW(in,2).eq.0) then
                IW(in  ,2)= -icol
                icou      = icou + 1
                IW(icou,1)= in
              endif
            enddo
            do k= 1, INU(i)
              in= IAU(k,i)
              if (IW(in,2).eq.0) then
                IW(in  ,2)= -icol
                icou      = icou + 1
                IW(icou,1)= in
              endif
            enddo
          endif
        enddo

        if (icou.eq.0) then
          do i= 1, N
            if (IW(i,2).eq.0) then
              icou= icou + 1
              IW(i   ,2)= -icol
              IW(icou,1)= i
              goto 850
            endif
          enddo
        endif
 850    continue
```

icouG: Global Counter

icou : Intra-Level Counter

Loop on Levels

cm (3/5)

```
!C
!C +----------+
!C | COLORING |
!C +----------+
!C===
      icouG= 1
      do icol= 2, N
        icou = 0
        do i= 1, N
          if (IW(i,2).eq.icol-1) then
            do k= 1, INL(i)
              in= IAL(k,i)
              if (IW(in,2).eq.0) then
                IW(in  ,2)= -icol
                icou      = icou + 1
                IW(icou,1)= in
              endif
            enddo
            do k= 1, INU(i)
              in= IAU(k,i)
              if (IW(in,2).eq.0) then
                IW(in  ,2)= -icol
                icou      = icou + 1
                IW(icou,1)= in
              endif
            enddo
          endif
        enddo

        if (icou.eq.0) then
          do i= 1, N
            if (IW(i,2).eq.0) then
              icou= icou + 1
              IW(i   ,2)= -icol
              IW(icou,1)= i
              goto 850
            endif
          enddo
        endif
 850    continue
```

icouG: Global Counter
icou : Intra-Level Counter

Loops for Each Element

If **in**th mesh is adjacent to **i**th mesh where **IW(i,2)=icol-1**, and level of **in**th mesh is not finalized, **in**th mesh could be a candidate for meshes in **icol**th level.

- **IW(in,2)= -icol**
- **icou= icou + 1**
- **IW(icou,1)= in**: This array indicates "when" this mesh was found, and nominated as a candidate.

What does it mean ?

13	14	15	16
9	10	11	12
5	6	7	8
1	2	3	4

```
icol=4
  IW(i,2)= icol-1=3: i=3,6,9
```

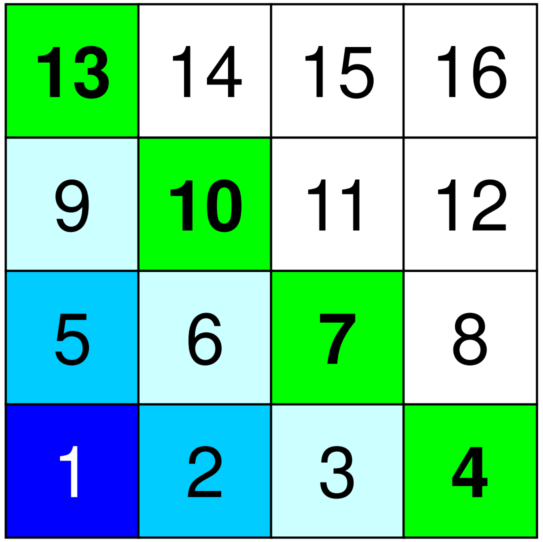
icouG: Global Counter
icou : Intra-Level Counter

Loops for Each Element

If **in**th mesh is adjacent to **i**th mesh where **IW(i,2)=icol-1**, and level of **in**th mesh is not finalized, **in**th mesh could be a candidate for meshes in **icol**th level.

- **IW(in,2)= -icol**
- **icou= icou + 1**
- **IW(icou,1)= in:** This array indicates “when” this mesh was found, and nominated as a candidate.

What does it mean ?




```
icol=4
   IW(i,2)= icol-1=3: i=3,6,9
```

```
IW( 4,2)= -4
IW( 7,2)= -4
IW(10,2)= -4
IW(13,2)= -4

IW(1,1)=  4
IW(2,1)=  7
IW(3,1)= 10
IW(4,1)= 13
```

icouG: Global Counter
icou : Intra-Level Counter

Loops for Each Element

If **in**th mesh is adjacent to **i**th mesh where **IW(i,2)=icol-1**, and level of **in**th mesh is not finalized, **in**th mesh could be a candidate for meshes in **icol**th level.

- **IW(in,2)= -icol**
- **icou= icou + 1**
- **IW(icou,1)= in**: This array indicates “when” this mesh was found, and nominated as a candidate.

cm (3/5)

icouG: Global Counter
icou : Intra-Level Counter

```
!C
!C +-----------+
!C | COLORING |
!C +-----------+
!C===
      icouG= 1
      do icol= 2, N
        icou = 0
        do i= 1, N
          if (IW(i,2).eq.icol-1) then
            do k= 1, INL(i)
              in= IAL(k,i)
              if (IW(in,2).eq.0) then
                IW(in  ,2)= -icol
                icou      = icou + 1
                IW(icou,1)= in
              endif
            enddo
            do k= 1, INU(i)
              in= IAU(k,i)
              if (IW(in,2).eq.0) then
                IW(in  ,2)= -icol
                icou      = icou + 1
                IW(icou,1)= in
              endif
            enddo
          endif
        enddo

        if (icou.eq.0) then
          do i= 1, N
            if (IW(i,2).eq.0) then
              icou= icou + 1
              IW(i   ,2)= -icol
              IW(icou,1)= i
              goto 850
            endif
          enddo
        endif
 850    continue
```

Loops for Each Element

If **icou=0**, a mesh, which satisfies the following conditions, is the candidate (usually, this does not happen):

- Level of this mesh is not finalized.
- Mesh ID according to the initial numbering is the smallest.

cm (4/5)

```
!C
!C +-----------+
!C | COLORING |
!C +-----------+
!C===

…

        do ic= 1, icou
          inC= IW(ic,1)
          if (IW(inC,2).ne.0) then
            do k= 1, INL(inC)
              in= IAL(k,inC)
              if (IW(in,2).le.0) IW(in,2)= 0
            enddo
            do k= 1, INU(inC)
              in= IAU(k,inC)
              if (IW(in,2).le.0) IW(in,2)= 0
            enddo
          endif
        enddo

        do ic= 1, icou
          inC= IW(ic,1)
          if (IW(inC,2).ne.0) then
            icouG      = icouG + 1
            IW(inC,2)= icol
          endif
        enddo

        if (icouG.eq.N) exit
      enddo
!C===
```

Candidates for **icol**[th] level are stored in:

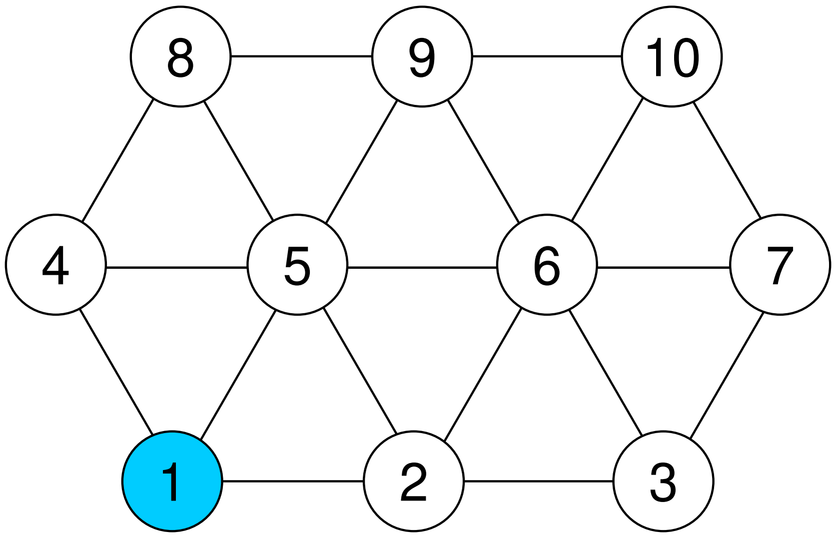
- **IW(ic,1), ic= 1, icou**

Remove such meshes that are adjacent to other candidates, because neighboring meshes cannot belong to same level.

If we have such removed mesh **in**, apply the following operations:

- **IW(in,2)= 0**

What does is mean ?



e.g.
Mesh (1) belongs to **(icol-1)th** level

Candidates for **icolth** level are stored in:

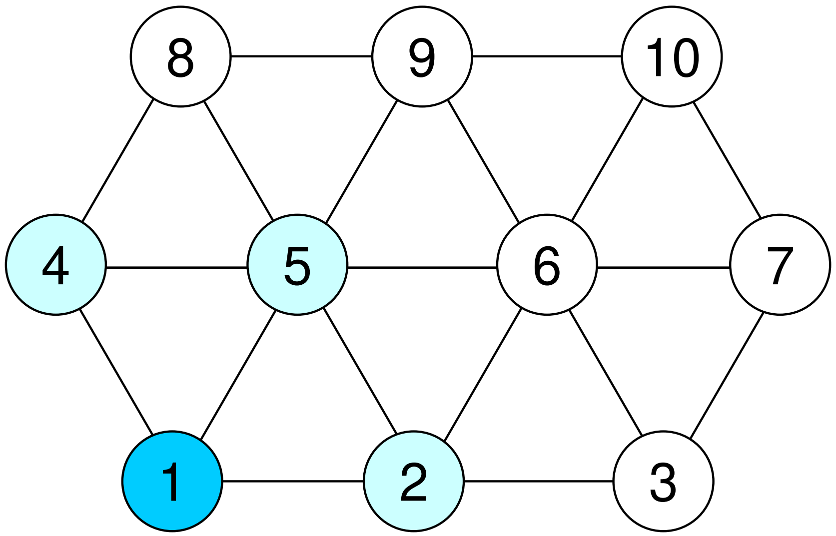
- **IW(ic,1), ic= 1, icou**

Remove such meshes that are adjacent to other candidates, because neighboring meshes cannot belong to same level.

If we have such removed mesh **in**, apply the following operations:

- **IW(in,2)= 0**

What does is mean ?



(2),(4) and (5) are candidates for **(icol)th** level

```
IW(2,2)= -icol
IW(4,2)= -icol
IW(5,2)= -icol

IW(1,1)= 2
IW(2,1)= 4
IW(3,1)= 5
```

Candidates for **icolth** level are stored in:

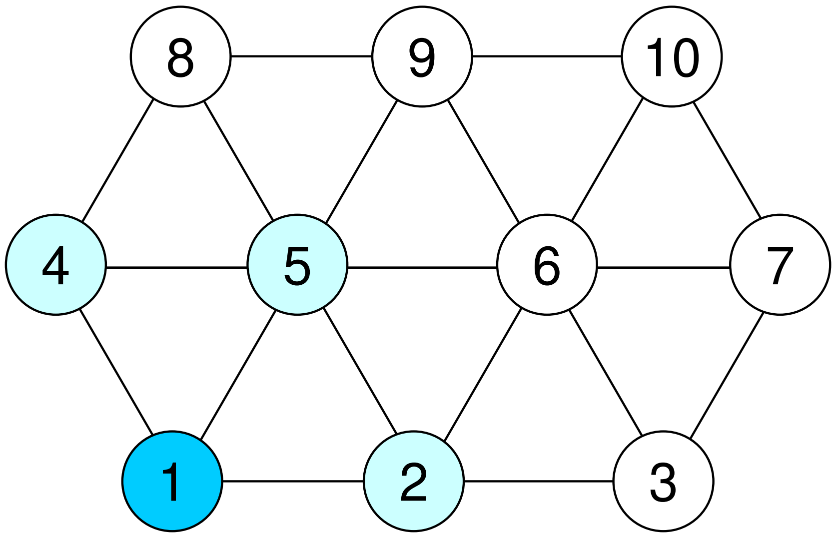
- **IW(ic,1), ic= 1, icou**

Remove such meshes that are adjacent to other candidates, because neighboring meshes cannot belong to same level.

If we have such removed mesh **in**, apply the following operations:

- **IW(in,2)= 0**

What does is mean ?



Considering dependency:

```
IW(2,2)= -icol
IW(4,2)= -icol
IW(5,2)= 0

IW(1,1)= 2
IW(2,1)= 4
IW(3,1)= 5
```

Candidates for **icol**th level are stored in:

- **IW(ic,1), ic= 1, icou**

Remove such meshes that are adjacent to other candidates, because neighboring meshes cannot belong to same level.

If we have such removed mesh **in**, apply the following operations:

- **IW(in,2)= 0**

cm (4/5)

```
!C
!C +----------+
!C | COLORING |
!C +----------+
!C===

...

        do ic= 1, icou
          inC= IW(ic,1)
          if (IW(inC,2).ne.0) then
            do k= 1, INL(inC)
              in= IAL(k,inC)
              if (IW(in,2).le.0) IW(in,2)= 0
            enddo
            do k= 1, INU(inC)
              in= IAU(k,inC)
              if (IW(in,2).le.0) IW(in,2)= 0
            enddo
          endif
        enddo

        do ic= 1, icou
          inC= IW(ic,1)
          if (IW(inC,2).ne.0) then
            icouG      = icouG + 1
            IW(inC,2)= icol
          endif
        enddo

        if (icouG.eq.N) exit
      enddo
!C===
```

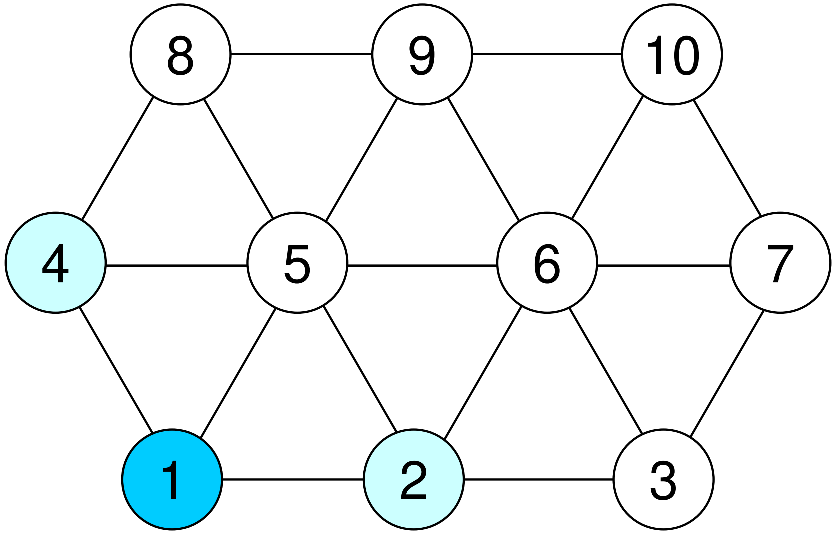
icouG: Global Counter
icou : Intra-Level Counter

Finally, meshes which satisfies **IW(inC,2)=-icol**, belong to **icol**th level.

For such meshes, apply **IW(inC,2)=icol**.

Finally, **icouG= icouG + 1**

What does is mean ?



Considering dependency:

```
IW(2,2)= -icol
IW(4,2)= -icol
IW(5,2)= 0
IW(1,1)= 2
IW(2,1)= 4
IW(3,1)= 5
```

Finally:

```
IW(2,2)= icol
IW(4,2)= icol
```

Finally, meshes which satisfies **IW(inC,2)=-icol**, belong to **icol**th level.

For such meshes, apply **IW(inC,2)=icol**.

Finally, **icouG= icouG + 1**

cm (4/5)

```
!C
!C +----------+
!C | COLORING |
!C +----------+
!C===

...

        do ic= 1, icou
          inC= IW(ic,1)
          if (IW(inC,2).ne.0) then
            do k= 1, INL(inC)
              in= IAL(k,inC)
              if (IW(in,2).le.0) IW(in,2)= 0
            enddo
            do k= 1, INU(inC)
              in= IAU(k,inC)
              if (IW(in,2).le.0) IW(in,2)= 0
            enddo
          endif
        enddo

        do ic= 1, icou
          inC= IW(ic,1)
          if (IW(inC,2).ne.0) then
            icouG     = icouG + 1
            IW(inC,2)= icol
          endif
        enddo

        if (icouG.eq.N) exit
      enddo
!C===
```

icouG: Global Counter
icou : Intra-Level Counter

if **icouG=N (ICELTOT)**:
- All meshes are colored (completed).

Otherwise, proceed to the next level.

cm (5/5)

```
!C
!C +----------------+
!C | FINAL COLORING |
!C +----------------+
!C===
 3000 continue
      NCOLORtot= icol
      icoug= 0
      do ic= 1, NCOLORtot
        icou= 0
        do i= 1, N
          if (IW(i,2).eq.ic) then
            icou = icou + 1
            icoug= icoug + 1
            NEWtoOLD(icoug)= i
            OLDtoNEW(i    )= icoug
          endif
        enddo
        COLORindex(ic)= icou
      enddo

      COLORindex(0)= 0
      do ic= 1, NCOLORtot
        COLORindex(ic)= COLORindex(ic-1) + COLORindex(ic)
      enddo
!C===

!C
!C +-----------------+
!C | MATRIX transfer |
!C +-----------------+
!C===
     …
!C===
      return
      end
```

NCOLORtot= NCOLORk:
Final number of colors.

NCOLORtot g.e. (Initial number of colors provided by user)

Renumber meshes in ascending orders according to level ID.

OLDtoNEW(OldID)= NewID
NEWtoOLD(NewID)= OldID

COLODindex(ic):
At this stage, number of meshes in each level (ic) is stored.

cm (5/5)

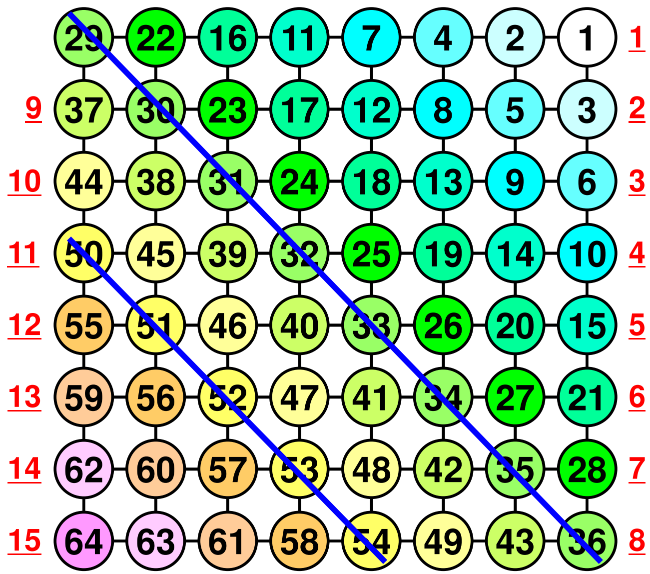
```
!C
!C +----------------+
!C | FINAL COLORING |
!C +----------------+
!C===
 3000 continue
      NCOLORtot= icol
      icoug= 0
      do ic= 1, NCOLORtot
        icou= 0
        do i= 1, N
          if (IW(i,2).eq.ic) then
            icou = icou + 1
            icoug= icoug + 1
            NEWtoOLD(icoug)= i
            OLDtoNEW(i    )= icoug
          endif
        enddo
        COLORindex(ic)= icou
      enddo

      COLORindex(0)= 0
      do ic= 1, NCOLORtot
        COLORindex(ic)= COLORindex(ic-1) + COLORindex(ic)
      enddo
!C===

!C
!C +-----------------+
!C | MATRIX transfer |
!C +-----------------+
!C===
     ...
!C===
      return
      end
```

COLODindex(ic):

Now it is 1D index.

Features of MC & CM/RCM

- MC
  - Good parallel performance & load balancing
  - More Colors -> Better Convergence
    - Smaller number of meshes per color, and per thread
    - Small Granularity（粒度）, Larger Synchronization Overhead
    - Finally, lower parallel performance
- CM/RCM
  - Faster convergence than MC.
  - Generally, many levels (and number is unknown before computation)
    - Same problems on parallel efficiency as MC
    - Number of meshes in each level is random
      - At the 1st/Last Level: Only One Mesh/Level



- Convenient method needed
  - Fast convergence
  - Low overhead with smaller number of colors

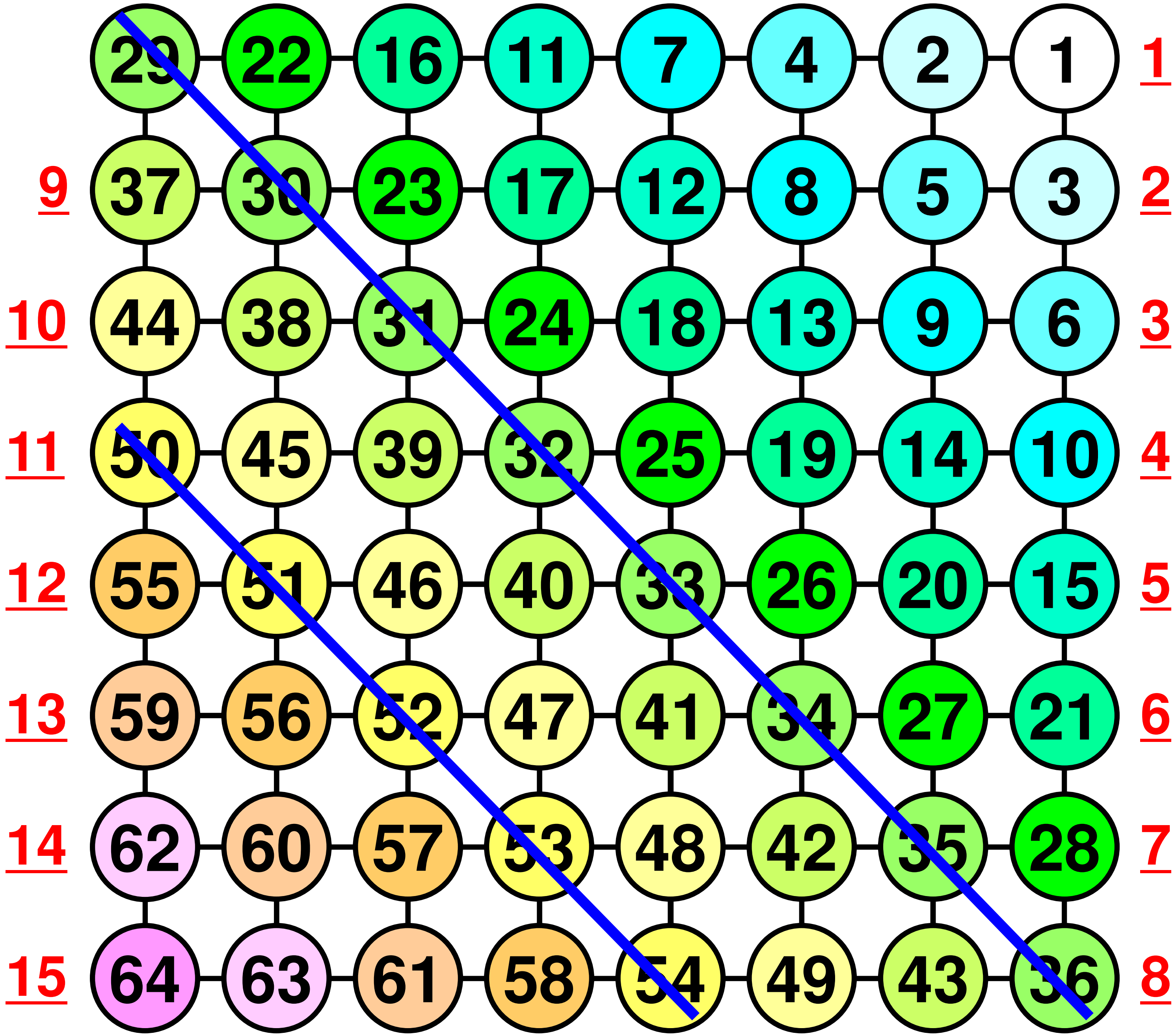
More Colors: Synch. Overhead

```
      do ic= 1, NCOLORtot
!$omp parallel do private(ip,ip1,i,WVAL,k)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
        enddo
!$omp end parallel do
      enddo
```

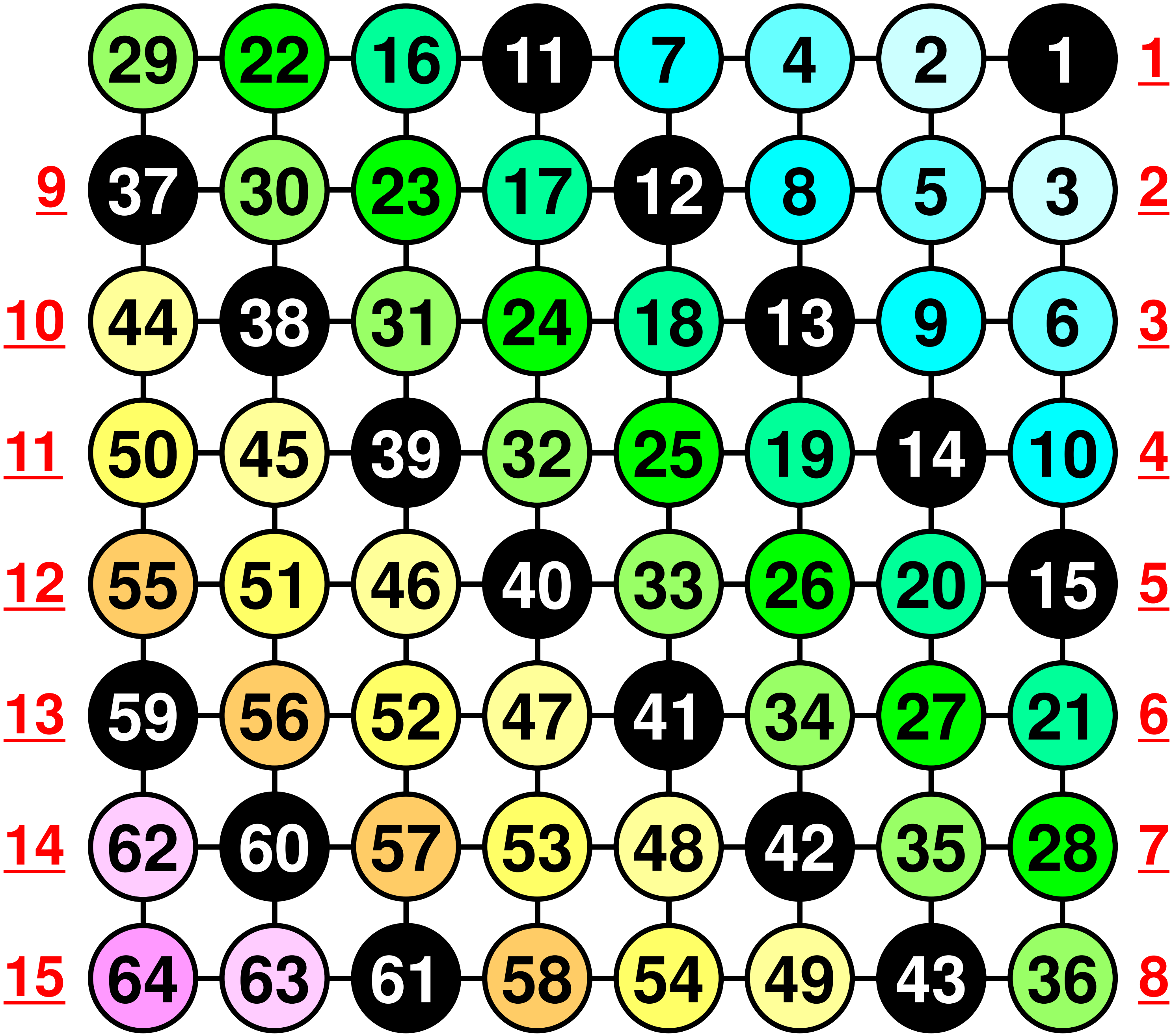
Remedy: CM-RCM

- RCM + Cyclic Mulricoloring [Doi, Osoda, Washio]
- Procedures
  - Apply RCM
  - Define "Nc" (Color number of Cyclic Multicoloring (CM))
    - 1st-Color in CM-RCM: 1st, (Nc+1)th, (2Nc+1) th ... levels in RCM
    - 2nd-Color in CM-RCM: 2nd, (Nc+2)th, (2Nc+2) th ... levels in RCM
    - kth-Color in CM-RCM: kth, (Nc+k)th, (2Nc+k) th ... levels in RCM
    - Each level of RCM is colored in cyclic manner (cycle=Nc).
  - If "k" reaches "Nc", and all levels of RCM are colored, it's completed.
    - Renumber meshes in ascending orders according to "Color" ID.
  - If dependency between levels in same color, start from the beginning of the cyclic multicoloring with Nc=Nc+1.

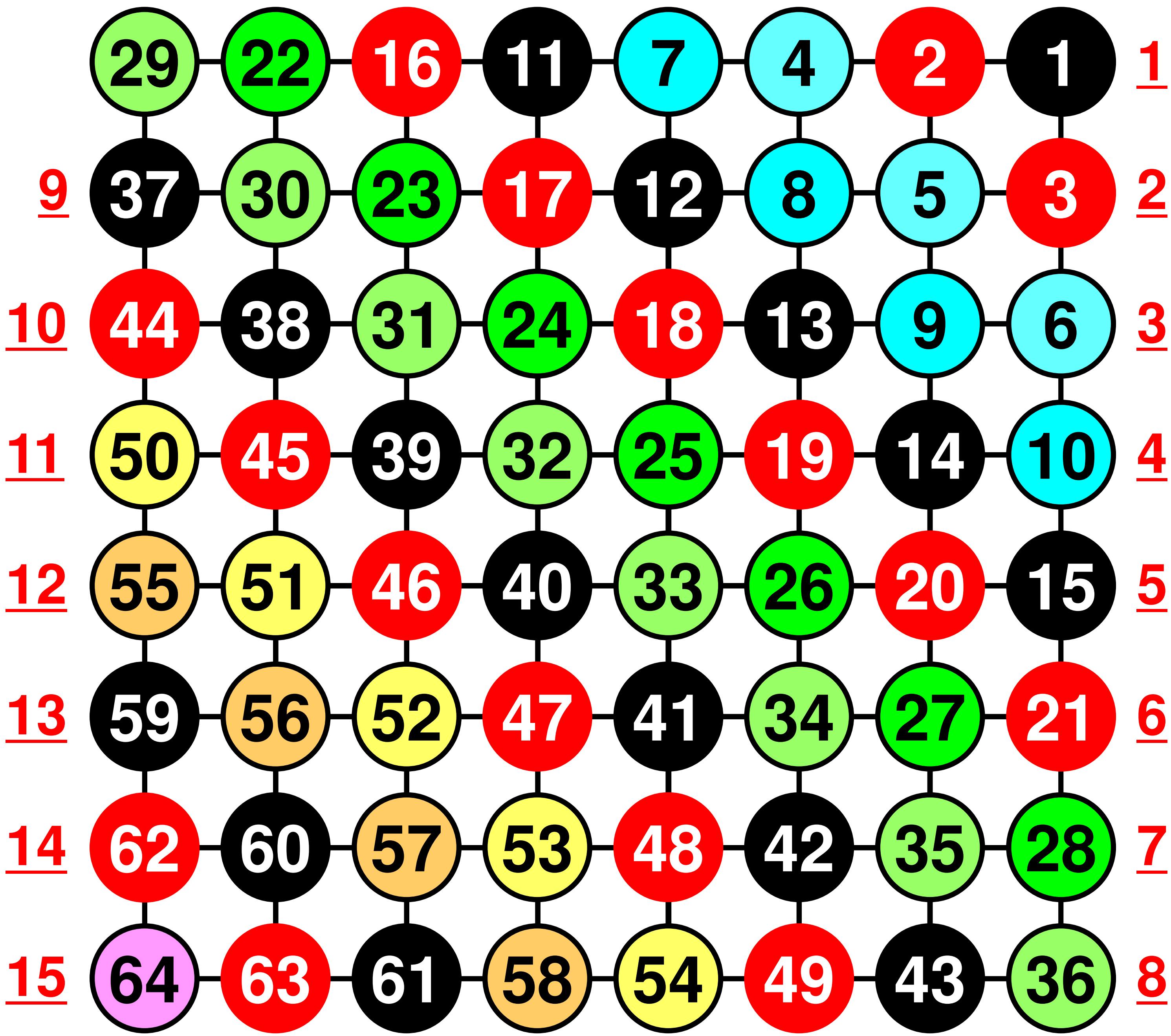
RCM: 1st/Last Level: Only 1 Mesh/Level



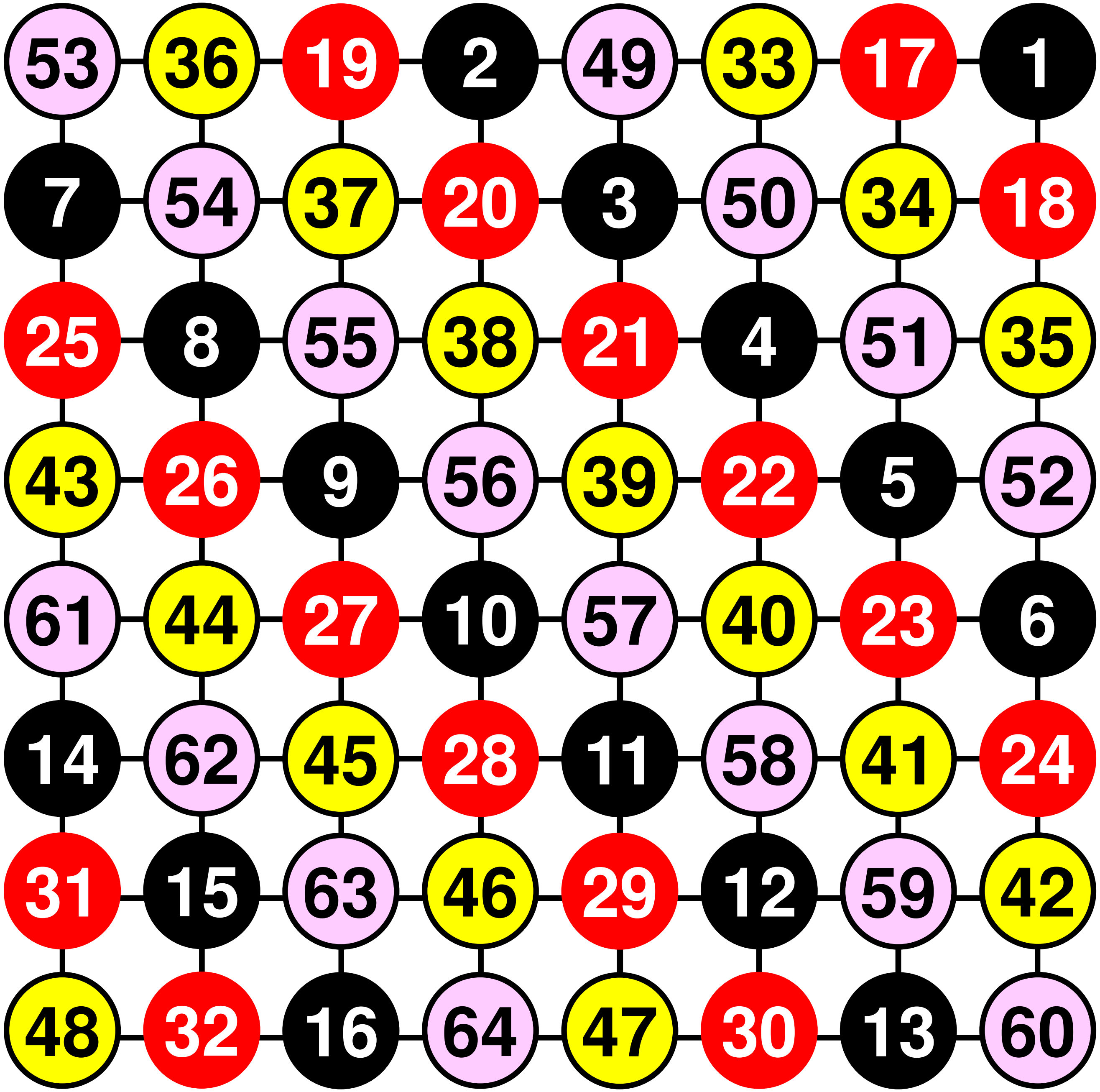
Nc=4, k=1, Level: 1,5,9,13



Nc=4, k=2, Level: 2,6,10,14



CM-RCM(Nc=4): Renumbering



k=1: 16
k=2: 16
k=3: 16
k=4: 16

CM-RCM

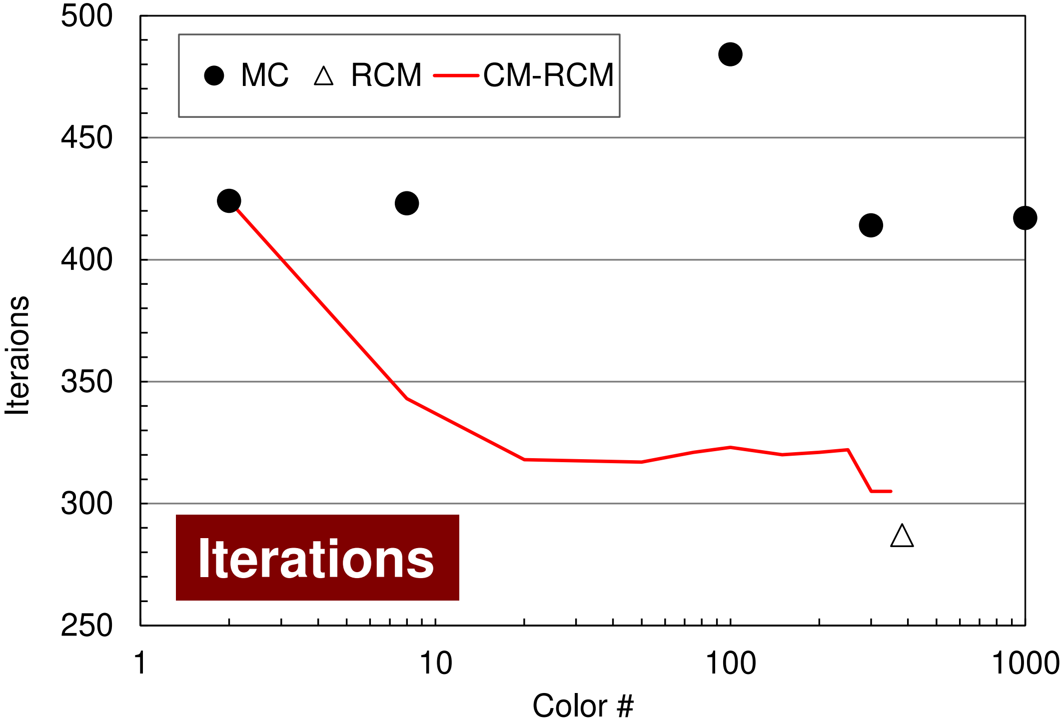
- How to run
  - ”**`NCOLORtot=-Nc`**” in INPUT.DAT
  - Already implemented in L2

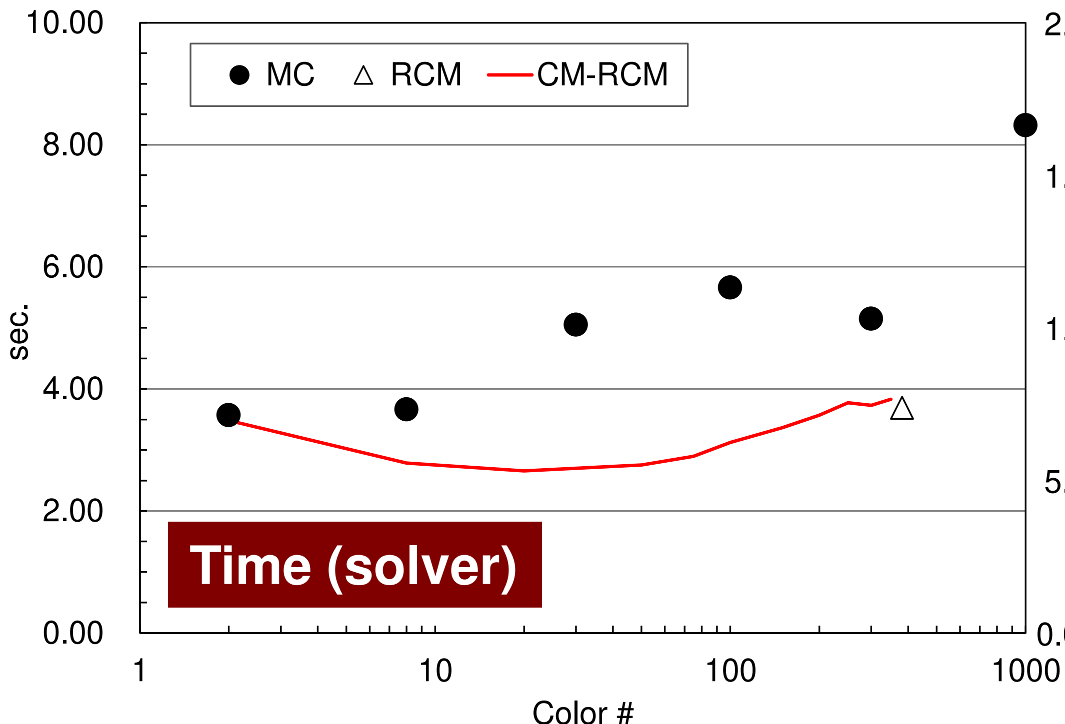
- cmrcm.f, cmrcm.c

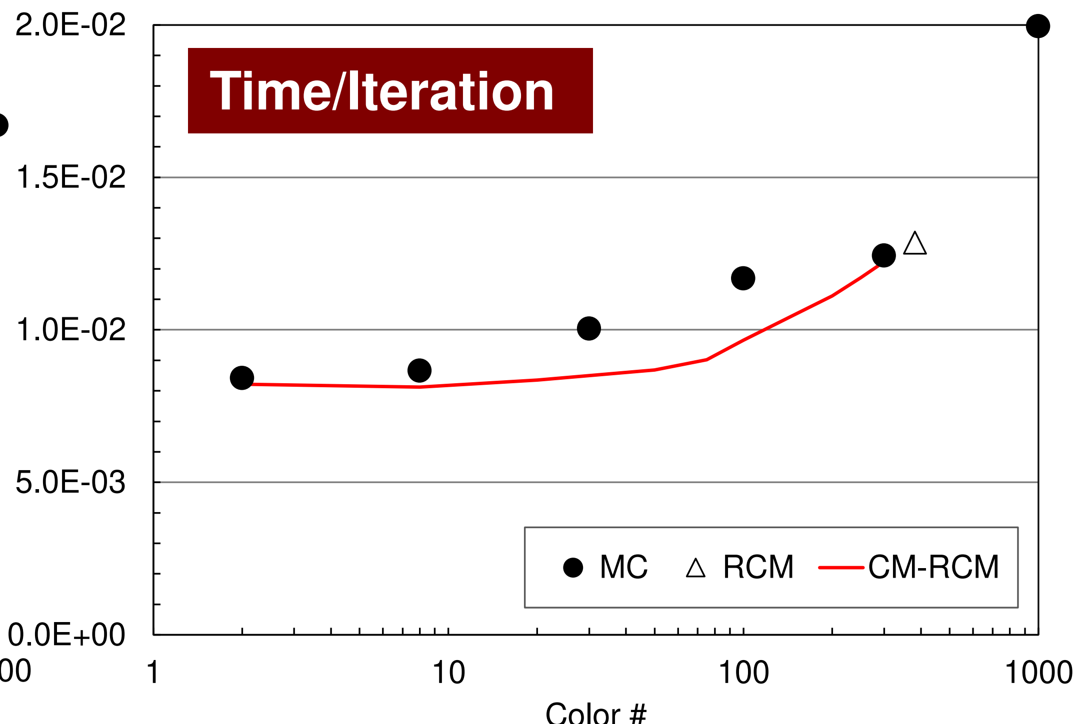
Odyssey

1-CMG/12-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)

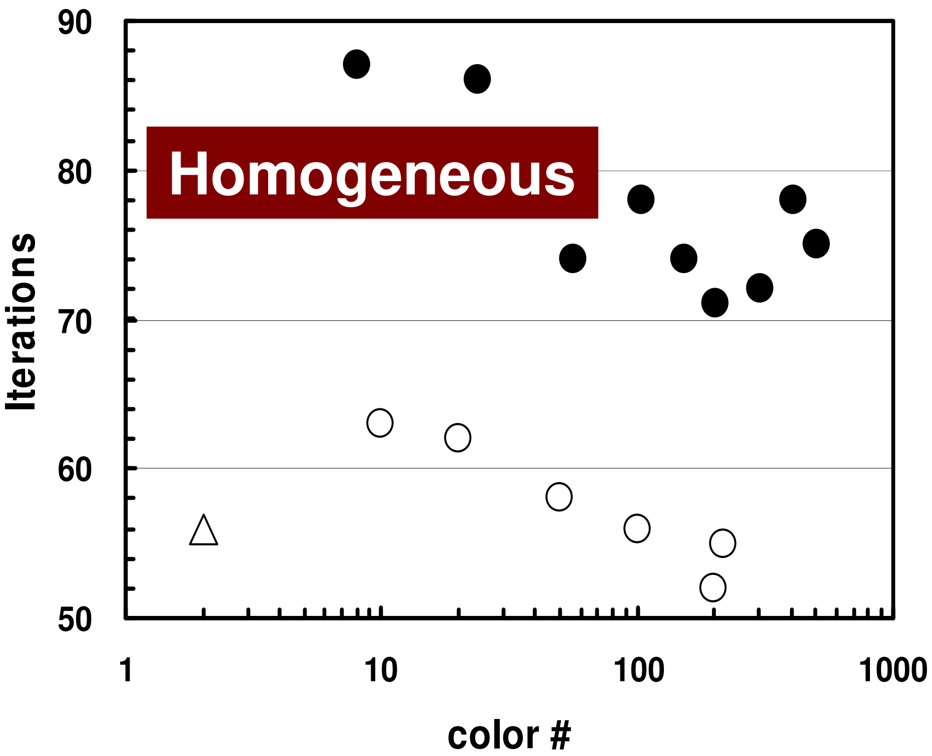


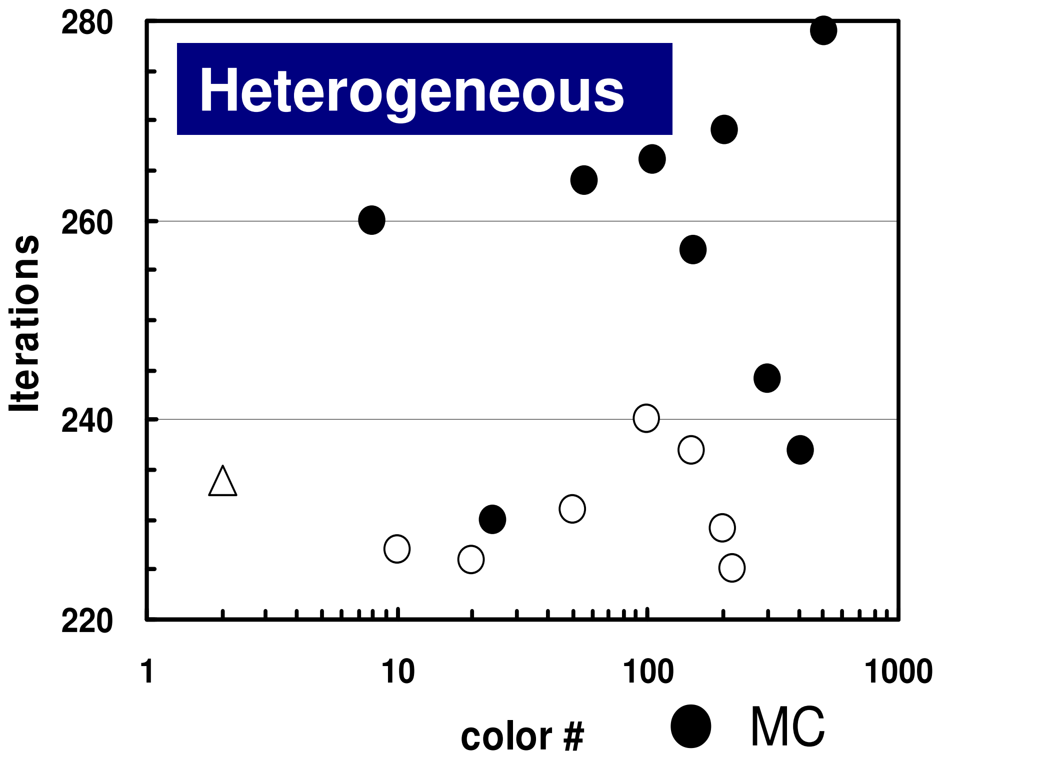




Comparison of Reordering Methods
3D Linear Elastic Problems

- MC: Slow convergence, unstable for heterogeneous cases (ill-conditioned problems).
- Cyclic-Mulricoloring + RCM (CM-RCM) is effective





3D Linear-Elastic Problems with 32,768 DOF

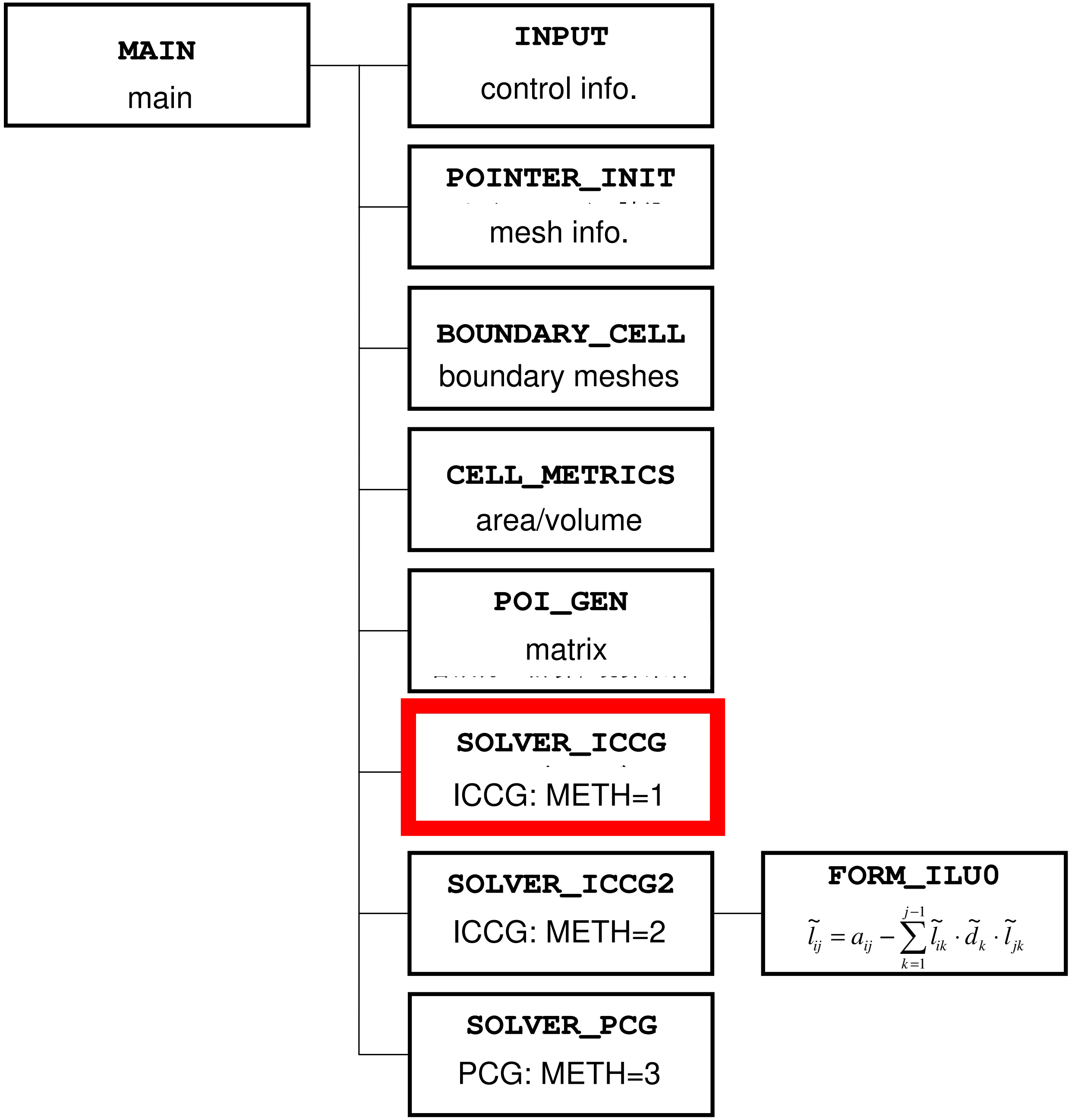
- Remedy for Data Dependency
- Ordering/Reordering
  - Red-Black, Multicoloring (MC)
  - Cuthill-McKee (CM), Reverse-CM (RCM)
  - Reordering and Convergence
- Implementation
- **ICCG with Reordering**

Implementation of Reordering to ICCG

- Apply “L2-color” to “L1-sol”

- Calling “mc”, “cm”, “rcm” and “cmrcm” after computation of “INU, INL, IAL, IAU” in “poi_gen”.
- Computing “AL,AU” by new numbering.
- B.C., and RHS are applied by new numbering.
- Calling “ICCG”
- Renumbering components of “PHI (results)” into initial numbering.
- OUPUT_UCD (UCD file)

L1-sol


MAIN
main
INPUT
control info.
POINTER_INIT
mesh info.
BOUNDARY_CELL
boundary meshes
CELL_METRICS
area/volume
POI_GEN
matrix
SOLVER_ICCG
ICCG: METH=1
SOLVER_ICCG2
ICCG: METH=2
FORM_ILU0
$\tilde{l}_{ij} = a_{ij} - \sum_{k=1}^{j-1} \tilde{l}_{ik} \cdot \tilde{d}_k \cdot \tilde{l}_{jk}$
SOLVER_PCG
PCG: METH=3

Minv{r}={z} (1/2)

Forward Substitution $(L)\{z\}=\{r\}$ $(M)\{z\}=(LDL^T)\{z\}=\{r\}$

```
do i= 1, N
  WVAL= R(i)
  do k= indexL(i-1)+1, indexL(i)
    WVAL= WVAL -  MAL(k) * Z(itemL(k))
  enddo
  Z(i)= WVAL / D(i)
enddo
```

Backward Substitution $(DL^T)\{z\}=\{z\}$

```
do i= N, 1, -1
  SW  = 0.0d0
  do k= indexU(i-1)+1, indexU(i)
    SW= SW + MAU(k) * Z(itemU(k))
  enddo
  Z(i)= Z(i) - SW / MD(i)
enddo
```

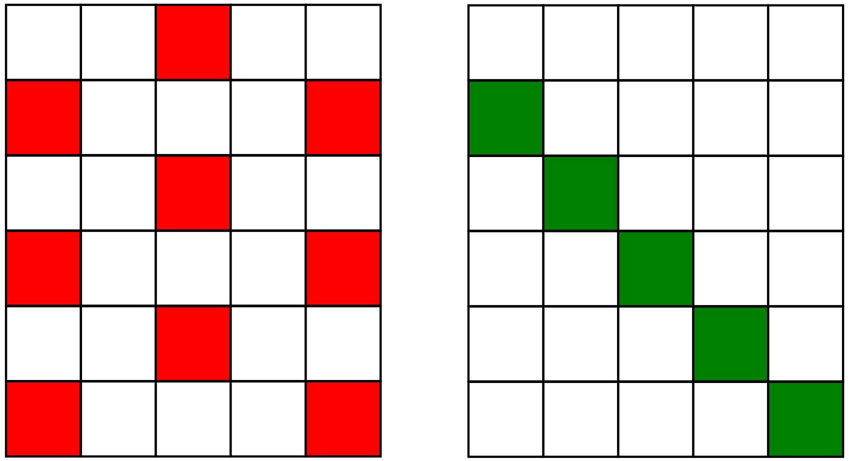
Data Dependency Z appears in both of LHS and RHS.

Reordering may eliminate this data dependency.

Minv{r}={z} (2/2)

Forward Substitution $(L)\{z\}=\{r\}$ $(M)\{z\}=(LDL^T)\{z\}=\{r\}$

```
do icol= 1, NCOLORtot
  do i= COLORindex(icol-1)+1, COLORindex(icol)
    WVAL= R(i)
    do k= indexL(i-1)+1, indexL(i)
      WVAL= WVAL -  MAL(k) * Z(itemL(k))
    enddo
    Z(i)= WVAL / D(i)
  enddo
enddo
```



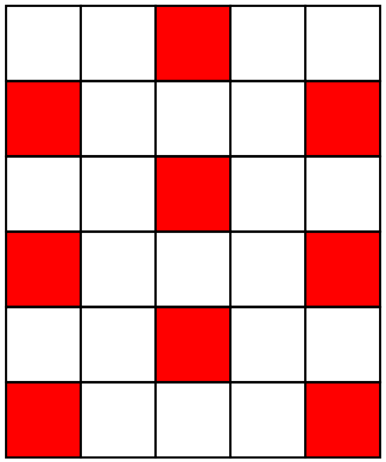
"Z" components in RHS do not belong to "icol-th" color.

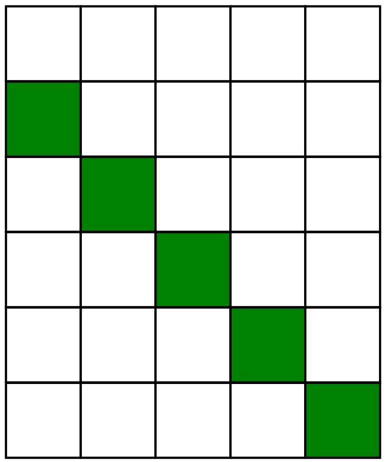
Meshes in same color are independent. (No Data Dependency)

Minv{r}={z} (2/2)

Forward Substitution $(L)\{z\}=\{r\}$ $(M)\{z\}=\left(LDL^T\right)\{z\}=\{r\}$

```
do icol= 1, NCOLORtot
  do i= COLORindex(icol-1)+1, COLORindex(icol)
    WVAL= R(i)
    do k= indexL(i-1)+1, indexL(i)
      WVAL= WVAL -  MAL(k) * Z(itemL(k))
    enddo
    Z(i)= WVAL / D(i)
  enddo
enddo
```



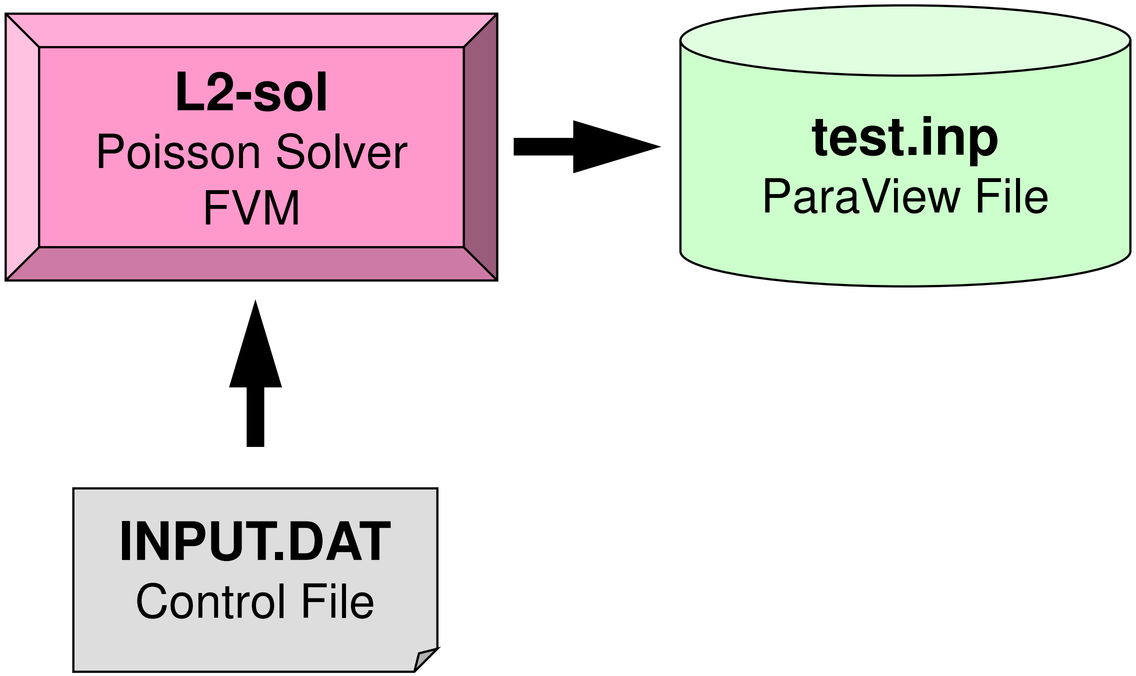


Parallel processing can be applied to these loops.

Files

```
$> cd multicore-f/L2/solver/src



$> make
$> ls ../run/L2-sol
   L2-sol
```

Running the Program <$P-L2>/solver/run

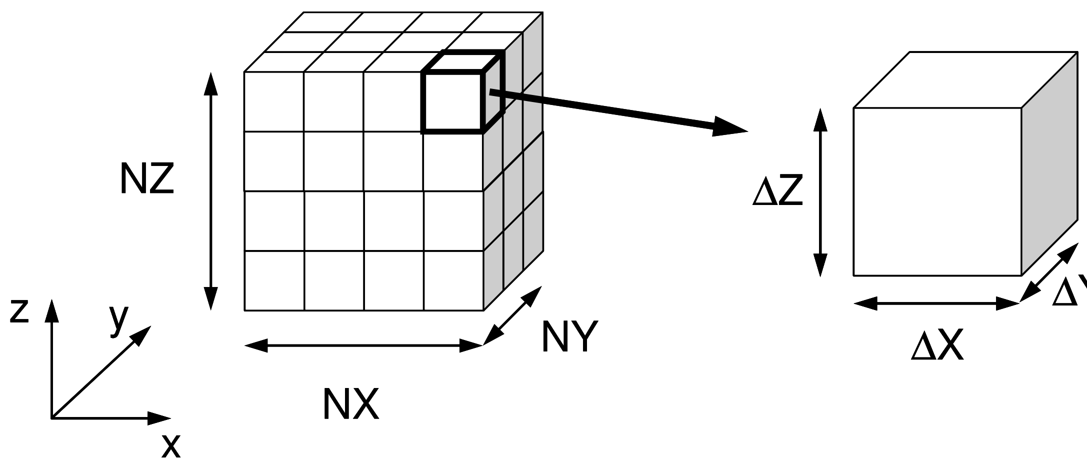


Running the Program

Control Data: <$P-L2>/solver/run/INPUT.DAT

```
32 32 32                                    NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00                  DX/DY/DZ
1.0e-08                                     EPSICCG
```

- NX, NY, NZ
  - Number of meshes in X/Y/Z dir.
- DX, DY, DZ
  - Size of meshes
- EPSICCG
  - Convergence Criteria for ICCG



Running the Program

<$P-L2>/solver/run/

```
$ cd <$P-L2>/solver/run
$ ./L2-sol

You have     8000 elements.
How many colors do you need ?
  #COLOR must be more than 2 and
  #COLOR must not be more than    8000
   CM if #COLOR .eq. 0
  RCM if #COLOR .eq.-1
CMRCM if #COLOR .le.-2

=> XXX

$ ls test.inp
```

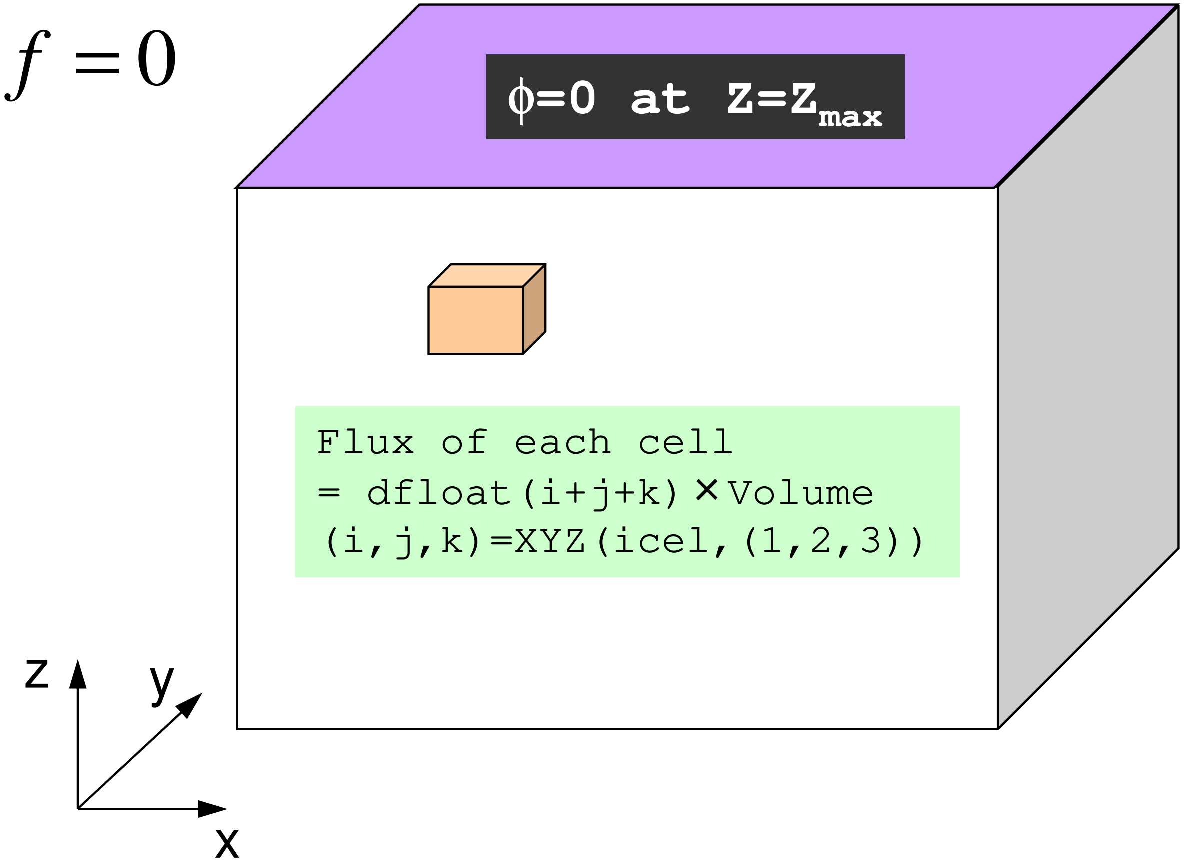
Target Problem: Variables are defined at cell-center’

Poisson Equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} + \frac{\partial^2 \phi}{\partial z^2} + f = 0$$

Boundary Conditions (B.C.) etc.

- Volume Flux
- $\phi = 0$ @ $Z = Z_{max}$

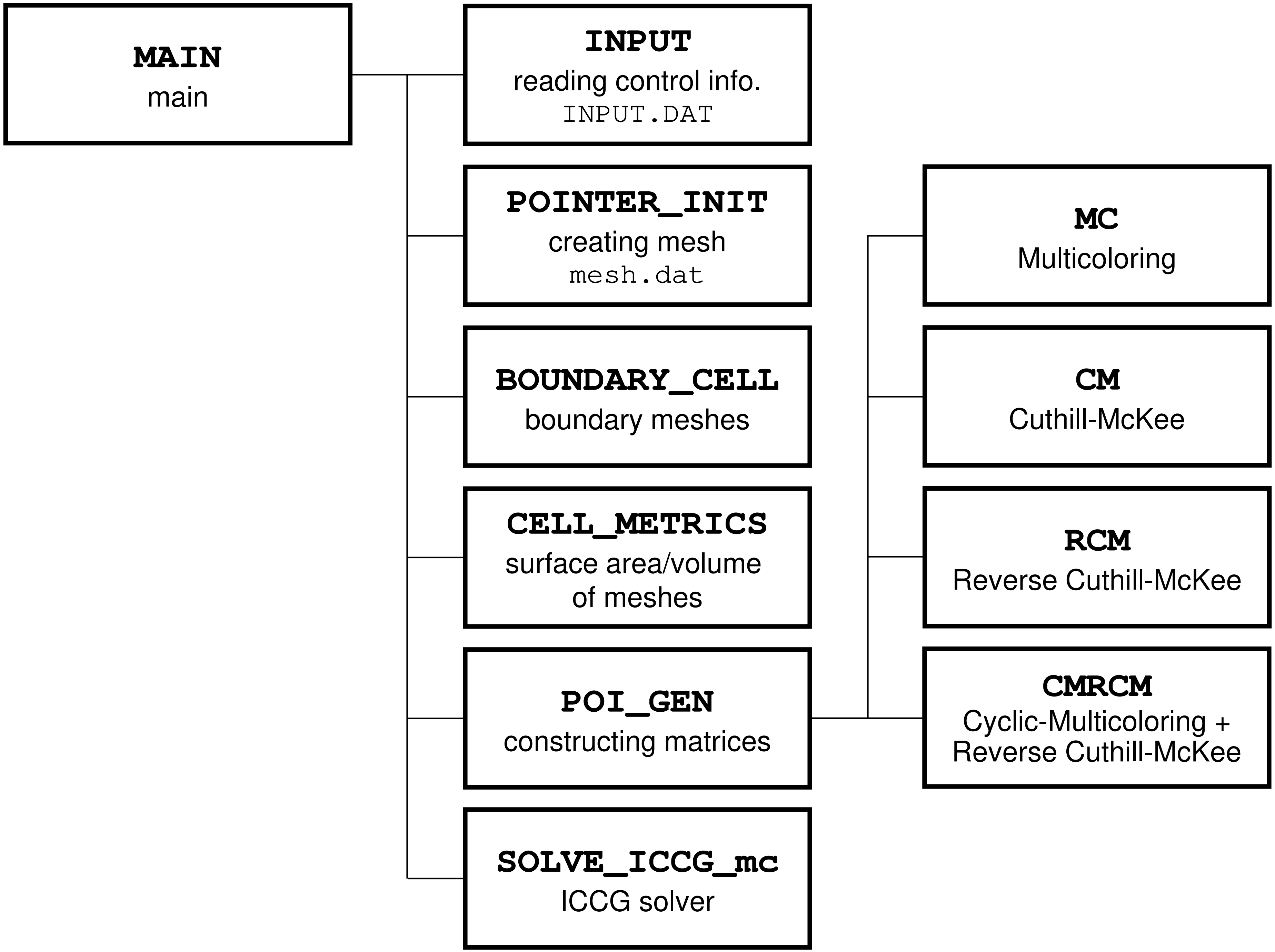


Main Program

```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

      implicit REAL*8 (A-H,O-Z)
      real(kind=8), dimension(:), allocatable :: WK

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0
      call solve_ICCG_mc                                             &
     &    ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,       &
     &      BFORCE,  PHI, AL, AU, NCOLORtot, COLORindex,              &
     &      EPSICCG, ITR, IER)

      allocate (WK(ICELTOT))

      do ic0= 1, ICELTOT
        icel= NEWtoOLD(ic0)
        WK(icel)= PHI(ic0)
      enddo

      do icel= 1, ICELTOT
        PHI(icel)= WK(icel)
      enddo

      call OUTUCD

      stop
      end
```

Renumbering of “PHI” to original numbering

Structure of L2-sol



Variables/Arrays for Matrix (1/2)

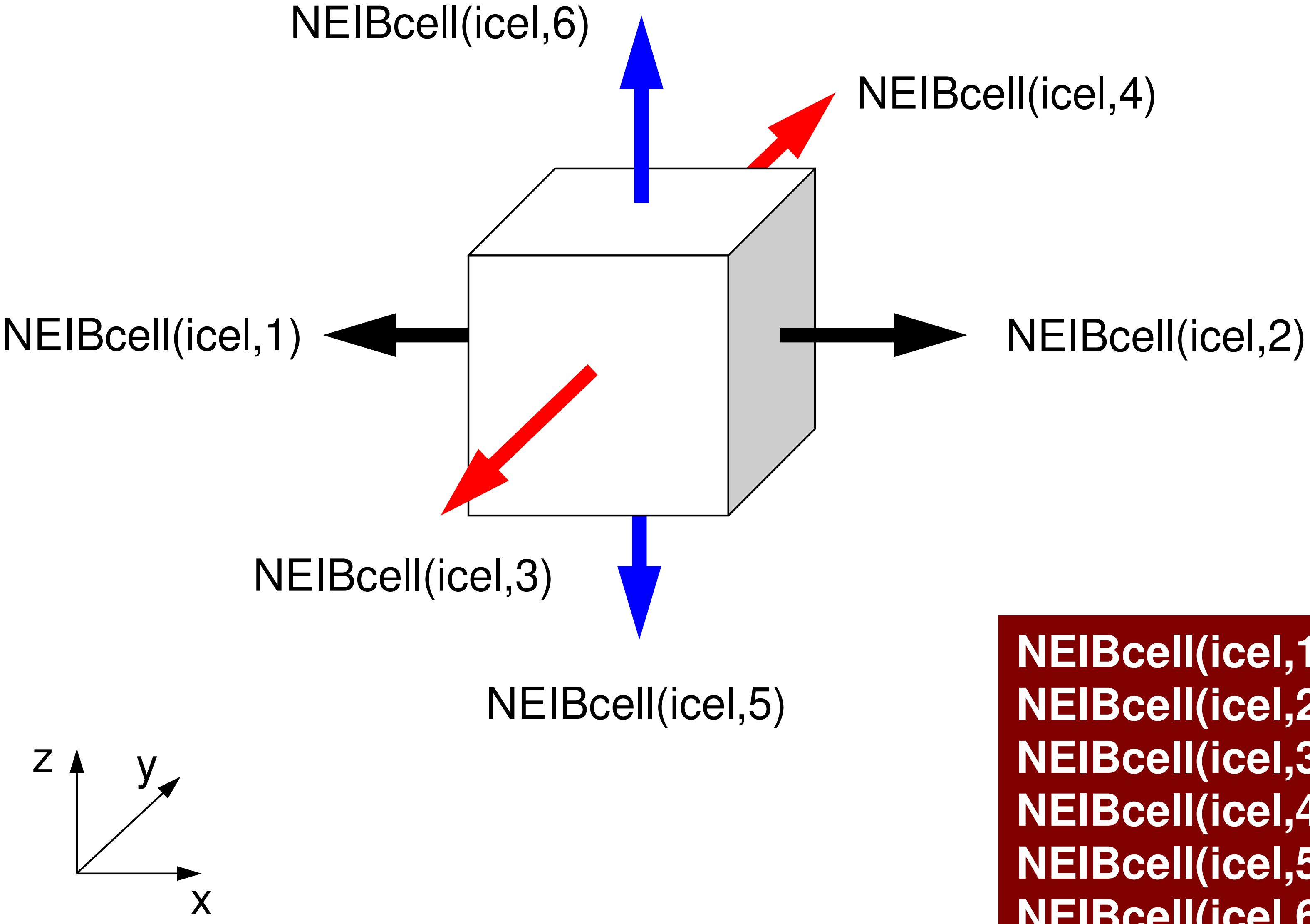
Name	Type	Content
D(N)	**R**	Diagonal components of the matrix `(N= ICELTOT)`
BFORCE(N)	**R**	RHS vector
PHI(N)	**R**	Unknown vector
indexL(0:N), indexU(0:N)	**I**	# of L/U non-zero off-diag. comp. (CRS)
NPL, NPU	**I**	Total # of L/U non-zero off-diag. comp. (CRS)
itemL(NPL), itemU(NPU)	**I**	Column ID of L/U non-zero off-diag. comp. (CRS)
AL(NPL), AU(NPU)	**R**	L/U non-zero off-diag. comp. (CRS)

Name	Type	Content
NL,NU	**I**	MAX. # of L/U non-zero off-diag. comp. for each mesh (=6)
INL(N), INU(N)	**I**	# of L/U non-zero off-diag. comp.
IAL(NL,N), IAU(NU,N)	**I**	Column ID of L/U non-zero off-diag. comp.

Variables/Arrays for Matrix (2/2)

Name	Type	Content
`NCOLORtot`	**`I`**	**<u>Input:</u>** reordering method + initial number of colors/levels ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM **<u>Output:</u>** Final number of colors/levels
`COLORindex (0:NCOLORtot)`	**`I`**	Number of meshes at each color/level 1D compressed array Meshes in **`icol`**th color/level are stored in this array from **`COLORindex(icol-1)+1`** to **`COLORindex(icol)`**
`NEWtoOLD(N)`	**`I`**	Reference array from New to Old numbering
`OLDtoNEW(N)`	**`I`**	Reference array from Old to New numbering

NEIBcell: ID of Neighboring Mesh/Cell =0: for Boundary Surface



NEIBcell(icel,1)= icel – 1
NEIBcell(icel,2)= icel + 1
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,4)= icel + NX
NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,6)= icel + NX*NY

Main Program

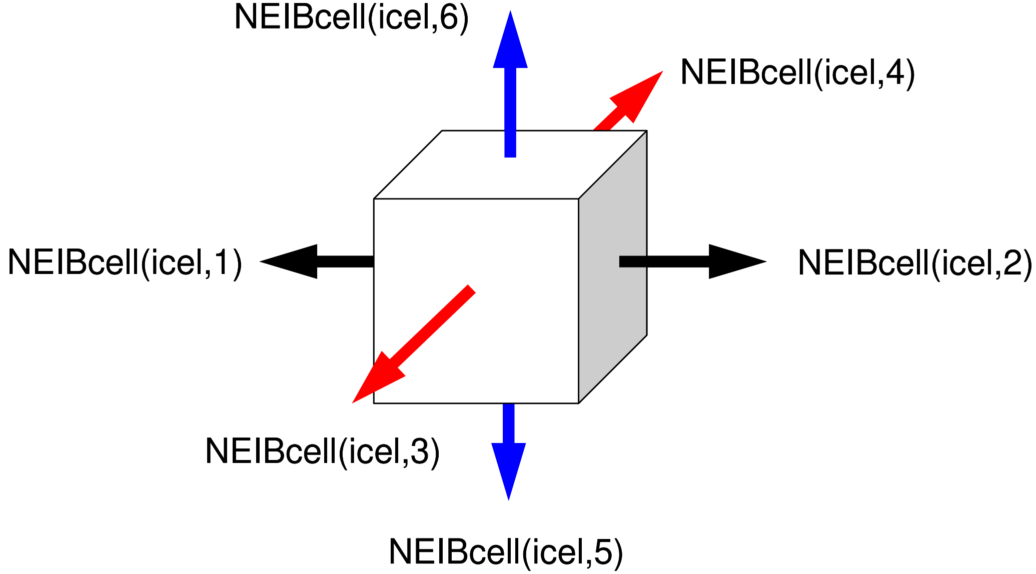
```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

      implicit REAL*8 (A-H,O-Z)
      real(kind=8), dimension(:), allocatable :: WK

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0
      call solve_ICCG_mc                                              &
     &     ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,       &
     &       BFORCE,  PHI, AL, AU, NCOLORtot, COLORindex,             &
     &       EPSICCG, ITR, IER)

      allocate (WK(ICELTOT))
      do ic0= 1, ICELTOT
        icel= NEWtoOLD(ic0)
        WK(icel)= PHI(ic0)
      enddo

      do icel= 1, ICELTOT
        PHI(icel)= WK(icel)
      enddo

      call OUTUCD

      stop
      end
```

poi_gen (1/8)

```
      subroutine POI_GEN

      use STRUCT
      use PCG

      implicit REAL*8 (A-H,O-Z)

!C
!C-- INIT.
      nn = ICELTOT

      NU= 6
      NL= 6

      allocate (BFORCE(nn), D(nn), PHI(nn))
      allocate (INL(nn), INU(nn), IAL(NL,nn), IAU(NU,nn))

         PHI= 0.d0
           D= 0.d0
      BFORCE= 0.d0

      INL= 0
      INU= 0
      IAL= 0
      IAU= 0
```

poi_gen (2/8)

```
!C
!C +--------------+
!C | CONNECTIVITY |
!C +--------------+
!C===
      do icel= 1, ICELTOT
        icN1= NEIBcell(icel,1)
        icN2= NEIBcell(icel,2)
        icN3= NEIBcell(icel,3)
        icN4= NEIBcell(icel,4)
        icN5= NEIBcell(icel,5)
        icN6= NEIBcell(icel,6)

        icouG= 0
        if (icN5.ne.0.and.icN5.le.ICELTOT) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN5
          INL(     icel)= icou
        endif

        if (icN3.ne.0.and.icN3.le.ICELTOT) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN3
          INL(     icel)= icou
        endif

        if (icN1.ne.0.and.icN1.le.ICELTOT) then
          icou= INL(icel) + 1
          IAL(icou,icel)= icN1
          INL(     icel)= icou
        endif
```

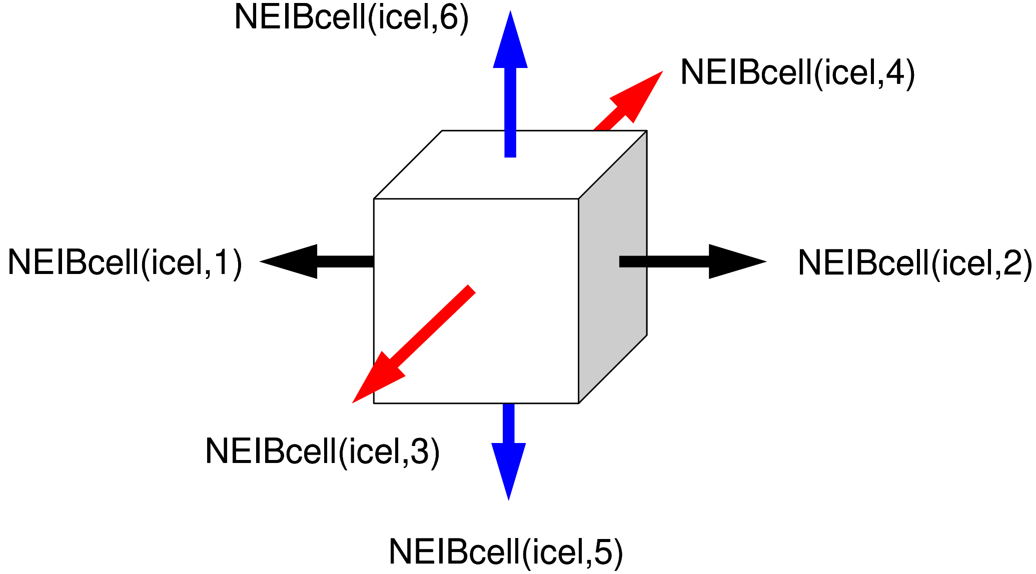


Lower Triangular Part

NEIBcell(icel,5)= icel – NX*NY
NEIBcell(icel,3)= icel – NX
NEIBcell(icel,1)= icel – 1

```
!C
!C +--------------+
!C | CONNECTIVITY |
!C +--------------+
!C===
      do icel= 1, ICELTOT
        icN1= NEIBcell(icel,1)
        icN2= NEIBcell(icel,2)
        icN3= NEIBcell(icel,3)
        icN4= NEIBcell(icel,4)
        icN5= NEIBcell(icel,5)
        icN6= NEIBcell(icel,6)

        icouG= 0
…

        if (icN2.ne.0.and.icN2.le.ICELTOT) then
          icou= INU(icel) + 1
          IAU(icou,icel)= icN2
          INU(     icel)= icou
        endif

        if (icN4.ne.0.and.icN4.le.ICELTOT) then
          icou= INU(icel) + 1
          IAU(icou,icel)= icN4
          INU(     icel)= icou
        endif

        if (icN6.ne.0.and.icN6.le.ICELTOT) then
          icou= INU(icel) + 1
          IAU(icou,icel)= icN6
          INU(     icel)= icou
        endif
      enddo
!C===
```

poi_gen (3/8)



Upper Triangular Part
- NEIBcell(icel,2)= icel + 1
- NEIBcell(icel,4)= icel + NX
- NEIBcell(icel,6)= icel + NX*NY

poi_gen (4/8)

```
!C
!C +---------------+
!C | MULTICOLORING |
!C +---------------+
!C===
      allocate (OLDtoNEW(ICELTOT), NEWtoOLD(ICELTOT))
      allocate (COLORindex(0:ICELTOT))

 111    continue
        write (*,'(//a,i8,a)') 'You have', ICELTOT, ' elements.'
        write (*,'(  a      )') 'How many colors do you need ?'
        write (*,'(  a      )') '  #COLOR must be more than 2 and'
        write (*,'(  a,i8   )') '  #COLOR must not be more than', ICELTOT
        write (*,'(  a      )') '   CM if #COLOR .eq. 0'
        write (*,'(  a      )') '  RCM if #COLOR .eq.-1'
        write (*,'(  a      )') 'CMRCM if #COLOR .le.-2'
        write (*,'(  a      )') '=>'
        read  (*,*)             NCOLORtot
        if (NCOLORtot.eq.1.or.NCOLORtot.gt.ICELTOT) goto 111

      if (NCOLORtot.gt.0) then
        call MC   (ICELTOT, NL, NU, INL, IAL, INU, IAU,                  &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.eq.0) then
        call  CM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.eq.-1) then
        call RCM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                   &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif
      if (NCOLORtot.lt.-1) then
        call CMRCM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                 &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif

      write (*,'(//a,i8,// )') '### FINAL COLOR NUMBER', NCOLORtot
!C===
```

poi_gen (5/8)

New numbering is applied after this point

```
!C
!C-- 1D array

      allocate (indexL(0:nn), indexU(0:nn))
      indexL= 0
      indexU= 0

      do icel= 1, ICELTOT
        indexL(icel)= INL(icel)
        indexU(icel)= INU(icel)
      enddo

      do icel= 1, ICELTOT
        indexL(icel)= indexL(icel) + indexL(icel-1)
        indexU(icel)= indexU(icel) + indexU(icel-1)
      enddo

      NPL= indexL(ICELTOT)
      NPU= indexU(ICELTOT)

      allocate (itemL(NPL), AL(NPL))
      allocate (itemU(NPU), AU(NPU))

      itemL= 0
      itemU= 0

         AL= 0.d0
         AU= 0.d0
!C===
```

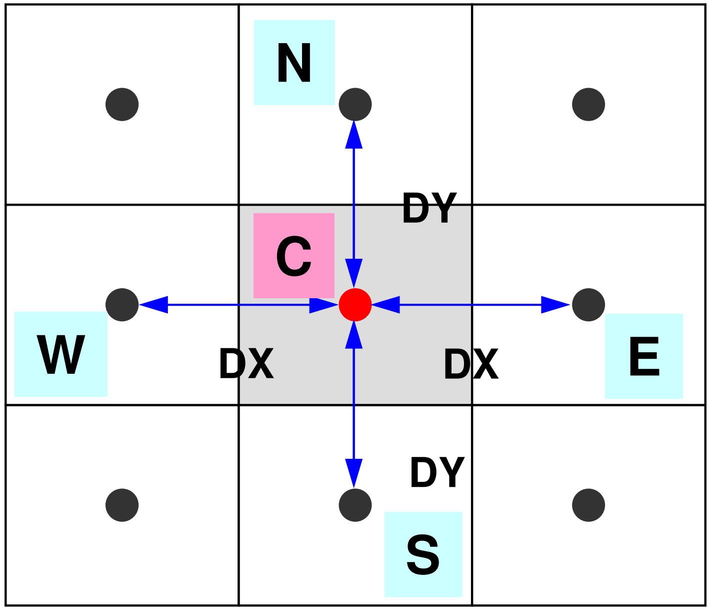
```
do i= 1, N

  VAL= D(i)*p(i)

  do k= indexL(i-1)+1, indexL(i)
    VAL= VAL + AL(k)*p(itemL(k))
  enddo

  do k= indexU(i-1)+1, indexU(i)
    VAL= VAL + AU(k)*p(itemU(k))
  enddo

  q(i)= VAL

enddo
```

Name	Type	Content
D(N)	**R**	Diagonal components of the matrix (N= ICELTOT)
BFORCE(N)	**R**	RHS vector
PHI(N)	**R**	Unknown vector
indexL(0:N), indexU(0:N)	**I**	# of L/U non-zero off-diag. comp. (CRS)
NPL, NPU	**I**	Total # of L/U non-zero off-diag. comp. (CRS)
itemL(NPL), itemU(NPU)	**I**	Column ID of L/U non-zero off-diag. comp. (CRS)
AL(NPL), AU(NPU)	**R**	L/U non-zero off-diag. comp. (CRS)

poi_gen (6/8)

```
!C
!C +-----------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-----------------------------------+
!C===
      icouG= 0
      do icol= 1, NCOLORtot
      do icel= COLORindex(icol-1)+1, COLORindex(icol)
        ic0 = NEWtoOLD(icel)
        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)
        VOL0= VOLCEL  (ic0)

        if (icN5.ne.0) then
          icN5= OLDtoNEW(icN5)
          coef= RDZ * ZAREA
          D(icel)= D(icel) - coef

          if (icN5.lt.icel) then
            do j= 1, INL(icel)
              if (IAL(j,icel).eq.icN5) then
                itemL(j+indexL(icel-1))= icN5
                   AL(j+indexL(icel-1))= coef
                exit
              endif
            enddo
           else
            do j= 1, INU(icel)
              if (IAU(j,icel).eq.icN5) then
                itemU(j+indexU(icel-1))= icN5
                   AU(j+indexU(icel-1))= coef
                exit
              endif
            enddo
          endif
        endif
```

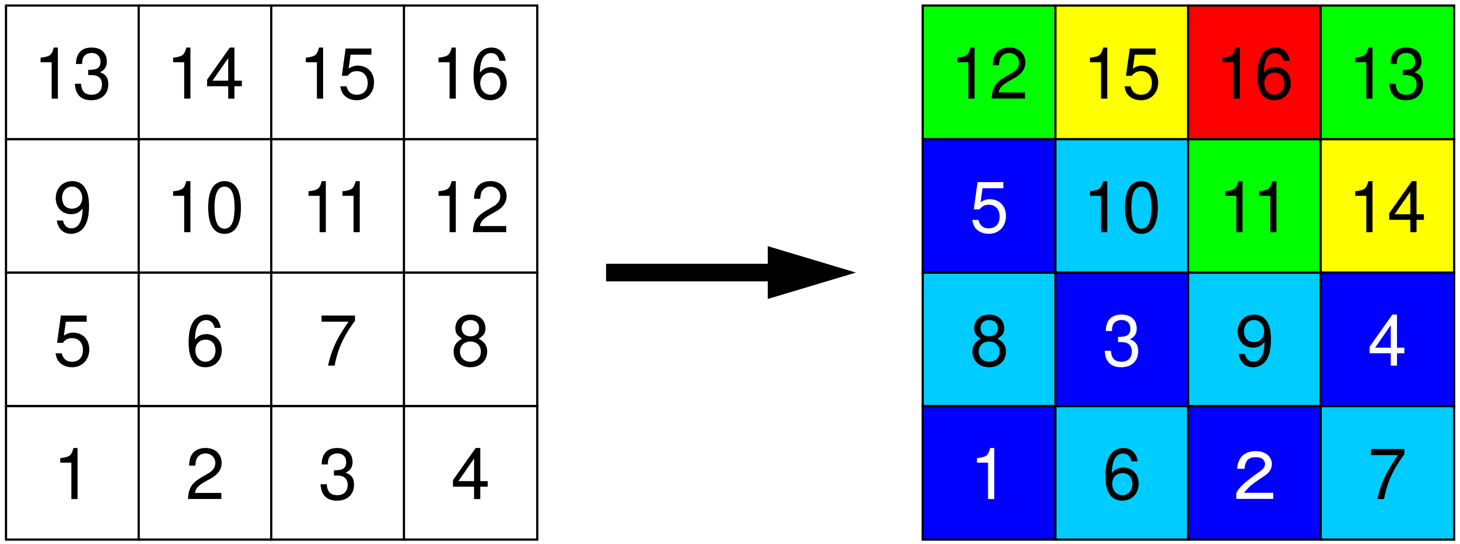
Calculation of Coefficients



$$\frac{\phi_E - \phi_i}{\Delta x}\Delta y + \frac{\phi_W - \phi_i}{\Delta x}\Delta y +$$

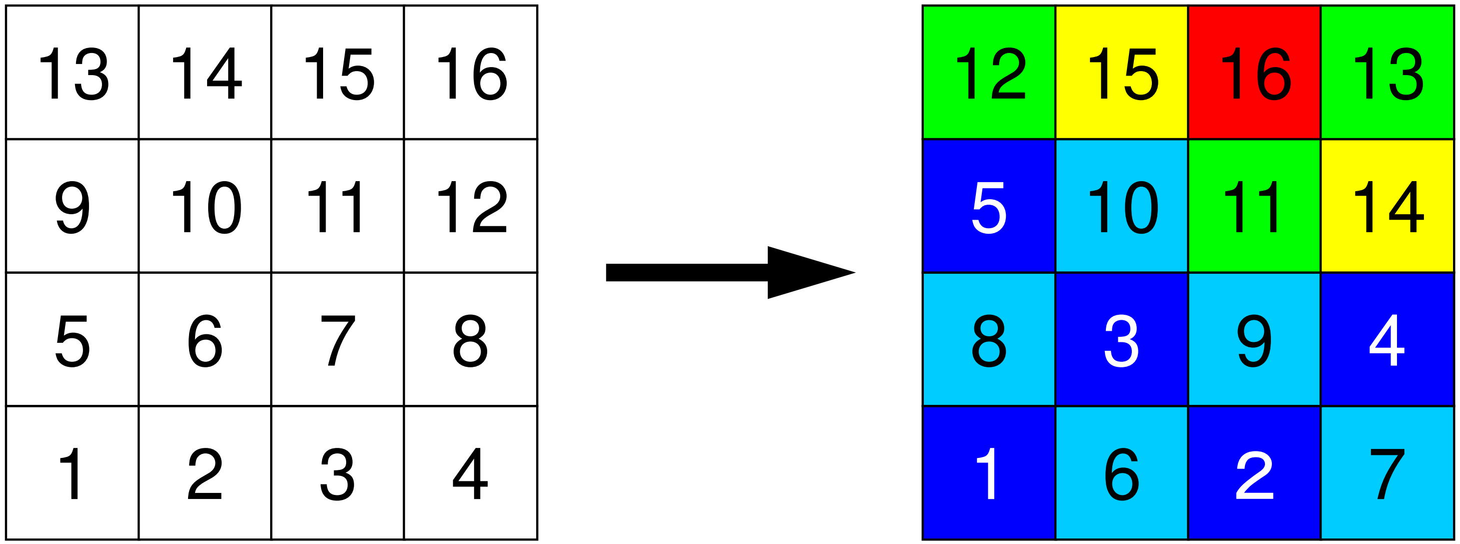
$$\frac{\phi_N - \phi_i}{\Delta y}\Delta x + \frac{\phi_S - \phi_i}{\Delta y}\Delta x = f_c \Delta x \Delta y$$

New Numbering



- Coloring by MC/CM/RCM/CM-RCM
- Renumber meshes in ascending orders according to "Level/Color" ID.
  - 1st-Color: 1,2,3,4,5 (Original: 1,3,6,8,9)
  - 2nd-Color: 6,7,8,9,10 (2,4,5,7,10)
  - 3rd-Color: 11,12,13 (11,13,16)
  - 4th-Color: 14,15 (12,14), 5th-Color: 16 (15)

New Numbering (cont.)




```
NCOLORtot= 5
COLORindex(0)=  0, COLORindex(1)=  5, COLORindex(2)= 10
COLORindex(3)= 13, COLORindex(4)= 15, COLORindex(5)= 16
```

- NEWtoOLD, OLDtoNEW
  - **`OLDtoNEW(6)=3, NEWtoOLD(3)=6`**

poi_gen (6/8)

```
!C
!C +-----------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-----------------------------------+
!C===
      icouG= 0
      do icol= 1, NCOLORtot
      do icel= COLORindex(icol-1)+1, COLORindex(icol)
        ic0 = NEWtoOLD(icel)
        icN1= NEIBcell(ic0, 1)
        icN2= NEIBcell(ic0, 2)
        icN3= NEIBcell(ic0, 3)
        icN4= NEIBcell(ic0, 4)
        icN5= NEIBcell(ic0, 5)
        icN6= NEIBcell(ic0, 6)
        VOL0= VOLCEL  (ic0)

        if (icN5.ne.0) then
          icN5= OLDtoNEW(icN5)
          coef= RDZ * ZAREA
          D(icel)= D(icel) - coef

          if (icN5.lt.icel) then
            do j= 1, INL(icel)
              if (IAL(j,icel).eq.icN5) then
                itemL(j+indexL(icel-1))= icN5
                   AL(j+indexL(icel-1))= coef
                exit
              endif
            enddo
           else
            do j= 1, INU(icel)
              if (IAU(j,icel).eq.icN5) then
                itemU(j+indexU(icel-1))= icN5
                   AU(j+indexU(icel-1))= coef
                exit
              endif
            enddo
          endif
        endif
```

$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\boxed{\frac{\phi_{neib(icel,5)}-\phi_{icel}}{\Delta z}\Delta x\Delta y+}$$

$$\frac{\phi_{neib(icel,6)}-\phi_{icel}}{\Delta z}\Delta x\Delta y=f_{icel}\Delta x\Delta y\Delta z$$

poi_gen (6/8)

```
!C
!C +------------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +------------------------------------+
!C===
      icouG= 0
      do icol= 1, NCOLORtot
      do icel= COLORindex(icol-1)+1, COLORindex(icol)
        ic0 = NEWtoOLD(icel)
        icN1= NEIBcell(ic0, 1)
        icN2= NEIBcell(ic0, 2)
        icN3= NEIBcell(ic0, 3)
        icN4= NEIBcell(ic0, 4)
        icN5= NEIBcell(ic0, 5)
        icN6= NEIBcell(ic0, 6)
        VOL0= VOLCEL  (ic0)

        if (icN5.ne.0) then
          icN5= OLDtoNEW(icN5)
          coef= RDZ * ZAREA
          D(icel)= D(icel) - coef

          if (icN5.lt.icel) then
            do j= 1, INL(icel)
              if (IAL(j,icel).eq.icN5) then
                itemL(j+indexL(icel-1))= icN5
                  AL(j+indexL(icel-1))= coef
                exit
              endif
            enddo
           else
            do j= 1, INU(icel)
              if (IAU(j,icel).eq.icN5) then
                itemU(j+indexU(icel-1))= icN5
                  AU(j+indexU(icel-1))= coef
                exit
              endif
            enddo
          endif
        endif
```

icN5 < icel
Lower Part

$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib(icel,5)}-\phi_{icel}}{\Delta z}\Delta x\Delta y+$$

$$\frac{\phi_{neib(icel,6)}-\phi_{icel}}{\Delta z}\Delta x\Delta y=f_{icel}\Delta x\Delta y\Delta z$$

poi_gen (6/8)

```
!C
!C +-----------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-----------------------------------+
!C===
      icouG= 0
      do icol= 1, NCOLORtot
      do icel= COLORindex(icol-1)+1, COLORindex(icol)
        ic0 = NEWtoOLD(icel)
        icN1= NEIBcell(ic0, 1)
        icN2= NEIBcell(ic0, 2)
        icN3= NEIBcell(ic0, 3)
        icN4= NEIBcell(ic0, 4)
        icN5= NEIBcell(ic0, 5)
        icN6= NEIBcell(ic0, 6)
        VOL0= VOLCEL  (ic0)

        if (icN5.ne.0) then
          icN5= OLDtoNEW(icN5)
          coef= RDZ * ZAREA
          D(icel)= D(icel) - coef

          if (icN5.lt.icel) then
            do j= 1, INL(icel)
              if (IAL(j,icel).eq.icN5) then
                itemL(j+indexL(icel-1))= icN5
                   AL(j+indexL(icel-1))= coef
                exit
              endif
            enddo
           else
            do j= 1, INU(icel)
              if (IAU(j,icel).eq.icN5) then
                itemU(j+indexU(icel-1))= icN5
                   AU(j+indexU(icel-1))= coef
                exit
              endif
            enddo
          endif
        endif
```

icN5 > icel
Upper Part

$$\frac{\phi_{neib(icel,1)} - \phi_{icel}}{\Delta x}\Delta y\Delta z +$$

$$\frac{\phi_{neib(icel,2)} - \phi_{icel}}{\Delta x}\Delta y\Delta z +$$

$$\frac{\phi_{neib(icel,3)} - \phi_{icel}}{\Delta y}\Delta z\Delta x +$$

$$\frac{\phi_{neib(icel,4)} - \phi_{icel}}{\Delta y}\Delta z\Delta x +$$

$$\frac{\phi_{neib(icel,5)} - \phi_{icel}}{\Delta z}\Delta x\Delta y +$$

$$\frac{\phi_{neib(icel,6)} - \phi_{icel}}{\Delta z}\Delta x\Delta y = f_{icel}\Delta x\Delta y\Delta z$$

poi_gen (7/8)

```
          if (icN6.ne.0) then
            icN6= OLDtoNEW(icN6)
            coef= RDZ * ZAREA
            D(icel)= D(icel) - coef

            if (icN6.lt.icel) then
              do j= 1, INL(icel)
                if (IAL(j,icel).eq.icN6) then
                  itemL(j+indexL(icel-1))= icN6
                     AL(j+indexL(icel-1))= coef
                  exit
                endif
              enddo
             else
              do j= 1, INU(icel)
                if (IAU(j,icel).eq.icN6) then
                  itemU(j+indexU(icel-1))= icN6
                     AU(j+indexU(icel-1))= coef
                  exit
                endif
              enddo
            endif
          endif

          ii= XYZ(ic0,1)
          jj= XYZ(ic0,2)
          kk= XYZ(ic0,3)

          BFORCE(icel)= -dfloat(ii+jj+kk) * VOL0

        enddo
        enddo
!C===
```

BFORCE using original mesh ID

$$\frac{\phi_{neib(icel,1)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,2)}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib(icel,3)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib(icel,4)}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

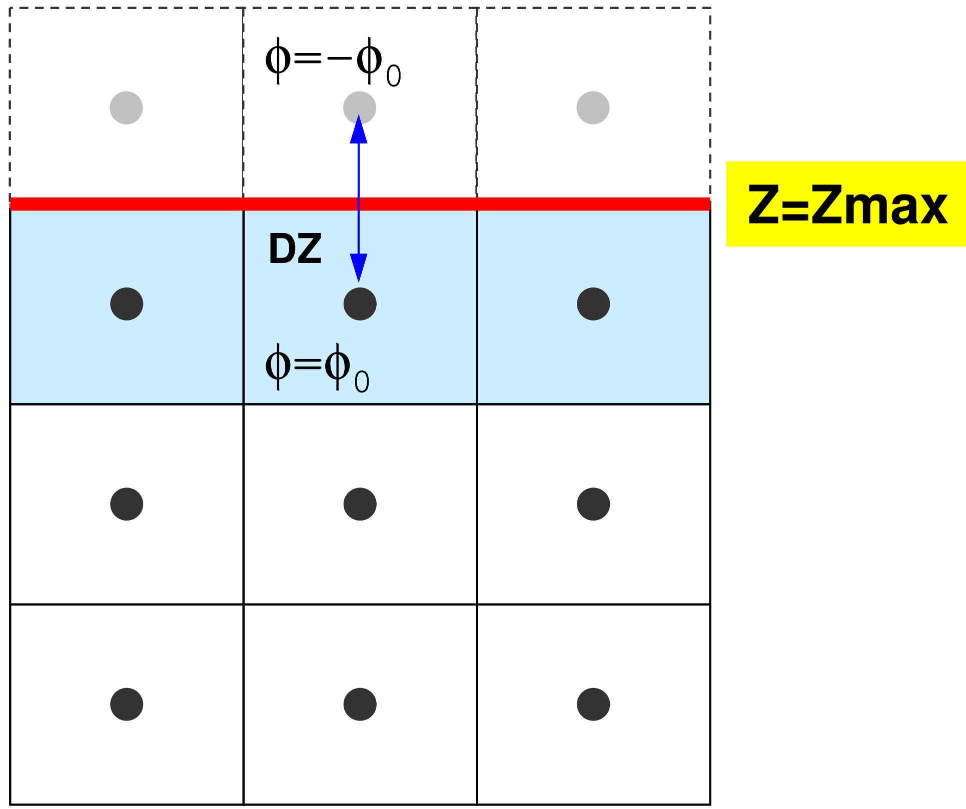
$$\frac{\phi_{neib(icel,5)}-\phi_{icel}}{\Delta z}\Delta x\Delta y+$$

$$\frac{\phi_{neib(icel,6)}-\phi_{icel}}{\Delta z}\Delta x\Delta y=f_{icel}\Delta x\Delta y\Delta z$$

poi_gen (8/8)

Calculation of Coefficients on Boundary Surface @ $Z=Z_{max}$

```
!C
!C +--------------------------+
!C | DIRICHLET BOUNDARY CELLs |
!C +--------------------------+
!C   TOP SURFACE
!C===
      do ib= 1, ZmaxCELtot
        ic0= ZmaxCEL(ib)
        coef= 2.d0 * RDZ * ZAREA
        icel= OLDtoNEW(ic0)
        D(icel)= D(icel) - coef
      enddo
!C===

      return
      end
```



<u>1st Order Approximation:</u>

Mirror Image according to $Z=Z_{max}$ surface.

$\phi=-\phi_0$ at the center of the (virtual) mesh

$\phi=0$ @ $Z=Z_{max}$ surface

Main Program

```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

      implicit REAL*8 (A-H,O-Z)
      real(kind=8), dimension(:), allocatable :: WK

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0
      call solve_ICCG_mc                                              &
     &     ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,      &
     &       BFORCE,  PHI, AL, AU, NCOLORtot, COLORindex,             &
     &       EPSICCG, ITR, IER)
      allocate (WK(ICELTOT))

      do ic0= 1, ICELTOT
        icel= NEWtoOLD(ic0)
        WK(icel)= PHI(ic0)
      enddo

      do icel= 1, ICELTOT
        PHI(icel)= WK(icel)
      enddo

      call OUTUCD

      stop
      end
```

Matrix, RHS are calculated according to new numbering

solve_ICCG_mc (1/7)

```
!C***
!C*** module solver_ICCG_mc
!C***
!
      module solver_ICCG_mc
      contains
!C
!C*** solve_ICCG
!C
 subroutine solve_ICCG_mc                                               &
     &          ( N, NPL, NPU, indexL, itemL, indexU, itemU, D, B, X,     &
     &            AL, AU, NCOLORtot, COLORindex, EPS, ITR, IER)

      implicit REAL*8 (A-H,O-Z)

      integer :: N, NL, NU, NCOLOR

      real(kind=8), dimension(N)   :: D
      real(kind=8), dimension(N)   :: B
      real(kind=8), dimension(N)   :: X
      real(kind=8), dimension(NPL) :: AL
      real(kind=8), dimension(NPU) :: AU

      integer, dimension(0:N)   :: indexL, indexU
      integer, dimension(NPL):: itemL
      integer, dimension(NPU):: itemU

      integer, dimension(0:NCOLORtot) :: COLORindex

      real(kind=8), dimension(:,:), allocatable :: W

      integer, parameter ::  R= 1
      integer, parameter ::  Z= 2
      integer, parameter ::  Q= 2
      integer, parameter ::  P= 3
      integer, parameter :: DD= 4
```

solve_ICCG_mc (2/7)

```
!C
!C +-------+
!C | INIT |
!C +-------+
!C===
      allocate (W(N,4))

      do i= 1, N
        X(i)   = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,4)= 0.0D0
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          VAL= D(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
          enddo
          W(i,DD)= 1.d0/VAL
        enddo
      enddo
!C===
```

Incomplete "Modified" Cholesky Factorization

Compute $r^{(0)}= b-[A]x^{(0)}$

<u>for</u> i= 1, 2, …
- solve $[M]z^{(i-1)}= r^{(i-1)}$
- $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
- <u>if</u> i=1
  - $p^{(1)}= z^{(0)}$
- <u>else</u>
  - $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
  - $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
- <u>endif</u>
- $q^{(i)}= [A]p^{(i)}$
- $\alpha_i\ = \rho_{i-1}/p^{(i)}q^{(i)}$
- $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
- $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
- check convergence $|r|$

<u>end</u>

solve_ICCG_mc (2/7)

```
!C
!C +-------+
!C | INIT |
!C +-------+
!C===
      allocate (W(N,4))

      do i= 1, N
        X(i)   = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,4)= 0.0D0
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          VAL= D(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
          enddo
          W(i,DD)= 1.d0/VAL
        enddo
      enddo
!C===
```

Incomplete "Modified" Cholesky Factorization

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} l_{ik}{}^2 \cdot d_k \right)^{-1} = l_{ii}{}^{-1}$$

↓

$$d_i = \left(a_{ii} - \sum_{k=1}^{i-1} a_{ik}{}^2 \cdot d_k \right)^{-1} = l_{ii}{}^{-1}$$

W(i,DD):	d_i
D(i):	a_{ii}
itemL(j):	k
AL(j):	a_{ik}

Incomplete “Modified” Cholesky Factorization

```
do i= 1, N
  VAL= D(i)
  do k= indexL(i-1)+1, indexL(i)
    VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
  enddo
  W(i,DD)= 1.d0/VAL
enddo
```

↓

```
do ic= 1, NCOLORtot
  do i= COLORindex(ic-1)+1, COLORindex(ic)
    VAL= D(i)
    do k= indexL(i-1)+1, indexL(i)
      VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
    enddo
    W(i,DD)= 1.d0/VAL
  enddo
enddo
```

Mesh “i” and “itemL(k)” in RHS belong to different “colors”.

NO data dependency.

solve_ICCG_mc (3/7)

```
!C
!C +----------------------+
!C | {r0}= {b} - [A]{xini} |
!C +----------------------+
!C===
      do i= 1, N
        VAL= D(i)*X(i)
        do k= indexL(i-1)+1, indexL(i)
          VAL= VAL + AL(k)*X(itemL(k))
        enddo
        do k= indexU(i-1)+1, indexU(i)
          VAL= VAL + AU(k)*X(itemU(k))
         enddo
        W(i,R)= B(i) - VAL
      enddo

      BNRM2= 0.0D0
      do i= 1, N
        BNRM2 = BNRM2 + B(i)  **2
      enddo
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$

<u>for</u> i= 1, 2, …
- solve $[M]z^{(i-1)}= r^{(i-1)}$
- $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
- <u>if</u> i=1
  - $p^{(1)}= z^{(0)}$
- <u>else</u>
  - $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
  - $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
- <u>endif</u>
- $q^{(i)}= [A]p^{(i)}$
- $\alpha_i\ = \rho_{i-1}/p^{(i)}q^{(i)}$
- $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
- $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
- check convergence $|r|$

<u>end</u>

solve_ICCG_mc (4/7)

```
!C
!C*************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
      enddo

      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$
<u>for</u> i= 1, 2, …
    solve $[M]z^{(i-1)}= r^{(i-1)}$
    $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
    <u>if</u> i=1
        $p^{(1)}= z^{(0)}$
    <u>else</u>
        $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
        $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
    <u>endif</u>
    $q^{(i)}= [A]p^{(i)}$
    $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
    $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
    $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
    check convergence $|r|$
<u>end</u>

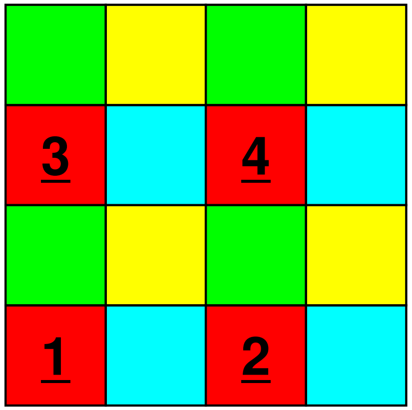
solve_ICCG_mc (4/7)

```
!C
!C*********************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
      enddo

      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

$$(M)\{z\}=\left(LDL^T\right)\{z\}=\{r\}$$

$$(L)\{z\}=\{r\}$$

Forward Substitution



ic=1

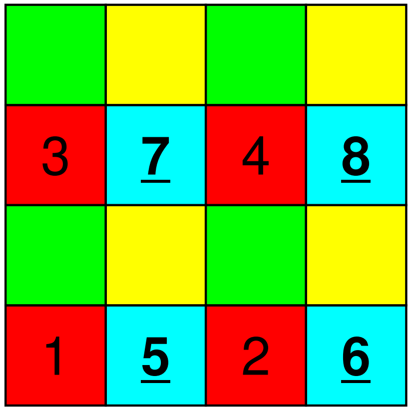
solve_ICCG_mc (4/7)

$$(M)\{z\}=(LDL^T)\{z\}=\{r\}$$

$$(L)\{z\}=\{r\}$$

```
!C
!C*************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
      enddo

      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

Forward Substitution



ic=2

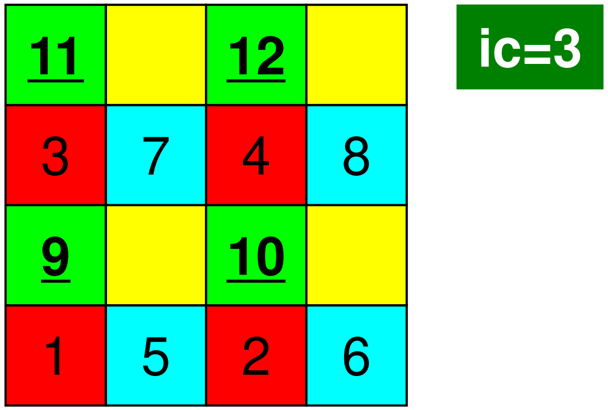
solve_ICCG_mc (4/7)

```
!C
!C*************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
      enddo

      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

$$(M)\{z\}=(LDL^T)\{z\}=\{r\}$$

$$(L)\{z\}=\{r\}$$

Forward Substitution



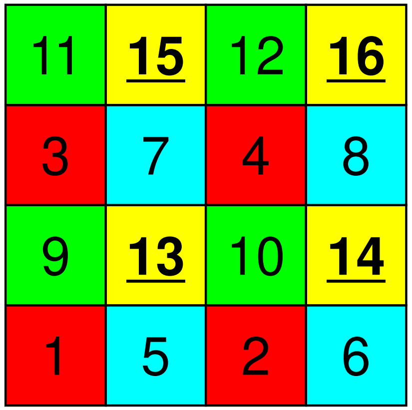
solve_ICCG_mc (4/7)

```
!C
!C************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
      enddo

      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW   = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

$$(M)\{z\}=\left(LDL^T\right)\{z\}=\{r\}$$

$$(L)\{z\}=\{r\}$$

Forward Substitution



ic=4

solve_ICCG_mc (4/7)

```
!C
!C************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
      enddo

      do ic= 1, NCOLORtot
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
      enddo

      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

$$(M)\{z\}=(LDL^T)\{z\}=\{r\}$$

$$(L)\{z\}=\{r\}$$

Forward Substitution

$$(DL^T)\{z\}=\{z\}$$

Backward Substitution

solve_ICCG_mc (4/7)

```
!C
!C************************************************** ITERATION
      ITR= N

      do L= 1, ITR
!C
!C +----------------+
!C | {z}= [Minv]{r} |
!C +----------------+
!C===
      do i= 1, N
        W(i,Z)= W(i,R)
```

$$(M)\{z\}=(LDL^T)\{z\}=\{r\}$$

$$(L)\{z\}=\{r\}$$

If order of computations in same color is changed: NO effect

i= COLOR(ic-1)+1, COLOR(ic)
i= COLOR(ic), COLOR(ic-1)+1, -1

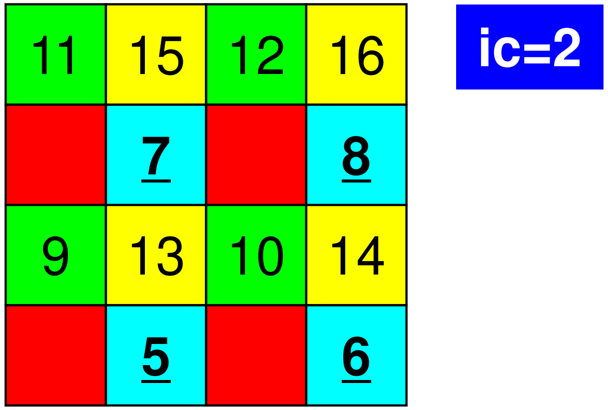
```
ic)
Z)
        enddo
      enddo
```

$$(DL^T)\{z\}=\{z\}$$

```
      do ic= NCOLORtot, 1, -1
        do i= COLORindex(ic-1)+1, COLORindex(ic)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
      enddo
!C===
```

Forward Substitution

Backward Substitution



Forward/Backward Substitution 前進後退代入

```
do i= 1, N
  WVAL= W(i,Z)
  do k= indexL(i-1)+1, indexL(i)
    WVAL= WVAL -  AL(k) * W(itemL(k),Z)
  enddo
  W(i,Z)= WVAL * W(i,DD)
enddo


do i= N, 1, -1
  SW= 0.0d0
  do k= indexU(i-1)+1, indexLU(i)
    SW= SW + AU(k) * W(itemU(k),Z)
  enddo
  W(i,Z)= W(i,Z) - W(i,DD) * SW
enddo
```

→

```
do ic= 1, NCOLORtot
  do i= COLORindex(ic-1)+1, COLORindex(ic)
    WVAL= W(i,Z)
    do k= indexL(i-1)+1, indexL(i)
      WVAL= WVAL -  AL(k) * W(itemL(k),Z)
    enddo
    W(i,Z)= WVAL * W(i,DD)
  enddo
enddo

do ic= NCOLORtot, 1, -1
  do i= COLORindex(ic-1)+1, COLORindex(ic)
    SW= 0.0d0
    do k= indexL(i-1)+1, indexL(i)
      SW= SW + AU(k) * W(itemU(k),Z)
    enddo
    W(i,Z)= W(i,Z) - W(i,DD) * SW
  enddo
enddo
```

solve_ICCG_mc (5/7)

```
!C
!C +-------------+
!C | RHO= {r}{z} |
!C +-------------+
!C===
      RHO= 0.d0
      do i= 1, N
        RHO= RHO + W(i,R)*W(i,Z)
      enddo
!C===

!C
!C +-----------------------------+
!C | {p} = {z} if      ITER=1    |
!C | BETA= RHO / RHO1  otherwise |
!C +-----------------------------+
!C===
      if ( L.eq.1 ) then
        do i= 1, N
          W(i,P)= W(i,Z)
        enddo
       else
         BETA= RHO / RHO1
         do i= 1, N
           W(i,P)= W(i,Z) + BETA*W(i,P)
         enddo
      endif
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$
<u>for</u> i= 1, 2, …
  solve $[M]z^{(i-1)}= r^{(i-1)}$
  $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
  <u>if</u> i=1
    $p^{(1)}= z^{(0)}$
   <u>else</u>
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  <u>endif</u>
  $q^{(i)}= [A]p^{(i)}$
  $\alpha_i\ = \rho_{i-1}/p^{(i)}q^{(i)}$
  $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
  $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
  check convergence $|r|$
<u>end</u>

solve_ICCG_mc (6/7)

```
!C
!C +-------------+
!C | {q}= [A]{p} |
!C +-------------+
!C===
      do i= 1, N
        VAL= D(i)*W(i,P)
        do k= indexL(i-1)+1, indexL(i)
          VAL= VAL + AL(k)*W(itemL(k),P)
        enddo
        do k= indexU(i-1)+1, indexU(i)
          VAL= VAL + AU(k)*W(itemU(k),P)
        enddo
        W(i,Q)= VAL
      enddo
!C===
```

Compute $r^{(0)}= b-[A]x^{(0)}$

<u>for</u> i= 1, 2, …

solve $[M]z^{(i-1)}= r^{(i-1)}$

$\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$

<u>if</u> i=1

$p^{(1)}= z^{(0)}$

<u>else</u>

$\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$

$p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$

<u>endif</u>

$q^{(i)}= [A]p^{(i)}$

$\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$

$x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$

$r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$

check convergence $|r|$

<u>end</u>

solve_ICCG_mc (7/7)

```
!C
!C +----------------------+
!C | ALPHA= RHO / {p}{q}  |
!C +----------------------+
!C===
      C1= 0.d0
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      ALPHA= RHO / C1
!C===
!C
!C +-----------------------+
!C | {x}= {x} + ALPHA*{p}  |
!C | {r}= {r} - ALPHA*{q}  |
!C +-----------------------+
!C===
      do i= 1, N
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
      DNRM2= 0.d0
      do i= 1, N
        DNRM2= DNRM2 + W(i,R)**2
      enddo
!C===
      ERR = dsqrt(DNRM2/BNRM2)
      if (ERR .lt. EPS) then
          IER = 0
          goto 900
         else
          RHO1 = RHO
        endif
      enddo
      IER = 1

  900 continue
```

Compute $r^{(0)}= b-[A]x^{(0)}$

<u>for</u> i= 1, 2, …

solve $[M]z^{(i-1)}= r^{(i-1)}$

$\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$

<u>if</u> i=1

$p^{(1)}= z^{(0)}$

<u>else</u>

$\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$

$p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$

<u>endif</u>

$q^{(i)}= [A]p^{(i)}$

$\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$

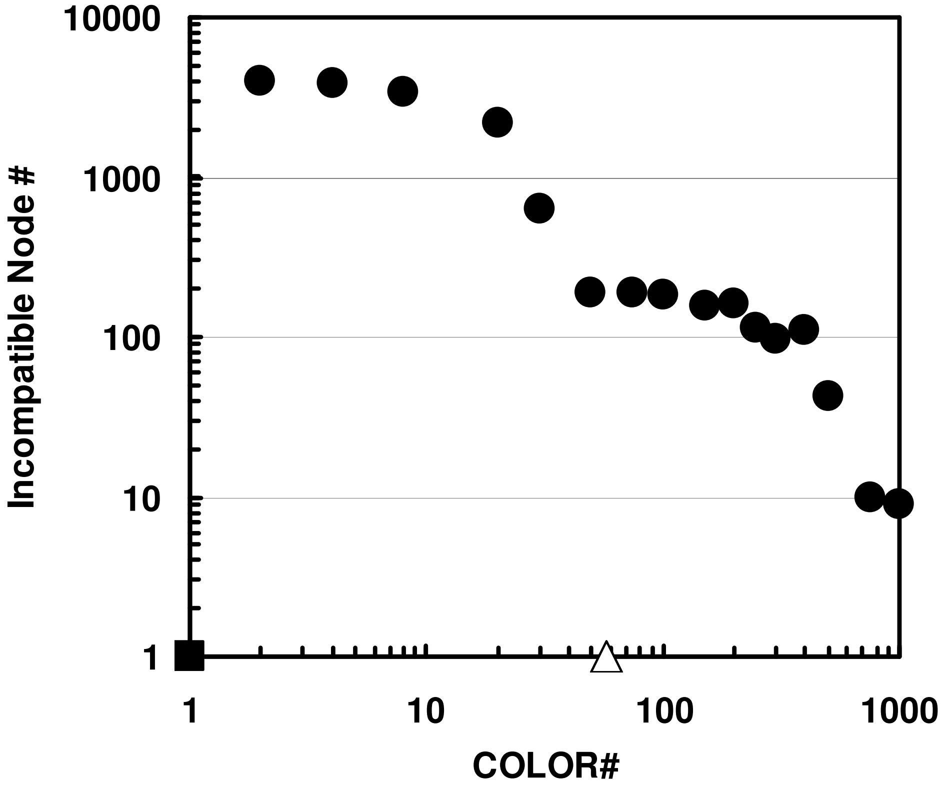
$x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$

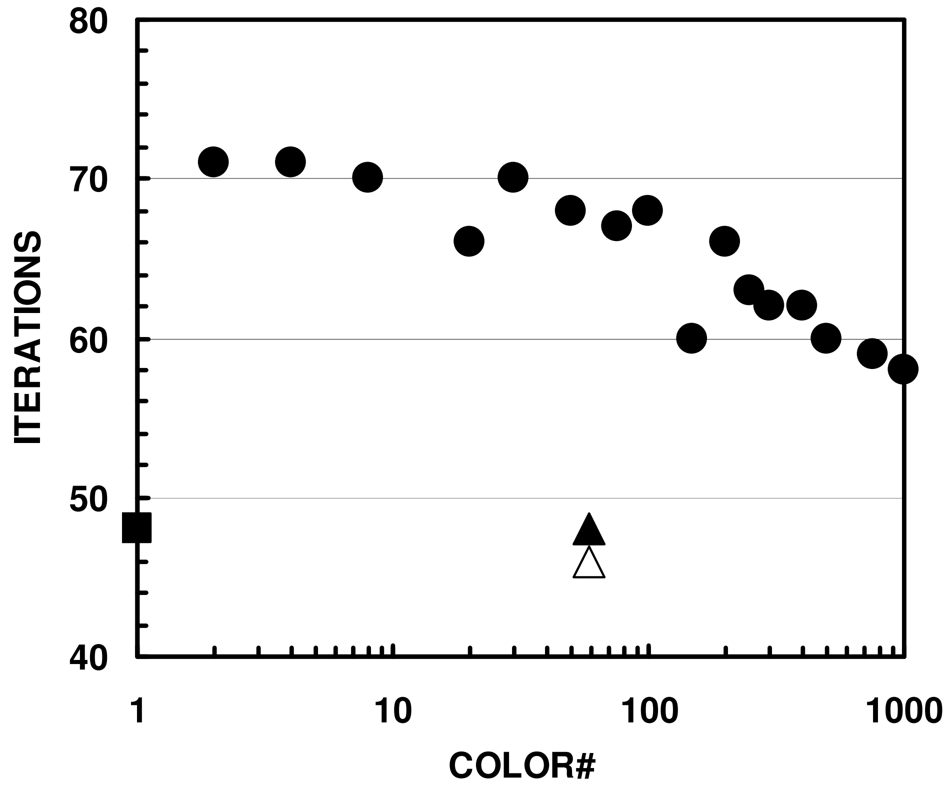
$r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$

check convergence $|r|$

<u>end</u>

Effect of Color Number on Convergence of ICCG





(20^3=8,000 meshe, EPSICCG=10^{-8})

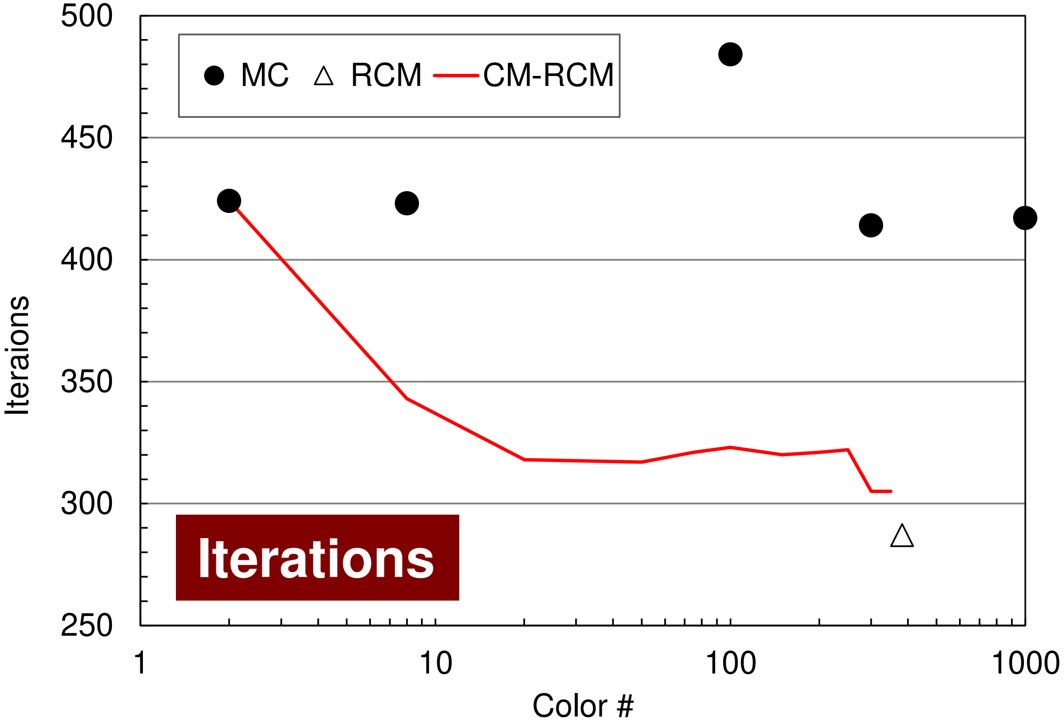
(■: ICCG(L1), ●: ICCG-MC, ▲: ICCG-CM, △: ICCG-RCM)

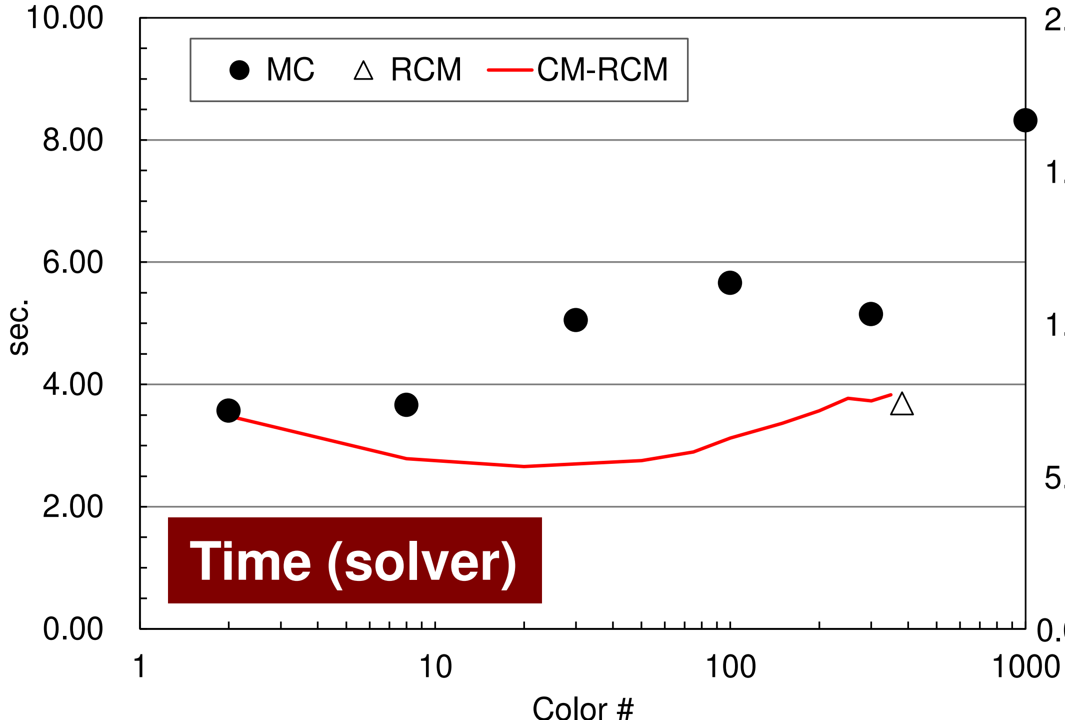
- Remedy for Data Dependency
- Ordering/Reordering
  - Red-Black, Multicoloring (MC)
  - Cuthill-McKee (CM), Reverse-CM (RCM)
  - Reordering and Convergence
- Implementation
- ICCG with Reordering
- **ICCG with Reordering on Multicores**
  - **Just apply OpenMP to L2-sol**

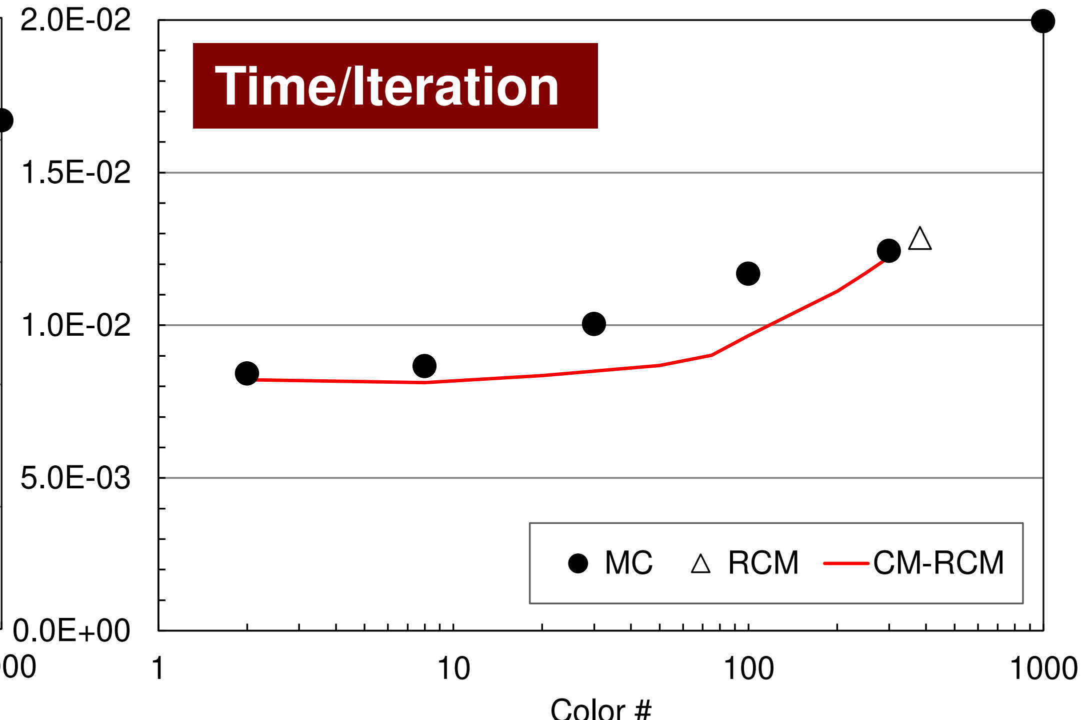
Odyssey

1-CMG/12-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)







OBCX

Intel Xeon CLX 1-soket/24-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)