Introduction to Parallel Programming for Multicore/Manycore Clusters

Part B3: Parallel ICCG by OpenMP

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Parallel Version: OpenMP

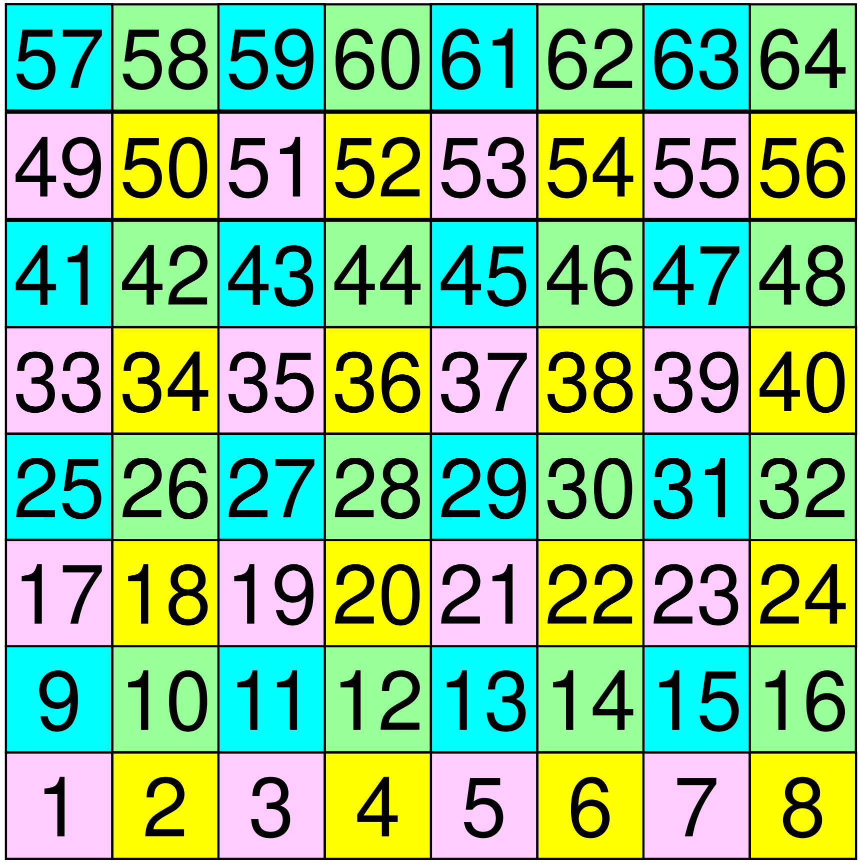
- OpenMP version of L2-sol
  - – Number of threads= “PEsmpTOT”
    - can be controlled in the program

- Fundamental Idea
  - – Meshes in a same color/level are independent, therefore parallel/concurrent processing is possible for these meshes.

4-Colors, 4-Threads
Initial Mesh

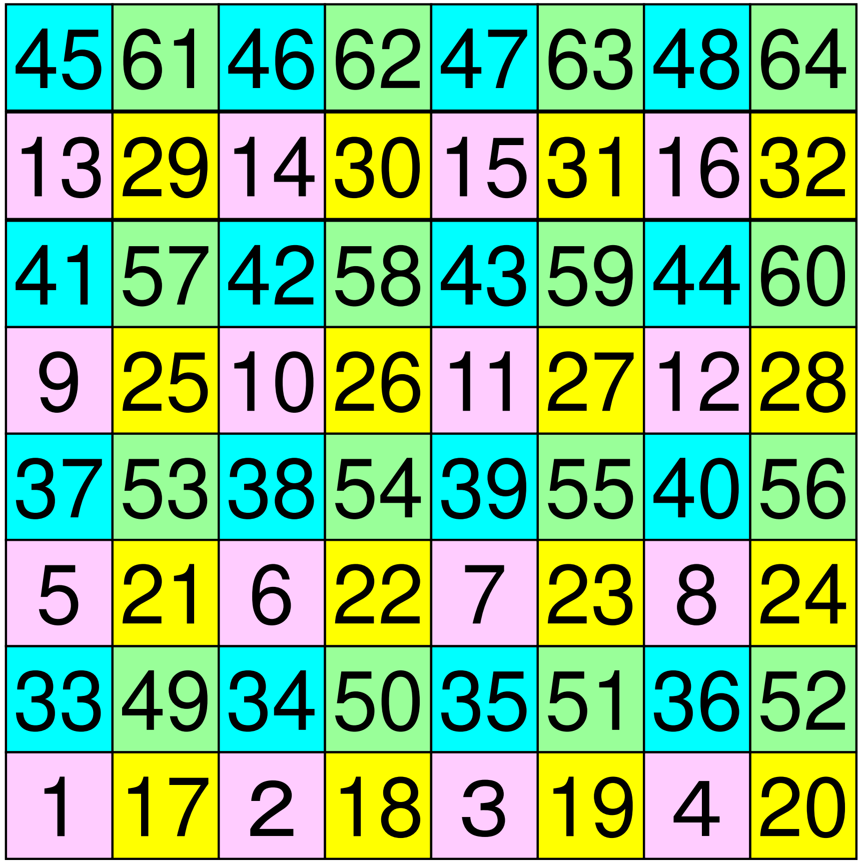
57	58	59	60	61	62	63	64
49	50	51	52	53	54	55	56
41	42	43	44	45	46	47	48
33	34	35	36	37	38	39	40
25	26	27	28	29	30	31	32
17	18	19	20	21	22	23	24
9	10	11	12	13	14	15	16
1	2	3	4	5	6	7	8

4-Colors, 4-Threads
Initial Mesh



57	58	59	60	61	62	63	64
49	50	51	52	53	54	55	56
41	42	43	44	45	46	47	48
33	34	35	36	37	38	39	40
25	26	27	28	29	30	31	32
17	18	19	20	21	22	23	24
9	10	11	12	13	14	15	16
1	2	3	4	5	6	7	8

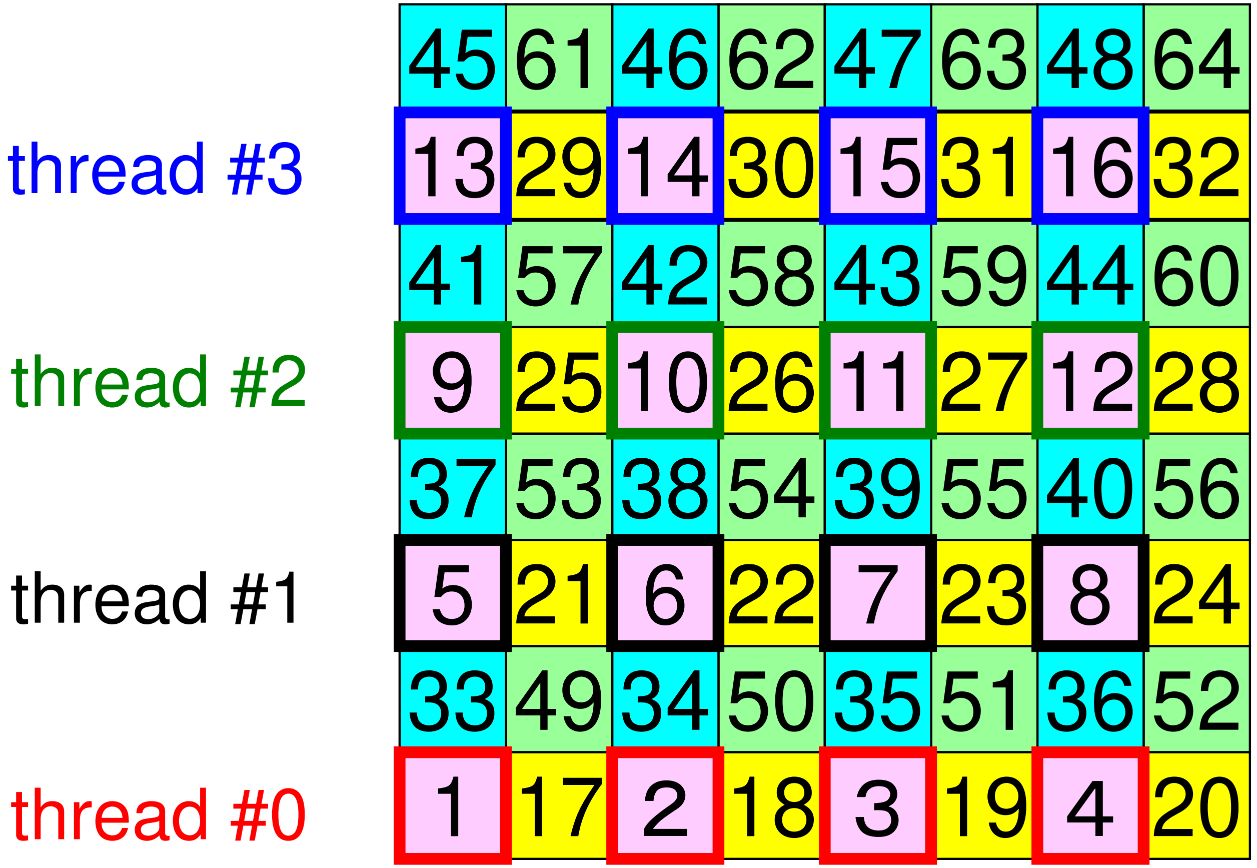
4-Colors, 4-Threads
Renumbering according to Color ID



45	61	46	62	47	63	48	64
13	29	14	30	15	31	16	32
41	57	42	58	43	59	44	60
9	25	10	26	11	27	12	28
37	53	38	54	39	55	40	56
5	21	6	22	7	23	8	24
33	49	34	50	35	51	36	52
1	17	2	18	3	19	4	20

4-Colors, 4-Threads

Meshes in a same color/level are independent, therefore parallel/concurrent processing is possible for these meshes, renumbered meshes are assigned to threads



	45	61	46	62	47	63	48	64
thread #3	13	29	14	30	15	31	16	32
	41	57	42	58	43	59	44	60
thread #2	9	25	10	26	11	27	12	28
	37	53	38	54	39	55	40	56
thread #1	5	21	6	22	7	23	8	24
	33	49	34	50	35	51	36	52
thread #0	1	17	2	18	3	19	4	20

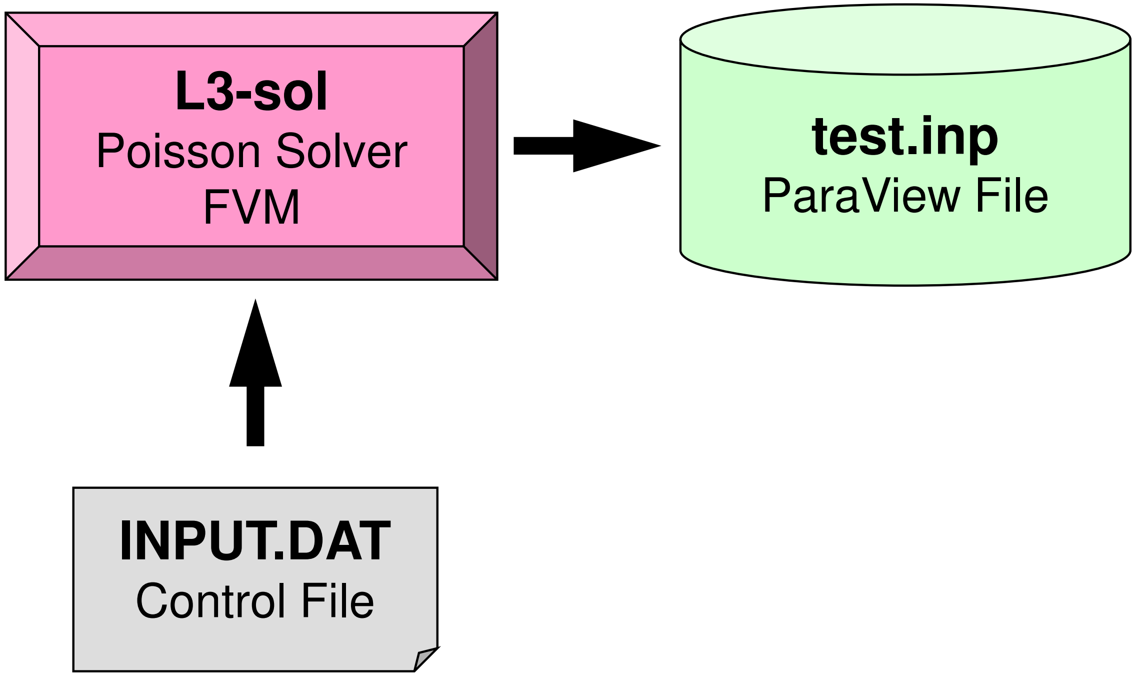
How to Run

```
>$ cd /work/gt89/t89XXX

>$ cp /work/gt00/z30088/ompc.tar .
>$ tar xvf ompc.tar

>$ cd ompc
>$ ls
     run   src  src0  reorder0

>$ cd src
>$ module load fj
>$ make
>$ cd ../run
>$ ls L3-sol
     L3-sol

<modify "INPUT.DAT">
<modify "go1.sh">

>$ pjsub go1.sh
```

Files on Odyssey

- Location
  - **`<$O-L3>: /work/gt89/t89XXX/ompc`**
  - `<$O-L3>/src`, `<$O-L3>/run`
- Compile & Run
  - Source Code
    - `cd <$O-L3>/src`
    - `make`
    - `<$O-L3>/run/L3-sol` execution file
  - Control Data
    - `<$O-L3>/run/INPUT.DAT`
  - Shell Script
    - `<$O-L3>/run/go1.sh`

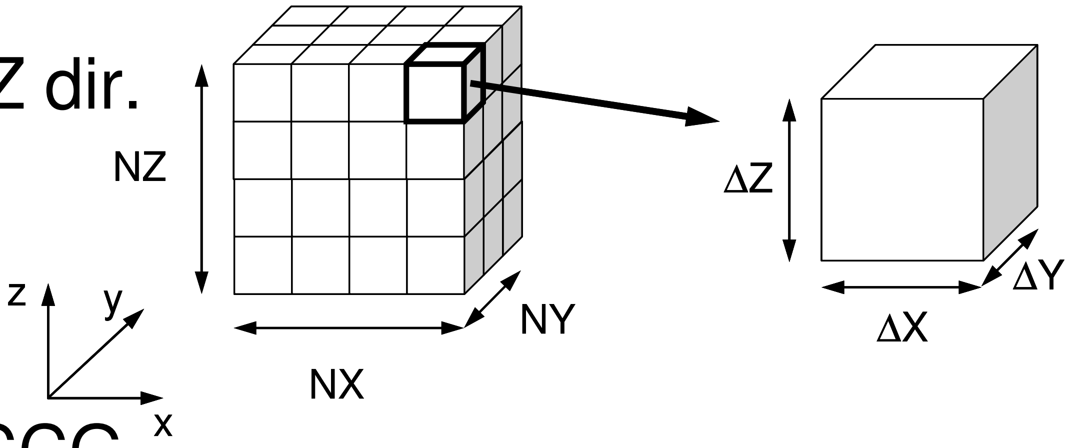
Running the Program



Control Data: INPUT.DAT

```
128 128 128                                 NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00                  DX/DY/DZ
1.0e-08                                     EPSICCG
12                                          PEsmpTOT
-10                                         NCOLORtot
```

- **NX,NY,NZ**
  - Number of meshes in X/Y/Z dir.
- **DX,DY,DZ**
  - Size of meshes
- **EPSICCG**
  - Convergence Criteria for ICCG
- **PEsmpTOT**
  - Thread Number **(--omp thread=XX)**
- **NCOLORtot**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM



Job Script: go1.sh

- /work/gt89/t89XXX/ompc/run/go1.sh
- Scheduling + Shell Script

```
#!/bin/sh
#PJM -N “go1”                 Job Name (not required)
#PJM -L rscgrp=lecture9-o     Name of Queue (Resource Group)
#PJM -L node=1                Node # (=1)
#PJM --omp thread=12          Thread # (= PEsmpTOT)
#PJM -L elapse=00:15:00       Elapsed Computation Time
#PJM -g gt89                  Group Name (Wallet)
#PJM -j
#PJM -e err                   Standard Error
#PJM -o test1.lst             Standard Output

module load fj
export OMP_NUM_THREADS=12     Thread #(--omp thread=XX)
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl ./L3-sol
numactl -C 12-23 -m 4 ./L3-sol
```

- Applying OpenMP to L2-sol
- Examples
- Optimization + Exercise

Applying OpenMP to “L2-sol”

- on ICCG solver

- Dot Products, DAXPY, Mat-Vec
  - NO data dependency: Just insert directives
- Preconditioning (IC Factorization, Forward/Backward Substitution)
  - NO data dependency in same color: Parallel processing is possible for meshes in same color

Just inserting directives works fine, but ... (1/2) (Mat-Vec)

```
#pragma omp parallel for private(i,VAL,j)
for(i=0; i<N; i++) {
     VAL = D[i] * W[P][i];
     for(j=indexL[i]; j<indexL[i+1]; j++) {
          VAL += AL[j] * W[P][itemL[j]-1];
     }
     for(j=indexU[i]; j<indexU[i+1]; j++) {
          VAL += AU[j] * W[P][itemU[j]-1];
     }
     W[Q][i] = VAL;
}
```

- Thread number cannot be handled in the program
- This may work better on GPU and manycore’s

Just inserting directives works fine, but ... (2/2) (Forward Substitution)

```
for(ic=0; ic<NCOLORtot; ic++){

#pragma omp parallel for private (i,WVAL,j)
    for(i=COLORindex[ic]; i<COLORindex[ic+1]; i++) {
        WVAL = W[Z][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            WVAL -= AL[j] * W[Z][itemL[j]-1];
        }
        W[Z][i] = WVAL * W[DD][i];
    }
}
```

- Thread number cannot be handled in the program
- This may work better on GPU and manycore's

Parallelize ICCG Method by OpenMP

- Dot Product: OK
- DAXPY: OK
- Matrix-Vector Multiply: OK
- Preconditioning

Main Program

```
#include <stdio.h> ...

int
main()
{
        double *WK;
        int NPL, NPU; ISET, ITR, IER; icel, ic0, i;
        double xN, xL, xU; Stime, Etime;

        if(INPUT()) goto error;
        if(POINTER_INIT()) goto error;
        if(BOUNDARY_CELL()) goto error;
        if(CELL_METRICS()) goto error;
        if(POI_GEN()) goto error;

        ISET = 0;
        WK = (double *)malloc(sizeof(double)*ICELTOT);
        if(WK == NULL) {
           fprintf(stderr, "Error: %s¥n", strerror(errno));
           goto error;}
           Stime = omp_get_wtime();
           if(solve_ICCG_mc(ICELTOT, NL, NU, indexL, itemL, indexU, itemU,
                            D, BFORCE, PHI, AL, AU, NCOLORtot, PEsmpTOT,
                            SMPindex, SMPindexG, EPSICCG, &ITR, &IER)) goto error;
           Etime = omp_get_wtime();
        for(ic0=0; ic0<ICELTOT; ic0++) {
            icel = NEWtoOLD[ic0];
            WK[icel-1] = PHI[ic0];
        }
        for(icel=0; icel<ICELTOT; icel++) {
            PHI[icel] = WK[icel];
        }
        if(OUTUCD()) goto error;
        return 0;
error:
        return -1;
}
```

struct.h

```
#ifndef __H_STRUCT
#define __H_STRUCT

#include <omp.h>

int ICELTOT, ICELTOTp, N;
int NX, NY, NZ, NXP1, NYP1, NZP1, IBNODTOT;
int NXc, NYc, NZc;

double DX, DY, DZ, XAREA, YAREA, ZAREA;
double RDX, RDY, RDZ, RDX2, RDY2, RDZ2, R2DX, R2DY, R2DZ;
double *VOLCEL, *VOLNOD, *RVC, *RVN;

int **XYZ, **NEIBcell;

int ZmaxCELtot;
int *BC_INDEX, *BC_NOD;
int *ZmaxCEL;

int **IWKX;
double **FCV;

int my_rank, PETOT, PEsmpTOT;

#endif /* __H_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

PEsmpTOT:

Number of threads

pcg.h

```
#ifndef __H_PCG
#define __H_PCG
        static int N2 = 256;
        int NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL;
        int METHOD, ORDER_METHOD;
        double EPSICCG;

        double *D, *PHI, *BFORCE;
        double *AL, *AU;

        int *INL, *INU, *COLORindex;
        int *indexL, *indexU;
        int *SMPindex, *SMPindexG;
        int *OLDtoNEW, *NEWtoOLD;
        int **IAL, **IAU;
        int *itemL, *itemU;
        int NPL, NPU;
#endif /* __H_PCG */
```

NCOLORtot Total number of colors/levels

COLORindex [NCOLORtot+1] Index of number of meshes in each color/level (COLORindex[icol+1]- COLORindex[icol])

SMPindex [NCOLORtot*PEsmpTOT+1]

SMPindexG[PEsmpTOT+1]

OLDtoNEW, NEWtoOLD Reference table before/after renumbering

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[N+1] **indexU[N+1]**	**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[N][NL] **IAU[N][NU]**	**I**	Column ID of L/U non-zero off-diag. comp.

Variables/Arrays for Matrix (2/2)

Name	Type	Content
NCOLORtot	**I**	**Input:** reordering method + initial number of colors/levels ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM **Output:** Final number of colors/levels
COLORindex **[NCOLORtot+1]**	**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]** to **COLORindex[icol+1]-1**
NEWtoOLD[N]	**I**	Reference array from New to Old numbering
OLDtoNEW[N]	**I**	Reference array from Old to New numbering
PEsmpTOT	**I**	Number of Threads
SMPindex **[NCOLORtot*PEsmpTOT+1]**	**I**	Array for OpenMP Operations (for Loops with Data Dependency)
SMPindexG[PEsmpTOT+1]	**I**	Array for OpenMP Operations (for Loops without Data Dependency)

Main Program

```
#include <stdio.h> ...

int
main()
{
        double *WK;
        int NPL, NPU; ISET, ITR, IER; icel, ic0, i;
        double xN, xL, xU; Stime, Etime;

        if(INPUT()) goto error;
        if(POINTER_INIT()) goto error;
        if(BOUNDARY_CELL()) goto error;
        if(CELL_METRICS()) goto error;
        if(POI_GEN()) goto error;

        ISET = 0;
        WK = (double *)malloc(sizeof(double)*ICELTOT);
        if(WK == NULL) {
           fprintf(stderr, "Error: %s¥n", strerror(errno));
           goto error;}
           Stime = omp_get_wtime();
           if(solve_ICCG_mc(ICELTOT, NL, NU, indexL, itemL, indexU, itemU,
                            D, BFORCE, PHI, AL, AU, NCOLORtot, PEsmpTOT,
                            SMPindex, SMPindexG, EPSICCG, &ITR, &IER)) goto error;
           Etime = omp_get_wtime();
        for(ic0=0; ic0<ICELTOT; ic0++) {
            icel = NEWtoOLD[ic0];
            WK[icel-1] = PHI[ic0];
        }
        for(icel=0; icel<ICELTOT; icel++) {
            PHI[icel] = WK[icel];
        }
        if(OUTUCD()) goto error;
        return 0;
error:
        return -1;
}
```

input: reading INPUT.DAT

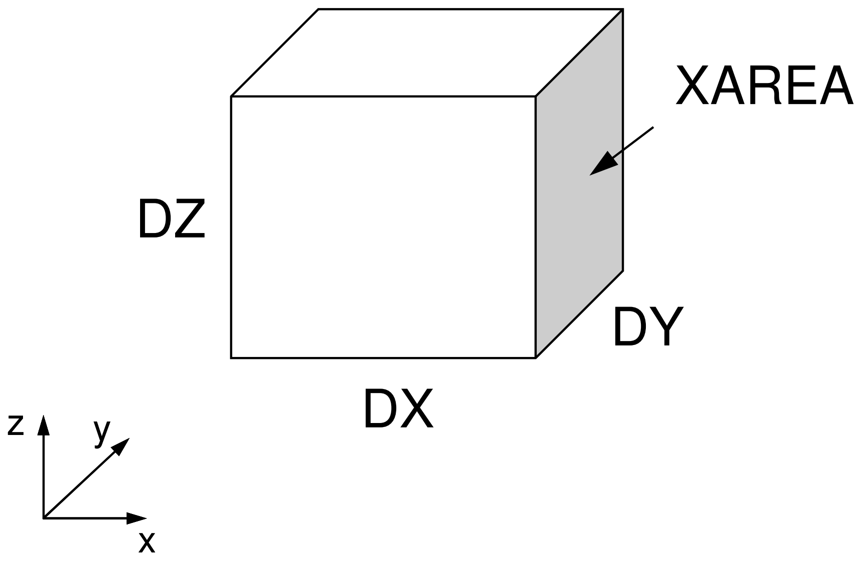
```
#include <stdio.h>; <stdlib.h>; <string.h>; <errno.h>
#include "struct_ext.h "; "pcg_ext.h "; "input.h"

extern int
INPUT(void)
{
#define BUF_SIZE 1024

char line[BUF_SIZE];
char CNTFIL[81];
double OMEGA;
FILE *fp11;

if((fp11 = fopen("INPUT.DAT", "r")) == NULL) {
           fprintf(stderr, "Error: %s¥n", strerror(errno));
           return -1;
}
sscanf(line, "%d%d%d", &NX, &NY, &NZ);
sscanf(line, "%d", &METHOD);
sscanf(line, "%le%le%le", &DX, &DY, &DZ);
sscanf(line, "%le", &EPSICCG);
sscanf(line, "%d", &PEsmpTOT);
sscanf(line, "%d", &NCOLORtot);

fclose(fp11);
return 0;
}
```

- **PEsmpTOT**
  - Thread Number
- **NCOLORtot**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC
  - =0: CM
  - =-1: RCM
  - -2≧: CMRCM

```
100 100 100                       NX/NY/NZ
1.00e-02 5.00e-02 1.00e-02        DX/DY/DZ
1.00e-08                          EPSICCG
24                                 PEsmpTOT
100                                NCOLORtot
```

cell_metrics

```
#include <stdio.h> ...

extern int
CELL_METRICS(void)
{        double V0, RV0;
         int i;
VOLCEL =
(double *)allocate_vector(sizeof(double),ICELTOT);
RVC    =
(double *)allocate_vector(sizeof(double),ICELTOT);

XAREA = DY * DZ;
YAREA = DZ * DX;
ZAREA = DX * DY;

RDX = 1.0 / DX;
RDY = 1.0 / DY;
RDZ = 1.0 / DZ;

RDX2 = 1.0 / (pow(DX, 2.0));
RDY2 = 1.0 / (pow(DY, 2.0));
RDZ2 = 1.0 / (pow(DZ, 2.0));
R2DX = 1.0 / (0.5 * DX);
R2DY = 1.0 / (0.5 * DY);
R2DZ = 1.0 / (0.5 * DZ);

V0  = DX * DY * DZ;
RV0 = 1.0 / V0;

for(i=0; i<ICELTOT; i++) {
    VOLCEL[i] = V0;
    RVC[i]    = RV0;
}
return 0; }
```



Main Program

```
#include <stdio.h> ...

int
main()
{
        double *WK;
        int NPL, NPU; ISET, ITR, IER; icel, ic0, i;
        double xN, xL, xU; Stime, Etime;

        if(INPUT()) goto error;
        if(POINTER_INIT()) goto error;
        if(BOUNDARY_CELL()) goto error;
        if(CELL_METRICS()) goto error;
        if(POI_GEN()) goto error;

        ISET = 0;
        WK = (double *)malloc(sizeof(double)*ICELTOT);
        if(WK == NULL) {
           fprintf(stderr, "Error: %s¥n", strerror(errno));
           goto error;}
           Stime = omp_get_wtime();
           if(solve_ICCG_mc(ICELTOT, NL, NU, indexL, itemL, indexU, itemU,
                            D, BFORCE, PHI, AL, AU, NCOLORtot, PEsmpTOT,
                            SMPindex, SMPindexG, EPSICCG, &ITR, &IER)) goto error;
           Etime = omp_get_wtime();
        for(ic0=0; ic0<ICELTOT; ic0++) {
            icel = NEWtoOLD[ic0];
            WK[icel-1] = PHI[ic0];
        }
        for(icel=0; icel<ICELTOT; icel++) {
            PHI[icel] = WK[icel];
        }
        if(OUTUCD()) goto error;
        return 0;
error:
        return -1;
}
```

poi_gen (1/9)

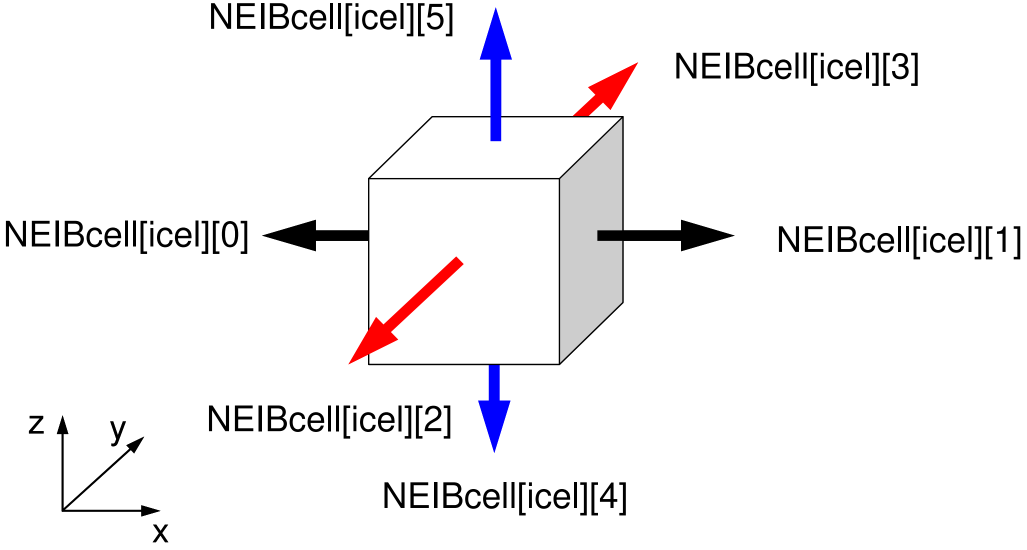
```
#include "allocate.h"
extern int
POI_GEN(void)
{ int nn;
  int ic0, icN1, icN2, icN3, icN4, icN5, icN6;
  int i, j, k, ib, ic, ip, icel, icou, icol, icouG;
  int ii, jj, kk, nn1, num, nr, j0, j1;
  double coef, VOL0, S1t, E1t;
  int isL, ieL, isU, ieU;
  NL=6; NU= 6;
  IAL = (int **)allocate_matrix(sizeof(int),ICELTOT,NL);
  IAU = (int **)allocate_matrix(sizeof(int),ICELTOT,NU);
  BFORCE = (double *)allocate_vector(sizeof(double),ICELTOT);
  D      = (double *)allocate_vector(sizeof(double),ICELTOT);
  PHI    = (double *)allocate_vector(sizeof(double),ICELTOT);
  INL = (int *)allocate_vector(sizeof(int),ICELTOT);
  INU = (int *)allocate_vector(sizeof(int),ICELTOT);

  for (i = 0; i <ICELTOT ; i++) {
       BFORCE[i]=0.0;
       D[i]  =0.0; PHI[i]=0.0;
       INL[i] = 0; INU[i] = 0;
       for(j=0;j<6;j++){
           IAL[i][j]=0; IAU[i][j]=0;
       }
  }
  for (i = 0; i <=ICELTOT ; i++) {
       indexL[i] = 0; indexU[i] = 0;
  }
```

allocate.c

```
/***************************
  allocate matrix
***************************/
void** allocate_matrix(int size,int m,int n)
{
  void **aa;
  int i;
  if ( ( aa=(void ** )malloc( m * sizeof(void*) ) ) == NULL ) {
     fprintf(stdout,"Error:Memory does not enough! aa in matrix ¥n");
     exit(1);
  }
  if ( ( aa[0]=(void * )malloc( m * n * size ) ) == NULL ) {
     fprintf(stdout,"Error:Memory does not enough! in matrix ¥n");
     exit(1);
  }
         for(i=1;i<m;i++) aa[i]=(char*)aa[i-1]+size*n;
  return aa;
}
```

poi_gen (2/9)

```
 for(icel=0; icel<ICELTOT; icel++) {
     icN1 = NEIBcell[icel][0];
     icN2 = NEIBcell[icel][1];
     icN3 = NEIBcell[icel][2];
     icN4 = NEIBcell[icel][3];
     icN5 = NEIBcell[icel][4];
     icN6 = NEIBcell[icel][5];

     if(icN5 != 0)  {
        icou = INL[icel] + 1;
        IAL[icel][icou-1] = icN5;
        INL[icel]         = icou;
      }

      if(icN3 != 0)  {
        icou = INL[icel] + 1;
        IAL[icel][icou-1] = icN3;
        INL[icel]         = icou;
      }
      if(icN1 != 0)  {
        icou = INL[icel] + 1;
        IAL[icel][icou-1] = icN3;
        INL[icel]         = icou;
      }
      if(icN2 != 0)  {
        icou = INU[icel] + 1;
        IAU[icel][icou-1] = icN2;
        INU[icel]         = icou;
      }

      if(icN4 != 0)  {
        icou = INU[icel] + 1;
        IAU[icel][icou-1] = icN4;
        INU[icel]         = icou;
      }

      if(icN6 != 0)  {
        icou = INU[icel] + 1;
        IAU[icel][icou-1] = icN6;
        INU[icel]         = icou;
      }
}
```



Lower Triangular Part
NEIBcell[icel][4]= icel – NX*NY + 1
NEIBcell[icel][2]= icel – NX + 1
NEIBcell[icel][0]= icel – 1 + 1

“icel” starts at 0

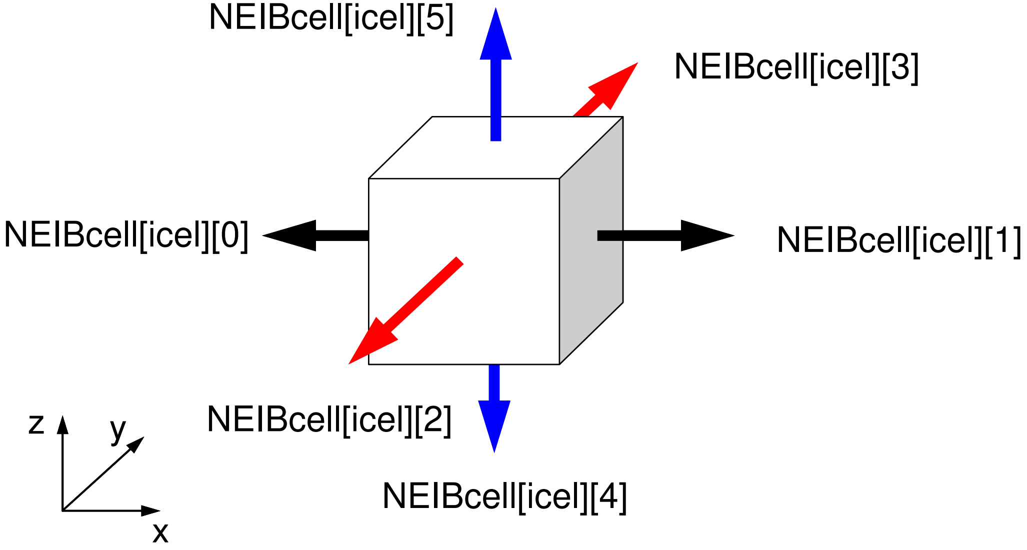
12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3

“IAL” starts at 1

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

poi_gen (2/9)

```
 for(icel=0; icel<ICELTOT; icel++) {
     icN1 = NEIBcell[icel][0];
     icN2 = NEIBcell[icel][1];
     icN3 = NEIBcell[icel][2];
     icN4 = NEIBcell[icel][3];
     icN5 = NEIBcell[icel][4];
     icN6 = NEIBcell[icel][5];

     if(icN5 != 0) {
        icou = INL[icel] + 1;
        IAL[icel][icou-1] = icN5;
        INL[icel]         = icou;
      }
      if(icN3 != 0) {
        icou = INL[icel] + 1;
        IAL[icel][icou-1] = icN3;
        INL[icel]         = icou;
      }

      if(icN1 != 0) {
        icou = INL[icel] + 1;
        IAL[icel][icou-1] = icN3;
        INL[icel]         = icou;
      }
      if(icN2 != 0) {
        icou = INU[icel] + 1;
        IAU[icel][icou-1] = icN2;
        INU[icel]         = icou;
      }

      if(icN4 != 0) {
        icou = INU[icel] + 1;
        IAU[icel][icou-1] = icN4;
        INU[icel]         = icou;
      }

      if(icN6 != 0) {
        icou = INU[icel] + 1;
        IAU[icel][icou-1] = icN6;
        INU[icel]         = icou;
      }
}
```



Upper Triangular Part
NEIBcell[icel][1]= icel + 1 + 1
NEIBcell[icel][3]= icel + NX + 1
NEIBcell[icel][5]= icel + NX*NY + 1

“icel” starts at 0

12	13	14	15
8	9	10	11
4	5	6	7
0	1	2	3

“IAU” starts at 1

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

poi_gen (3/9)

```
N111:
        fprintf(stderr, "¥n¥nYou have%8d elements¥n", ICELTOT);
        fprintf(stderr, "How many colors do you need ?¥n");
        fprintf(stderr, "  #COLOR must be more than 2 and¥n");
        fprintf(stderr, "  #COLOR must not be more than%8d¥n", ICELTOT);
        fprintf(stderr, "  if #COLOR= 0 then CM  ordering¥n");
        fprintf(stderr, "  if #COLOR=-1 then RCM ordering¥n");
        fprintf(stderr, "  if #COLOR<-1 then CMRCM ordering¥n");
        fprintf(stderr, "=>¥n");
        fscanf(stdin, "%d", &NCOLORtot);
        if(NCOLORtot == 1 && NCOLORtot > ICELTOT) goto N111;

        OLDtoNEW = (int *)calloc(ICELTOT, sizeof(int));
        if(OLDtoNEW == NULL) {
                fprintf(stderr, "Error: %s¥n", strerror(errno));
                return -1;
        }
        NEWtoOLD = (int *)calloc(ICELTOT, sizeof(int));
        if(NEWtoOLD == NULL) {
                fprintf(stderr, "Error: %s¥n", strerror(errno));
                return -1;
        }
        COLORindex = (int *)calloc(ICELTOT+1, sizeof(int));
        if(COLORindex == NULL) {
                fprintf(stderr, "Error: %s¥n", strerror(errno));
                return -1;
        }

        if(NCOLORtot > 0) {
                MC(ICELTOT, NL, NU, INL, IAL, INU, IAU,
                                &NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW);
        } else if(NCOLORtot == 0) {
                CM(ICELTOT, NL, NU, INL, IAL, INU, IAU,
                                &NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW);
        } else if(NCOLORtot ==-1) {
                RCM(ICELTOT, NL, NU, INL, IAL, INU, IAU,
                                &NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW);
        } else if(NCOLORtot <-1) {
                CMRCM(ICELTOT, NL, NU, INL, IAL, INU, IAU,
                                &NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW);
        }

        fprintf(stderr, "¥n# TOTAL COLOR number%8d¥n", NCOLORtot);
        return 0;
}
```

Reordering

NCOLORtot > 1: Multicolor
NCOLORtot = 0: CM
NCOLORtot =-1: RCM
NCOLORtot <-1: CM-RCM

poi_gen (4/9)

SMPindex:

for preconditioning

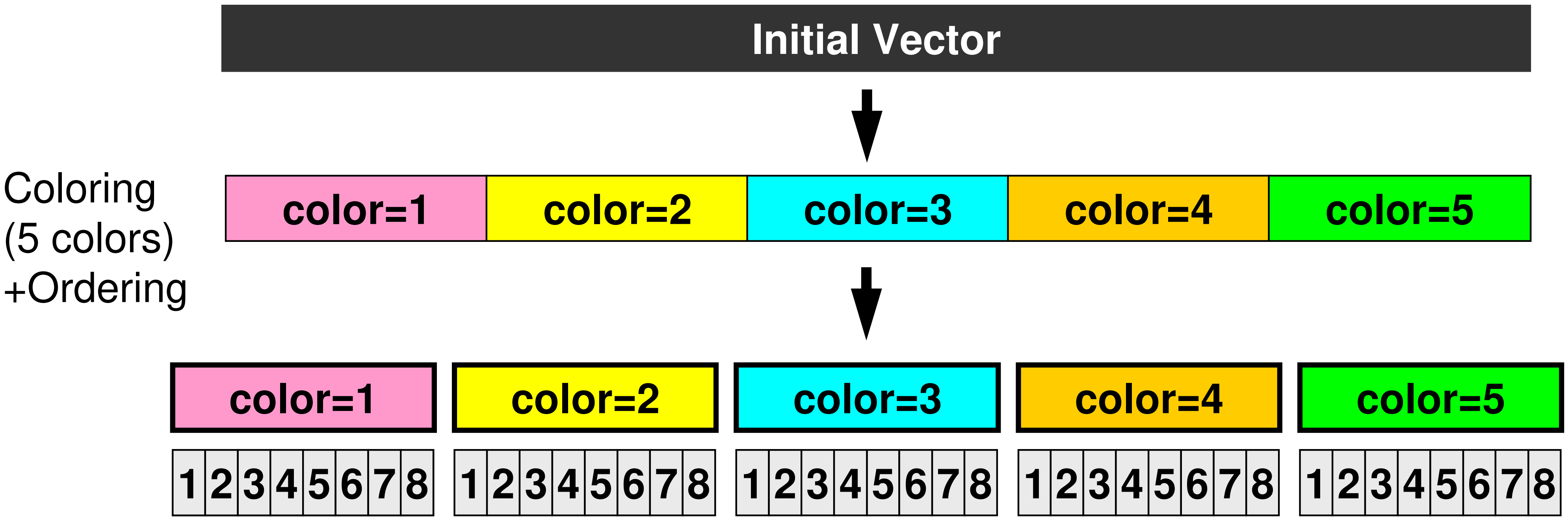
```
SMPindex = (int *) allocate_vector(sizeof(int),
NCOLORtot*PEsmpTOT+1);
memset(SMPindex, 0,
sizeof(int)*(NCOLORtot*PEsmpTOT+1));

for(ic=1; ic<=NCOLORtot; ic++) {
    nn1 = COLORindex[ic] - COLORindex[ic-1];
    num = nn1 / PEsmpTOT;
    nr  = nn1 - PEsmpTOT * num;
    for(ip=1; ip<=PEsmpTOT; ip++) {
        if(ip <= nr) {
          SMPindex[(ic-1)*PEsmpTOT+ip] = num + 1;
        } else {
          SMPindex[(ic-1)*PEsmpTOT+ip] = num;
        }
    }
}

for(ic=1; ic<=NCOLORtot; ic++) {
    for(ip=1; ip<=PEsmpTOT; ip++) {
        j1 = (ic-1) * PEsmpTOT + ip;
        j0 = j1 - 1;
        SMPindex[j1] += SMPindex[j0];
    }
}

SMPindexG = (int *) allocate_vector
                         PEsmpTOT+1);
memset(SMPindexG, 0, sizeof(int)*(PE

nn = ICELTOT / PEsmpTOT;
nr = ICELTOT - nn * PEsmpTOT;
for(ip=1; ip<=PEsmpTOT; ip++) {
    SMPindexG[ip] = nn;
    if(ip <= nr) {SMPindexG[ip] +=
}
for(ip=1; ip<=PEsmpTOT; ip++) {
    SMPindexG[ip] += SMPindexG[ip-1];
}
```

```
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for ...
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
            (...)
        }
    }
}
```

SMPindex:

for preconditioning

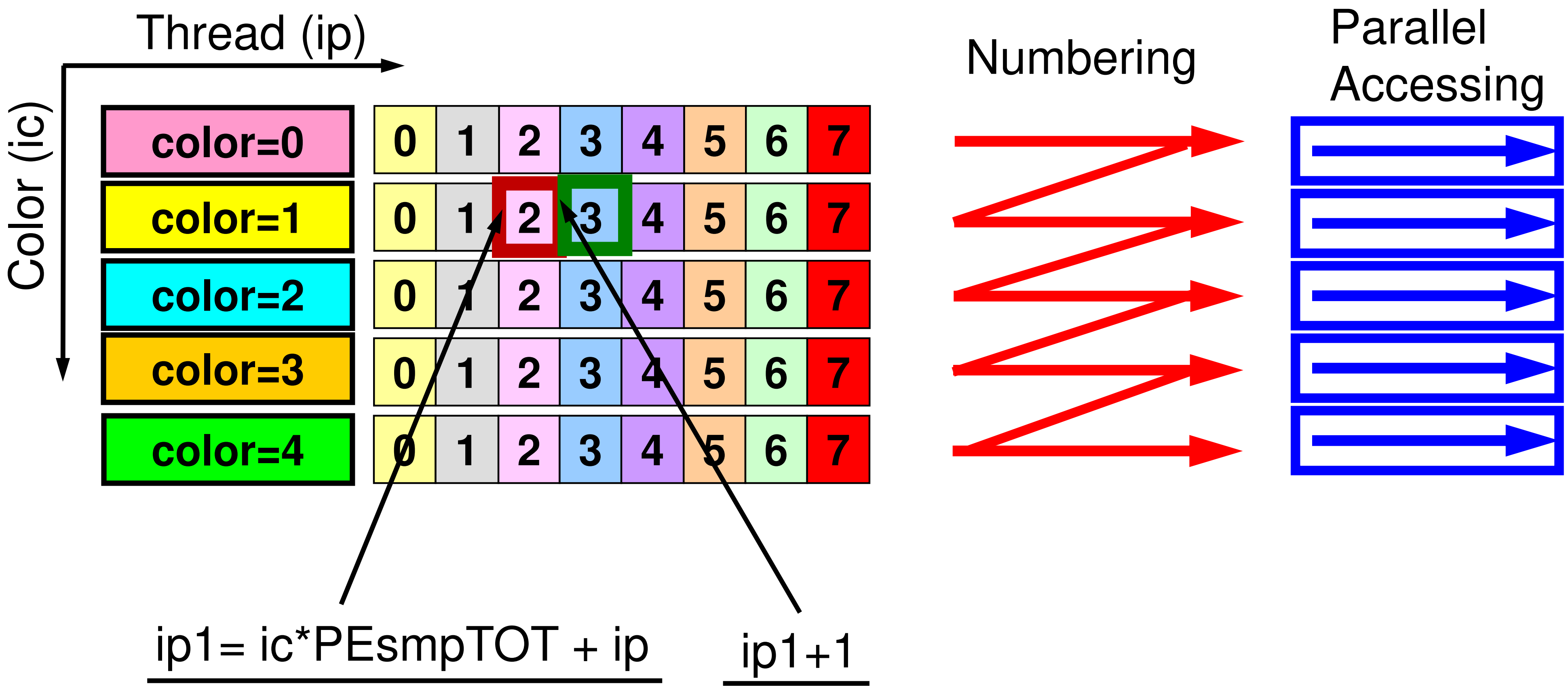
```
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for ...
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
            (...)
        }
    }
}
```



- 5-colors, 8-threads
- Meshes in same color are independent: parallel processing
- Reordering in ascending order according to color ID

SMPindex

```
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip,ip1,i,WVAL,j)
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {…
```



SMPindex

```
COLORindex[ic  ]= 100
COLORindex[ic+1]= 200
PEsmpTOT        =   8

nn1= 200-100   = 100
num= 100 / 8   =  12 (12.5)
nr = 100 - 12*8=   4
ip0= ic*PEsmpTOT (ic: starting at 0)

SMPindex[ip0  ]= 100
SMPindex[ip0+1]= 113 (13 elements in the 1st thread)
SMPindex[ip0+2]= 126 (13 elements in the 2nd thread)
SMPindex[ip0+3]= 139 (13 elements in the 3rd thread)
SMPindex[ip0+4]= 152 (13 elements in the 4th thread)
SMPindex[ip0+5]= 164 (12 elements in the 5th thread)
SMPindex[ip0+6]= 176 (12 elements in the 6th thread)
SMPindex[ip0+7]= 188 (12 elements in the 7th thread)
SMPindex[ip0+8]= 200 (12 elements in the 8th thread)
```

poi_gen (4/9)

```
SMPindex = (int *) allocate_vector(sizeof(int),
NCOLORtot*PEsmpTOT+1);
memset(SMPindex, 0,
sizeof(int)*(NCOLORtot*PEsmpTOT+1));

for(ic=1; ic<=NCOLORtot; ic++) {
    nn1 = COLORindex[ic] - COLORindex[ic-1];
    num = nn1 / PEsmpTOT;
    nr  = nn1 - PEsmpTOT * num;
    for(ip=1; ip<=PEsmpTOT; ip++) {
        if(ip <= nr) {
          SMPindex[(ic-1)*PEsmpTOT+ip] = num + 1;
        } else {
          SMPindex[(ic-1)*PEsmpTOT+ip] = num;
        }
    }
}

for(ic=1; ic<=NCOLORtot; ic++) {
    for(ip=1; ip<=PEsmpTOT; ip++) {
        j1 = (ic-1) * PEsmpTOT + ip;
        j0 = j1 - 1;
        SMPindex[j1] += SMPindex[j0];
    }
}

SMPindexG = (int *) allocate_vector(sizeof(int),
                    PEsmpTOT+1);
memset(SMPindexG, 0, sizeof(int)*(PEsmpTOT+1));

nn = ICELTOT / PEsmpTOT;
nr = ICELTOT - nn * PEsmpTOT;
for(ip=1; ip<=PEsmpTOT; ip++) {
    SMPindexG[ip] = nn;
    if(ip <= nr) {SMPindexG[ip] += 1;}
}
for(ip=1; ip<=PEsmpTOT; ip++) {
    SMPindexG[ip] += SMPindexG[ip-1];
}
```

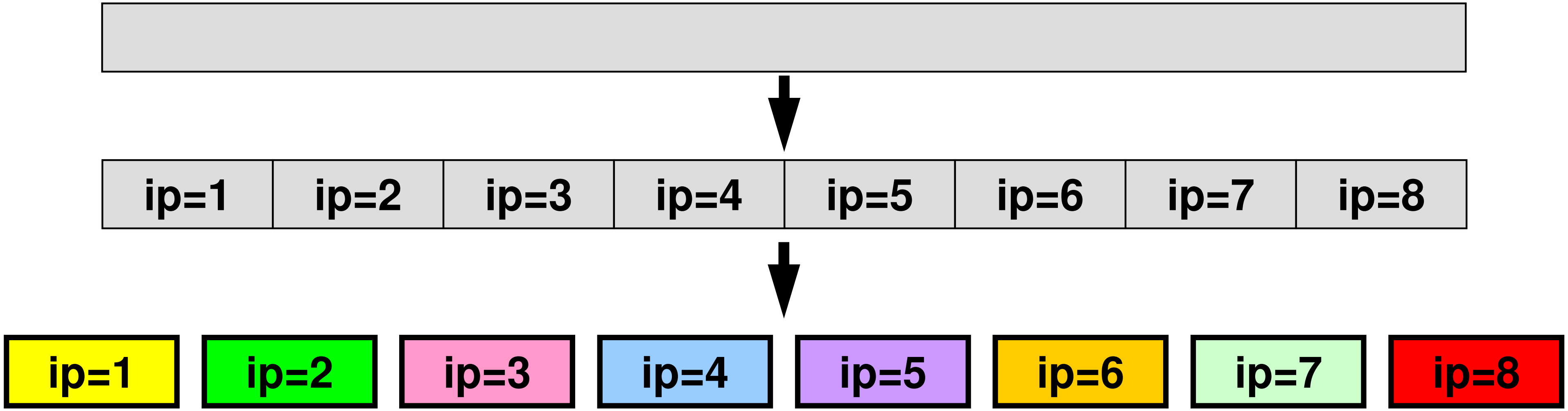
```
#pragma omp parallel for ...
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        (...)
    }
}
```

SMPindexG:

for Dot-products, DAXPY, Mat-vec, and Poi-gen

SMPindexG

```
#pragma omp parallel for ...
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        (...)
    }
}
```



for Dot-products, DAXPY, Mat-vec, and Poi-gen

poi_gen (5/9)

New numbering is applied after this point

```
indexL =
(int *)allocate_vector(sizeof(int),ICELTOT+1);
indexU =
(int *)allocate_vector(sizeof(int),ICELTOT+1);

for(i=0; i<ICELTOT; i++){
    indexL[i+1]=indexL[i]+INL[i];
    indexU[i+1]=indexU[i]+INU[i];
}
NPL = indexL[ICELTOT];
NPU = indexU[ICELTOT];

itemL = (int *)allocate_vector(sizeof(int),NPL);
itemU = (int *)allocate_vector(sizeof(int),NPU);
AL =
(double *)allocate_vector(sizeof(double),NPL);
AU =
(double *)allocate_vector(sizeof(double),NPU);

memset(itemL, 0, sizeof(int)*NPL);
memset(itemU, 0, sizeof(int)*NPU);
memset(AL, 0.0, sizeof(double)*NPL);
memset(AU, 0.0, sizeof(double)*NPU);

for(i=0; i<ICELTOT; i++){
    for(k=0;k<INL[i];k++){
        kk= k + indexL[i];
        itemL[kk]= IAL[i][k];
    }
    for(k=0;k<INU[i];k++){
        kk= k + indexU[i];
        itemU[kk]= IAU[i][k];
    }
}

free(INL); free(INU);
free(IAL); free(IAU);
```

Name	Type	Content
D[N]	**R**	Diagonal components of the matrix (N= ICELTOT)
BFORCE[N]	**R**	RHS vector
PHI[N]	**R**	Unknown vector
indexL[N+1] **indexU[N+1]**	**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)

“itemL” /”itemU” start at 1

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

```
for (i=0; i<N; i++) {
    q[i]= D[i] * p[i];
    for (j=indexL[i]; j<indexL[i+1]; j++) {
        q[i] += AL[j] * p[itemL[j]-1];
    }
    for (j=indexU[i]; j<indexU[i+1]; j++) {
        q[i] += AU[j] * p[itemU[j]-1];
    }
}
```

poi_gen (6/9)

New numbering applied

```
S1t = omp_get_wtime();
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6, coef, j,
ii, jj, kk, isL, ieL, isU, ieU)

for(ip=0; ip<PEsmpTOT; ip++) {
for(icel=SMPindexG[ip]; icel<SMPindexG[ip+1]; icel++) {

    ic0  = NEWtoOLD[icel];
    icN1 = NEIBcell[ic0-1][0];
    icN2 = NEIBcell[ic0-1][1];
    icN3 = NEIBcell[ic0-1][2];
    icN4 = NEIBcell[ic0-1][3];
    icN5 = NEIBcell[ic0-1][4];
    icN6 = NEIBcell[ic0-1][5];

    isL =indexL[icel  ];       ieL =indexL[icel+1];
    isU =indexU[icel  ];       ieU =indexU[icel+1];

    if(icN5 != 0) {
       icN5 = OLDtoNEW[icN5-1];
       coef = RDZ * ZAREA;
       D[icel] -= coef;

       if(icN5-1 < icel) {
          for(j=isL; j<ieL; j++) {
              if(itemL[j] == icN5) {
                 AL[j] = coef;
                 break;
              }
          }
       } else {
          for(j=isU; j<ieU; j++) {
              if(itemU[j] == icN5) {
                 AU[j] = coef;
                 break;
              }
           }
        }
      }
...
```

icel: New ID
ic0: Old ID

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\boxed{\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+}$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

Coef. Matrix: Parallel, “SMPindexG”

“private”

```
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6, coef, j, ii,
jj, kk, isL, ieL, isU, ieU)

for(ip=0; ip<PEsmpTOT; ip++) {
for(icel=SMPindexG[ip]; icel<SMPindexG[ip+1]; icel++) {

    ic0  = NEWtoOLD[icel];
    icN1 = NEIBcell[ic0-1][0];
```

poi_gen (6/9)

New numbering applied

```
S1t = omp_get_wtime();
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6, coef, j,
ii, jj, kk, isL, ieL, isU, ieU)

for(ip=0; ip<PEsmpTOT; ip++) {
for(icel=SMPindexG[ip]; icel<SMPindexG[ip+1]; icel++) {

     ic0  = NEWtoOLD[icel];
     icN1 = NEIBcell[ic0-1][0];
     icN2 = NEIBcell[ic0-1][1];
     icN3 = NEIBcell[ic0-1][2];
     icN4 = NEIBcell[ic0-1][3];
     icN5 = NEIBcell[ic0-1][4];
     icN6 = NEIBcell[ic0-1][5];

     isL =indexL[icel  ];    ieL =indexL[icel+1];
     isU =indexU[icel  ];    ieU =indexU[icel+1];

     if(icN5 != 0) {
        icN5 = OLDtoNEW[icN5-1];
        coef = RDZ * ZAREA;
        D[icel] -= coef;

        if(icN5-1 < icel) {
           for(j=isL; j<ieL; j++) {
               if(itemL[j] == icN5) {
                  AL[j] = coef;
                  break;
               }
           }
        } else {
           for(j=isU; j<ieU; j++) {
               if(itemU[j] == icN5) {
                  AU[j] = coef;
                  break;
               }
           }
        }
     }
...
```

icel: New ID
ic0: Old ID

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\boxed{\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+}$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

```
S1t = omp_get_wtime();
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6, coef, j,
ii, jj, kk, isL, ieL, isU, ieU)

for(ip=0; ip<PEsmpTOT; ip++) {
for(icel=SMPindexG[ip]; icel<SMPindexG[ip+1]; icel++) {

    ic0  = NEWtoOLD[icel];
    icN1 = NEIBcell[ic0-1][0];
    icN2 = NEIBcell[ic0-1][1];
    icN3 = NEIBcell[ic0-1][2];
    icN4 = NEIBcell[ic0-1][3];
    icN5 = NEIBcell[ic0-1][4];
    icN6 = NEIBcell[ic0-1][5];

    isL =indexL[icel  ];     ieL =indexL[icel+1];
    isU =indexU[icel  ];     ieU =indexU[icel+1];

    if(icN5 != 0) {
       icN5 = OLDtoNEW[icN5-1];
       coef = RDZ * ZAREA;
       D[icel] -= coef;

       if(icN5-1 < icel) {
          for(j=isL; j<ieL; j++) {
              if(itemL[j] == icN5) {
                 AL[j] = coef;
                 break;
              }
          }
       } else {
          for(j=isU; j<ieU; j++) {
              if(itemU[j] == icN5) {
                 AU[j] = coef;
                 break;
              }
            }
         }
       }
...
```

poi_gen (6/9)

New numbering applied

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\boxed{\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+}$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

poi_gen (6/9)

New numbering applied

```
S1t = omp_get_wtime();
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6, coef, j,
ii, jj, kk, isL, ieL, isU, ieU)

for(ip=0; ip<PEsmpTOT; ip++) {
for(icel=SMPindexG[ip]; icel<SMPindexG[ip+1]; icel++) {

    ic0  = NEWtoOLD[icel];
    icN1 = NEIBcell[ic0-1][0];
    icN2 = NEIBcell[ic0-1][1];
    icN3 = NEIBcell[ic0-1][2];
    icN4 = NEIBcell[ic0-1][3];
    icN5 = NEIBcell[ic0-1][4];
    icN6 = NEIBcell[ic0-1][5];

    isL =indexL[icel  ];     ieL =indexL[icel+1];
    isU =indexU[icel  ];     ieU =indexU[icel+1];

    if(icN5 != 0) {
       icN5 = OLDtoNEW[icN5-1];
       coef = RDZ * ZAREA;
       D[icel] -= coef;

       if(icN5-1 < icel) {
          for(j=isL; j<ieL; j++) {
              if(itemL[j] == icN5) {
                 AL[j] = coef;
                 break;
              }
          }
       } else {
          for(j=isU; j<ieU; j++) {
              if(itemU[j] == icN5) {
                 AU[j] = coef;
                 break;
              }
           }
        }
     }
...
```

$$\mathrm{RDZ}=\frac{1}{\Delta z}$$

$$\mathrm{ZAREA}=\Delta x\Delta y$$

icN5 < icel
Lower Part

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\boxed{\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+}$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

poi_gen (6/9)

New numbering applied

```
S1t = omp_get_wtime();
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6, coef, j,
ii, jj, kk, isL, ieL, isU, ieU)

for(ip=0; ip<PEsmpTOT; ip++) {
for(icel=SMPindexG[ip]; icel<SMPindexG[ip+1]; icel++) {

    ic0  = NEWtoOLD[icel];
    icN1 = NEIBcell[ic0-1][0];
    icN2 = NEIBcell[ic0-1][1];
    icN3 = NEIBcell[ic0-1][2];
    icN4 = NEIBcell[ic0-1][3];
    icN5 = NEIBcell[ic0-1][4];
    icN6 = NEIBcell[ic0-1][5];

    isL =indexL[icel  ];     ieL =indexL[icel+1];
    isU =indexU[icel  ];     ieU =indexU[icel+1];

    if(icN5 != 0) {
       icN5 = OLDtoNEW[icN5-1];
       coef = RDZ * ZAREA;
       D[icel] -= coef;

       if(icN5-1 < icel) {
          for(j=isL; j<ieL; j++) {
              if(itemL[j] == icN5) {
                 AL[j] = coef;
                 break;
              }
          }
       } else {
          for(j=isU; j<ieU; j++) {
              if(itemU[j] == icN5) {
                 AU[j] = coef;
                 break;
              }
           }
        }
      }
...
```

$$RDZ = \frac{1}{\Delta z}$$

$$ZAREA = \Delta x \Delta y$$

icN5 > icel
Upper Part

$$\frac{\phi_{neib[icel][0]} - \phi_{icel}}{\Delta x}\Delta y \Delta z +$$

$$\frac{\phi_{neib[icel][1]} - \phi_{icel}}{\Delta x}\Delta y \Delta z +$$

$$\frac{\phi_{neib[icel][2]} - \phi_{icel}}{\Delta y}\Delta z \Delta x +$$

$$\frac{\phi_{neib[icel][3]} - \phi_{icel}}{\Delta y}\Delta z \Delta x +$$

$$\boxed{\frac{\phi_{neib[icel][4]} - \phi_{icel}}{\Delta z}\Delta x \Delta y +}$$

$$\frac{\phi_{neib[icel][5]} - \phi_{icel}}{\Delta z}\Delta x \Delta y + f_{icel}\Delta x \Delta y \Delta z = 0$$

poi_gen (7/9)

```
if(icN3 != 0) {
   icN3 = OLDtoNEW[icN3-1];
   coef = RDY * YAREA;
   D[icel] -= coef;

   if(icN3-1 < icel) {
      for(j=isL; j<ieL; j++) {
          if(itemL[j] == icN3) {
             AL[j] = coef;
             break; }
      }
   } else {
      for(j=isU; j<ieU; j++) {
          if(itemU[j] == icN3) {
             AU[j] = coef;
             break; }
      }
   }
}

if(icN1 != 0) {
   icN1 = OLDtoNEW[icN1-1];
   coef = RDX * XAREA;
   D[icel] -= coef;

   if(icN1-1 < icel) {
      for(j=isL; j<ieL; j++) {
          if(itemL[j] == icN1) {
             AL[j] = coef;
             break;}
      }
   } else {
      for(j=isU; j<ieU; j++) {
          if(itemU[j] == icN1) {
             AU[j] = coef;
             break;}
      }
   }
}
```

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

poi_gen (8/9)

```
if(icN2 != 0) {
   icN2 = OLDtoNEW[icN2-1];
   coef = RDX * XAREA;
   D[icel] -= coef;

   if(icN2-1 < icel) {
      for(j=isL; j<ieL; j++) {
          if(itemL[j] == icN2) {
             AL[j] = coef;
             break;}
      }
   } else {
      for(j=isU; j<ieU; j++) {
          if(itemU[j] == icN2) {
             AU[j] = coef;
             break;}
      }
   }
}

if(icN4 != 0) {
   icN4 = OLDtoNEW[icN4-1];
   coef = RDY * YAREA;
   D[icel] -= coef;

   if(icN4-1 < icel) {
      for(j=isL; j<ieL; j++) {
          if(itemL[j] == icN4) {
             AL[j] = coef;
             break; }
      }
   } else {
      for(j=isU; j<ieU; j++) {
          if(itemU[j] == icN4) {
             AU[j] = coef;
             break; }
      }
   }
}
```

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

poi_gen (9/9)

```
#pragma omp parallel for private
(ip, icel, ic0, icN1, icN2, icN3, icN4, icN5, icN6,
coef, j, ii, jj, kk, isL, ieL, isU, ieU)

…

    if(icN6 != 0) {
       icN6 = OLDtoNEW[icN5-1];
       coef = RDZ * ZAREA;
       D[icel] -= coef;

       if(icN6-1 < icel) {
          for(j=isL; j<ieL; j++) {
              if(itemL[j] == icN6) {
                 AL[j] = coef;
                 break;
              }
          }
       } else {
          for(j=isU; j<ieU; j++) {
              if(itemU[j] == icN6) {
                 AU[j] = coef;
                 break;
              }
           }
        }
      }

     ii = XYZ[ic0-1][0];
     jj = XYZ[ic0-1][1];
     kk = XYZ[ic0-1][2];

     BFORCE[icel]= -(double)(ii+jj+kk) * VOL0;

}
```

BFORCE using original mesh ID

ii,jj,kk,VOL0: private

$$\frac{\phi_{neib[icel][0]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][1]}-\phi_{icel}}{\Delta x}\Delta y\Delta z+$$

$$\frac{\phi_{neib[icel][2]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][3]}-\phi_{icel}}{\Delta y}\Delta z\Delta x+$$

$$\frac{\phi_{neib[icel][4]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+$$

$$\frac{\phi_{neib[icel][5]}-\phi_{icel}}{\Delta z}\Delta x\Delta y+f_{icel}\Delta x\Delta y\Delta z=0$$

Main Program

```
#include <stdio.h> ...

int
main()
{
        double *WK;
        int NPL, NPU; ISET, ITR, IER; icel, ic0, i;
        double xN, xL, xU; Stime, Etime;

        if(INPUT()) goto error;
        if(POINTER_INIT()) goto error;
        if(BOUNDARY_CELL()) goto error;
        if(CELL_METRICS()) goto error;
        if(POI_GEN()) goto error;

        ISET = 0;
        WK = (double *)malloc(sizeof(double)*ICELTOT);
        if(WK == NULL) {
           fprintf(stderr, "Error: %s¥n", strerror(errno));
           goto error;}
           Stime = omp_get_wtime();
           if(solve_ICCG_mc(ICELTOT, NL, NU, indexL, itemL, indexU, itemU,
                            D, BFORCE, PHI, AL, AU, NCOLORtot, PEsmpTOT,
                            SMPindex, SMPindexG, EPSICCG, &ITR, &IER)) goto error;
           Etime = omp_get_wtime();
        for(ic0=0; ic0<ICELTOT; ic0++) {
             icel = NEWtoOLD[ic0];
            WK[icel-1] = PHI[ic0];
        }
        for(icel=0; icel<ICELTOT; icel++) {
            PHI[icel] = WK[icel];
        }
        if(OUTUCD()) goto error;
        return 0;
error:
        return -1;
}
```

solve_ICCG_mc (1/6)

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>
#include <math.h> etc.

#include ”solver_ICCG.h”

extern int
solve_ICCG_mc(int N, int NL, int NU, int *indexL, int *itemL, int *indexU,
              int *itemU,
              double *D, double *B, double *X, double *AL, double *AU,
              int NCOLORtot, int *COLORindex,
              int PEsmpTOT, int *SMPindex, int *SMPindexG,
              double EPS, int *ITR, int *IER)
{

        double **W;
        double VAL, BNRM2, WVAL, SW, RHO, BETA, RHO1, C1, DNRM2, ALPHA, ERR;
        int i, j, ic, ip, L, ip1;
        int R = 0;
        int Z = 1;
        int Q = 1;
        int P = 2;
        int DD = 3;
```

solve_ICCG_mc (2/6)

```
W =
(double **)allocate_matrix(sizeof(double *), 4, N+128);


#pragma omp parallel for private (ip, i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        X[i] = 0.0;
        W[1][i] = 0.0;
        W[2][i] = 0.0;
        W[3][i] = 0.0;
    }
}

for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip, ip1, i, VAL, j)
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
            VAL = D[i];
            for(j=indexL[i]; j<indexL[i+1]; j++) {
                VAL-= AL[j]*AL[j]*W[DD][itemL[j] - 1];
            }
            W[DD][i] = 1.0 / VAL;
        }
    }
}
```

Incomplete “Modified” Cholesky Factorization

Incomplete “Modified” Cholesky Factorization

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

W[DD][i]:	d_i
D[i]:	a_{ii}
itemL[j]:	k
AL[j]:	a_{ik}

```
for(i=0; i<N; i++) {
    VAL = D[i];
    for(j=indexL[i]; j<indexL[i+1]; j++) {
        VAL-= AL[j]*AL[j]*W[DD][itemL[j] - 1];
    }
    W[DD][i] = 1.0 / VAL;
}
```

Incomplete “Modified” Cholesky Factorization: Parallel Version

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

W[DD][i]:	d_i
D[i]:	a_{ii}
itemL[j]:	k
AL[j]:	a_{ik}

```
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip,ip1,i,VAL,j)
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
            VAL = D[i];
            for(j=indexL[i]; j<indexL[i+1]; j++) {
                VAL-= AL[j]*AL[j]*W[DD][itemL[j] - 1];
            }
            W[DD][i] = 1.0 / VAL;
        }
    }
}
```

solve_ICCG_mc (3/6)

```
#pragma omp parallel for private (ip,i,VAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        VAL = D[i] * X[i];

        for(j=indexL[i]; j<indexL[i+1]; j++) {
            VAL += AL[j] * X[itemL[j]-1];
        }
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            VAL += AU[j] * X[itemU[j]-1];
        }
    }
    W[R][i] = B[i] - VAL;
}

BNRM2 = 0.0;
#pragma omp parallel for private (ip, i)
                              reduction (+:BNRM2)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        BNRM2 += B[i]*B[i];
    }
}
```

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

Mat-Vec

NO Data Dependency: SMPindexG

```
#pragma omp parallel for private (ip,i,VAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        VAL = D[i] * X[i];

        for(j=indexL[i]; j<indexL[i+1]; j++) {
            VAL += AL[j] * X[itemL[j]-1];
        }
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            VAL += AU[j] * X[itemU[j]-1];
        }
    }
    W[R][i] = B[i] - VAL;
}
```

solve_ICCG_mc (3/6)

```
#pragma omp parallel for private (ip,i,VAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        VAL = D[i] * X[i];

        for(j=indexL[i]; j<indexL[i+1]; j++) {
            VAL += AL[j] * X[itemL[j]-1];
        }
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            VAL += AU[j] * X[itemU[j]-1];
        }
    }
    W[R][i] = B[i] - VAL;
}

BNRM2 = 0.0;
#pragma omp parallel for private (ip, i)
                        reduction (+:BNRM2)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        BNRM2 += B[i]*B[i];
    }
}
```

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

Dot Products: SMPindexG, reduction

```
BNRM2 = 0.0;
#pragma omp parallel for private (ip,i) reduction (+:BNRM2)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        BNRM2 += B[i]*B[i];
    }
}
```

solve_ICCG_mc (4/6)

```
*ITR = N;
for(L=0; L<(*ITR); L++) {

#pragma omp parallel for private(ip, i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        W[Z][i] = W[R][i];
    }
}

for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip,ip1,i,WVAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        WVAL = W[Z][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            WVAL -= AL[j] * W[Z][itemL[j]-1];
        }
        W[Z][i] = WVAL * W[DD][i];
    }
}
}
for(ic=NCOLORtot-1; ic>=0; ic--){
#pragma omp parallel for private (ip,ip1,i,SW,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        SW = 0.0;
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            SW += AU[j] * W[Z][itemU[j]-1];
        }
        W[Z][i]= W[Z][i]  - W[DD][i] * SW;
     }
}
}
```

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

solve_ICCG_mc (4/6)

```
*ITR = N;
for(L=0; L<(*ITR); L++) {

#pragma omp parallel for private(ip, i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        W[Z][i] = W[R][i];
    }
}

for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip,ip1,i,WVAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        WVAL = W[Z][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            WVAL -= AL[j] * W[Z][itemL[j]-1];
        }
        W[Z][i] = WVAL * W[DD][i];
    }
}
}
for(ic=NCOLORtot-1; ic>=0; ic--){
#pragma omp parallel for private (ip,ip1,i,SW,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        SW = 0.0;
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            SW += AU[j] * W[Z][itemU[j]-1];
        }
        W[Z][i]= W[Z][i]  - W[DD][i] * SW;
     }
}
}
```

SMPindex

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

solve_ICCG_mc (4/6)

```
*ITR = N;
for(L=0; L<(*ITR); L++) {

#pragma omp parallel for private(ip, i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        W[Z][i] = W[R][i];
    }
}

for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip,ip1,i,WVAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        WVAL = W[Z][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            WVAL -= AL[j] * W[Z][itemL[j]-1];
        }
        W[Z][i] = WVAL * W[DD][i];
    }
}
}
for(ic=NCOLORtot-1; ic>=0; ic--){
#pragma omp parallel for private (ip,ip1,i,SW,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        SW = 0.0;
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            SW += AU[j] * W[Z][itemU[j]-1];
        }
        W[Z][i]= W[Z][i]  - W[DD][i] * SW;
     }
}
}
```

SMPindex

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

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

Forward Substitution

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

Backward Substitution

Forward Substitution: SMPindex

```
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip,ip1,i,WVAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    ip1 = ic * PEsmpTOT + ip;
    for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
        WVAL = W[Z][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            WVAL -= AL[j] * W[Z][itemL[j]-1];
        }
        W[Z][i] = WVAL * W[DD][i];
    }
}
}
```

solve_ICCG_mc (5/6)

```
/*********************************
 * {p}  = {z} if      ITER=0    *
 * BETA = RHO / RHO1  otherwise *
 *********************************/

if(L == 0) {
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
           W[P][i] = W[Z][i];
       }
   }
} else {
   BETA = RHO / RHO1;
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip];]; i++) {
           W[P][i] = W[Z][i] + BETA * W[P][i];
       }
   }
}

/****************
 * {q} = [A]{p} *
 ****************/

#pragma omp parallel for private(ip, i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        VAL = D[i] * W[P][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            VAL += AL[j] * W[P][itemL[j]-1];
        }
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            VAL += AU[j] * W[P][itemU[j]-1];
        }
        W[Q][i] = VAL;
    }
}
```

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

solve_ICCG_mc (5/6)

```
/**********************************
 * {p}  = {z} if      ITER=0    *
 * BETA = RHO / RHO1  otherwise *
 **********************************/

if(L == 0) {
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
        for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
            W[P][i] = W[Z][i];
        }
   }
} else {
   BETA = RHO / RHO1;
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
        for(i=SMPindexG[ip];]; i++) {
            W[P][i] = W[Z][i] + BETA * W[P][i];
        }
   }
}

/****************
 * {q} = [A]{p} *
 ****************/

#pragma omp parallel for private(ip,i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        VAL = D[i] * W[P][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            VAL += AL[j] * W[P][itemL[j]-1];
        }
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            VAL += AU[j] * W[P][itemU[j]-1];
        }
        W[Q][i] = VAL;
    }
}
```

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

solve_ICCG_mc (6/6)

```
/*************************
 * ALPHA = RHO / {p}{q} *
 *************************/
   C1 = 0.0;
#pragma omp parallel for private(ip,i)reduction(+:C1)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           C1 += W[P][i] * W[Q][i];
       }
   }
   ALPHA = RHO / C1;

/***************************
 * {x} = {x} + ALPHA * {p} *
 * {r} = {r} - ALPHA * {q} *
 ***************************/
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           X[i]    += ALPHA * W[P][i];
           W[R][i] -= ALPHA * W[Q][i];
   }
}

   DNRM2 = 0.0;
#pragma omp parallel for private(ip,i)
                         reduction(+:DNRM2)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           DNRM2 += W[R][i]*W[R][i];
       }
   }
```

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

solve_ICCG_mc (6/6)

```
/*************************
 * ALPHA = RHO / {p}{q} *
 *************************/
   C1 = 0.0;
#pragma omp parallel for private(ip,i)reduction(+:C1)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           C1 += W[P][i] * W[Q][i];
       }
   }
   ALPHA = RHO / C1;

/***************************
 * {x} = {x} + ALPHA * {p} *
 * {r} = {r} - ALPHA * {q} *
 ***************************/
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           X[i]    += ALPHA * W[P][i];
           W[R][i] -= ALPHA * W[Q][i];
   }
}

   DNRM2 = 0.0;
#pragma omp parallel for private(ip,i)
                              reduction(+:DNRM2)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           DNRM2 += W[R][i]*W[R][i];
       }
   }
```

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

solve_ICCG_mc (6/6)

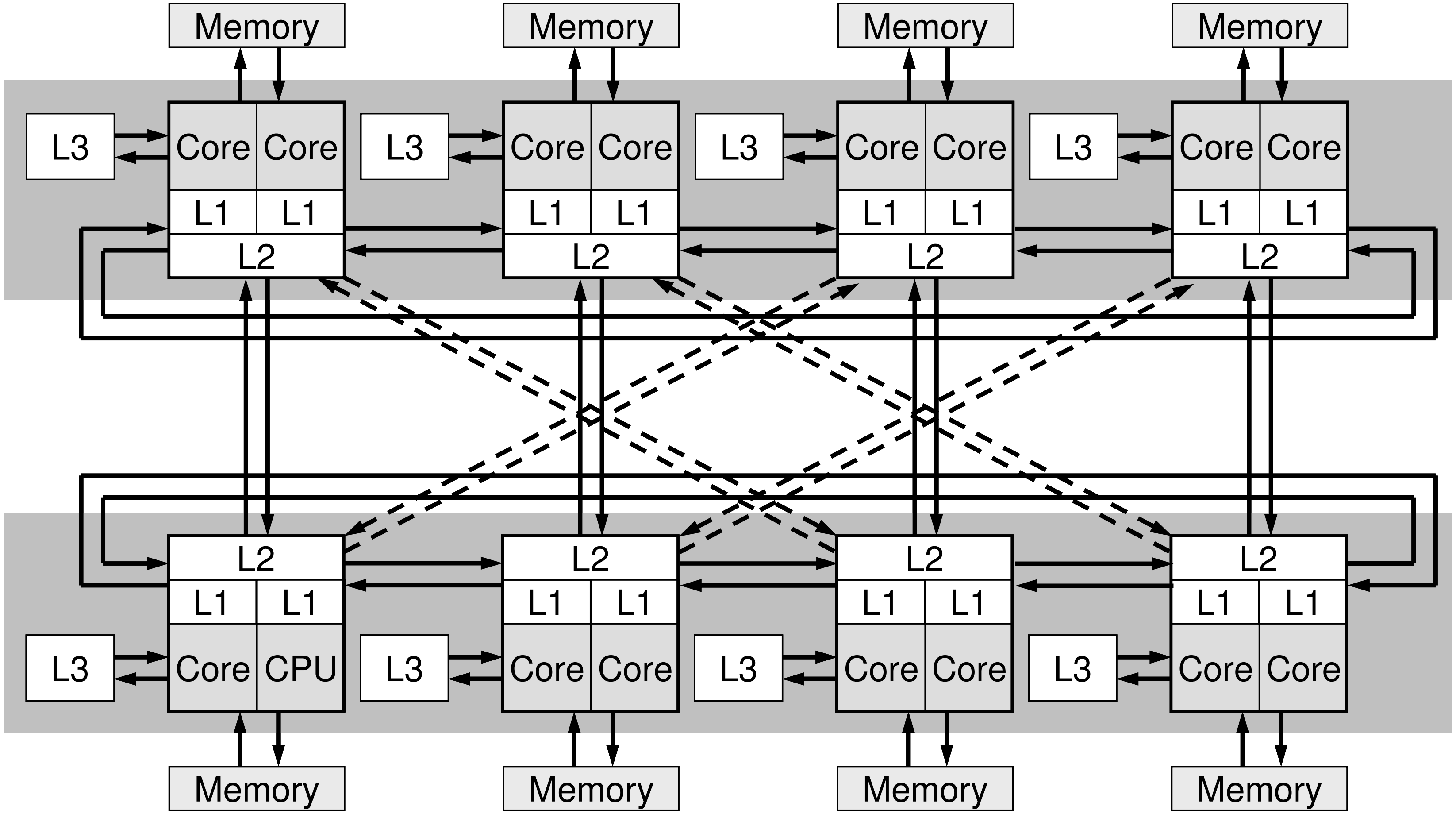
```
/************************
 * ALPHA = RHO / {p}{q} *
 ************************/
   C1 = 0.0;
#pragma omp parallel for private(ip,i)reduction(+:C1)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           C1 += W[P][i] * W[Q][i];
       }
   }
   ALPHA = RHO / C1;

/***************************
 * {x} = {x} + ALPHA * {p} *
 * {r} = {r} - ALPHA * {q} *
 ***************************/
#pragma omp parallel for private(ip,i)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           X[i]    += ALPHA * W[P][i];
           W[R][i] -= ALPHA * W[Q][i];
   }
}

   DNRM2 = 0.0;
#pragma omp parallel for private(ip,i)
                         reduction(+:DNRM2)
   for(ip=0; ip<PEsmpTOT; ip++) {
       for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
           DNRM2 += W[R][i]*W[R][i];
       }
   }
```

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

- Applying OpenMP to L2-sol
- **Examples**
- Optimization + Exercise

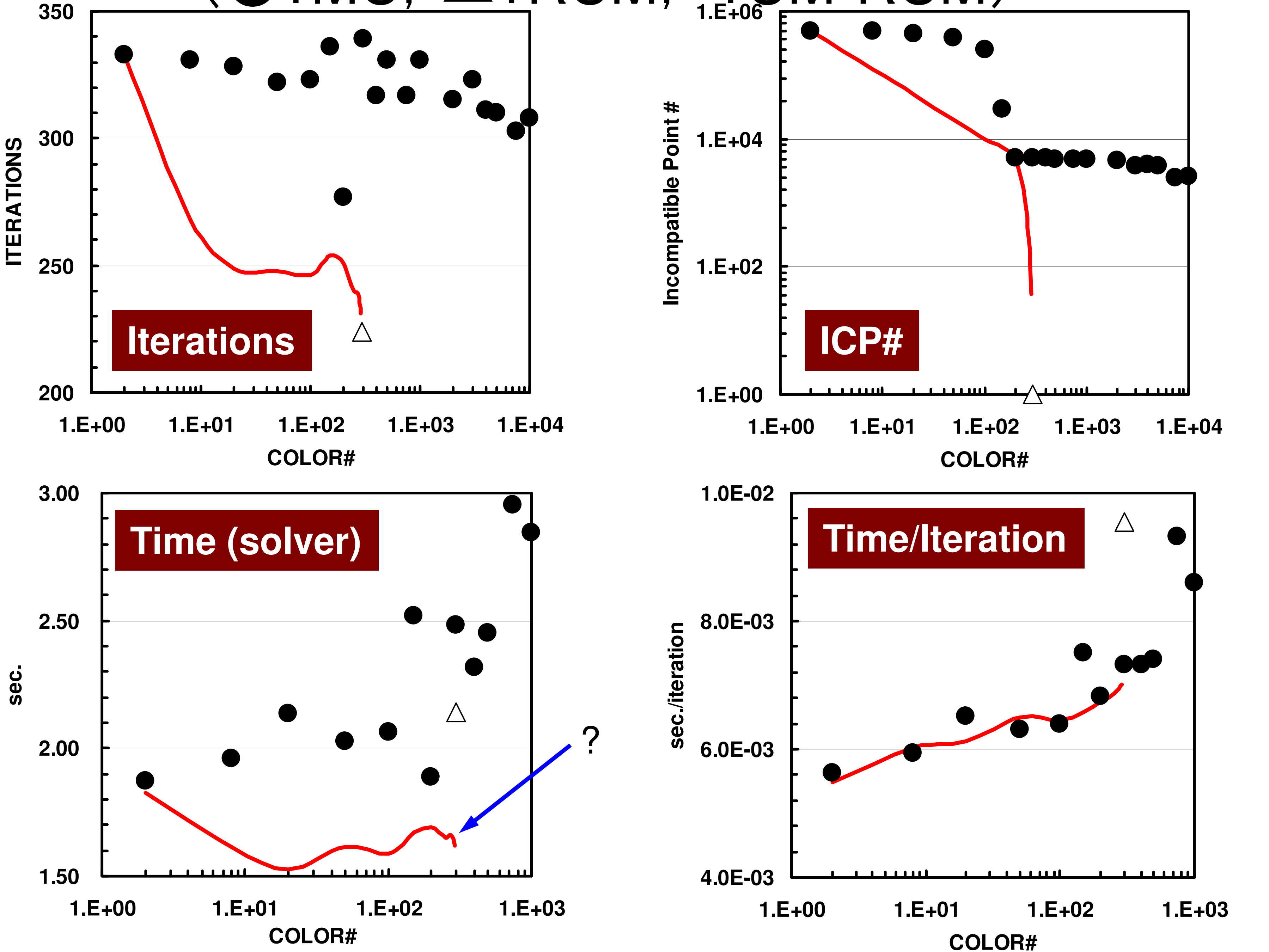
Results

- Hitachi SR11000/J2 1-node, 16-cores
  - – Retired in Fall 2011, based on IBM’s Power 5+
- 100^3 Meshes



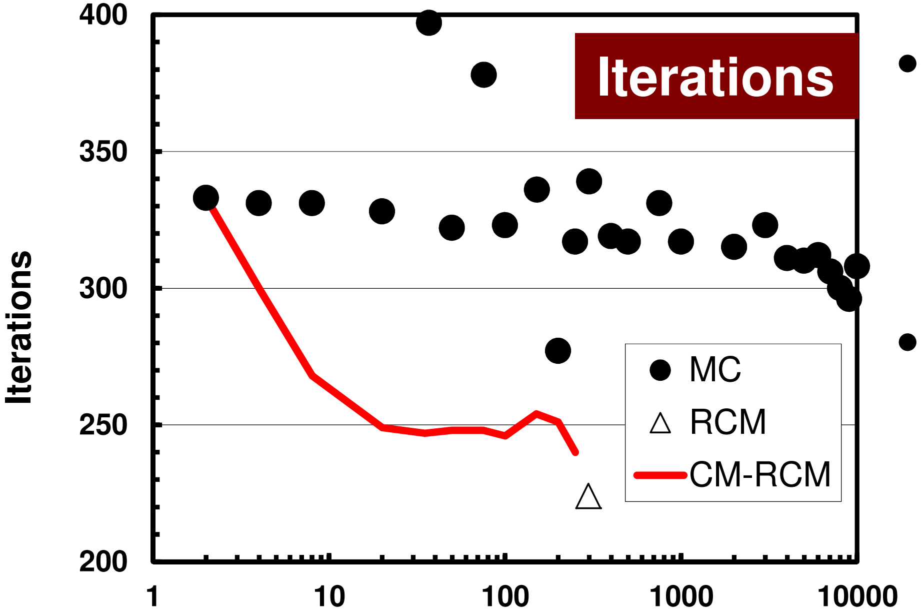
SR11000, 1-node/16-cores, 100^3

(●：MC, △：RCM, -：CM-RCM)

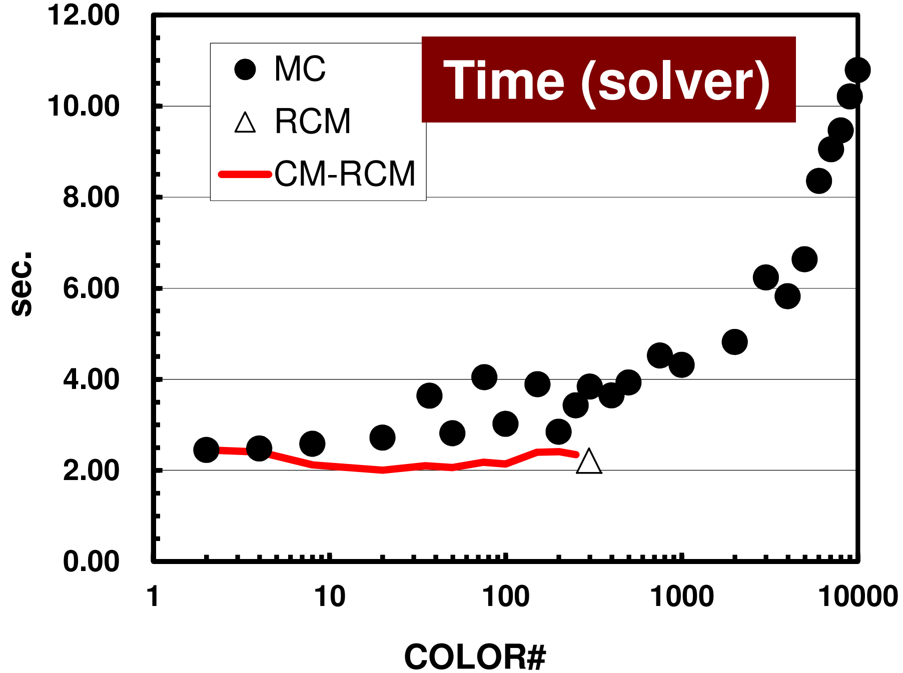


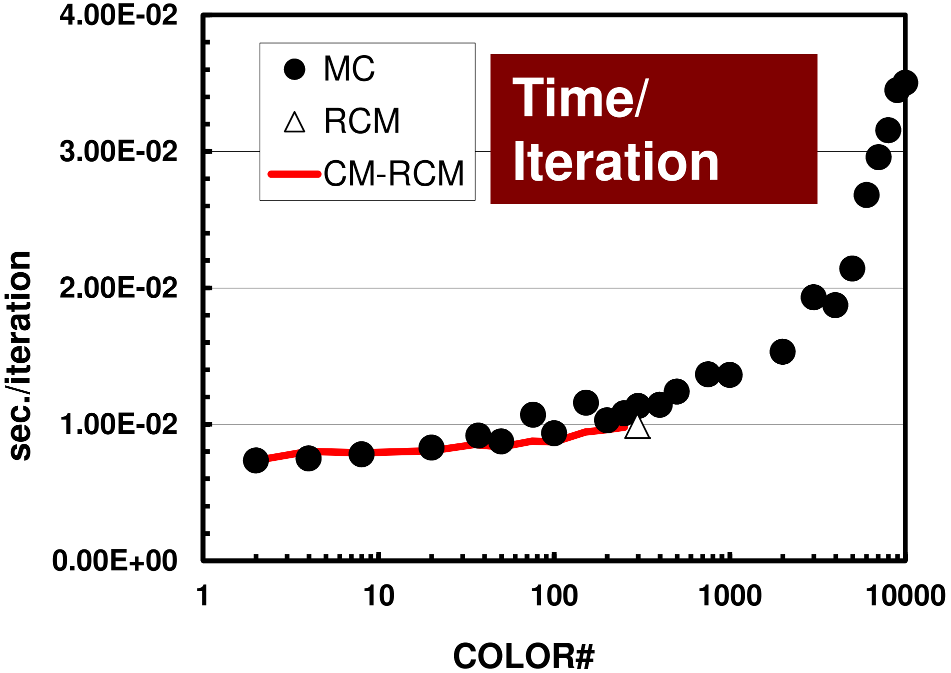
FX10, 1-node/16-cores, 100^3

（●：MC, △：RCM, -：CM-RCM）



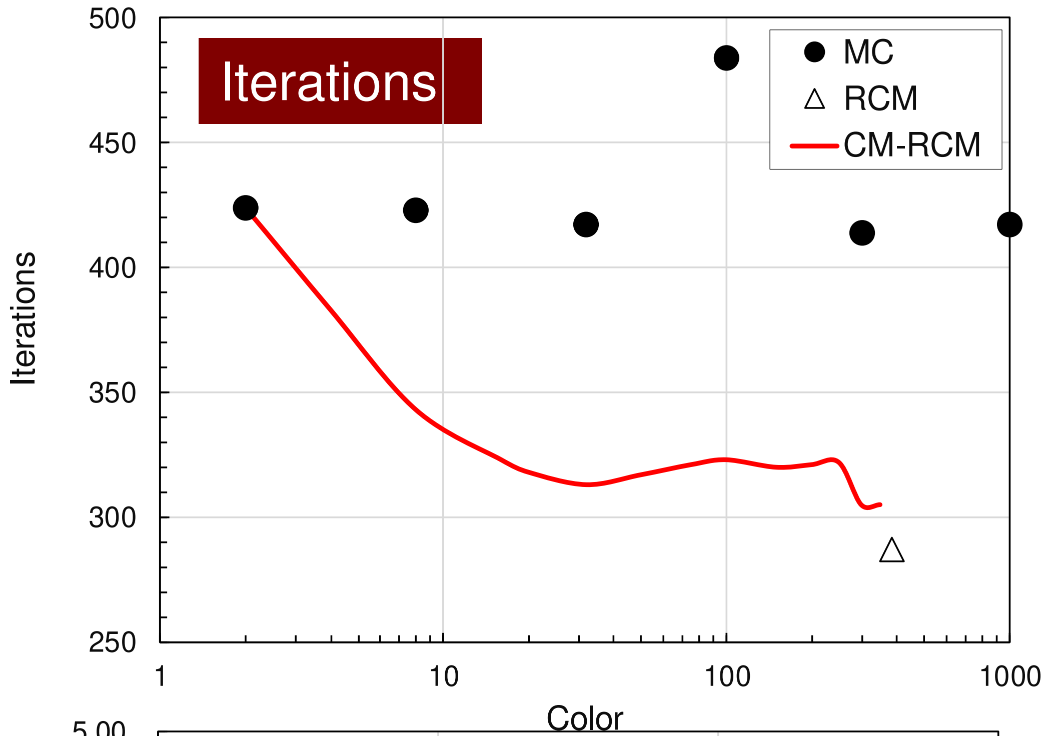
- Fujitsu PRIMEHPC FX10
  - ✓ Oakleaf-FX, Oakbridge-CX
  - ✓ Commercial Version of K
- Apr. 2012-Mar. 2018

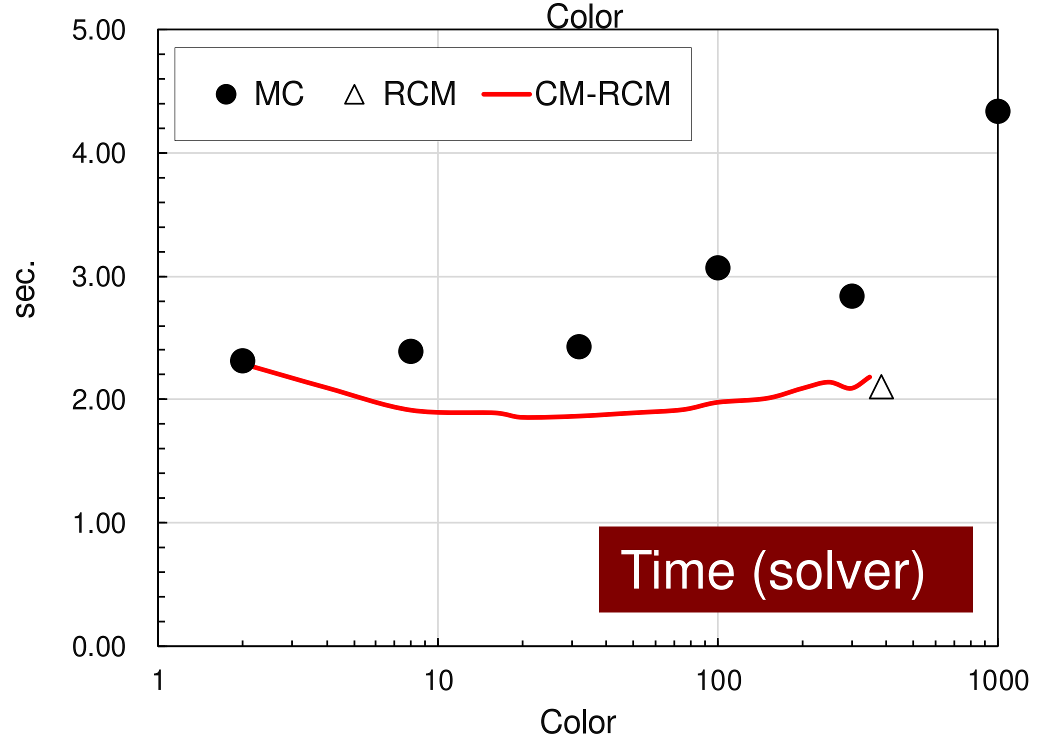


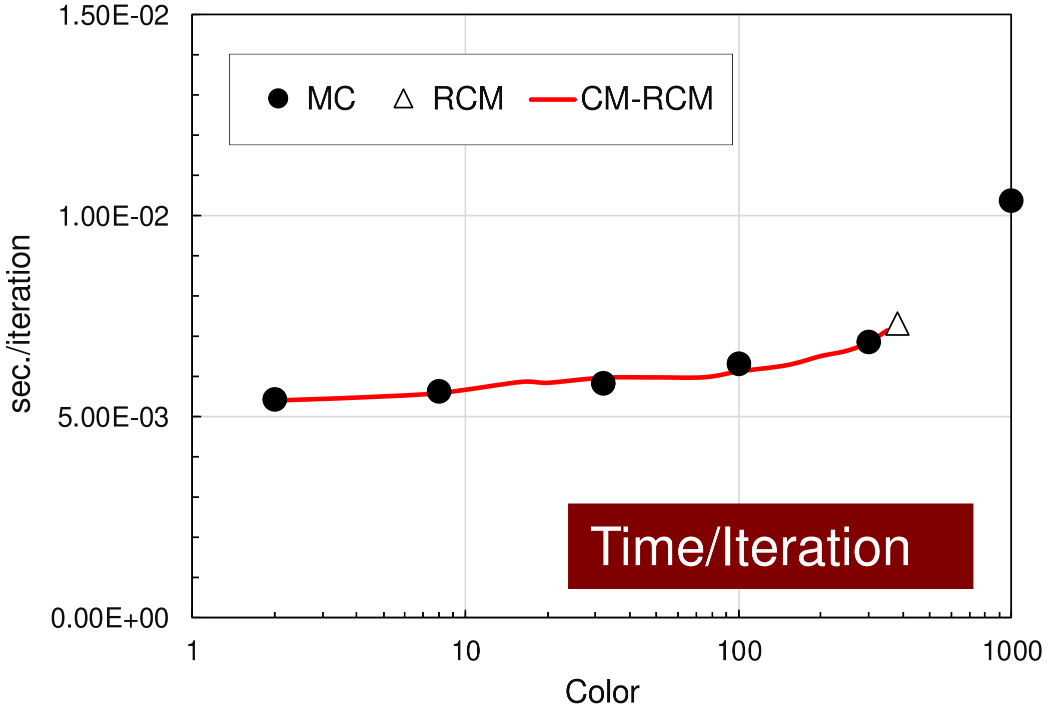


OBCX, 1-soket/24-cores, 128^3

（●：MC, △：RCM, -：CM-RCM）



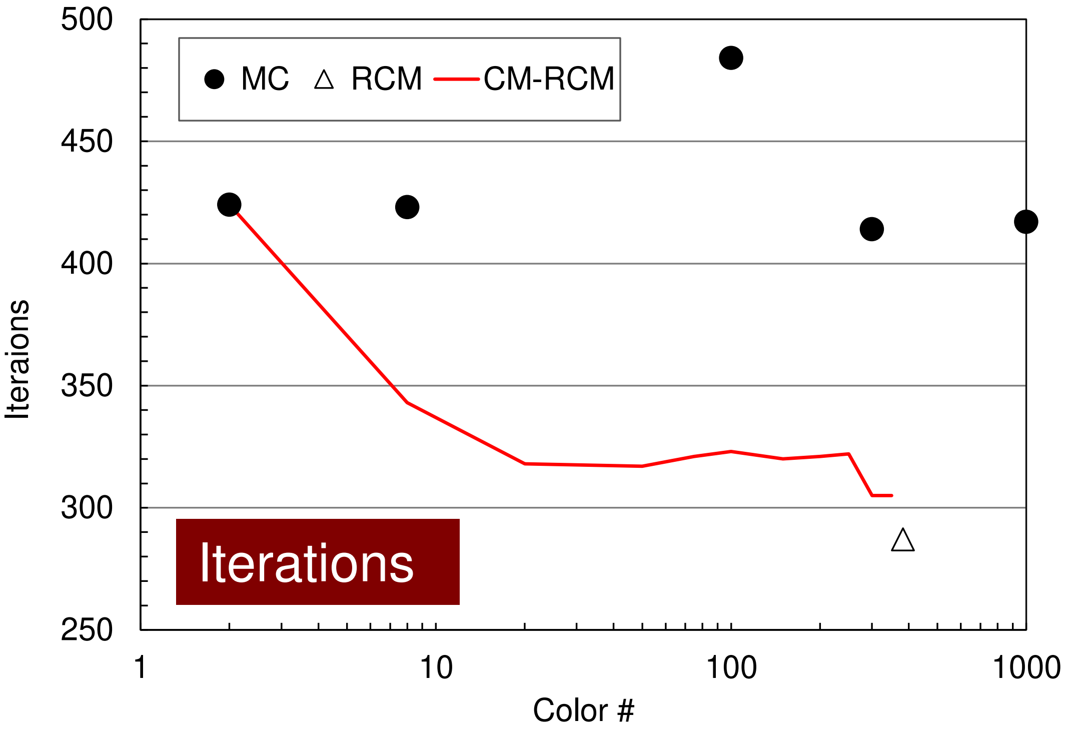


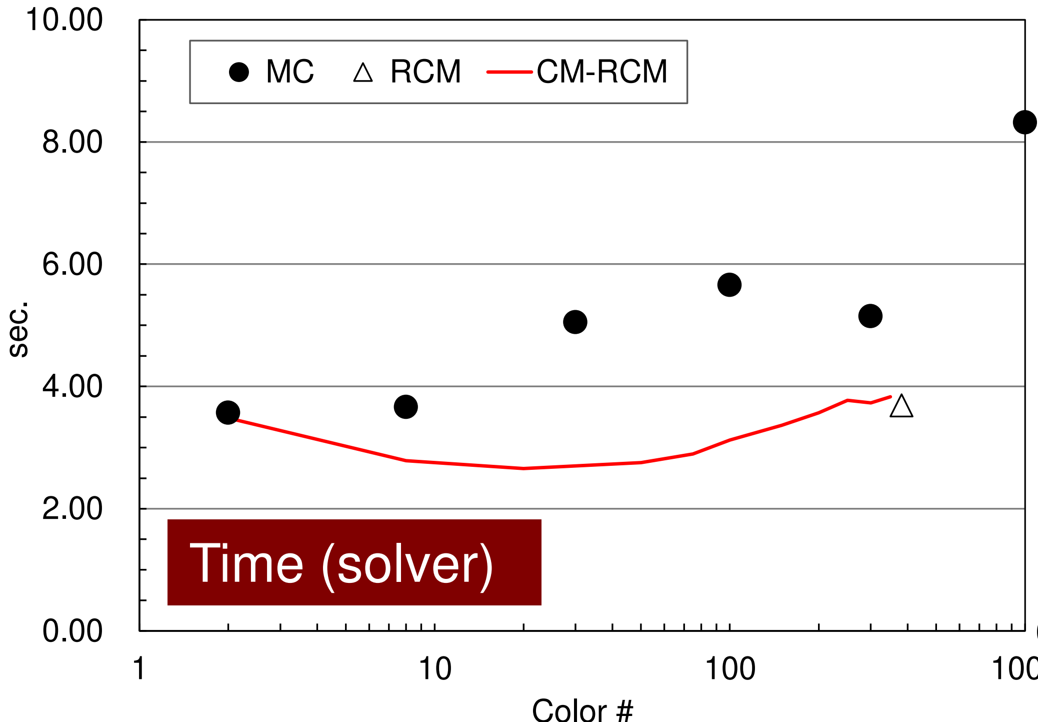


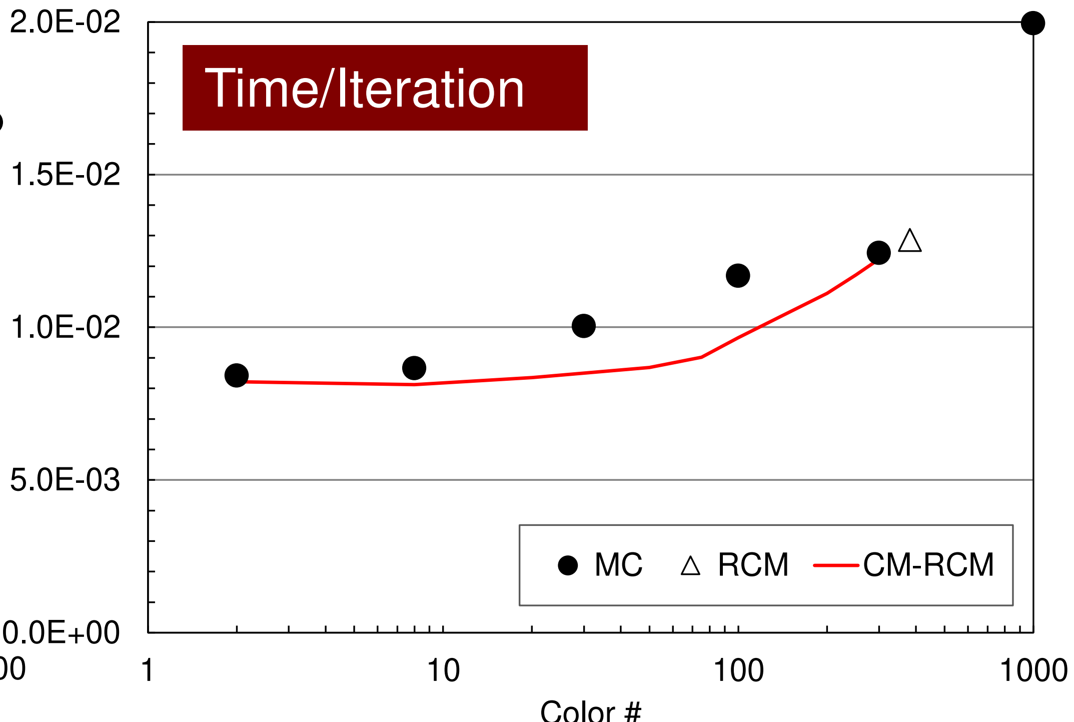
Odyssey

1-CMG/12-cores, 128^3

(●：MC, △：RCM, -：CM-RCM)







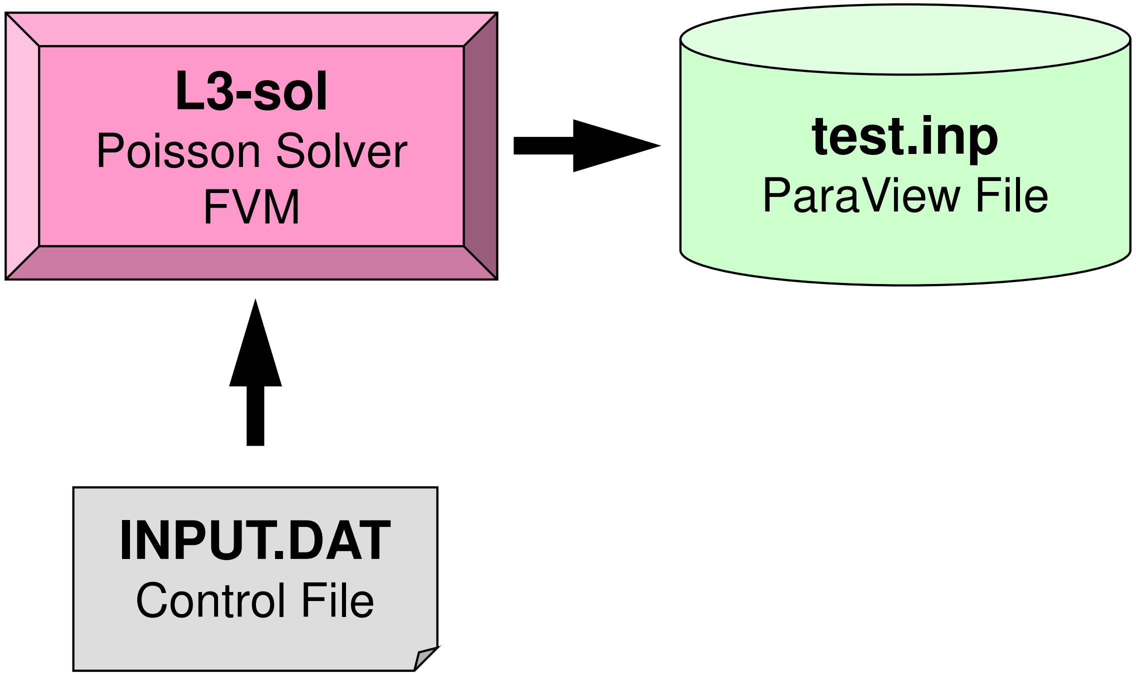
- Applying OpenMP to L2-sol
- Examples
- **Optimization + Exercise**

- Running the Code
- Further Optimization

Compile & Run

```
>$ cd /work/gt89/t89XXX/ompc/src
>$ module load fj

>$ make
>$ ls ../run/L3-sol

  L3-sol

>$ cd ../run

(modify INPUT.DAT, go1.sh)

>$ pjsub go1.sh
```

Running L3-sol



L3-sol
Poisson Solver
FVM

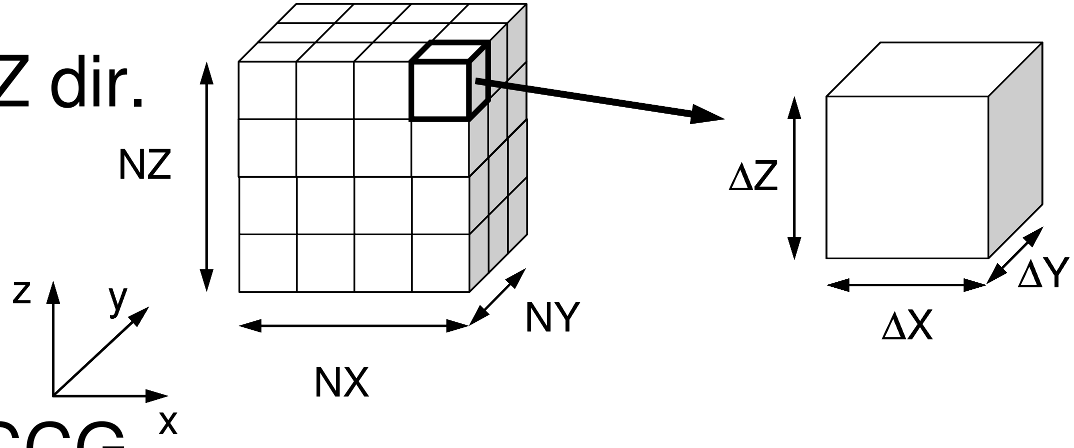
test.inp
ParaView File

INPUT.DAT
Control File

Control Data: INPUT.DAT

```
128 128 128                              NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00               DX/DY/DZ
1.0e-08                                  EPSICCG
12                                       PEsmpTOT
-10                                      NCOLORtot
```

- **NX,NY,NZ**
  - Number of meshes in X/Y/Z dir.
- **DX,DY,DZ**
  - Size of meshes
- **EPSICCG**
  - Convergence Criteria for ICCG
- **PEsmpTOT**
  - Thread Number **(--omp thread=XX)**
- **NCOLORtot**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM



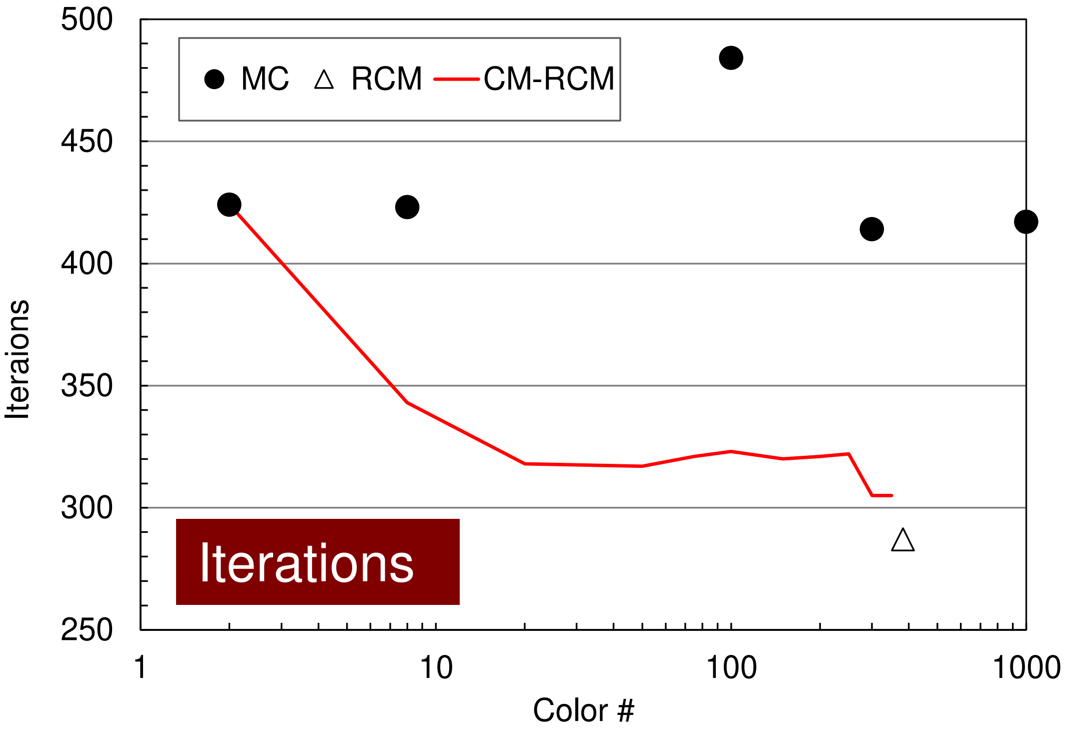
go1.sh

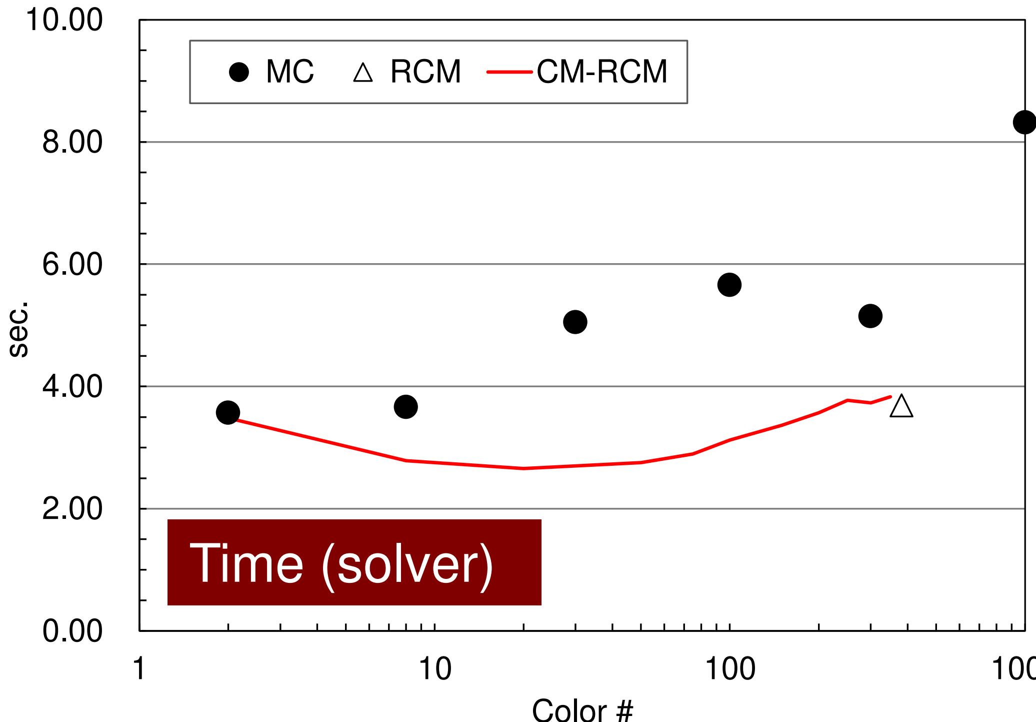
```
#!/bin/sh
#PJM -N "go1"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=12          (=PEsmpTOT)
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o test1.lst

module load fj
export OMP_NUM_THREADS=12     (=PEsmpTOT)
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl -l ./L3-sol
numactl -C 12-23 -m 4 ./L3-sol
```

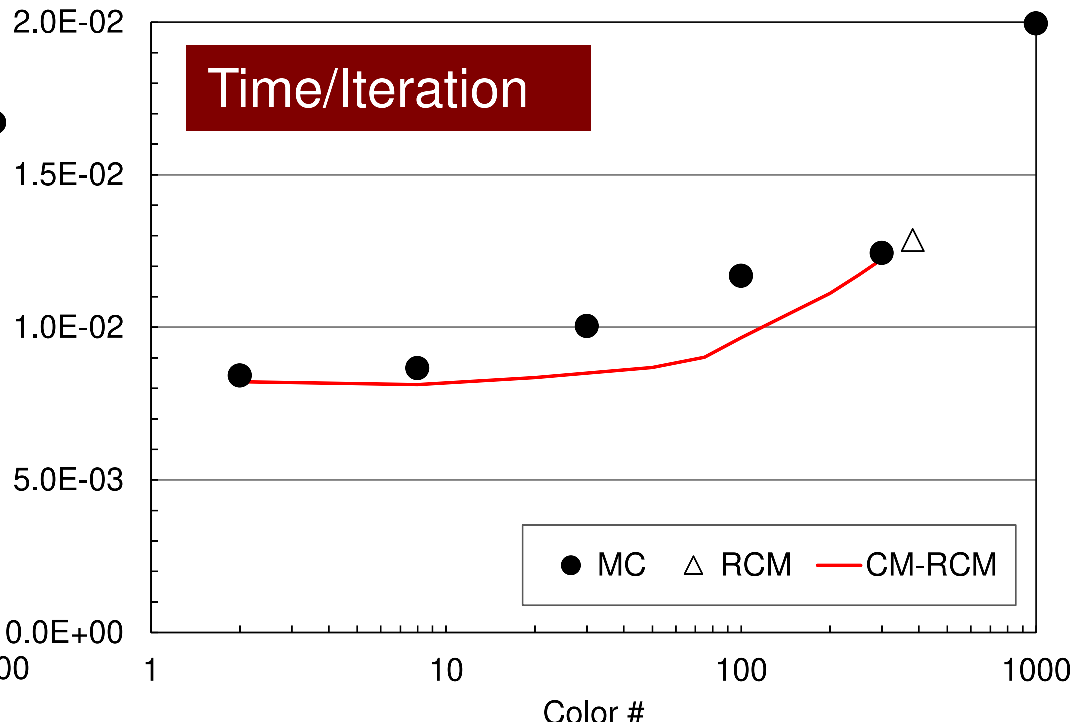
Odyssey

1-CMG/12-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)







- Running the Code
- **Further Optimization**
  - **OpenMP Statement**
  - Sequential Reordering

Forward Subst.: Current Impl. (C)

```
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp parallel for private (ip, ip1, i, WVAL, j)
        for(ip=0; ip<PEsmpTOT; ip++) {
                ip1 = ic * PEsmpTOT + ip;
                for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++){
                        WVAL = W[Z][i];
                        for(j=indexL[i]; j<indexL[i+1]; j++){
                                WVAL -= AL[j] * W[Z][itemL[j]-1];
                        }
                        W[Z][i] = WVAL * W[DD][i];
                }
        }
}
```

- At “`!omp parallel`”, generation and corruption of threads (up to 28) occurs: Fork-Join
  - In each color, this occurs
  - Some overhead
- Overhead increases, if number of color increases.

For. Subst.: Reduced Overhead (C)

```
#pragma omp parallel private (ic, ip, ip1, i, WVAL, j)
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp for
        for(ip=0; ip<PEsmpTOT; ip++) {
                ip1 = ic * PEsmpTOT + ip;
                for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++){
                        WVAL = W[Z][i];
                        for(j=indexL[i]; j<indexL[i+1]; j++){
                                WVAL -= AL[j] * W[Z][itemL[j]-1];
                        }
                        W[Z][i] = WVAL * W[DD][i];
                }
        }
}
```

- Generation of threads occurs just once before starting forward substitutions.
- Loops with “**`#pragma omp for`**” are parallelized.

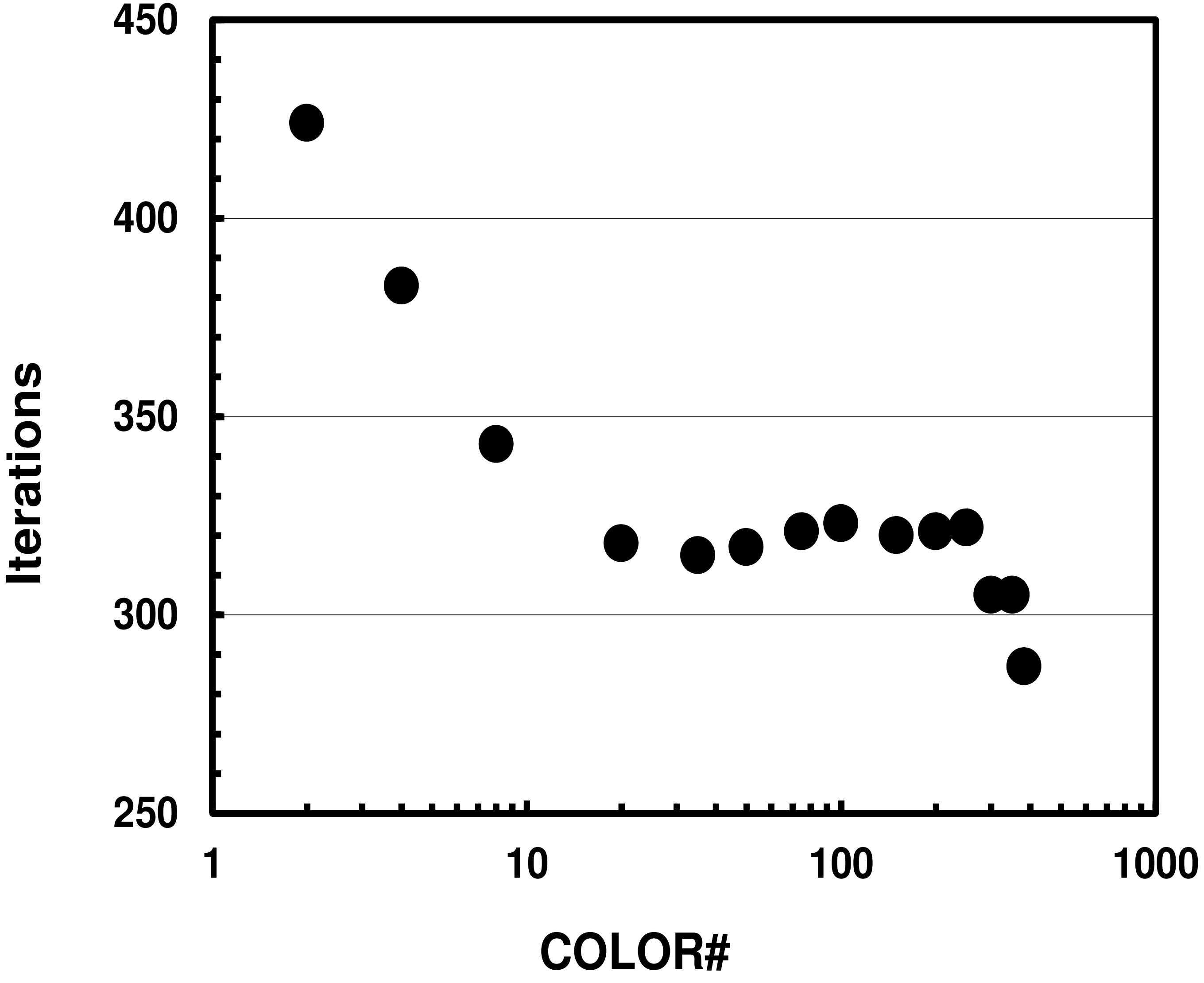
Programs (src0)

```
% cd /work/gt89/t89XXX/ompc/src0
% module load fj

% make
% cd ../run
% ls L3-sol0
    L3-sol0

<modify “INPUT.DAT”>
<modify “go0.sh”>

% pjsub go0.sh
```

go0.sh

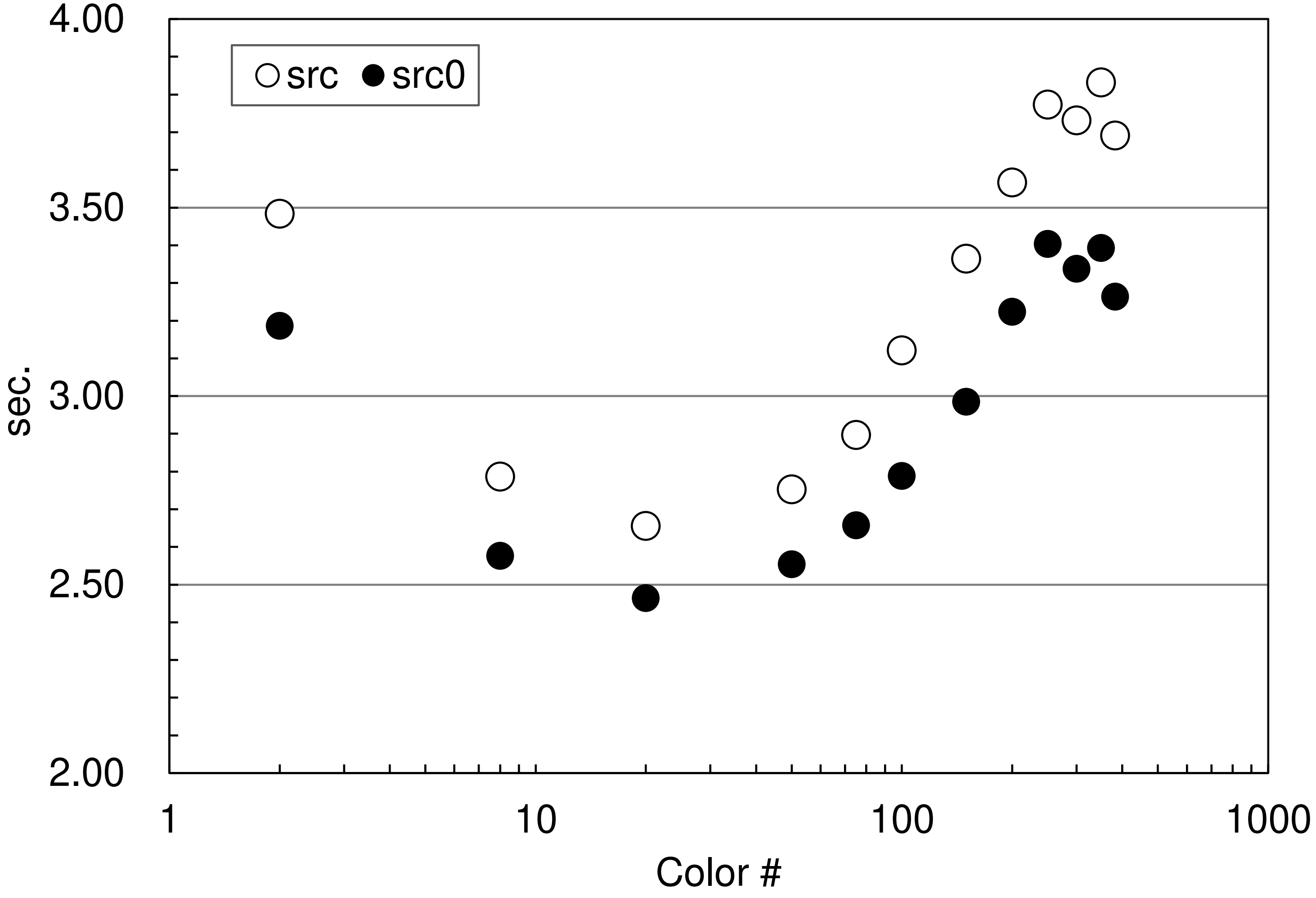
```
#!/bin/sh
#PJM -N "go0"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=12          (=PEsmpTOT)
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o test0.lst

module load fj
export OMP_NUM_THREADS=12     (=PEsmpTOT)
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl -l ./L3-sol0
numactl -C 12-23 -m 4 ./L3-sol0
```

Color#~Iterations for CM-RCM 128^3 case



Time for ICCG Solver: CM-RCM

“src” becomes slower if color# is larger: overhead of fork-join, unstable for many colors (12 threads, C)



- Running the Code
- **Further Optimization**
  - OpenMP Statement
  - **Sequential Reordering**

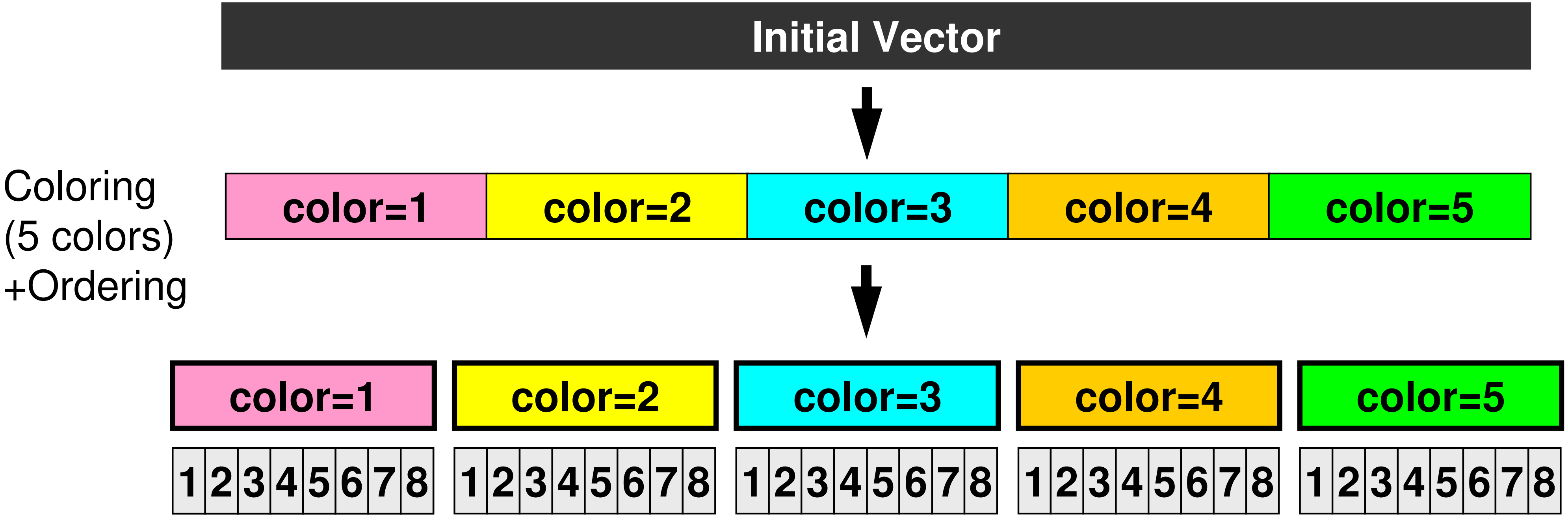
Problems in Reordering

- Coloring
  - MC
  - RCM
  - CM-RCM
- Renumbering is according to color/level ID
- On each thread, numbering is not continuous
  - reduced performance

SMPindex:

for preconditioning

```
  do ic= 1, NCOLORtot
!$omp parallel do …
    do ip= 1, PEsmpTOT
      ip1= (ic-1)*PEsmpTOT+ip
    do i= SMPindex(ip1-1)+1, SMPindex(ip1)
      (…)
    enddo
    enddo
!omp end parallel do
  enddo
```



Initial Vector

Coloring
(5 colors)
+Ordering

color=1 color=2 color=3 color=4 color=5

color=1 color=2 color=3 color=4 color=5

1 2 3 4 5 6 7 8 | 1 2 3 4 5 6 7 8 | 1 2 3 4 5 6 7 8 | 1 2 3 4 5 6 7 8 | 1 2 3 4 5 6 7 8

- 5-colors, 8-threads
- Meshes in same color are independent: parallel processing
- Reordering in ascending order according to color ID

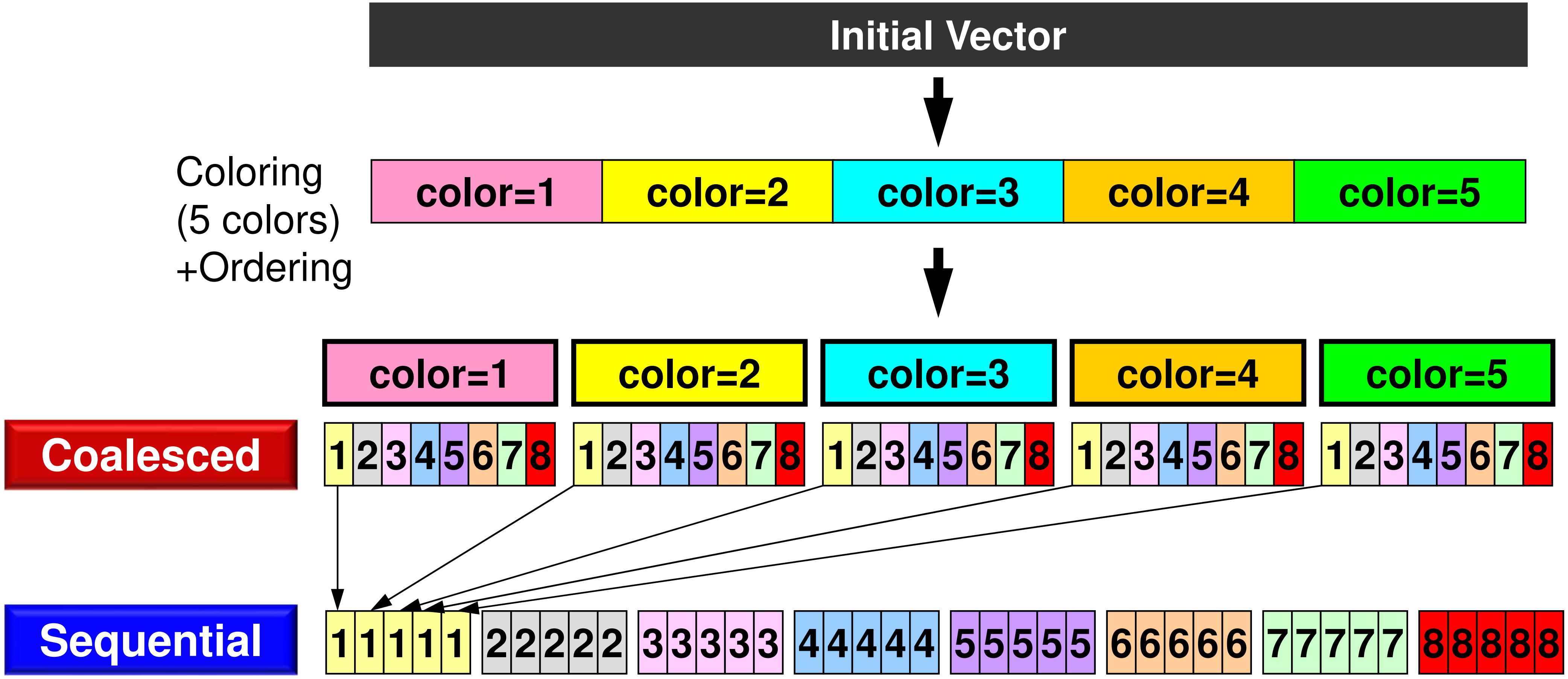
Sequential Reordering

- Reordering for continuous memory access on each thread (core)
  - Performance is expected to be better.
    - Continuous address of arrays, such as coefficient matrices
    - Locality (2-page later)

- Inconsistent numbering
  - **`itemL(k) > icel`**
  - **`indexL(icel-1)+1≦k≦indexL(icel)`**

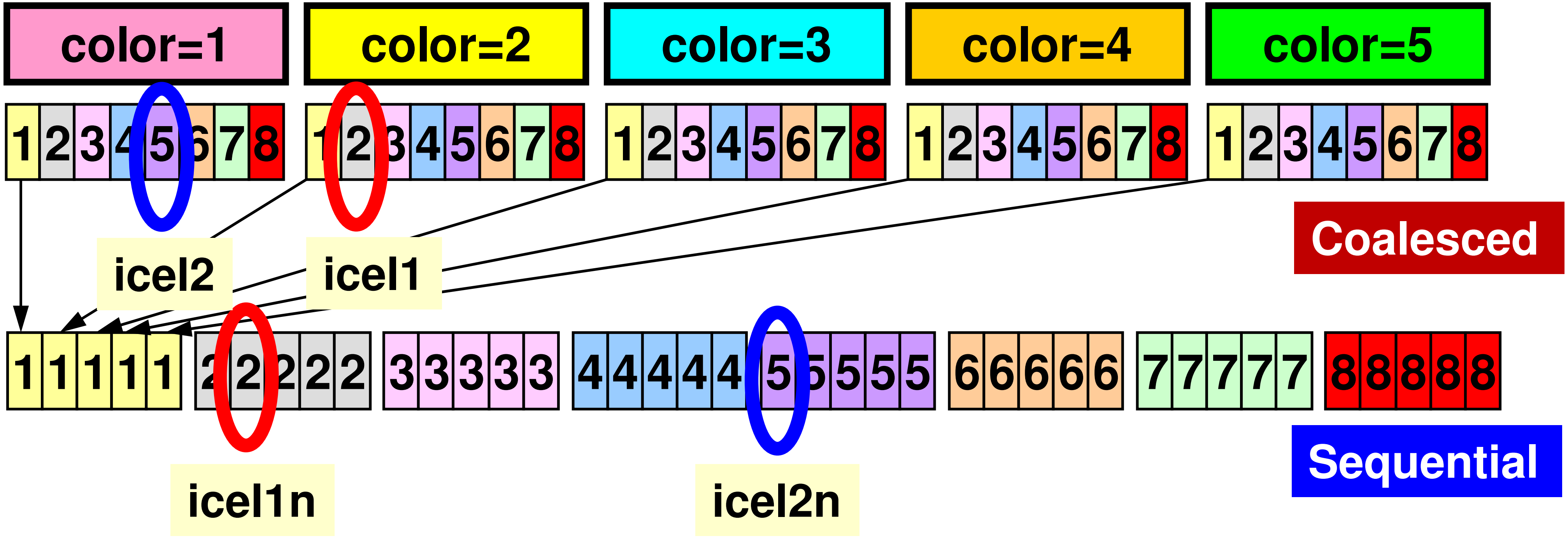
Sequential Reordering

Further reordering for continuous memory access on each thread, 5-color, 8-threads



Inconsistent numbering may occur

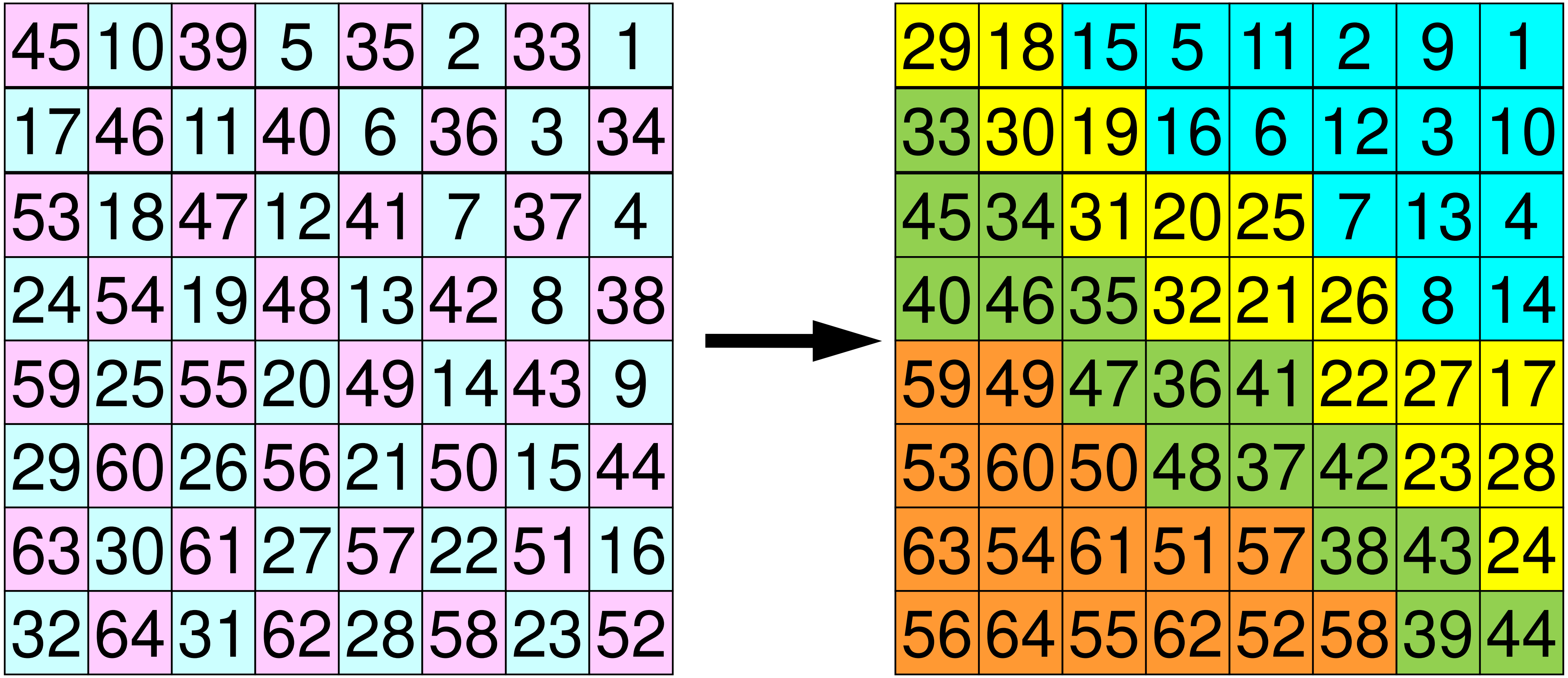
- Coalesced
  - **icel1 > icel2**, therefore, **icel2= itemL[k]**, where **indexL[icel1]≦k＜indexL[icel1+1]**
- Sequential
  - **icel1n < icel2n**, but still **icel2n= itemL[k]**, where **indexL[icel1n]≦k＜indexL[icel1n+2]**



Sequential Reordering

CM-RCM(2), 4-threads

Continuous Data Access on a Thread: Utilization of Cache, Prefetching



45	10	39	5	35	2	33	1
17	46	11	40	6	36	3	34
53	18	47	12	41	7	37	4
24	54	19	48	13	42	8	38
59	25	55	20	49	14	43	9
29	60	26	56	21	50	15	44
63	30	61	27	57	22	51	16
32	64	31	62	28	58	23	52

CM-RCM(2)

29	18	15	5	11	2	9	1
33	30	19	16	6	12	3	10
45	34	31	20	25	7	13	4
40	46	35	32	21	26	8	14
59	49	47	36	41	22	27	17
53	60	50	48	37	42	23	28
63	54	61	51	57	38	43	24
56	64	55	62	52	58	39	44

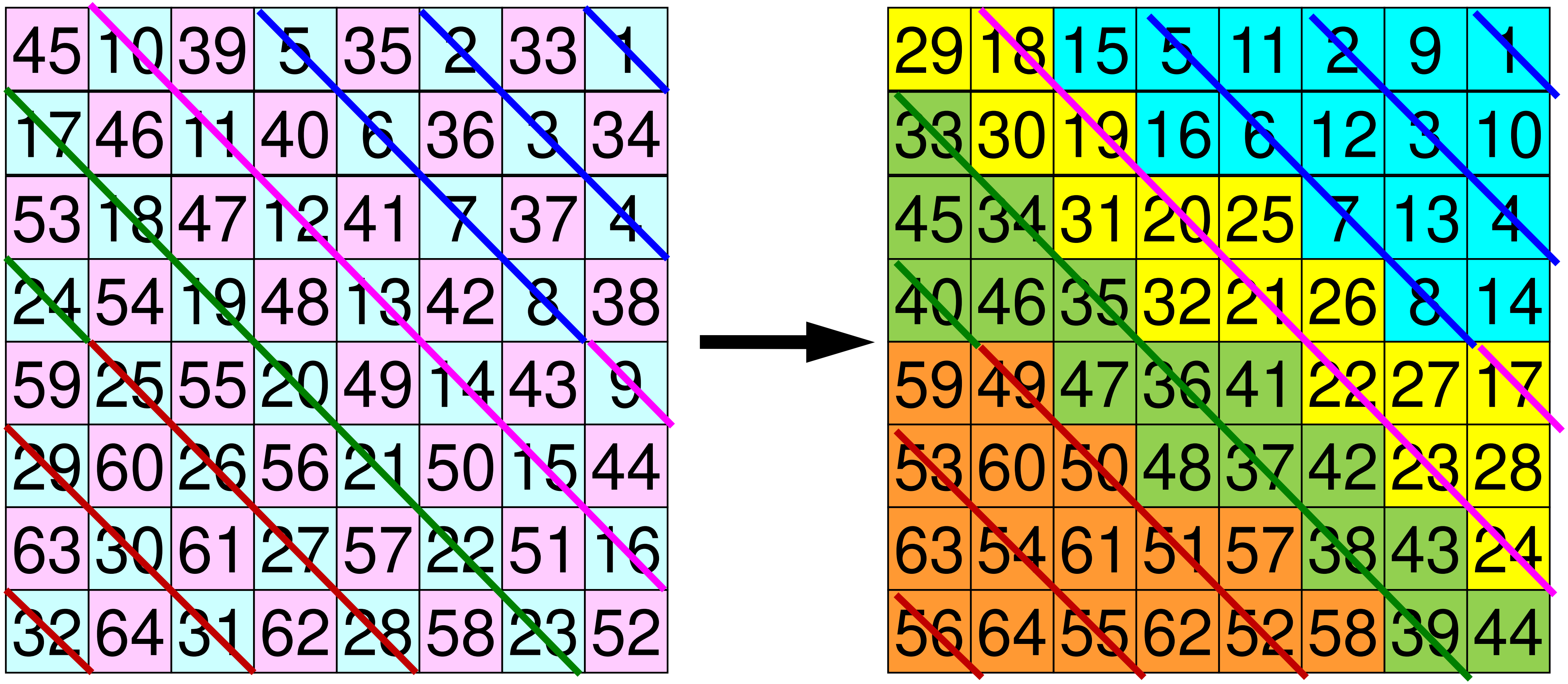
Sequential Reordering, 4-threads

Sequential Reordering

CM-RCM(2), 4-threads

1st-Color

🟦 #0 thread, 🟨 #1, 🟩 #2, 🟧 #3



45	10	39	5	35	2	33	1
17	46	11	40	6	36	3	34
53	18	47	12	41	7	37	4
24	54	19	48	13	42	8	38
59	25	55	20	49	14	43	9
29	60	26	56	21	50	15	44
63	30	61	27	57	22	51	16
32	64	31	62	28	58	23	52

CM-RCM(2)

29	18	15	5	11	2	9	1
33	30	19	16	6	12	3	10
45	34	31	20	25	7	13	4
40	46	35	32	21	26	8	14
59	49	47	36	41	22	27	17
53	60	50	48	37	42	23	28
63	54	61	51	57	38	43	24
56	64	55	62	52	58	39	44

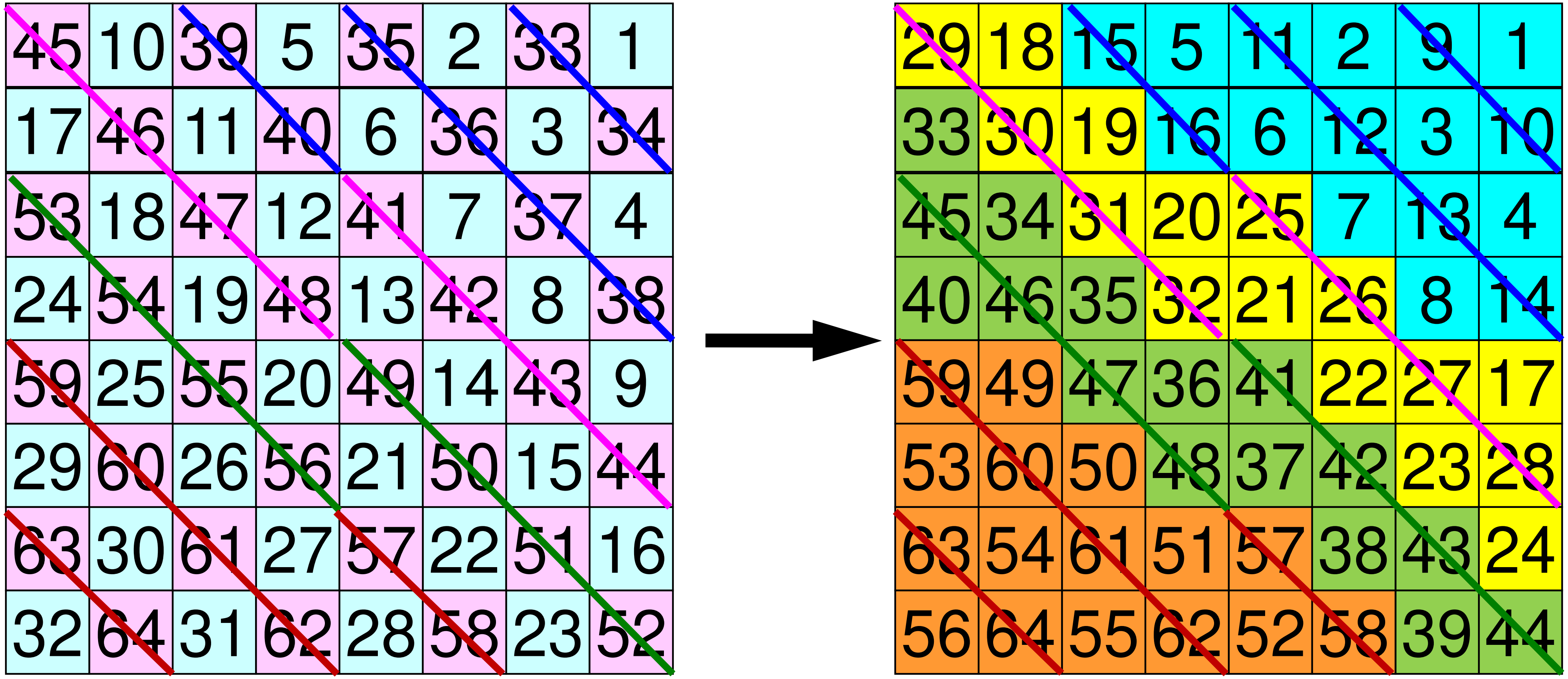
Sequential Reordering, 4-threads

Sequential Reordering

CM-RCM(2), 4-threads

2nd-Color

🟦 #0 thread, 🟨 #1, 🟩 #2, 🟧 #3



45	10	39	5	35	2	33	1
17	46	11	40	6	36	3	34
53	18	47	12	41	7	37	4
24	54	19	48	13	42	8	38
59	25	55	20	49	14	43	9
29	60	26	56	21	50	15	44
63	30	61	27	57	22	51	16
32	64	31	62	28	58	23	52

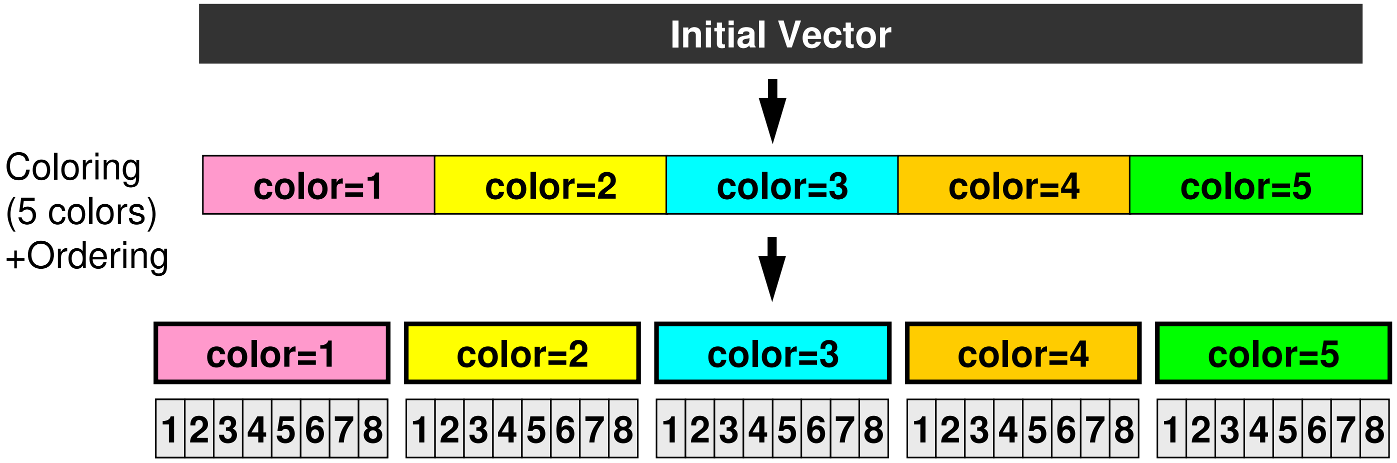
CM-RCM(2)

29	18	15	5	11	2	9	1
33	30	19	16	6	12	3	10
45	34	31	20	25	7	13	4
40	46	35	32	21	26	8	14
59	49	47	36	41	22	27	17
53	60	50	48	37	42	23	28
63	54	61	51	57	38	43	24
56	64	55	62	52	58	39	44

Sequential Reordering, 4-threads

Sequential Reordering

Coalesced Good for GPU



Initial Vector

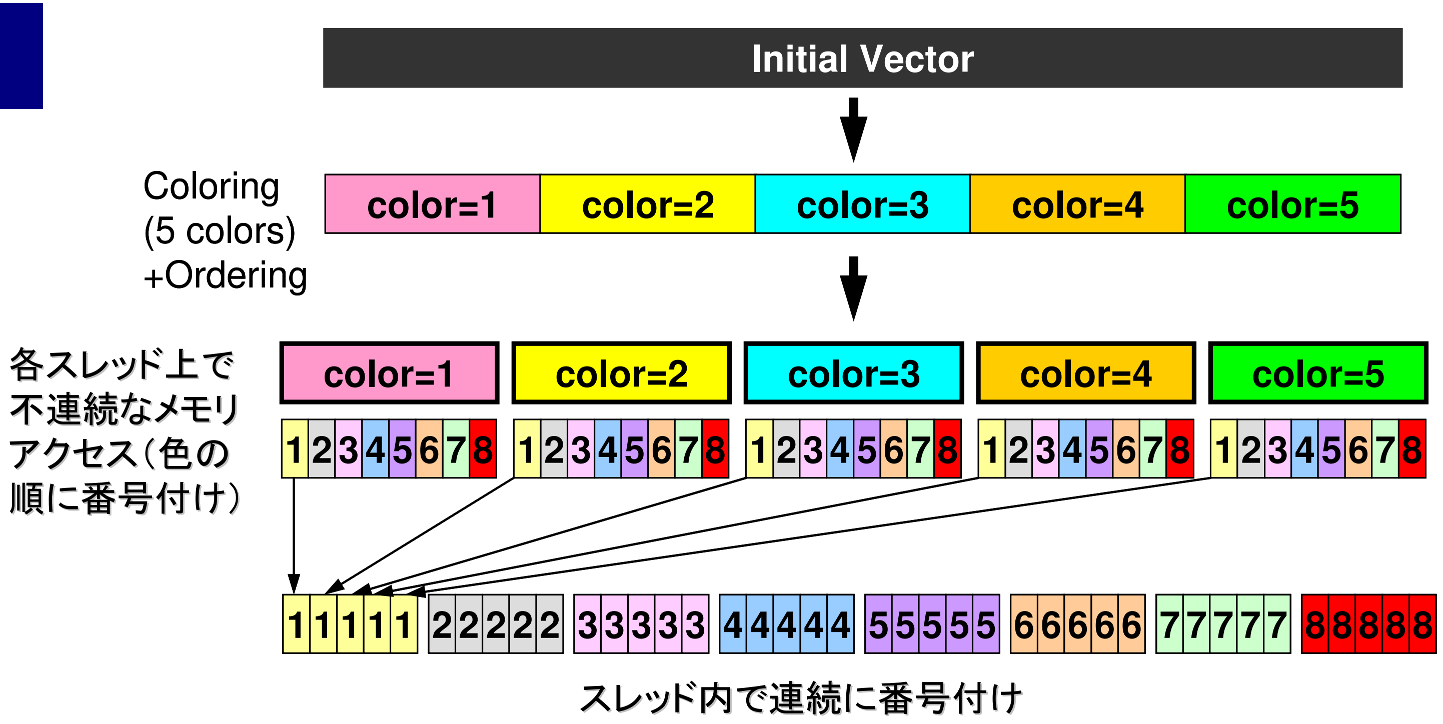
Coloring (5 colors) +Ordering

color=1 color=2 color=3 color=4 color=5

color=1 color=2 color=3 color=4 color=5

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

Sequential



Initial Vector

Coloring (5 colors) +Ordering

color=1 color=2 color=3 color=4 color=5

各スレッド上で不連続なメモリアクセス（色の順に番号付け）

color=1 color=2 color=3 color=4 color=5

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

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

スレッド内で連続に番号付け

Programs (reorder0)

```
% cd /work/gt89/t89XXX/ompc/reorder0
% module load fj

% make
% cd ../run
% ls L3-rsol0
    L3-rsol0

<modify "INPUT.DAT">
<modify "gor.sh">

% pjsub gor.sh
```

gor.sh

```
#!/bin/sh
#PJM -N "gor"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=12           (=PEsmpTOT)
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o testr.lst

module load fj
export OMP_NUM_THREADS=12      (=PEsmpTOT)
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl -l ./L3-rsol0
numactl -C 12-23 -m 4 ./L3-rsol0
```

INPUT.DAT

```
128 128 128                             NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00              DX/DY/DZ
1.0e-08                                 EPSICC
12                                      PEsmpTOT
-10                                     NCOLORtot
0                                       NFLAG
0                                       METHOD
```

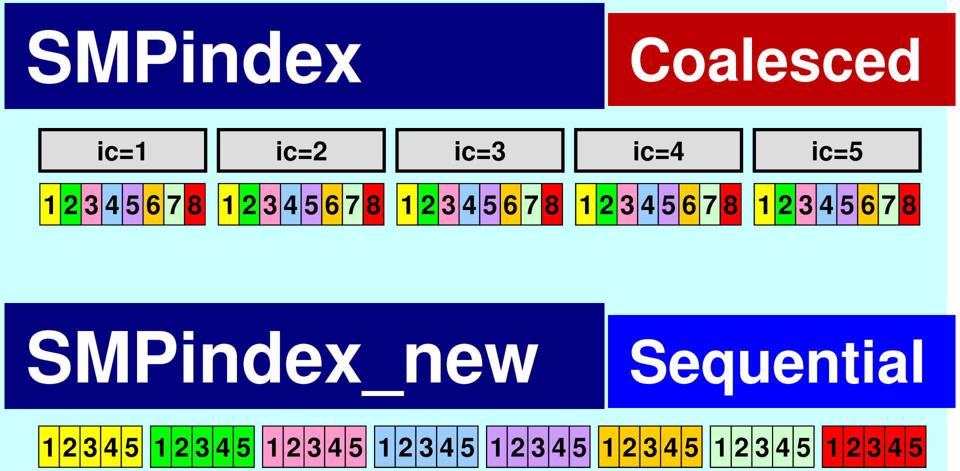
- **`PEsmpTOT`**
  - Thread Number **`(--omp thread=XX)`**
- **`NCOLORtot`**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM
- **`NFLAG`**
  - =0: without first-touch, =1: with first-touch
- **`METHOD`**
  - Loop structure for Mat-Vec
  - =0: conventional way, =1: similar to forward/backward substitution

Sequential Reordering (1/5) Main

```c
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>

#include "struct.h"
#include "pcg.h"
(…)

int main(){
        double *WK;
        int ISET, ITR, IER;
        int icel, ic0, i;
        double Stime, Etime;

        if(INPUT()) goto error;
        if(POINTER_INIT()) goto error;
        if(BOUNDARY_CELL()) goto error;
        if(CELL_METRICS()) goto error;
        if(POI_GEN()) goto error;

        ISET = 0;
        if(METHOD == 0 ){
                if(solve_ICCG_mc(ICELTOT, NL, NU, indexLnew, itemLnew,
                        indexUnew, itemUnew, D, BFORCE, PHI, ALnew, AUnew,
                        NCOLORtot, PEsmpTOT, SMPindex_new, EPSICCG,
                        &ITR, &IER)) goto error;
        }else if (METHOD == 1){
                if(solve_ICCG_mc_ft(ICELTOT, NL, NU, indexLnew, itemLnew,
                        indexUnew, itemUnew, D, BFORCE, PHI, ALnew, AUnew,
                        NCOLORtot, PEsmpTOT, SMPindex_new, EPSICCG,
                        &ITR, &IER)) goto error;
        }

        for(ic0=0; ic0<ICELTOT; ic0++){
                icel = NEWtoOLDnew[ic0];
                WK[icel-1] = PHI[ic0];
        }
        for(icel=0; icel<ICELTOT; icel++){
                PHI[icel] = WK[icel];
        }

        if(OUTUCD()) goto error;
        return 0;

error:
        return -1;
}
```

Sequential Reordering (2/5) poi_gen-1

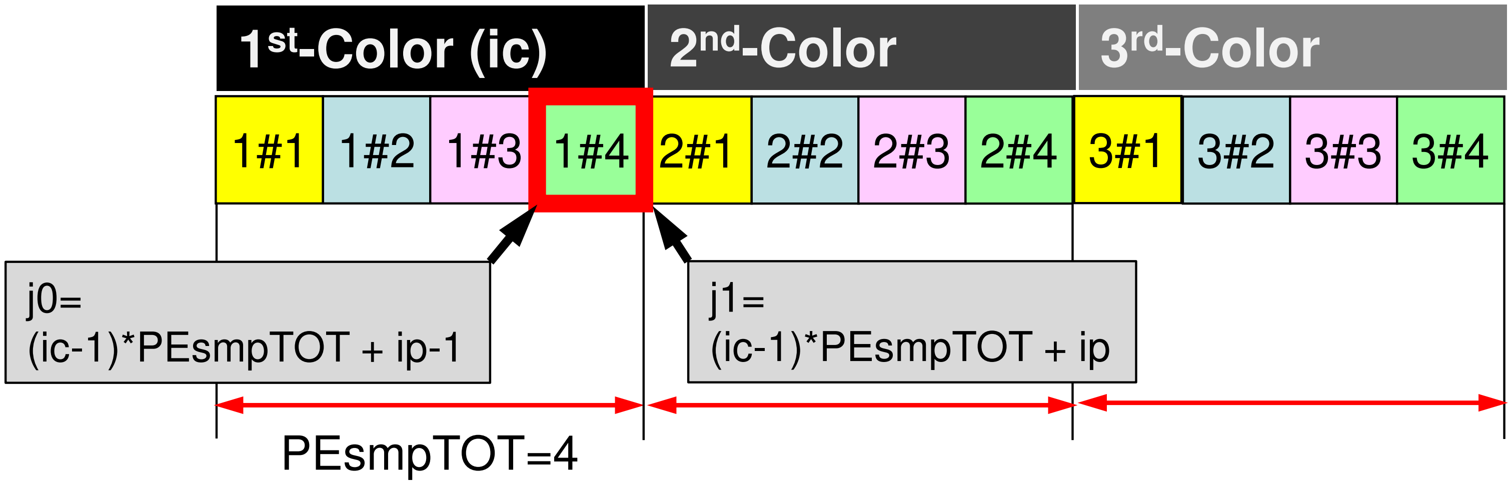
```
SMPindex = (int *) allocate_vector(sizeof(int), NCOLORtot * PEsmpTOT + 1);
memset(SMPindex, 0, sizeof(int)*(NCOLORtot*PEsmpTOT+1));

for(ic=1; ic<=NCOLORtot; ic++) {
    nn1 = COLORindex[ic] - COLORindex[ic-1];
    num = nn1 / PEsmpTOT;
    nr  = nn1 - PEsmpTOT * num;
    for(ip=1; ip<=PEsmpTOT; ip++) {
        if(ip <= nr) {
           SMPindex[(ic-1)*PEsmpTOT+ip] = num + 1;
        } else {
           SMPindex[(ic-1)*PEsmpTOT+ip] = num;
        }
    }
}

SMPindex_new = (int *) allocate_vector(sizeof(int), NCOLORtot * PEsmpTOT + 1);
memset(SMPindex_new, 0, sizeof(int)*(NCOLORtot*PEsmpTOT+1));

for(ic=1; ic<=NCOLORtot; ic++) {
    for(ip=1; ip<=PEsmpTOT; ip++) {
        j1 =(ic-1)*PEsmpTOT + ip;
        j0 =j1-1;
        SMPindex_new[(ip-1)*NCOLORtot+ic] = SMPindex[j1];
        SMPindex[j1] = SMPindex[j0] + SMPindex[j1];
    }
}

for(ip=1; ip<=PEsmpTOT; ip++) {
    for(ic=1; ic<=NCOLORtot; ic++) {
        j1 = (ip-1) * NCOLORtot + ic;
        j0 = j1 - 1;
        SMPindex_new[j1] += SMPindex_new[j0];
    }
}
```



ic#ip

ic: 1~ NCOLORtot
ip: 1~ PEsmpTOT

SMPindex



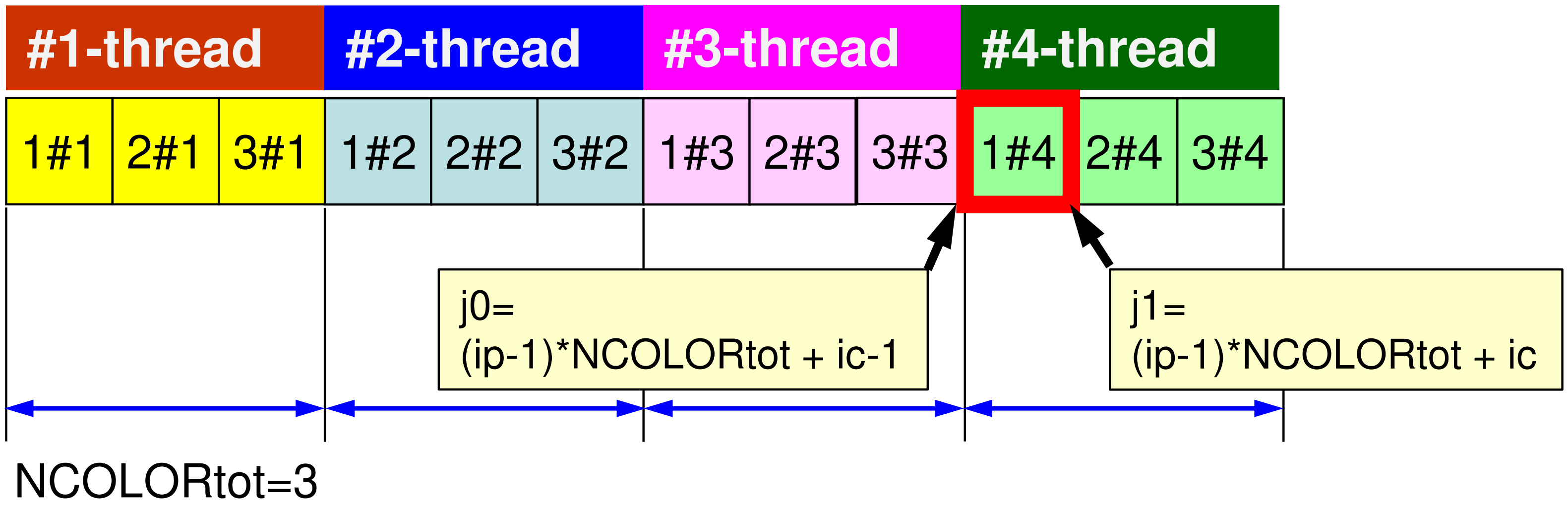
1st-Color (ic)				2nd-Color				3rd-Color			
1#1	1#2	1#3	1#4	2#1	2#2	2#3	2#4	3#1	3#2	3#3	3#4

j0=
(ic-1)*PEsmpTOT + ip-1

j1=
(ic-1)*PEsmpTOT + ip

PEsmpTOT=4

SMPindex_new



#1-thread			#2-thread			#3-thread			#4-thread		
1#1	2#1	3#1	1#2	2#2	3#2	1#3	2#3	3#3	1#4	2#4	3#4

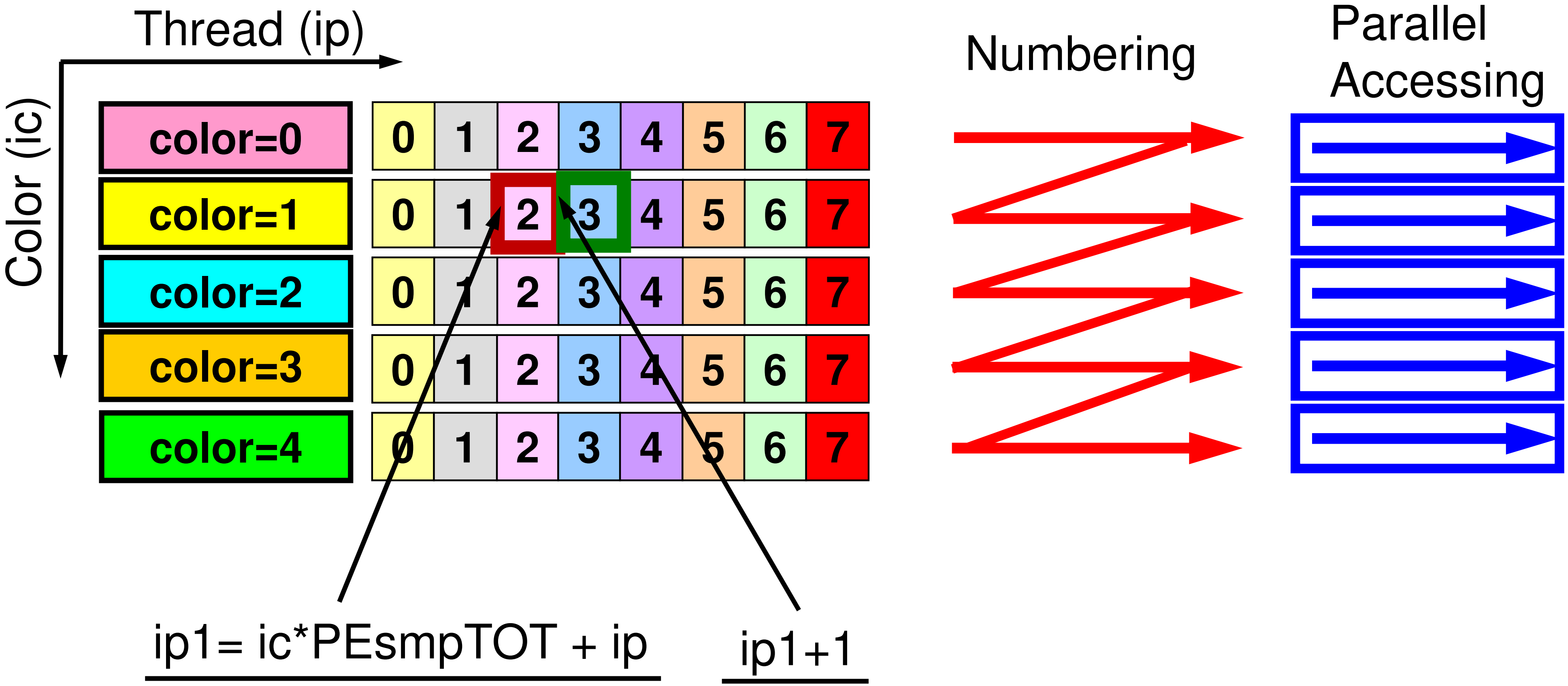
j0=
(ip-1)*NCOLORtot + ic-1

j1=
(ip-1)*NCOLORtot + ic

NCOLORtot=3

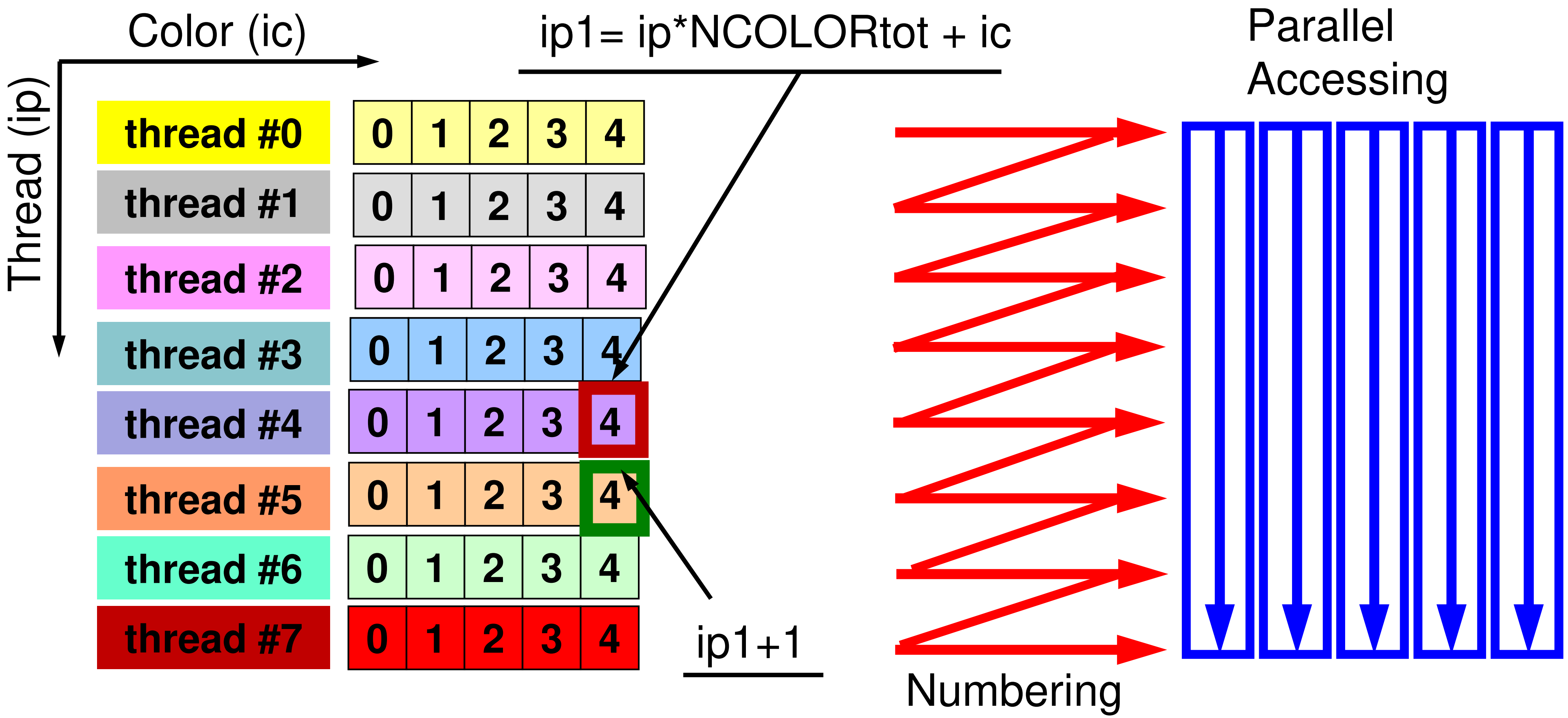
Coalesced

```
#pragma omp parallel private (ic,ip,ip1,i,WVAL,j)
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp for
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {…
```



Sequential

```
#pragma omp parallel private (ic, ip, ip1, i, WVAL, j)
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp for
   for(ip=0; ip<PEsmpTOT; ip++) {
       ip1 = ip * NCOLORtot + ic;
       for(i=SMPindex_new[ip1]; i<SMPindex_new[ip1+1]; i++) {…
```



Sequential Reordering (3/5) poi_gen-2

```
for(ip=0; ip<PEsmpTOT; ip++){
    for(ic=0; ic<NCOLORtot; ic++){
        icNS = SMPindex_new[ip*NCOLORtot + ic];
        ic01 = SMPindex[ic*PEsmpTOT + ip];
        ic02 = SMPindex[ic*PEsmpTOT + ip+1];
        icou = 0;
        for(k=ic01; k<ic02; k++){
            icel=NEWtoOLD[k];
            icou = icou +1;
            icelN=icNS+icou;
            OLDtoNEWnew[icel-1] = icelN;
            NEWtoOLDnew[icelN-1]= icel;
        }
    }
}
```

OLDtoNEWnew: Original -> Sequential
NEWtoOLDnew: Sequential -> Original
-Original: Initial icel
-Sequential icelN

```
indexLnew = (int *)allocate_vector(sizeof(int),ICELTOT+1);
indexUnew = (int *)allocate_vector(sizeof(int),ICELTOT+1);
INLnew = (int *)allocate_vector( sizeof(int),ICELTOT);
INUnew = (int *)allocate_vector( sizeof(int),ICELTOT);
indexLnew_org = (int *)allocate_vector(sizeof(int),ICELTOT+1);
indexUnew_org = (int *)allocate_vector(sizeof(int),ICELTOT+1);

for(ip=1; ip<=PEsmpTOT; ip++) {
    id1 = ip     *NCOLORtot;
    id2 = (ip-1)*NCOLORtot;

    for(icel=SMPindex_new[id2]+1; icel<=SMPindex_new[id1]; icel++) {
        ic0  = NEWtoOLDnew[icel-1];
        ik0  = OLDtoNEW[ic0-1];
        INLnew[icel-1] =INL[ik0-1];
        INUnew[icel-1] =INU[ik0-1];
    }
}
```

Sequential **Coalesced**

-Original: Initial ic0
-Coalesced ik0
-Sequential icel

```
for(i=1; i<=ICELTOT; i++){
    indexLnew_org[i]=indexLnew_org[i-1]+INLnew[i-1];
    indexUnew_org[i]=indexUnew_org[i-1]+INUnew[i-1];
}
```

Sequential Reordering (4/5) poi_gen-3

```
/************
* ARRAY init.
*************/
        if(NFLAG == 0){
                for(i=0; i<ICELTOT; i++) {
                        BFORCE[i] = 0.0;
                        D[i]      = 0.0;
                        PHI[i]    = 0.0;
                }
                for(i=0; i<=ICELTOT; i++) {
                        indexLnew[i] = indexLnew_org[i];
                        indexUnew[i] = indexUnew_org[i];

                }
                for(i=0; i<NPL; i++) {
                        itemLnew[i] = 0;
                        ALnew[i] = 0.0;
                }
                for(i=0; i<NPU; i++) {
                        itemUnew[i] = 0;
                        AUnew[i] = 0.0;
                }

        }else {
                indexLnew[0]=0;
                indexUnew[0]=0;
#pragma omp parallel for private (icel, j)
                for(ip=1; ip<=PEsmpTOT; ip++){
                        for(icel = SMPindex_new[(ip-1)*NCOLORtot]+1; icel<=SMPindex_new[ip*NCOLORtot]; icel++){
                                BFORCE[icel-1] = 0.0;
                                PHI[icel-1] = 0.0;
                                D[icel-1] = 0.0;
                                indexLnew[icel]=indexLnew_org[icel];
                                indexUnew[icel]=indexUnew_org[icel];

                                for(j=indexLnew_org[icel-1];j<indexLnew_org[icel];j++){
                                        itemLnew[j]=0;
                                        ALnew[j] = 0.0;
                                }
                                for(j=indexUnew_org[icel-1];j<indexUnew_org[icel];j++){
                                        itemUnew[j]=0;
                                        AUnew[j] = 0.0;
                                }
                        }
                }
        }
```

Sequential Reordering (5/5) poi_gen-4

```
#pragma omp parallel for private (icel, id1, id2 …)
for(ip=1; ip<=PEsmpTOT; ip++) {
    id1= ip    *NCOLORtot; id2= (ip-1)*NCOLORtot;
    for(icel=SMPindex_new[id2]+1; icel<=SMPindex_new[id1]; icel++) {
        ic0   = NEWtoOLDnew[icel-1];
        ik0   = OLDtoNEW[ic0-1];
        icN10 = NEIBcell[ic0-1][0];
(…)

        icN50 = NEIBcell[ic0-1][4];
        icN60 = NEIBcell[ic0-1][5];
        isL=indexL[ik0-1]; ieL=indexL[ik0  ];
        isU=indexU[ik0-1]; ieU=indexU[ik0  ];

        if(icN50 != 0) {
           icN5 = OLDtoNEW[icN50-1];
           coef = RDZ * ZAREA;
           D[icel-1] -= coef;
           if(icN5 < ik0) {
              for(j=isL; j<ieL; j++) {
                  if(itemL[j] == icN5) {
                     j_new=indexLnew[icel-1]+j-isL;
                     ALnew[j_new]     = coef;
                     itemLnew[j_new] = OLDtoNEWnew[icN50-1];
                     break;
                  }
              }
           } else {
              for(j=isU; j<ieU; j++) {
                  if(itemU[j] == icN5) {
                     j_new=indexUnew[icel-1]+j-isU;
                     AUnew[j_new] = coef;
                     itemUnew[j_new] = OLDtoNEWnew[icN50-1];
                     break;
                  }
              }
           }
    }
```

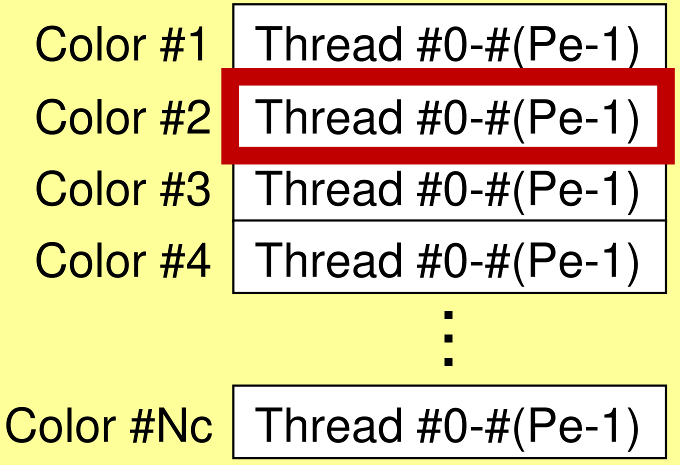
icel: Sequential
ic0: Original
ik0: Coalesced

icN50: Original
icN5 : Coalesced

icN5>ik0: Upper (AU)
icN5<ik0: Lower (AL)

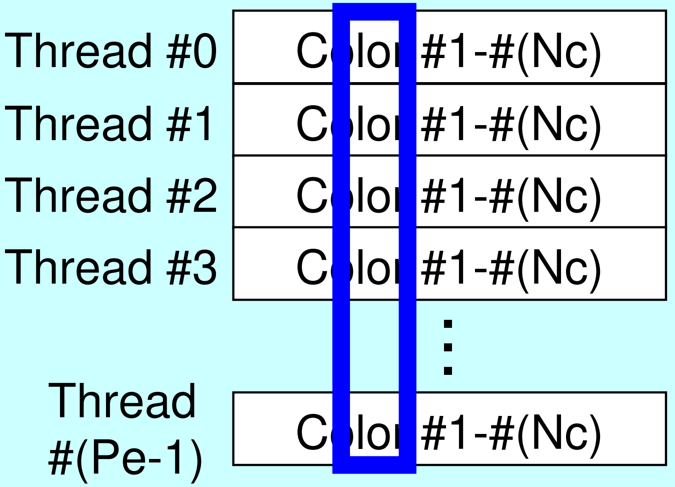
Forward Substitution

```
#pragma omp parallel private (ic,ip,ip1,i,WVAL,j)
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp for
    for(ip=0; ip<PEsmpTOT; ip++) {
        ip1 = ic * PEsmpTOT + ip;
        for(i=SMPindex[ip1]; i<SMPindex[ip1+1]; i++) {
            WVAL = W[Z][i];
            for(j=indexL[i]; j<indexL[i+1]; j++) {
                WVAL -= AL[j] * W[Z][itemL[j]-1];
            }
            W[Z][i] = WVAL * W[DD][i];
        }
    }
}
```



Coalesced

```
#pragma omp parallel private (ic,ip,ip1,i,WVAL,j)
for(ic=0; ic<NCOLORtot; ic++) {
#pragma omp for
   for(ip=0; ip<PEsmpTOT; ip++) {
       ip1 = ip * NCOLORtot + ic;
       for(i=SMPindex_new[ip1]; i<SMPindex_new[ip1+1]; i++) {
           WVAL = W[Z][i];
           for(j=indexLnew[i]; j<indexLnew[i+1]; j++) {
               WVAL -= ALnew[j] * W[Z][itemLnew[j]-1];
           }
           W[Z][i] = WVAL * W[DD][i];
       }
   }
}
```



Sequential

Mat-Vec

```
#pragma omp parallel for private(ip,i)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++) {
        VAL = D[i] * W[P][i];
        for(j=indexL[i]; j<indexL[i+1]; j++) {
            VAL += AL[j] * W[P][itemL[j]-1];
        }
        for(j=indexU[i]; j<indexU[i+1]; j++) {
            VAL += AU[j] * W[P][itemU[j]-1];
        }
        W[Q][i] = VAL;
    }
}
```

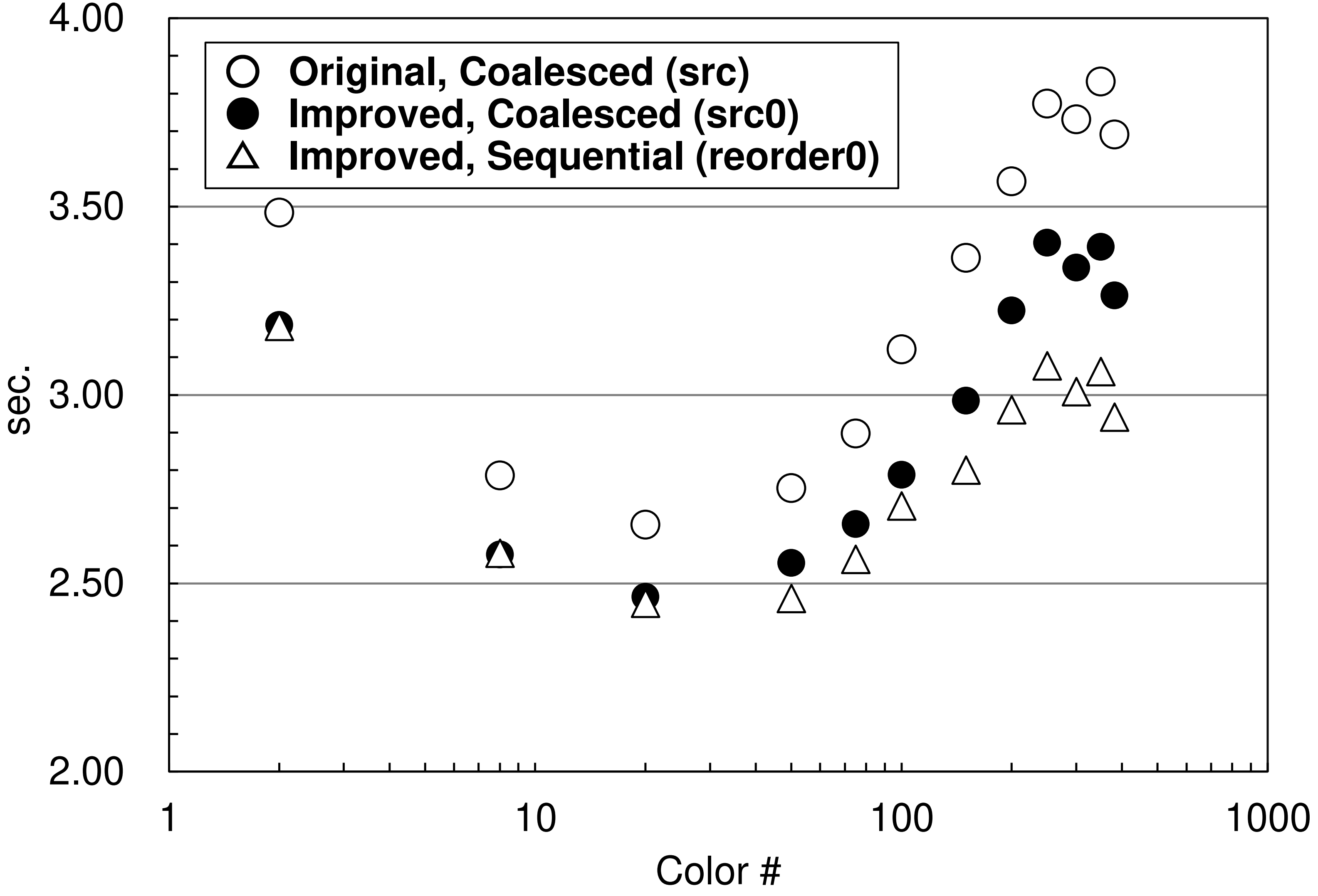
METHOD=0

```
#pragma omp parallel for private (ip1,i,VAL,j)
for(ip=0; ip<PEsmpTOT; ip++) {
    for(i=SMPindex_new[ip*NCOLORtot]; i<SMPindex_new[(ip+1)*NCOLORtot];i++){
        VAL = D[newi] * W[P][i];
        for(j=indexLnew[i]; j<indexLnew[i+1]; j++) {
            VAL += ALnew[j] * W[P][itemLnew[j]-1];
        }
        for(j=indexUnew[i]; j<indexUnew[i+1]; j++) {
            VAL += AUnew[j] * W[P][itemUnew[j]-1];
        }
        W[Q][i] = VAL;
    }
}
```

METHOD=1

Comp. Time for ICCG, CM-RCM

Generally “sequential (reorder0)” is stable and faster than “coalesced (src, src0)”. Effects aremore significant in cases with more colors (12 threads, C)



First Touch Data Placement

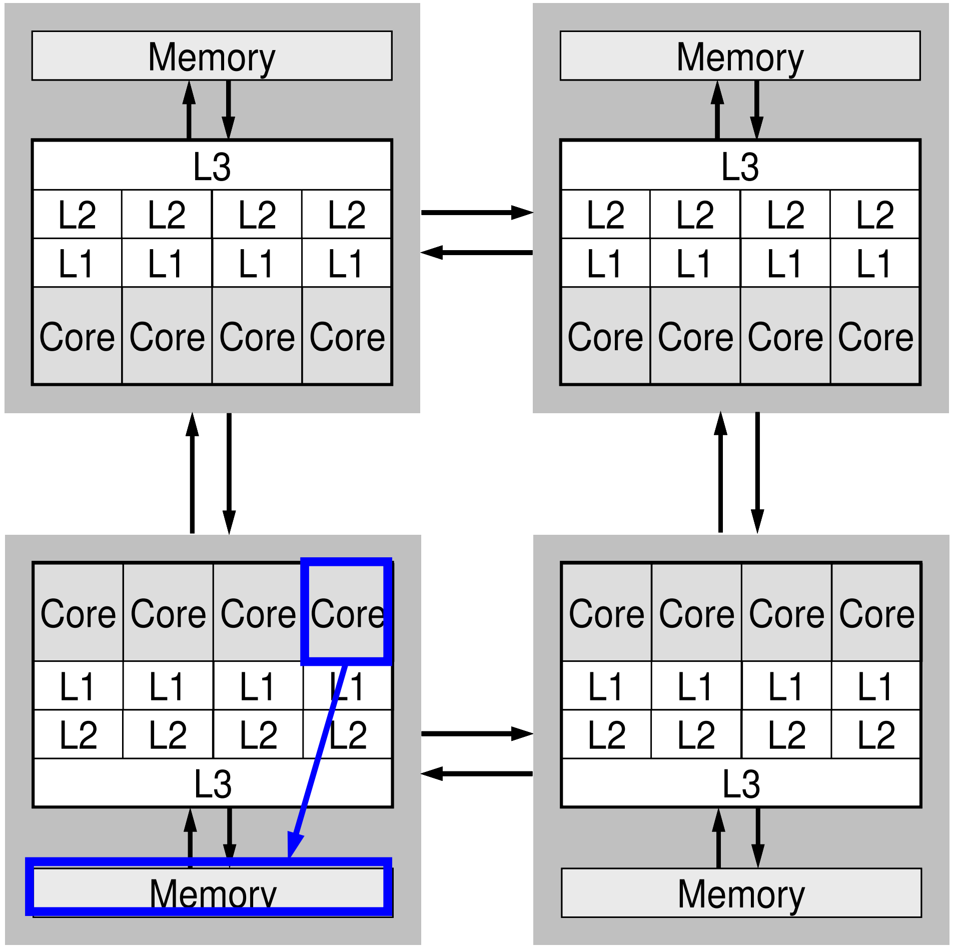
"Patterns for Parallel Programming" Mattson, T.G. et al.

- To reduce memory traffic in the system, it is important to keep the data close to the PEs that will work with the data (e.g. NUMA control).
- On NUMA computers, this corresponds to making sure the pages of memory are allocated and "owned" by the PEs that will be working with the data contained in the page.
  - ✓ Page/Memory Page/Virtual Page: A fixed-length continuous block of virtual memory, smallest unit of data for memory management in a virtual memory OS
- The most common NUMA page-placement algorithm is the "first touch" algorithm, in which the PE first referencing a region of memory will have the page holding that memory assigned to it.
- A very common technique in OpenMP program for optimization is to initialize data in parallel using the same loop schedule as will be used later in the computations.

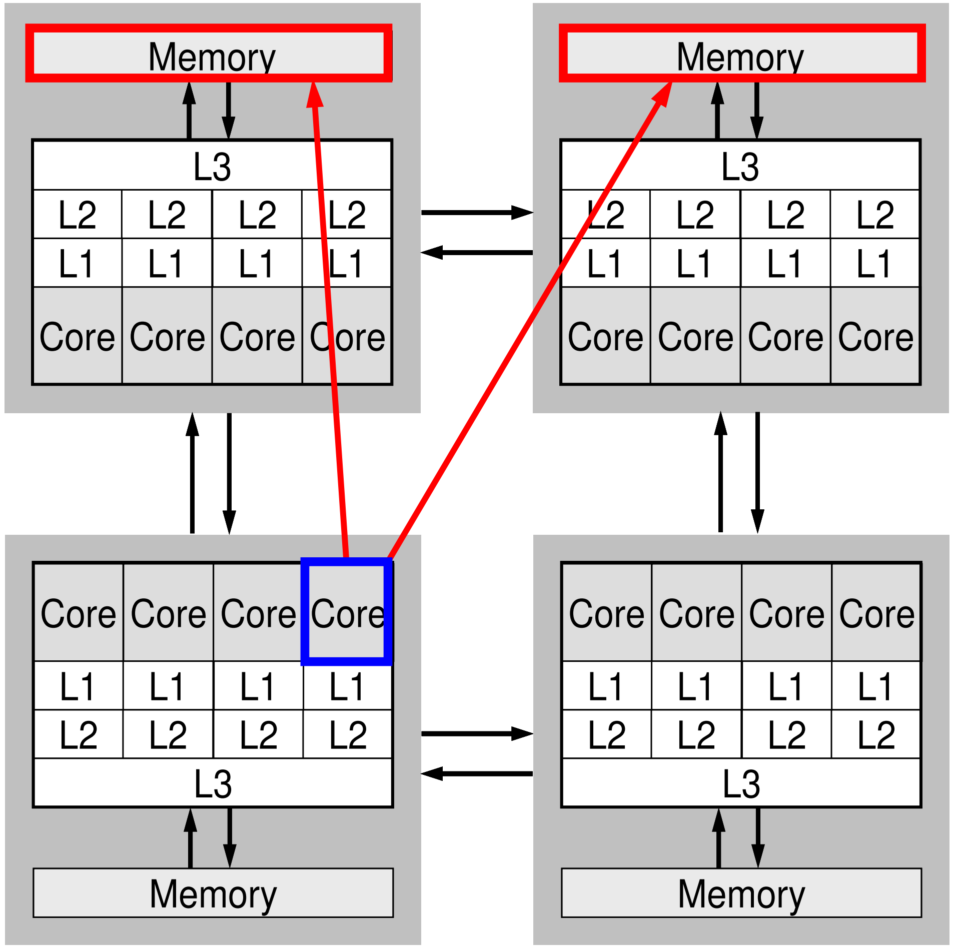
Summary: First Touch Data Placement

- On NUMA architecture (Non-Uniform Memory Access), "pages of memory" are not allocated when variables and arrays are declared/allocated in the program.
- "Pages" are allocated at the local memory of the "socket" for the "core/thread" that first touches the variables and/or arrays.
- If the pages are not on the local memory of the socket for each thread, performance of the program is very bad.
- A very common technique in OpenMP program for optimization is to initialize data in parallel using the same loop schedule as will be used later in the computations.
- You have to consider this if you use multiple CMG's of the Odyssey system for a single OpenMP program
  - If you don't care, all pages are crated at the local memory of CMG#0
  - Not needed for a single CMG case

Local/Remote Memory



Local Memory



Remote Memory

Control Data: INPUT.DAT

```
128 128 128                          NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00          DX/DY/DZ
1.0e-08                             EPSICC
48                                  PEsmpTOT
-50                                 NCOLORtot
0                                   NFLAG (0 or 1)
0                                   METHOD
```

- **PEsmpTOT**
  - Thread Number **(--omp thread=XX)**
- **NCOLORtot**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM
- **NFLAG**
  - =0: without first-touch, =1: with first-touch
- **METHOD**
  - Loop structure for Mat-Vec
  - =0: conventional way, =1: similar to forward/backward substitution

g.sh: reorder0

```
#!/bin/sh
#PJM -N "go0"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=48          (=PEsmpTOT)
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o test1.lst

module load fj
export OMP_NUM_THREADS=48     (=PEsmpTOT)
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl -l ./L3-rsol0
numactl -C 12-59 -m 4-7 ./L3-rsol0
```

Array Initialization: NFLAG=0/1 (1/3) poi_gen.c

```
 if(NFLAG == 0){
                for(i=0; i<ICELTOT; i++) {
                        OLDtoNEWnew[i] = 0;
                        NEWtoOLDnew[i] = 0;
                }
        }else {
#pragma omp parallel for private (icel, j)
                for(ip=1; ip<=PEsmpTOT; ip++){
                        for(icel = SMPindex_new[(ip-1)*NCOLORtot]+1;
                            icel<= SMPindex_new[ip*NCOLORtot]; icel++){
                                OLDtoNEWnew[icel-1] = 0;
                                NEWtoOLDnew[icel-1] = 0;
                        }
                }
        }
```

Pages are allocated at the local memory of the master thread

Pages are allocated at the local memory of each thread

A very common technique in OpenMP program for optimization is to initialize data in parallel using the same loop schedule as will be used later in the computations.

Array Initialization: NFLAG=0/1 (2/3)

```
if(NFLAG == 0){
   for(i=0; i<ICELTOT; i++) {
       BFORCE[i] = 0.0;
       D[i]      = 0.0;
       PHI[i]    = 0.0;
   }
   for(i=0; i<=ICELTOT; i++) {
       indexLnew[i] = indexLnew_org[i];
       indexUnew[i] = indexUnew_org[i];
   }
   for(i=0; i<NPL; i++) {
       itemLnew[i] = 0;
       ALnew[i] = 0.0;
   }
   for(i=0; i<NPU; i++) {
       itemUnew[i] = 0;
       AUnew[i] = 0.0;
   }

   }else {
```

Pages are allocated at the local memory of the master thread

A very common technique in OpenMP program for optimization is to initialize data in parallel using the same loop schedule as will be used later in the computations.

Array Initialization: NFLAG=0/1 (3/3)

```
    }else {
            indexLnew[0]=0;
            indexUnew[0]=0;
#pragma omp parallel for private (icel, j)
     for(ip=1; ip<=PEsmpTOT; ip++){
         for(icel = SMPindex_new[(ip-1)*NCOLORtot]+1;
             icel<=SMPindex_new[ip*NCOLORtot]; icel++){
             BFORCE[icel-1] = 0.0;
             PHI[icel-1] = 0.0;
             D[icel-1] = 0.0;
             indexLnew[icel]=indexLnew_org[icel];
             indexUnew[icel]=indexUnew_org[icel];

             for(j=indexLnew_org[icel-1];j<indexLnew_org[icel];j++){
                 itemLnew[j]=0;
                 ALnew[j] = 0.0;
             }
             for(j=indexUnew_org[icel-1];j<indexUnew_org[icel];j++){
                 itemUnew[j]=0;
                 AUnew[j] = 0.0;
             }
         }
     }
  }
```

Pages are allocated at the local memory of each thread

A very common technique in OpenMP program for optimization is to initialize data in parallel using the same loop schedule as will be used later in the computations.

Sequential Reordering (4/5) poi_gen-3

```
/*************
* ARRAY init.
*************/
        if(NFLAG == 0){
                for(i=0; i<ICELTOT; i++)  {
                        BFORCE[i] = 0.0;
                        D[i]      = 0.0;
                        PHI[i]    = 0.0;
                }
                for(i=0; i<=ICELTOT; i++)  {
                        indexLnew[i] = indexLnew_org[i];
                        indexUnew[i] = indexUnew_org[i];

                }
                for(i=0; i<NPL; i++)  {
                        itemLnew[i] = 0;
                        ALnew[i] = 0.0;
                }
                for(i=0; i<NPU; i++)  {
                        itemUnew[i] = 0;
                        AUnew[i] = 0.0;
                }

        }else {
                indexLnew[0]=0;
                indexUnew[0]=0;
#pragma omp parallel for private (icel, j)
                for(ip=1; ip<=PEsmpTOT; ip++){
                        for(icel = SMPindex_new[(ip-1)*NCOLORtot]+1; icel<=SMPindex_new[ip*NCOLORtot]; icel++){
                                BFORCE[icel-1] = 0.0;
                                PHI[icel-1] = 0.0;
                                D[icel-1] = 0.0;
                                indexLnew[icel]=indexLnew_org[icel];
                                indexUnew[icel]=indexUnew_org[icel];

                                for(j=indexLnew_org[icel-1];j<indexLnew_org[icel];j++){
                                        itemLnew[j]=0;
                                        ALnew[j] = 0.0;
                                }
                                for(j=indexUnew_org[icel-1];j<indexUnew_org[icel];j++){
                                        itemUnew[j]=0;
                                        AUnew[j] = 0.0;
                                }
                        }
                }
        }
```

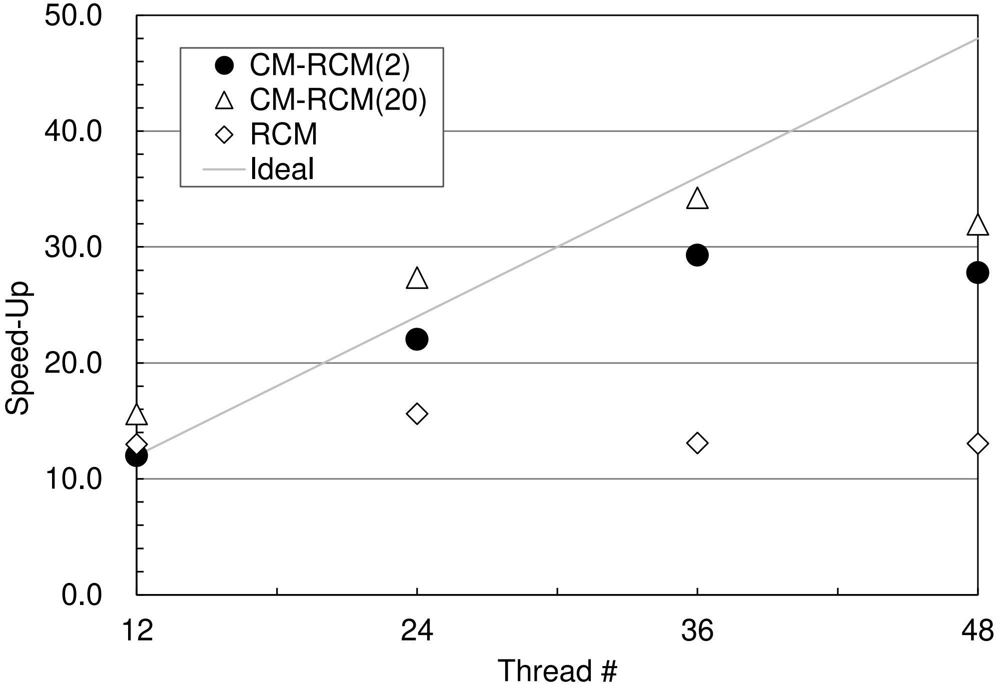
Pages are allocated at the local memory of the master thread

Pages are allocated at the local memory of each thread

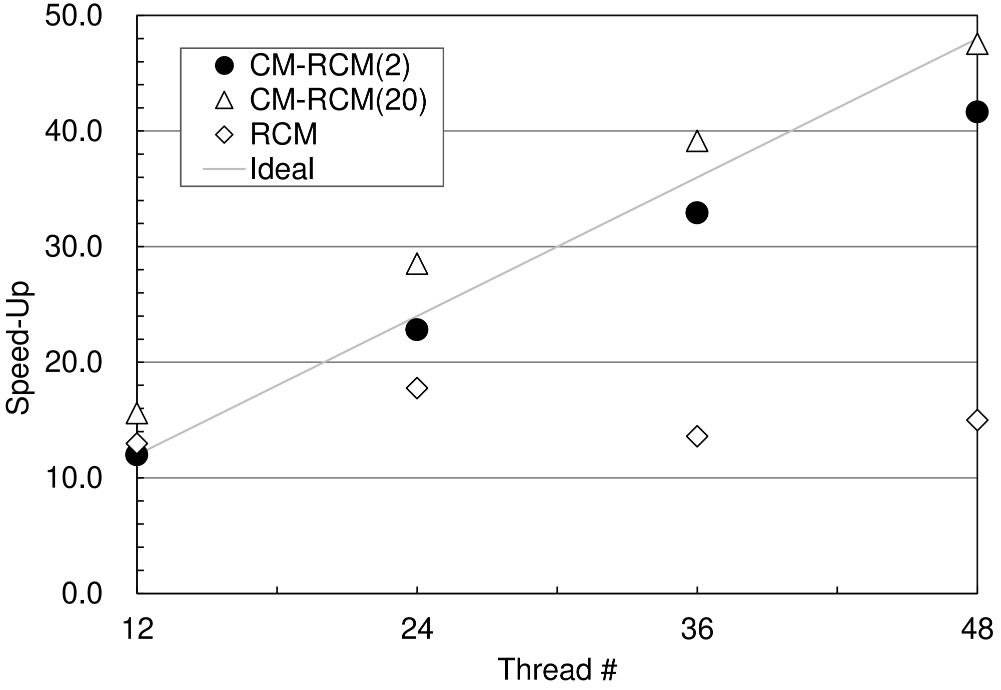
Results: reoder0, L3-rsol0, N=128^3, C

based on the performance of CM-RCM(2) with 12 threads/without First Touch

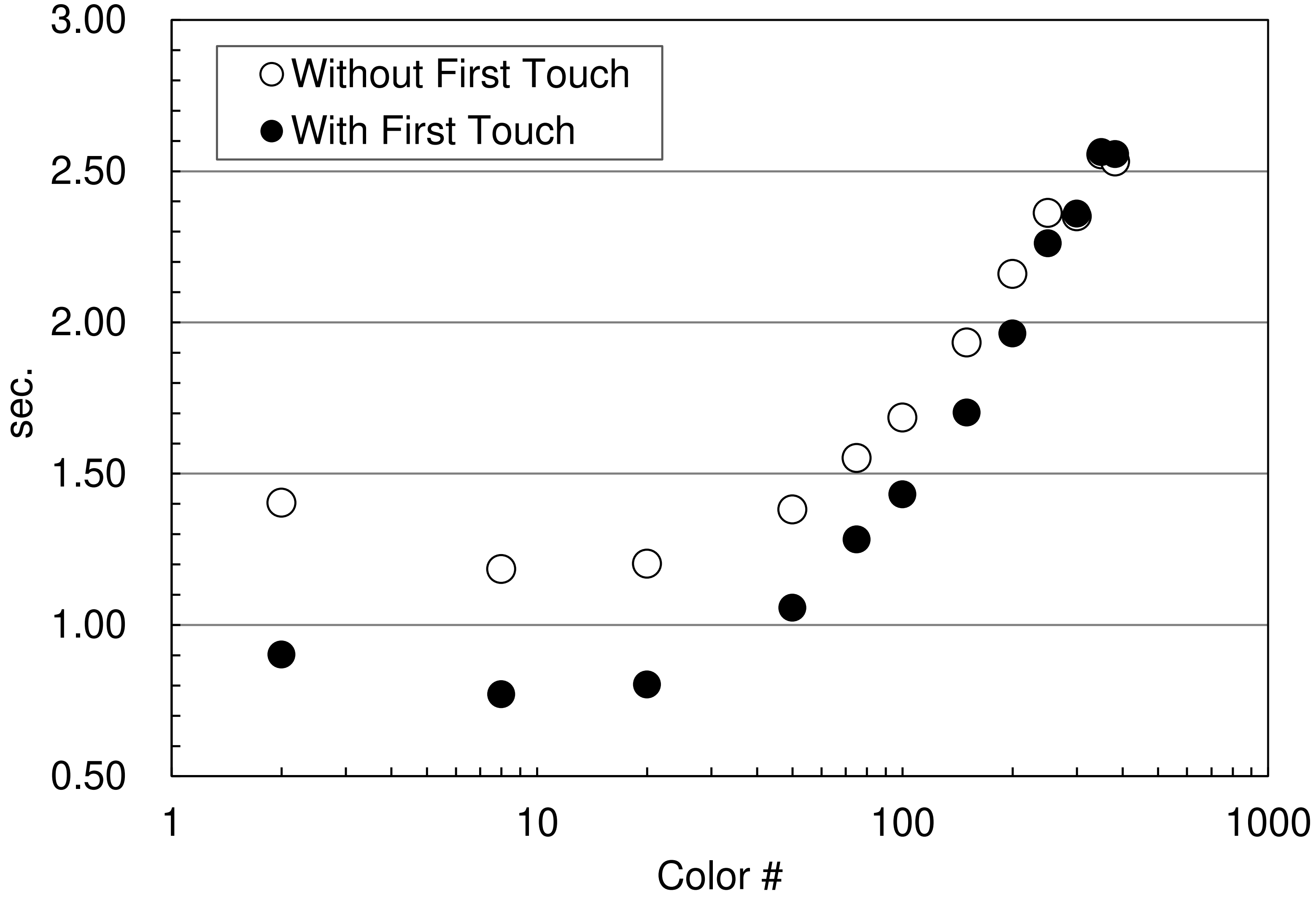
Without First-Touch



With First-Touch



Results: reoder0, L3-rsol0, N=128^3, C 48 threads



Summary

- Material: ICCG solver for sparse matrices derived from FVM applications (Finite Volume Method).
- Parallelization on a single node of Odyssey using OpenMP
  - Data Placement
  - Reordering

- Effects of reordering
- First-Touch Data Placement

Future Directions

- Gap between performance of CPU & memory
  - BYTE/FLOP
- Multicore/Manycore
  - Intel Xeon/Phi, GPU with OpenACC
- Supercomputer system with >10^5 cores
  - Exascale：＞10^8
- Reordering/Ordering
  - Intensity of components of matrices should be also considered (not only the connectivity information)
  - Selection of optimum number of colors: research topic, especially for ill-conditioned problems
- OpenMP/MPI Hybrid -> One of effective choices
  - Optimization for OpenMP is the most critical
  - **Winter School: Parallel FEM using OpenMP/MPI**

Fortran Code

```
% cd /work/gt89/t89XXX
% module load fj

% cp /work/gt00/z30088/makeNEW.tar .
% tar xvf makeNEW.tar
% cd ompf/src
% make -f make-n clean
% make -f make-n
% cd ../src0
% make -f make-n clean
% make -f make-n
% cd ../reorder0
% make -f make-n clean
% make -f make-n

% cd ../run
% ls *NEW
    L3-rsol0-NEW  L3-sol0-NEW  L3-sol-NEW
```

make-n

```
F90    = frtpx
F90OPTFLAGS= -Knoswp,openmp,nosimd,nounroll
F90FLAGS =$(F90OPTFLAGS)

.SUFFIXES:
.SUFFIXES: .o .f .f90 .c
#
.f90.o:; $(F90) -c $(F90FLAGS)  $(F90OPTFLAG) $<
.f.o:; $(F90) -c -loglist $(F90FLAGS)  $(F90OPTFLAG) $<
#
OBJS = ¥
solver_ICCG_mc.o solver_ICCG_mc_ft.o struct.o pcg.o ¥
boundary_cell.o cell_metrics.o ¥
input.o main.o poi_gen.o pointer_init.o outucd.o mc.o cm.o rcm.o
cmrcm.o

TARGET = ../run/L3-rsol0-NEW

all: $(TARGET)

$(TARGET): $(OBJS)
        $(F90) $(F90FLAGS) -o $(TARGET) ¥
        $(OBJS) ¥
        $(F90FLAGS)

clean:
        rm -f *.o $(TARGET) *.mod *~ PI* *.log *.lst
```

All options for optimization are suppressed

Effects of Compiler Options

- Original: `–Kfast,openmp –KSVE`
- NEW: `–Knoswp,openmp,nosimd,nounroll`
- If the most inner-loop is small (3-6), optimization of Fujitsu's Fortran compiler does not work well.

- N=128^3, CM-RCM(20), 48-threads, First-Touch
  - reorder0
    - 1.484 sec. -> 1.354 sec.
- reorder0+ELL
    - 0.674. sec -> 1.467 sec.