Introduction to Parallel Programming for Multicore/Manycore Clusters

Part B3: Parallel ICCG by OpenMP

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Parallel Version: OpenMP

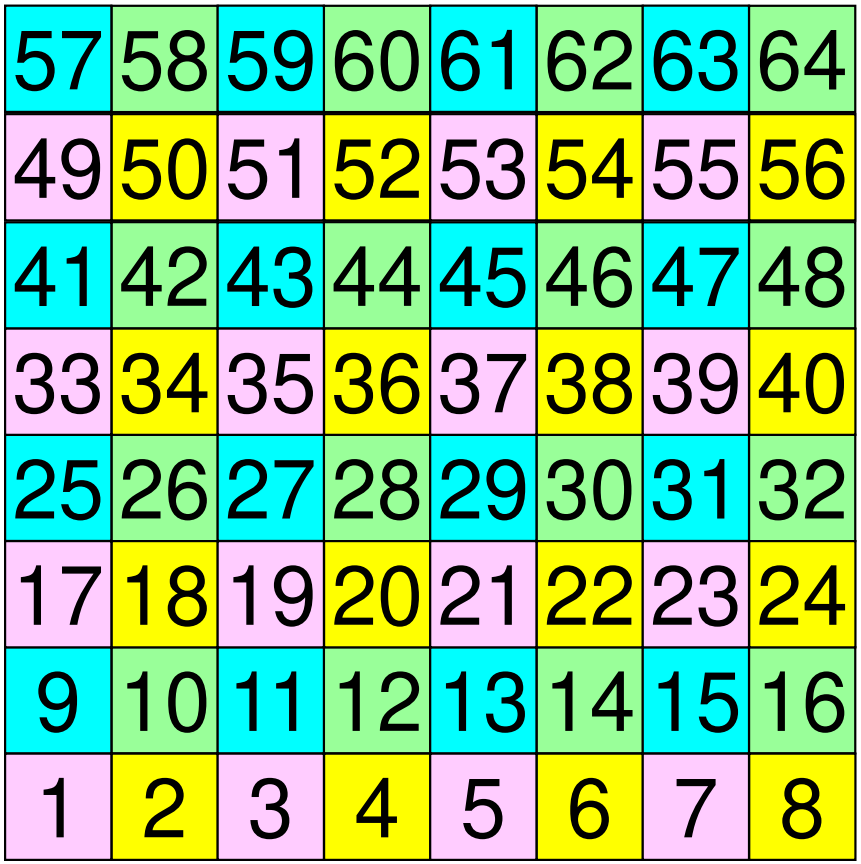
- OpenMP version of L2-sol
  - Number of threads= “PEsmpTOT”
    - can be controlled in the program

- 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

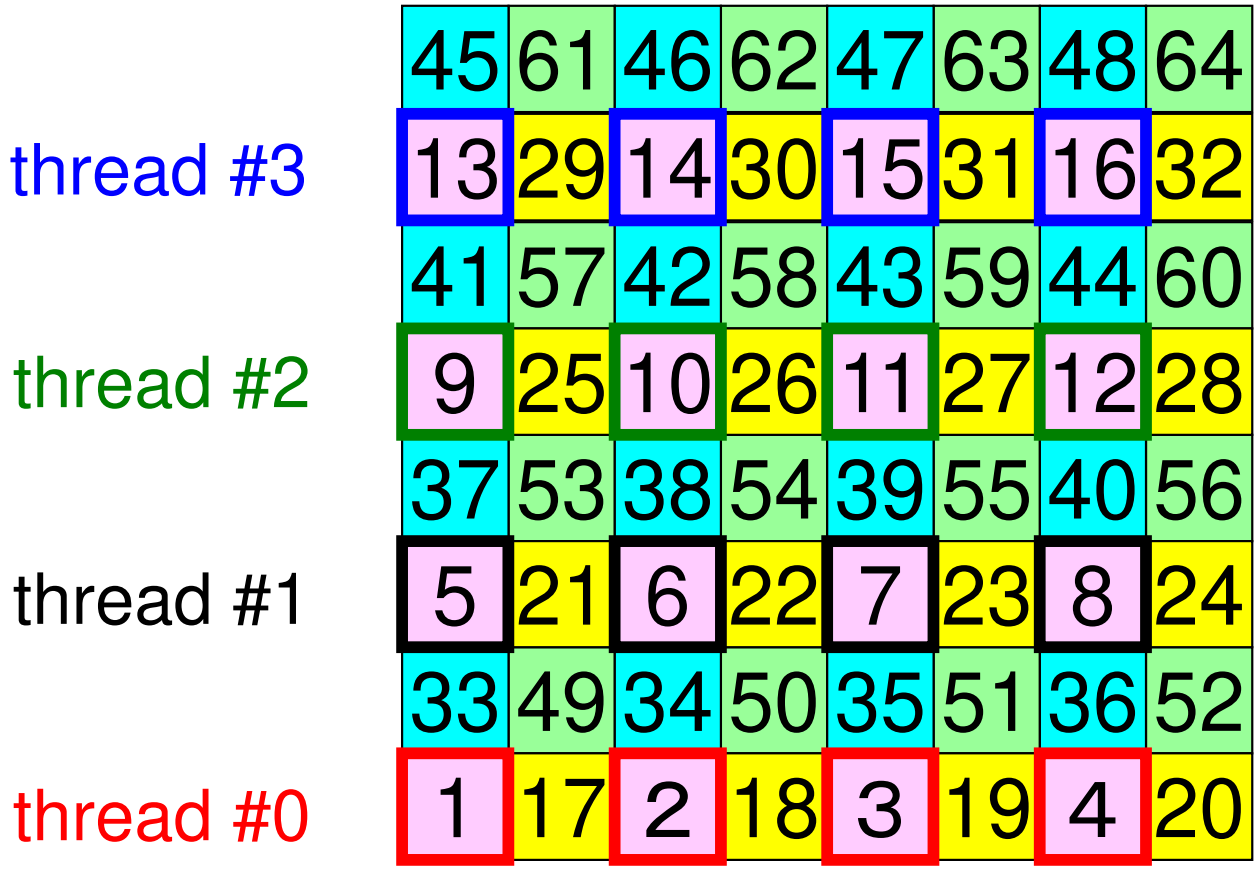


4-Colors, 4-Threads
Renumbering according to Color ID

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



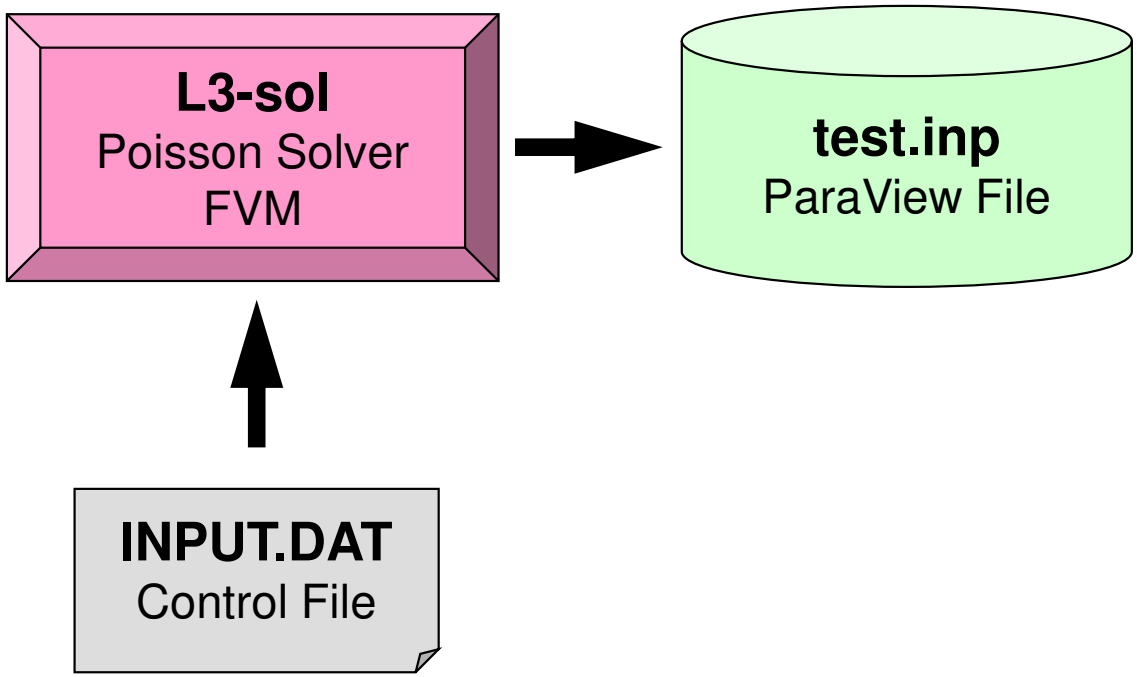
How to Run

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

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

>$ cd ompf
>$ 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
  - **<$O-L3>: /work/gt89/t89XXX/ompf**
  - <$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

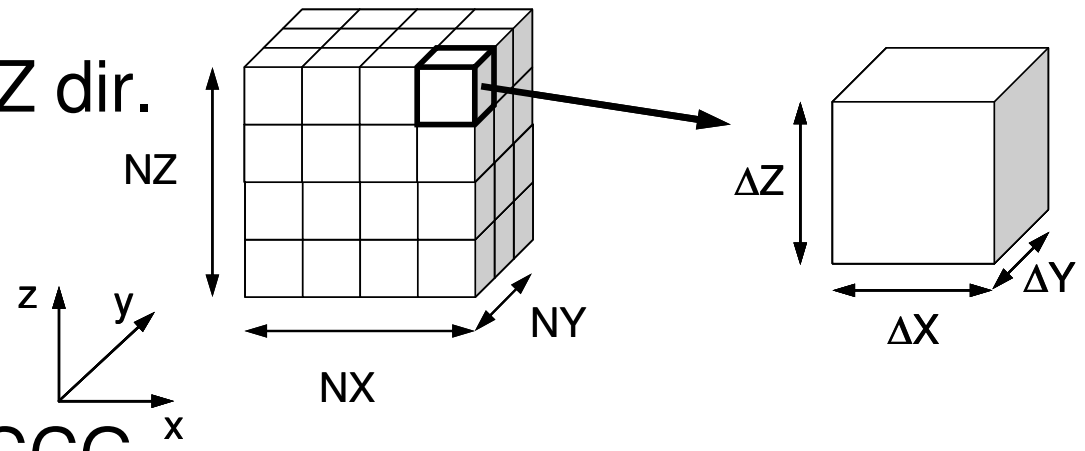
Running the Program



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
24                                   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/ompf/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)

```
!$omp parallel do private(i,VAL,k)
        do i = 1, N
          VAL= D(i)*W(i,P)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL + AL(k)*W(itemL(k),P)
          enddo
          do k= indexU(i-1)+1, indexU(i)
            VAL= VAL + AU(k)*W(itemU(k),P)
          enddo
          W(i,Q)= VAL
        enddo
!$omp end parallel do
```

- 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)

```
      do icol= 1, NCOLORtot
!$omp parallel do private (i, VAL, k)
        do i= COLORindex(icol-1)+1, COLORindex(icol)
          VAL= D(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL - (AL(k)**2) * DD(itemL(k))
          enddo
          DD(i)= 1.d0/VAL
        enddo
!$omp end parallel do
      enddo
```

- 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

```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

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

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0

      call solve_ICCG_mc                                                &
     &      ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,       &
     &        BFORCE,  PHI, AL, AU, NCOLORtot, PEsmpTOT,                &
     &        SMPindex, SMPindexG, EPSICCG, ITR, IER)

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

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

      call OUTUCD

      stop
      end
```

module STRUCT

```
      module STRUCT

      use omp_lib
      include 'precision.inc'

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

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

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

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

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

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

      integer (kind=kint) :: PEsmpTOT

      end module STRUCT
```

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

N:
Number of modes

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

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

IBNODTOT:
= NXP1 x NYP1

XYZ(ICELTOT,3):
Location of meshes

NEIBcell(ICELTOT,6):
Neighboring meshes

PEsmpTOT:
Number of threads

module PCG

```
module PCG

integer, parameter :: N2= 256
integer :: NUmax, NLmax, NCOLORtot, NCOLORk, NU, NL
integer :: NPL, NPU
integer :: METHOD, ORDER_METHOD

real(kind=8) :: EPSICCG

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

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

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

integer, dimension(:), allocatable :: indexL, itemL
integer, dimension(:), allocatable :: indexU, itemU
end module PCG
```

NCOLORtot Total number of colors/levels

COLORindex Index of number of meshes in each color/level

(0:NCOLORtot) (COLORindex(icol)- COLORindex(icol-1))

SMPindex (0:NCOLORtot*PEsmpTOT)

SMPindexG(0:PEsmpTOT)

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(0:N), indexU(0:N)	**I**	# of L/U non-zero off-diag. comp. (CRS)
NPL, NPU	**I**	Total # of L/U non-zero off-diag. comp. (CRS)
itemL(NPL), itemU(NPU)	**I**	Column ID of L/U non-zero off-diag. comp. (CRS)
AL(NPL), AU(NPU)	**R**	L/U non-zero off-diag. comp. (CRS)

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

Variables/Arrays for Matrix (2/2)

Name	Type	Content
NCOLORtot	**I**	**Input:** reordering method + initial number of colors/levels ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM **Output:** Final number of colors/levels
COLORindex (0:NCOLORtot)	**I**	Number of meshes at each color/level 1D compressed array Meshes in **icolth** color/level are stored in this array from **COLORindex(icol-1)+1** to **COLORindex(icol)**
NEWtoOLD(N)	**I**	Reference array from New to Old numbering
OLDtoNEW(N)	**I**	Reference array from Old to New numbering
PEsmpTOT	**I**	Number of Threads
SMPindex (0:NCOLORtot*PEsmpTOT)	**I**	Array for OpenMP Operations (for Loops with Data Dependency)
SMPindexG(0:PEsmpTOT)	**I**	Array for OpenMP Operations (for Loops without Data Dependency)

Main Program

```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

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

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0

      call solve_ICCG_mc                                                &
     &      ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,       &
     &        BFORCE,  PHI, AL, AU, NCOLORtot, PEsmpTOT,                &
     &        SMPindex, SMPindexG, EPSICCG, ITR, IER)
```

input: reading INPUT.DAT

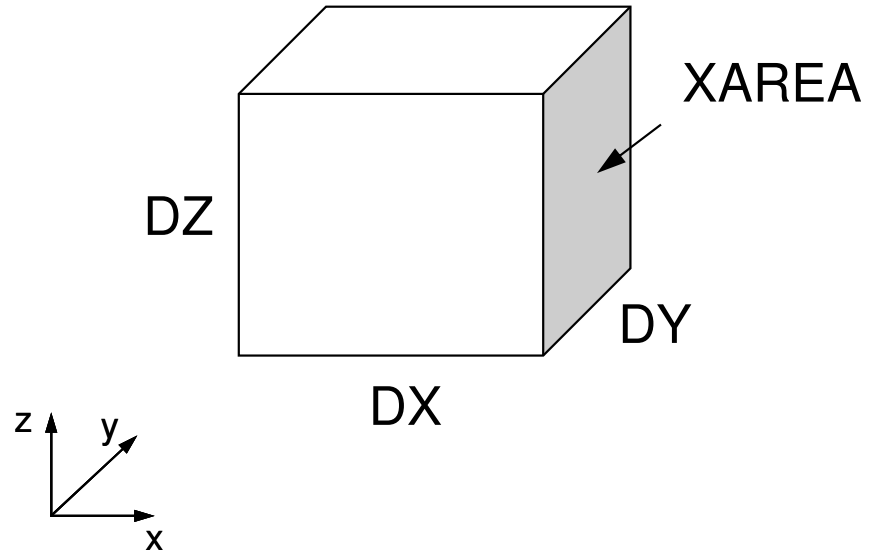
```
!C
!C***
!C*** INPUT
!C***
!C
!C    INPUT CONTROL DATA
!C
      subroutine INPUT
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)
      character*80 CNTFIL
!C
!C-- CNTL. file
      open  (11, file='INPUT.DAT', status='unknown')
        read (11,*) NX, NY, NZ
        read (11,*) DX, DY, DZ
        read (11,*) EPSICCG
        read (11,*) PEsmpTOT
        read (11,*) NCOLORtot
      close (11)
!C===
      return
      end
```

- **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

```
!C
!C***
!C*** CELL_METRICS
!C***
!C
      subroutine CELL_METRICS
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)

!C
!C-- ALLOCATE
      allocate (VOLCEL(ICELTOT))
      allocate (   RVC(ICELTOT))
!C
!C-- VOLUME, AREA, PROJECTION etc.
      XAREA= DY * DZ
      YAREA= DX * DZ
      ZAREA= DX * DY

      RDX= 1.d0 / DX
      RDY= 1.d0 / DY
      RDZ= 1.d0 / DZ

      RDX2= 1.d0 / (DX**2)
      RDY2= 1.d0 / (DY**2)
      RDZ2= 1.d0 / (DZ**2)

      R2DX= 1.d0 / (0.50d0*DX)
      R2DY= 1.d0 / (0.50d0*DY)
      R2DZ= 1.d0 / (0.50d0*DZ)

       V0= DX * DY * DZ
      RV0= 1.d0/V0

      VOLCEL=  V0
      RVC   = RV0

      return
      end
```



Main Program

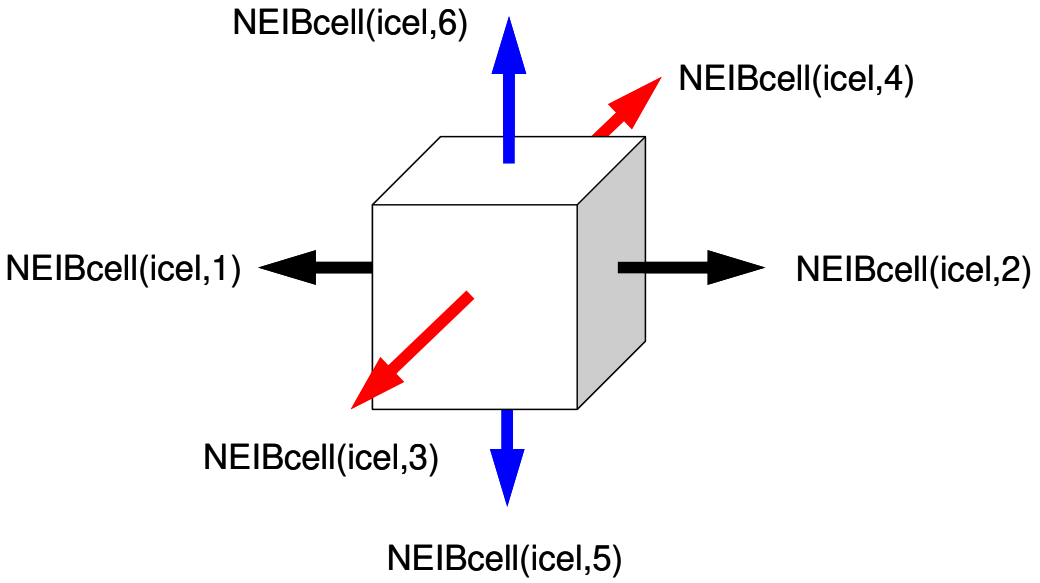
```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

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

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0

        call solve_ICCG_mc                                              &
     &       ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,      &
     &         BFORCE,  PHI, AL, AU, NCOLORtot, PEsmpTOT,               &
     &         SMPindex, SMPindexG, EPSICCG, ITR, IER)
```

poi_gen (1/9)

```
      subroutine POI_GEN

      use STRUCT
      use PCG

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

!C
!C-- INIT.
      nn = ICELTOT
      nnp= ICELTOTp

      NU= 6
      NL= 6

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

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

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

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

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

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

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

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

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

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

poi_gen (2/9)

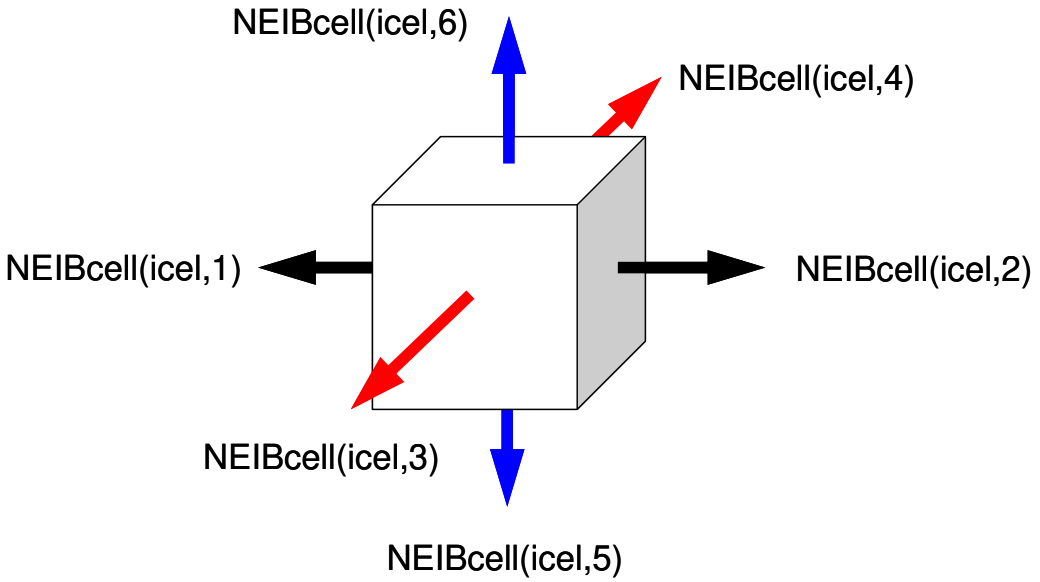


Lower Triangular Part

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

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

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

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

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

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

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

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

poi_gen (2/9)



Upper Triangular Part

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

poi_gen (3/9)

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

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

      if (NCOLORtot.gt.0) then
        call MC  (ICELTOT, NL, NU, INL, IAL, INU, IAU,                  &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif

      if (NCOLORtot.eq.0) then
        call  CM (ICELTOT, NL, NU, INL, IAL, INU, IAU,                  &
     &            NCOLORtot, COLORindex, NEWtoOLD, OLDtoNEW)
      endif

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

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

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

Reordering

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

poi_gen (4/9)

```
      allocate (SMPindex(0:PEsmpTOT*NCOLORtot))
      SMPindex= 0
      do ic= 1, NCOLORtot
        nn1= COLORindex(ic) - COLORindex(ic-1)
        num= nn1 / PEsmpTOT
        nr = nn1 - PEsmpTOT*num
        do ip= 1, PEsmpTOT
          if (ip.le.nr) then
            SMPindex((ic-1)*PEsmpTOT+ip)= num + 1
           else
            SMPindex((ic-1)*PEsmpTOT+ip)= num
          endif
        enddo
      enddo

      do ic= 1, NCOLORtot
        do ip= 1, PEsmpTOT
          j1= (ic-1)*PEsmpTOT + ip
          j0= j1 - 1
          SMPindex(j1)= SMPindex(j0) + SMPindex(j1)
        enddo
      enddo

      allocate (SMPindexG(0:PEsmpTOT))
      SMPindexG= 0
      nn= ICELTOT / PEsmpTOT
      nr= ICELTOT - nn*PEsmpTOT
      do ip= 1, PEsmpTOT
        SMPindexG(ip)= nn
        if (ip.le.nr) SMPindexG(ip)= nn + 1
      enddo

      do ip= 1, PEsmpTOT
        SMPindexG(ip)= SMPindexG(ip-1) + SMPindexG(ip)
      enddo

!C===
```

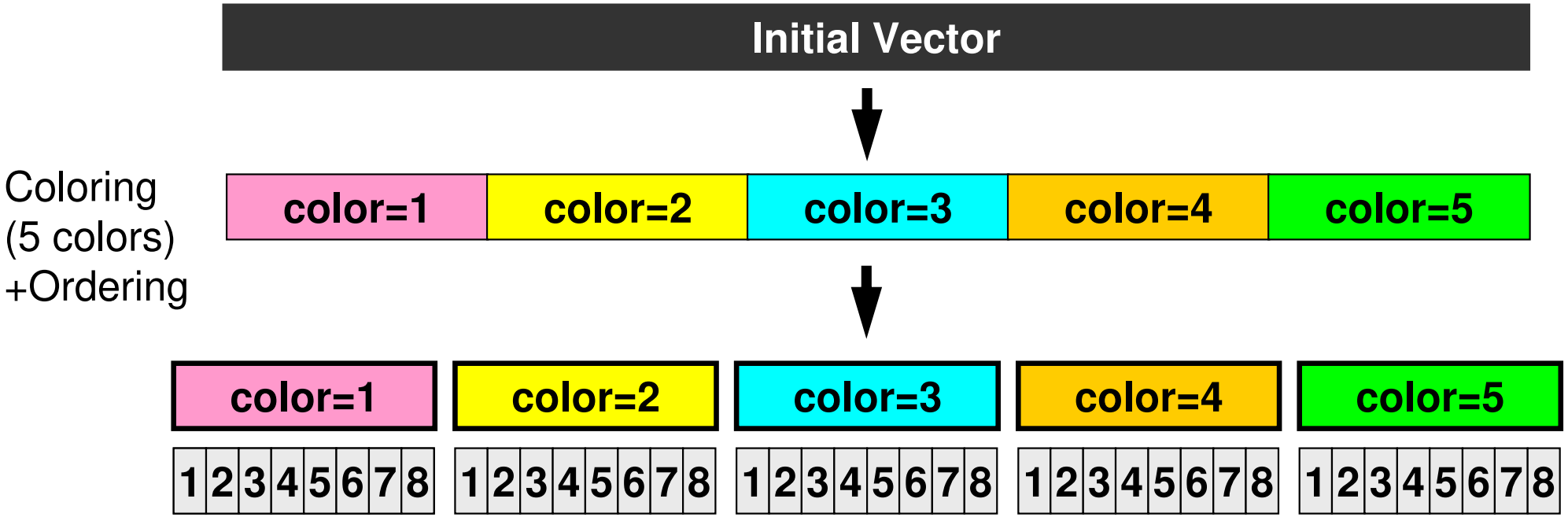
`SMPindex`:
for preconditioning

```
  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
```

SMPindex:

for preconditioning

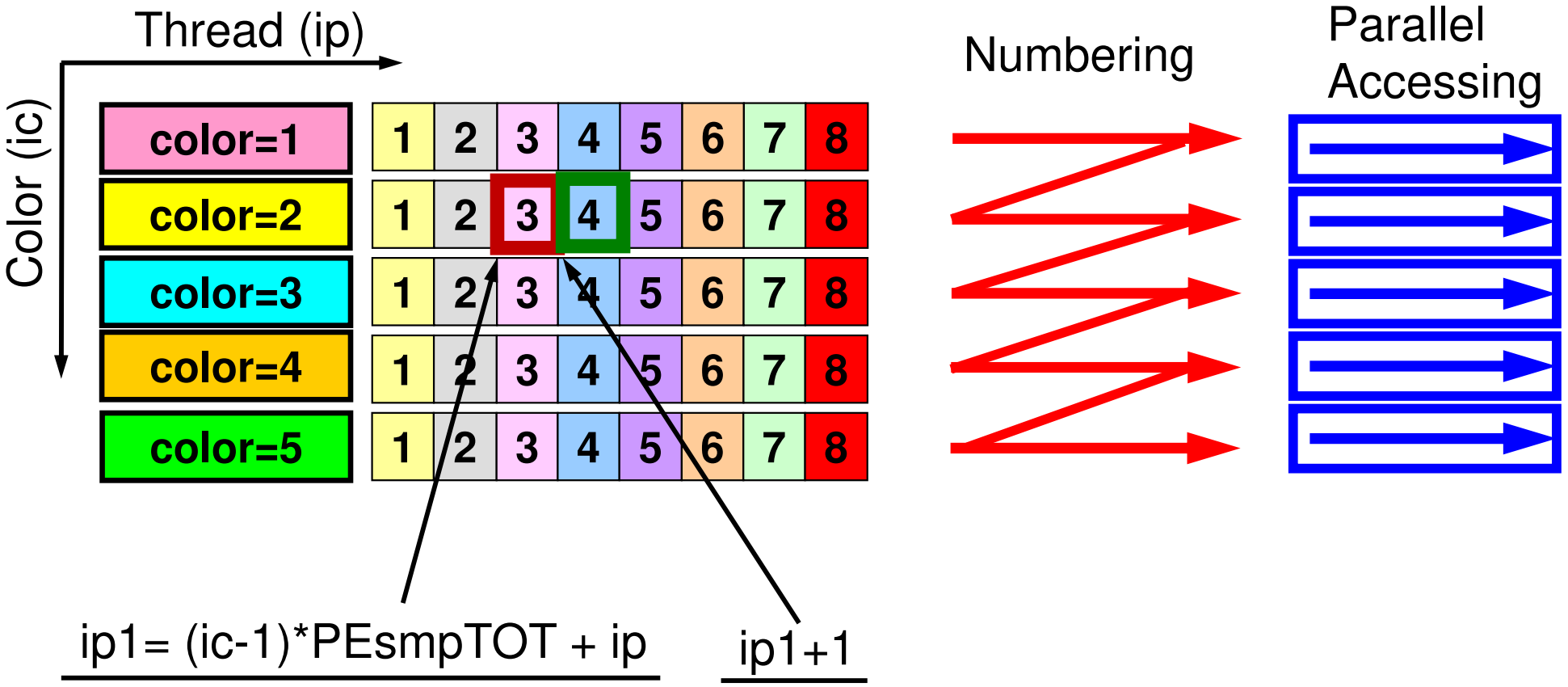
```
  do ic= 1, NCOLORtot
!$omp parallel do …
      do ip= 1, PEsmpTOT
        ip1= (ic-1)*PEsmpTOT+ip
      do i= SMPindex(ip1-1)+1, SMPindex(ip1)
        (…)
      enddo
      enddo
!omp end parallel do
  enddo
```



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

SMPindex

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



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-1)*PEsmpTOT    (ic: starting at 1)

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)

```
      allocate (SMPindex(0:PEsmpTOT*NCOLORtot))
      SMPindex= 0
      do ic= 1, NCOLORtot
        nn1= COLORindex(ic) - COLORindex(ic-1)
        num= nn1 / PEsmpTOT
        nr = nn1 - PEsmpTOT*num
        do ip= 1, PEsmpTOT
          if (ip.le.nr) then
            SMPindex((ic-1)*PEsmpTOT+ip)= num + 1
           else
            SMPindex((ic-1)*PEsmpTOT+ip)= num
          endif
        enddo
      enddo

      do ic= 1, NCOLORtot
        do ip= 1, PEsmpTOT
          j1= (ic-1)*PEsmpTOT + ip
          j0= j1 - 1
          SMPindex(j1)= SMPindex(j0) + SMPindex(j1)
        enddo
      enddo

      allocate (SMPindexG(0:PEsmpTOT))
      SMPindexG= 0
      nn= ICELTOT / PEsmpTOT
      nr= ICELTOT - nn*PEsmpTOT
      do ip= 1, PEsmpTOT
        SMPindexG(ip)= nn
        if (ip.le.nr) SMPindexG(ip)= nn + 1
      enddo

      do ip= 1, PEsmpTOT
        SMPindexG(ip)= SMPindexG(ip-1) + SMPindexG(ip)
      enddo

!C===
```

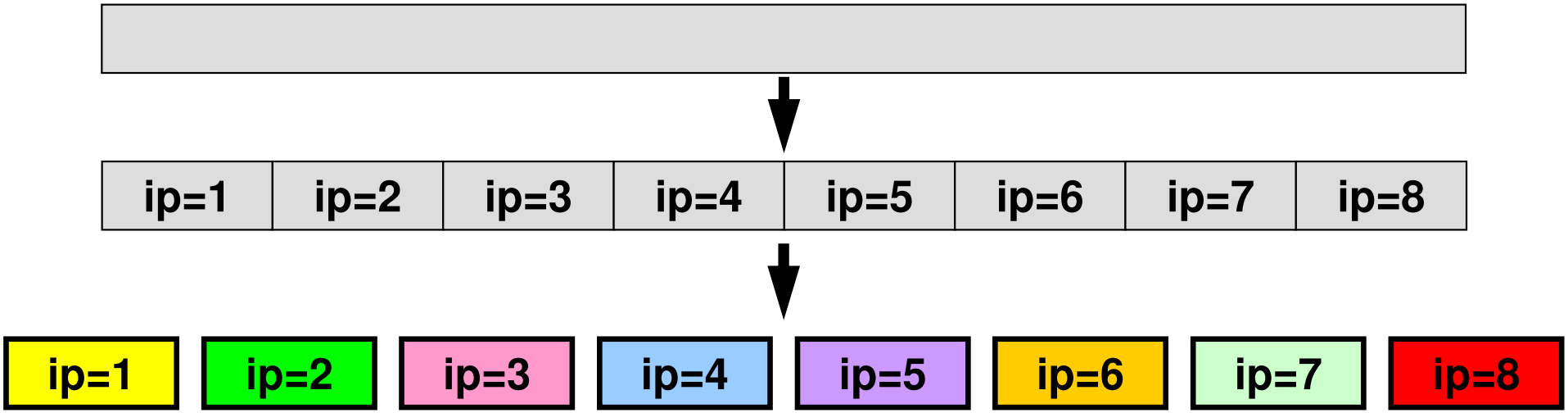
```
!$omp parallel do …
  do ip= 1, PEsmpTOT
  do i= SMPindexG(ip-1)+1, SMPindexG(ip)
    (…)
  enddo
  enddo
!$omp end parallel do
```

SMPindexG:

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

SMPindexG

```
!$omp parallel do …
  do ip= 1, PEsmpTOT
  do i= SMPindexG(ip-1)+1, SMPindexG(ip)
    (…)
  enddo
  enddo
!$omp end parallel do
```



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

poi_gen (5/9)

New numbering is applied after this point

```
!C
!C-- 1D array
      nn = ICELTOT
      allocate (indexL(0:nn), indexU(0:nn))
      indexL= 0
      indexU= 0

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

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

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

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

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

```
do i= 1, N

  VAL= D(i)*p(i)

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

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

  q(i)= VAL

enddo
```

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

poi_gen (6/9)

New numbering is applied

```
!C
!C +-------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-------------------------------+
!C===

!$omp parallel do private
(ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&            private (VOL0,coef,j,ii,jj,kk)

      do ip  = 1, PEsmpTOT
      do icel= SMPindexG(ip-1)+1, SMPindexG(ip)
        ic0 = NEWtoOLD(icel)

        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)

        VOL0= VOLCEL  (ic0)

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

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

icel: New ID
ic0: Old ID

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

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

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

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

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

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

Coef. Matrix: Parallel, “SMPindexG”

“private”

```
!C
!C +-------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-------------------------------+
!C===

!$omp parallel do private (ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&             private (VOL0,coef,j,ii,jj,kk)

      do ip  = 1, PEsmpTOT
      do icel= SMPindexG(ip-1)+1, SMPindexG(ip)
        ic0 = NEWtoOLD(icel)

        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)

        VOL0= VOLCEL  (ic0)
...
```

poi_gen (6/9)

New numbering is applied

```
!C
!C +-------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-------------------------------+
!C===

!$omp parallel do private
(ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&            private (VOL0,coef,j,ii,jj,kk)

      do ip  = 1, PEsmpTOT
      do icel= SMPindexG(ip-1)+1, SMPindexG(ip)
        ic0 = NEWtoOLD(icel)

        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)

        VOL0= VOLCEL  (ic0)

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

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

icel: New ID
ic0: Old ID

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

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

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

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

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

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

```
!C
!C +-------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-------------------------------+
!C===

!$omp parallel do private
(ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&            private (VOL0,coef,j,ii,jj,kk)

      do ip  = 1, PEsmpTOT
      do icel= SMPindexG(ip-1)+1, SMPindexG(ip)
        ic0 = NEWtoOLD(icel)

        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)

        VOL0= VOLCEL  (ic0)

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

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

poi_gen (6/9)

New numbering is applied

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

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

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

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

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

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

poi_gen (6/9)

New numbering is applied

```
!C
!C +-------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-------------------------------+
!C===

!$omp parallel do private
(ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&            private (VOL0,coef,j,ii,jj,kk)

      do ip  = 1, PEsmpTOT
      do icel= SMPindexG(ip-1)+1, SMPindexG(ip)
        ic0 = NEWtoOLD(icel)

        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)

        VOL0= VOLCEL  (ic0)

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

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

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

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

icN5 < icel
Lower Part

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

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

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

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

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

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

poi_gen (6/9)

New numbering is applied

```
!C
!C +-------------------------------+
!C | INTERIOR & NEUMANN BOUNDARY CELLs |
!C +-------------------------------+
!C===

!$omp parallel do private
(ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&            private (VOL0,coef,j,ii,jj,kk)

      do ip  = 1, PEsmpTOT
      do icel= SMPindexG(ip-1)+1, SMPindexG(ip)
        ic0 = NEWtoOLD(icel)

        icN1= NEIBcell(ic0,1)
        icN2= NEIBcell(ic0,2)
        icN3= NEIBcell(ic0,3)
        icN4= NEIBcell(ic0,4)
        icN5= NEIBcell(ic0,5)
        icN6= NEIBcell(ic0,6)

        VOL0= VOLCEL  (ic0)

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

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

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

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

icN5 > icel
Upper Part

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

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

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

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

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

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

```
      if (icN3.ne.0) then
        icN3= OLDtoNEW(icN3)
        coef= RDY * YAREA
        D(icel)= D(icel) - coef

        if (icN3.lt.icel) then
          do j= 1, INL(icel)
            if (IAL(j,icel).eq.icN3) then
              itemL(j+indexL(icel-1))= icN3
                 AL(j+indexL(icel-1))= coef
              exit
            endif
          enddo
         else
          do j= 1, INU(icel)
            if (IAU(j,icel).eq.icN3) then
              itemU(j+indexU(icel-1))= icN3
                 AU(j+indexU(icel-1))= coef
              exit
            endif
          enddo
        endif
      endif

      if (icN1.ne.0) then
        icN1= OLDtoNEW(icN1)
        coef= RDX * XAREA
        D(icel)= D(icel) - coef

        if (icN1.lt.icel) then
          do j= 1, INL(icel)
            if (IAL(j,icel).eq.icN1) then
              itemL(j+indexL(icel-1))= icN1
                 AL(j+indexL(icel-1))= coef
              exit
            endif
          enddo
         else
          do j= 1, INU(icel)
            if (IAU(j,icel).eq.icN1) then
              itemU(j+indexU(icel-1))= icN1
                 AU(j+indexU(icel-1))= coef
              exit
            endif
          enddo
        endif
      endif
```

poi_gen (7/9)

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

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

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

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

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

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

```
      if (icN2.ne.0) then
        icN2= OLDtoNEW(icN2)
        coef= RDX * XAREA
        D(icel)= D(icel) - coef

        if (icN2.lt.icel) then
          do j= 1, INL(icel)
            if (IAL(j,icel).eq.icN2) then
              itemL(j+indexL(icel-1))= icN2
                 AL(j+indexL(icel-1))= coef
              exit
            endif
          enddo
         else
          do j= 1, INU(icel)
            if (IAU(j,icel).eq.icN2) then
              itemU(j+indexU(icel-1))= icN2
                 AU(j+indexU(icel-1))= coef
              exit
            endif
          enddo
        endif
      endif

      if (icN4.ne.0) then
        icN4= OLDtoNEW(icN4)
        coef= RDY * YAREA
        D(icel)= D(icel) - coef

        if (icN4.lt.icel) then
          do j= 1, INL(icel)
            if (IAL(j,icel).eq.icN4) then
              itemL(j+indexL(icel-1))= icN4
                 AL(j+indexL(icel-1))= coef
              exit
            endif
          enddo
         else
          do j= 1, INU(icel)
            if (IAU(j,icel).eq.icN4) then
              itemU(j+indexU(icel-1))= icN4
                 AU(j+indexU(icel-1))= coef
              exit
            endif
          enddo
        endif
      endif
```

poi_gen (8/9)

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

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

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

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

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

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

poi_gen (9/9)

```
!$omp parallel do private
(ip,icel,ic0,icN1,icN2,icN3,icN4,icN5,icN6)  &
!$omp&            private (VOL0,coef,j,ii,jj,kk)

...

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

          if (icN6.lt.icel) then
            do j= 1, INL(icel)
              if (IAL(j,icel).eq.icN6) then
                itemL(j+indexL(icel-1))= icN6
                   AL(j+indexL(icel-1))= coef
                exit
              endif
            enddo
           else
            do j= 1, INU(icel)
              if (IAU(j,icel).eq.icN6) then
                itemU(j+indexU(icel-1))= icN6
                   AU(j+indexU(icel-1))= coef
                exit
              endif
            enddo
          endif
        endif
        ii= XYZ(ic0,1)
        jj= XYZ(ic0,2)
        kk= XYZ(ic0,3)

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

      enddo
      enddo
!$omp end parallel do
!C===
```

BFORCE using original mesh ID

ii,jj,kk,VOL0: private

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

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

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

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

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

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

Main Program

```
      program MAIN

      use STRUCT
      use PCG
      use solver_ICCG_mc

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

      call INPUT
      call POINTER_INIT
      call BOUNDARY_CELL
      call CELL_METRICS
      call POI_GEN

      PHI=  0.d0

        call solve_ICCG_mc                                              &
     &       ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU, D,      &
     &         BFORCE,  PHI, AL, AU, NCOLORtot, PEsmpTOT,               &
     &         SMPindex, SMPindexG, EPSICCG, ITR, IER)
```

solve_ICCG_mc (1/6)

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

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

      integer :: N, NL, NU, NCOLORtot, PEsmpTOT

      real(kind=8), dimension(N)   :: D
      real(kind=8), dimension(N)   :: B
      real(kind=8), dimension(N)   :: X

      real(kind=8), dimension(NPL) :: AL
      real(kind=8), dimension(NPU) :: AU

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

      integer, dimension(0:NCOLORtot*PEsmpTOT):: SMPindex
      integer, dimension(0:PEsmpTOT)          :: SMPindexG

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

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

solve_ICCG_mc (2/6)

```
!C
!C +------+
!C | INIT |
!C +------+
!C===
      allocate (W(N+128,4))

!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        X(i)   = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,4)= 0.0D0
      enddo
      enddo
!$omp end parallel do


      do ic= 1, NCOLORtot
!$omp parallel do private(ip,ip1,i,VAL,k)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          VAL= D(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL - (AL(k)**2) *
W(itemL(k),DD)
          enddo
          W(i,DD)= 1.d0/VAL
        enddo
        enddo
!$omp end parallel do
      enddo
```

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}

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

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}

```
      do ic= 1, NCOLORtot
!$omp parallel do private(ip,ip1,i,VAL,k)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          VAL= D(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL - (AL(k)**2) * W(itemL(k),DD)
          enddo
          W(i,DD)= 1.d0/VAL
        enddo
        enddo
!$omp end parallel do
      enddo
```

solve_ICCG_mc (3/6)

```
!C +---------------------+
!C | {r0}= {b} - [A]{xini} |
!C +---------------------+
!C===
!$omp parallel do private(ip,i,VAL,k)
        do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1,
     &         SMPindexG(ip)
          VAL= D(i)*X(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL + AL(k)*X(itemL(k))
          enddo
          do k= indexU(i-1)+1, indexU(i)
            VAL= VAL + AU(k)*X(itemU(k))
          enddo
          W(i,R)= B(i) - VAL
        enddo
        enddo
!$omp end parallel do

      BNRM2= 0.0D0
!$omp parallel do private(ip,i)
reduction(+:BNRM2)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        BNRM2 = BNRM2 + B(i)  **2
      enddo
      enddo
!$omp end parallel do
!C===
```

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

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

```
!$omp parallel do private(ip,i,VAL,k)
      do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          VAL= D(i)*X(i)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL + AL(k)*X(itemL(k))
          enddo
          do k= indexU(i-1)+1, indexU(i)
            VAL= VAL + AU(k)*X(itemU(k))
          enddo
          W(i,R)= B(i) - VAL
        enddo
      enddo
!$omp end parallel do
```

solve_ICCG_mc (3/6)

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

      BNRM2= 0.0D0
!$omp parallel do private(ip,i) reduction(+:BNRM2)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        BNRM2 = BNRM2 + B(i)  **2
      enddo
      enddo
!$omp end parallel do
!C===
```

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

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= 0.0D0
!$omp parallel do private(ip,i) reduction(+:BNRM2)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        BNRM2 = BNRM2 + B(i)  **2
      enddo
      enddo
!$omp end parallel do
```

solve_ICCG_mc (4/6)

```
      ITR= N
      do L= 1, ITR
!C
!C +---------------+
!C | {z}= [Minv]{r} |
!C +---------------+
!C===
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        W(i,Z)= W(i,R)
      enddo
      enddo
!$omp end parallel do

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

      do ic= NCOLORtot, 1, -1
!$omp parallel do private(ip,ip1,i,SW,j)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          SW  = 0.0d0
          do j= 1, INU(i)
            SW= SW + AU(j,i) * W(IAU(j,i),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
        enddo
!$omp end parallel do
      enddo
!C===
```

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)

SMPindex

```
      ITR= N
      do L= 1, ITR
!C
!C +---------------+
!C | {z}= [Minv]{r} |
!C +---------------+
!C===
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        W(i,Z)= W(i,R)
      enddo
      enddo
!$omp end parallel do

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

      do ic= NCOLORtot, 1, -1
!$omp parallel do private(ip,ip1,i,SW,k)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
        enddo
!$omp end parallel do
      enddo
!C===
```

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)

SMPindex

```
      ITR= N
      do L= 1, ITR
!C
!C +---------------+
!C | {z}= [Minv]{r} |
!C +---------------+
!C===
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        W(i,Z)= W(i,R)
      enddo
      enddo
!$omp end parallel do
 do ic= 1, NCOLORtot
!$omp parallel do private(ip,ip1,i,WVAL,k)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
        enddo
!$omp end parallel do
      enddo

      do ic= NCOLORtot, 1, -1
!$omp parallel do private(ip,ip1,i,SW,k)
        do ip= 1, PEsmpTOT
          ip1= (ic-1)*PEsmpTOT + ip
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          SW  = 0.0d0
          do k= indexU(i-1)+1, indexU(i)
            SW= SW + AU(k) * W(itemU(k),Z)
          enddo
          W(i,Z)= W(i,Z) - W(i,DD) * SW
        enddo
        enddo
!$omp end parallel do
      enddo
!C===
```

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

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

Forward Substitution

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

Backward Substitution

Forward Substitution: SMPindex

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

solve_ICCG_mc (5/6)

```
!C +----------------------------+
!C | {p} = {z} if      ITER=1   |
!C | BETA= RHO / RHO1  otherwise |
!C +----------------------------+
!C===
      if ( L.eq.1 ) then
!$omp parallel do private(ip,i)
        do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          W(i,P)= W(i,Z)
        enddo
        enddo
!$omp end parallel do
       else
        BETA= RHO / RHO1
!$omp parallel do private(ip,i)
        do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          W(i,P)= W(i,Z) + BETA*W(i,P)
        enddo
        enddo
!$omp end parallel do
      endif
!C===

!C +------------+
!C | {q}= [A]{p} |
!C +------------+
!C===
!$omp parallel do private(ip,i,VAL,k)
      do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          VAL= D(i)*W(i,P)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL + AL(k)*W(itemL(k),P)
          enddo
          do k= indexU(i-1)+1, indexU(i)
            VAL= VAL + AU(k)*W(itemU(k),P)
          enddo
          W(i,Q)= VAL
        enddo
      enddo
!$omp end parallel do
!C===
```

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)

```
!C +----------------------------+
!C | {p} = {z} if      ITER=1   |
!C | BETA= RHO / RHO1  otherwise |
!C +----------------------------+
!C===
      if ( L.eq.1 ) then
!$omp parallel do private(ip,i)
        do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          W(i,P)= W(i,Z)
        enddo
        enddo
!$omp end parallel do
       else
        BETA= RHO / RHO1
!$omp parallel do private(ip,i)
        do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          W(i,P)= W(i,Z) + BETA*W(i,P)
        enddo
        enddo
!$omp end parallel do
      endif
!C===

!C +------------+
!C | {q}= [A]{p} |
!C +------------+
!C===
!$omp parallel do private(ip,i,VAL,k)
      do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          VAL= D(i)*W(i,P)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL + AL(k)*W(itemL(k),P)
          enddo
          do k= indexU(i-1)+1, indexU(i)
            VAL= VAL + AU(k)*W(itemU(k),P)
          enddo
          W(i,Q)= VAL
        enddo
      enddo
!$omp end parallel do
!C===
```

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)

```
!C
!C +--------------------+
!C | ALPHA= RHO / {p}{q} |
!C +--------------------+
!C===
      C1= 0.d0
!$omp parallel do private(ip,i) reduction(+:C1)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      enddo
!$omp end parallel do

      ALPHA= RHO / C1
!C===


!C
!C +---------------------+
!C | {x}= {x} + ALPHA*{p} |
!C | {r}= {r} - ALPHA*{q} |
!C +---------------------+
!C===
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
      enddo
!$omp end parallel do

      DNRM2= 0.d0
!$omp parallel do private(ip,i) reduction(+:DNRM2)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        DNRM2= DNRM2 + W(i,R)**2
      enddo
      enddo
!$omp end parallel do
!C===
```

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)

```
!C
!C +--------------------+
!C | ALPHA= RHO / {p}{q} |
!C +--------------------+
!C===
      C1= 0.d0
!$omp parallel do private(ip,i) reduction(+:C1)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      enddo
!$omp end parallel do

      ALPHA= RHO / C1
!C===


!C
!C +---------------------+
!C | {x}= {x} + ALPHA*{p} |
!C | {r}= {r} - ALPHA*{q} |
!C +---------------------+
!C===
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        X(i)   = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
      enddo
!$omp end parallel do

      DNRM2= 0.d0
!$omp parallel do private(ip,i) reduction(+:DNRM2)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        DNRM2= DNRM2 + W(i,R)**2
      enddo
      enddo
!$omp end parallel do
!C===
```

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)

```
!C
!C +--------------------+
!C | ALPHA= RHO / {p}{q} |
!C +--------------------+
!C===
      C1= 0.d0
!$omp parallel do private(ip,i) reduction(+:C1)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      enddo
!$omp end parallel do

      ALPHA= RHO / C1
!C===


!C
!C +---------------------+
!C | {x}= {x} + ALPHA*{p} |
!C | {r}= {r} - ALPHA*{q} |
!C +---------------------+
!C===
!$omp parallel do private(ip,i)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo
      enddo
!$omp end parallel do

      DNRM2= 0.d0
!$omp parallel do private(ip,i) reduction(+:DNRM2)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        DNRM2= DNRM2 + W(i,R)**2
      enddo
      enddo
!$omp end parallel do
!C===
```

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

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

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

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

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

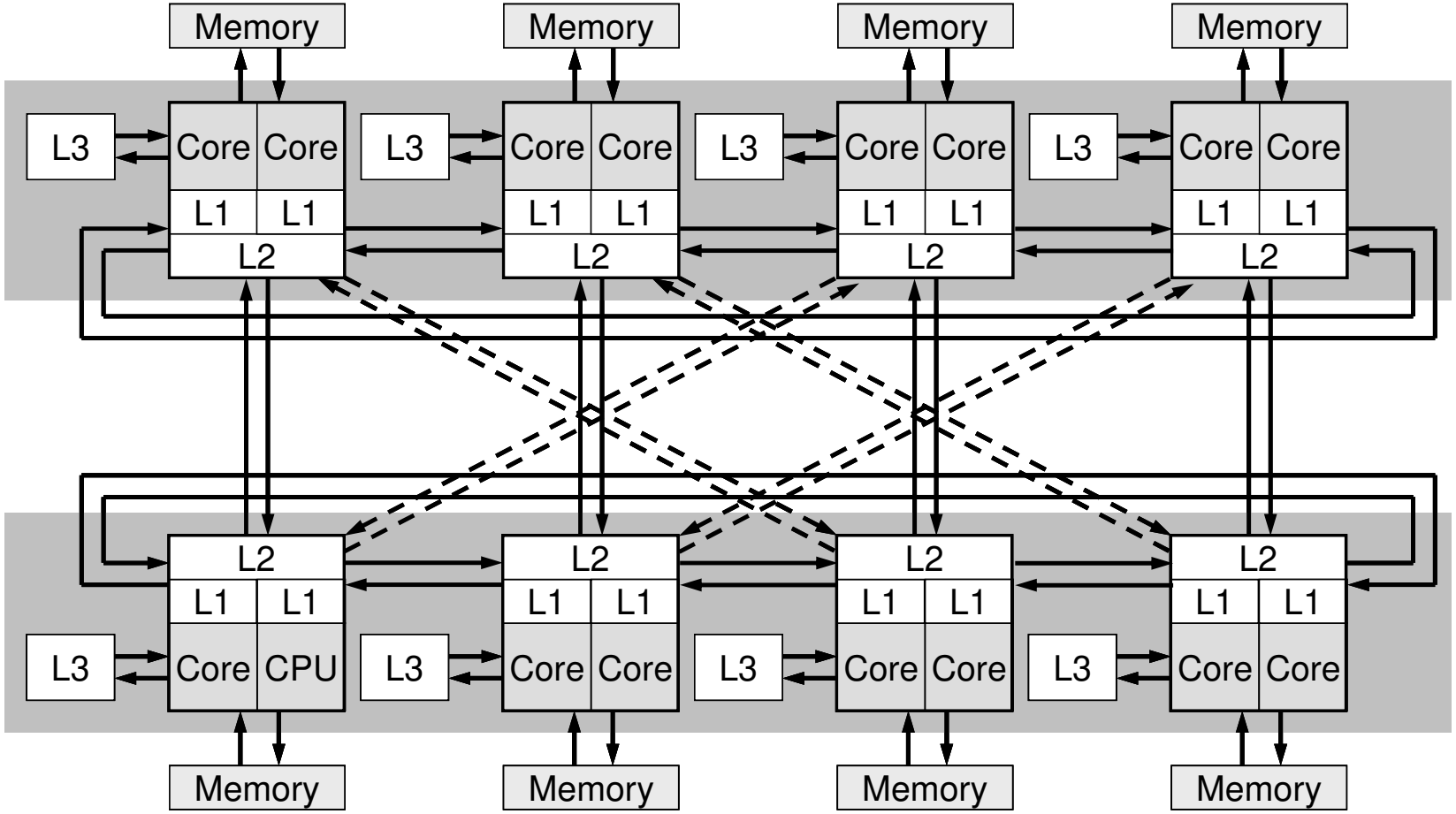
  check convergence |r|

end

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

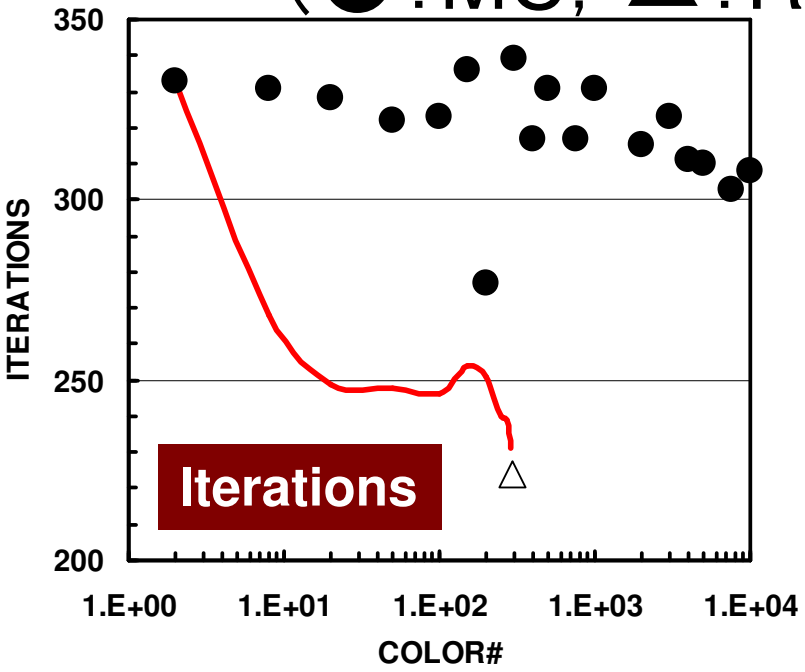
Results

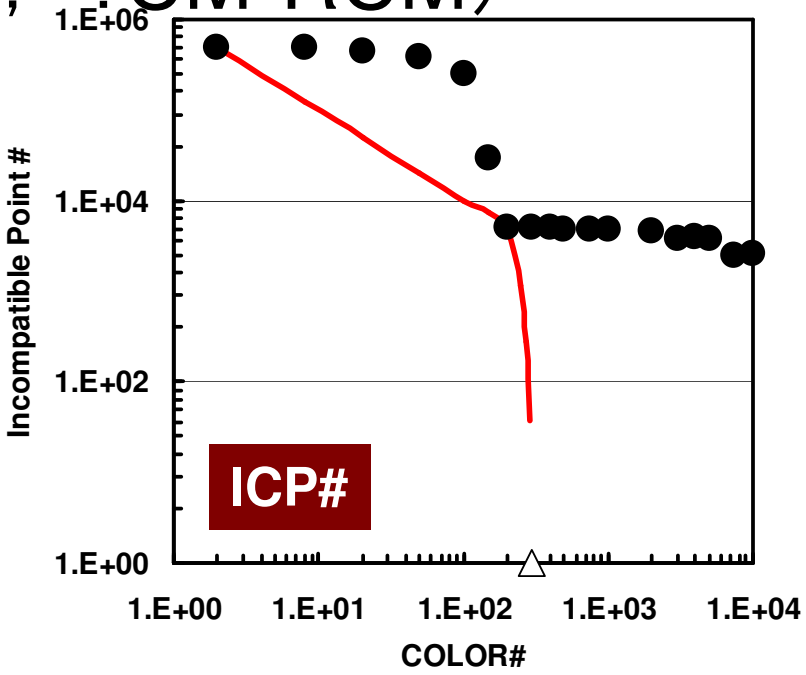
- Hitachi SR11000/J2 1-node, 16-cores
  - Retired in Fall 2011, based on IBM's Power 5+
- 100^3 Meshes

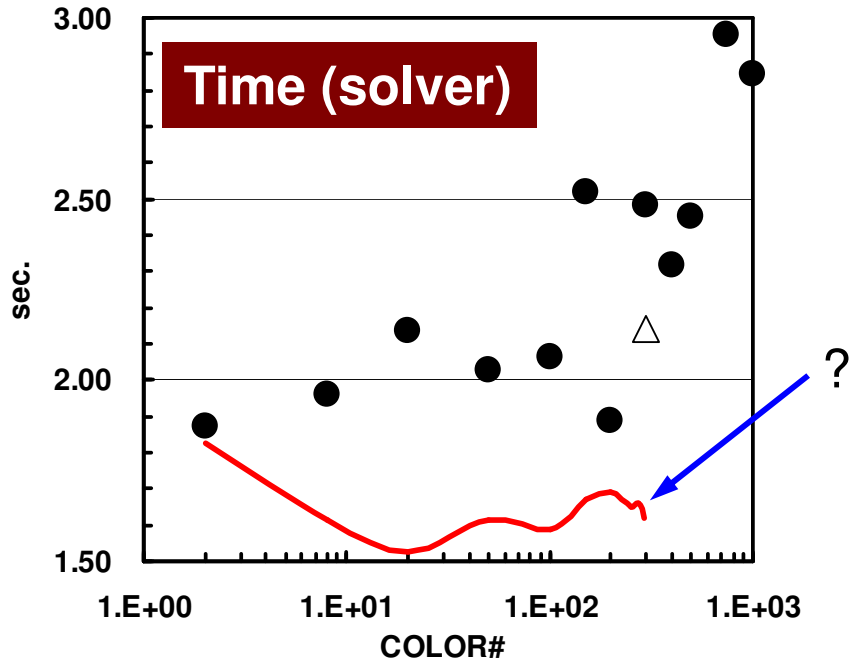


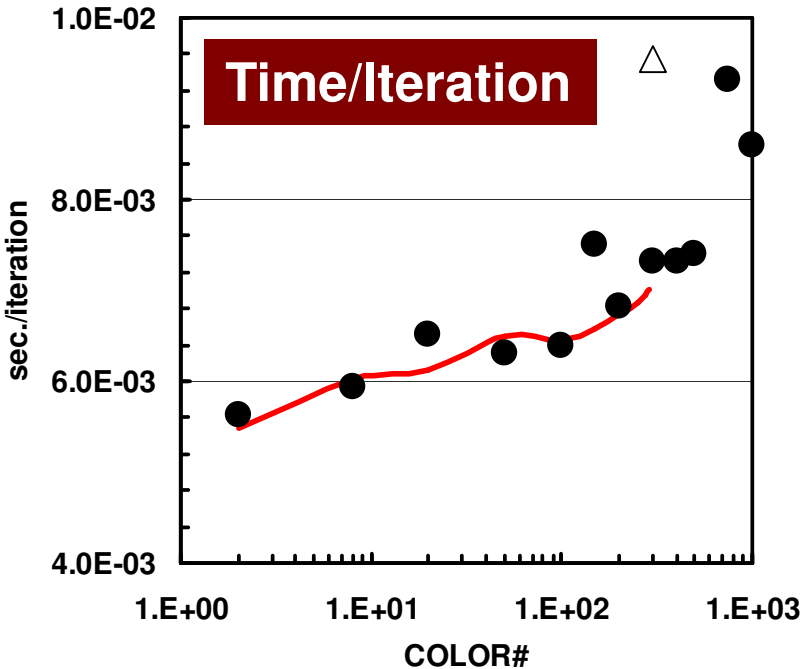
SR11000, 1-node/16-cores, 100^3

(●:MC, △:RCM, -:CM-RCM)



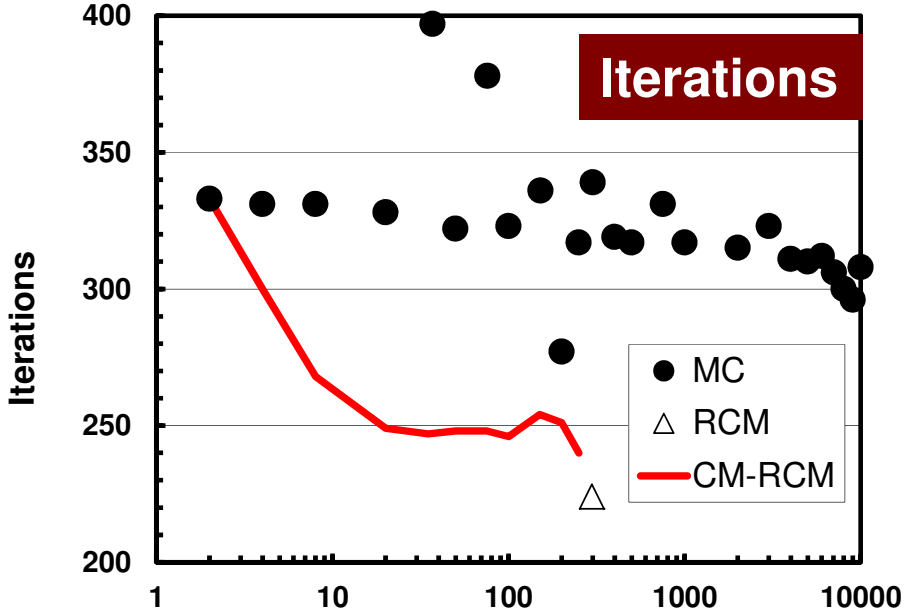




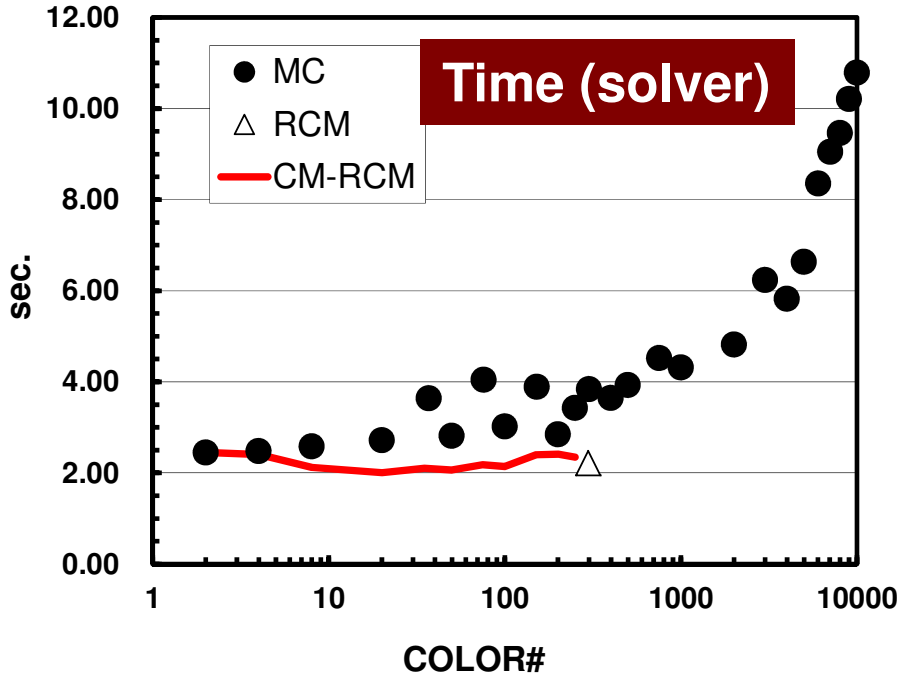


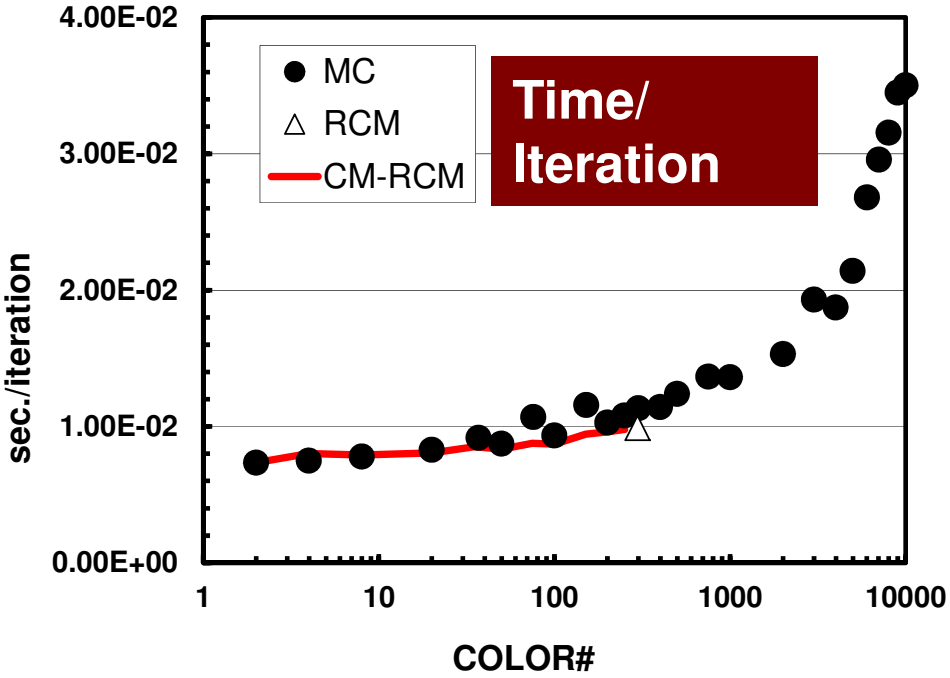
FX10, 1-node/16-cores, 100^3

(●:MC, △:RCM, -:CM-RCM)



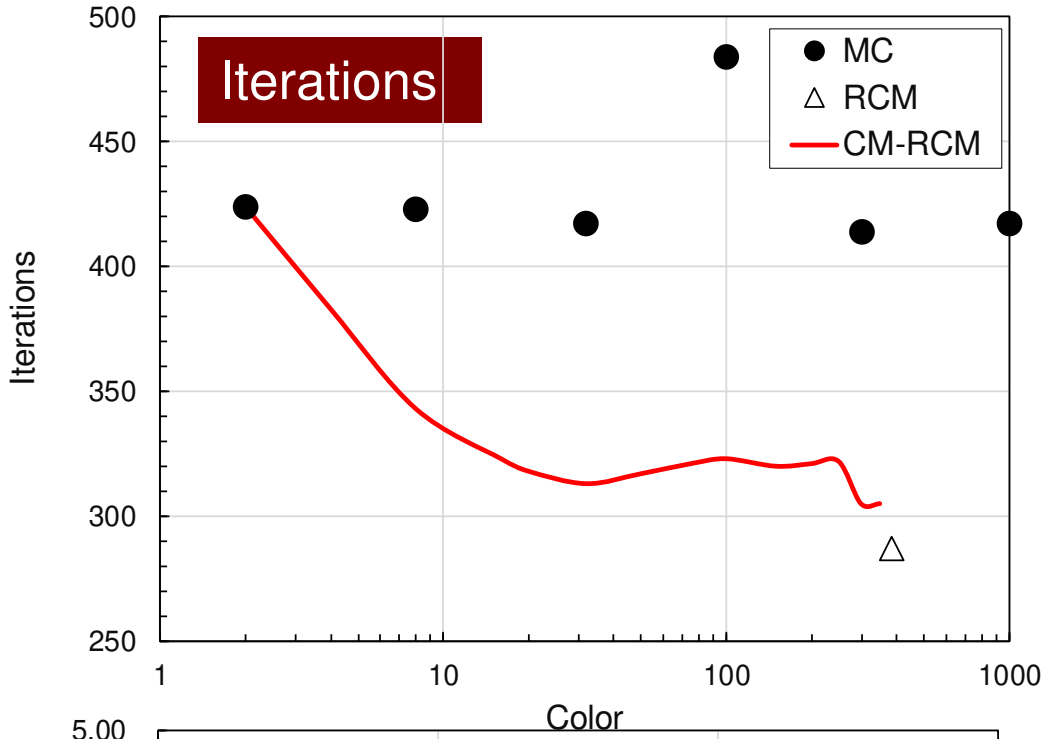
- Fujitsu PRIMEHPC FX10
  - ✓ Oakleaf-FX, Oakbridge-CX
  - ✓ Commercial Version of K
- Apr. 2012-Mar. 2018

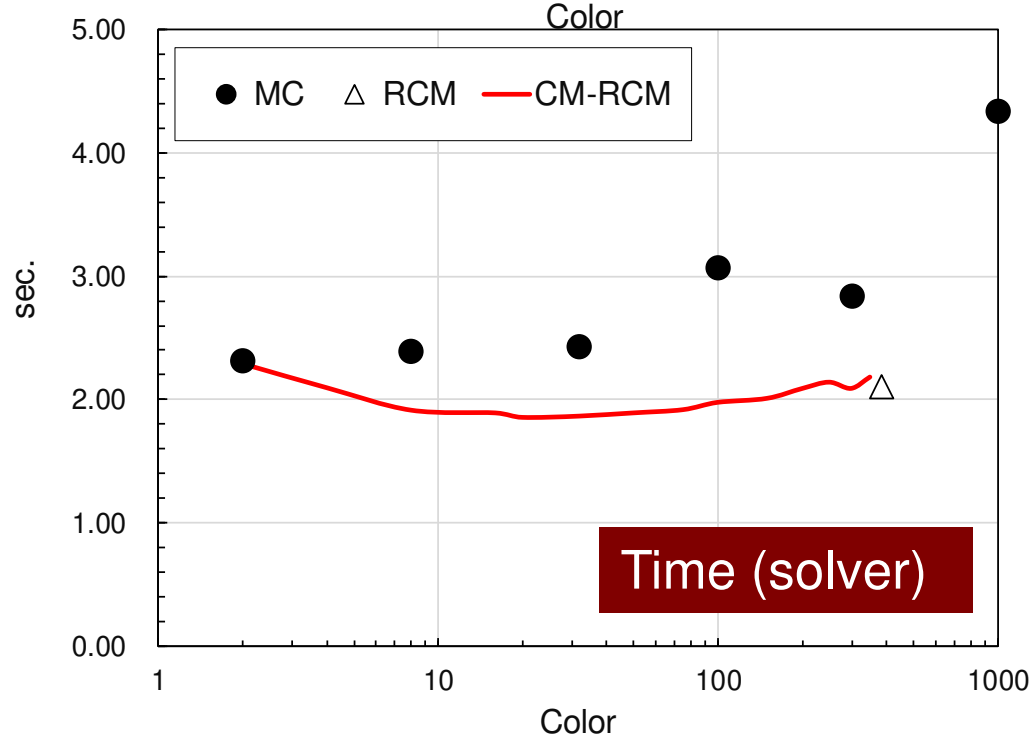


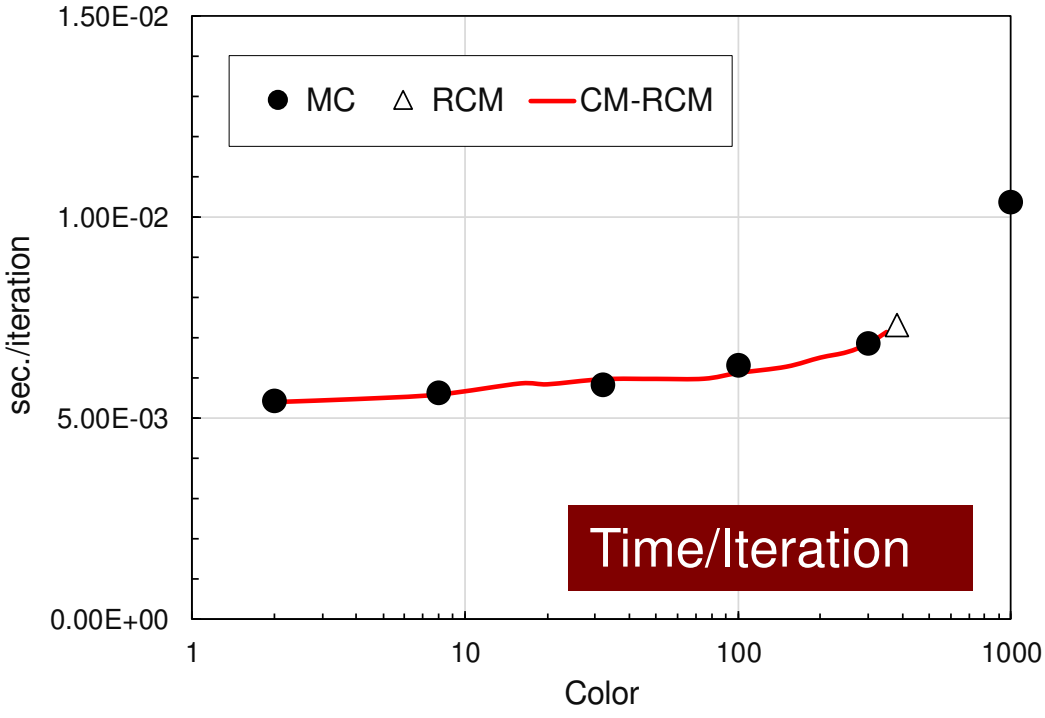


OBCX, 1-soket/24-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)



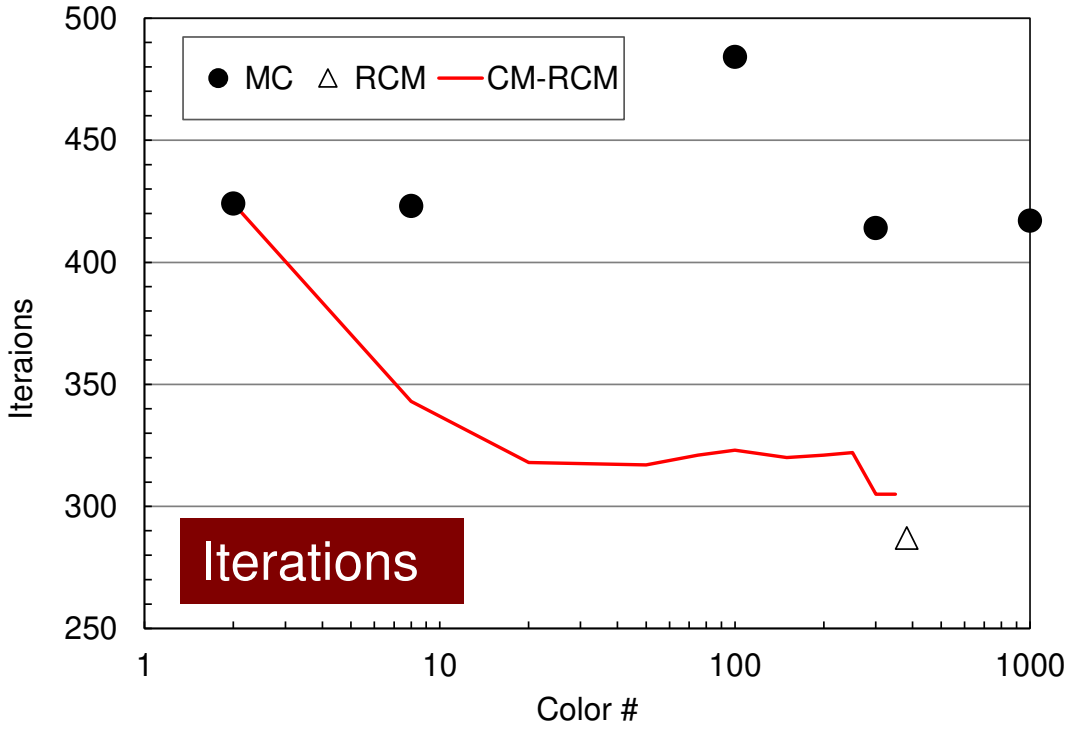


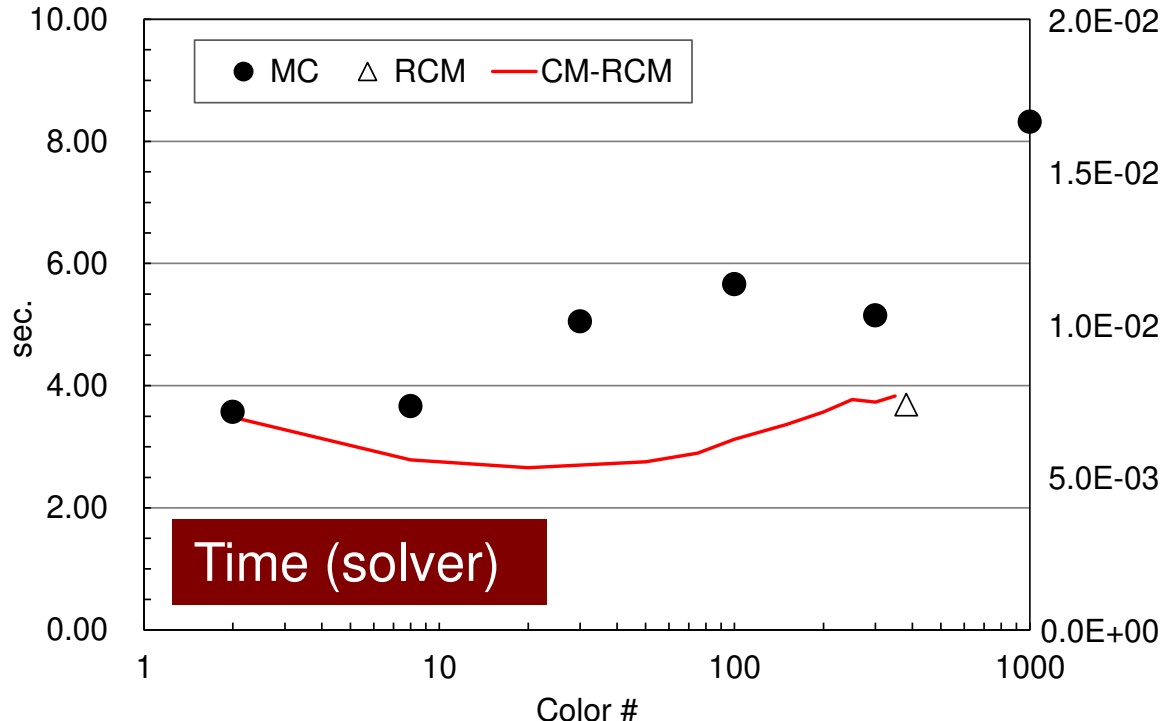


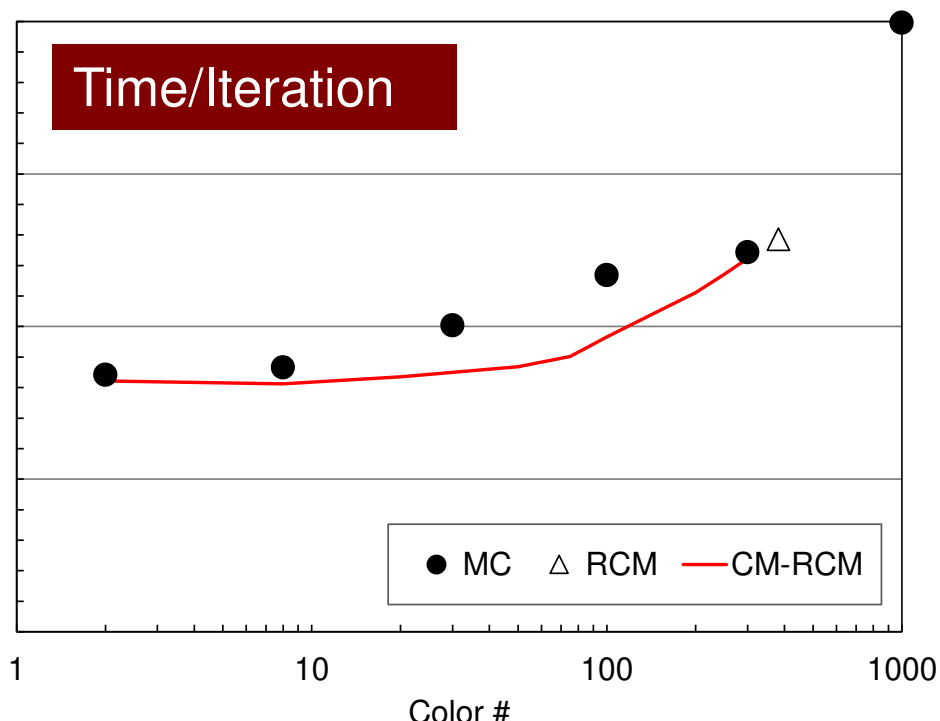
Odyssey

1-CMG/12-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)







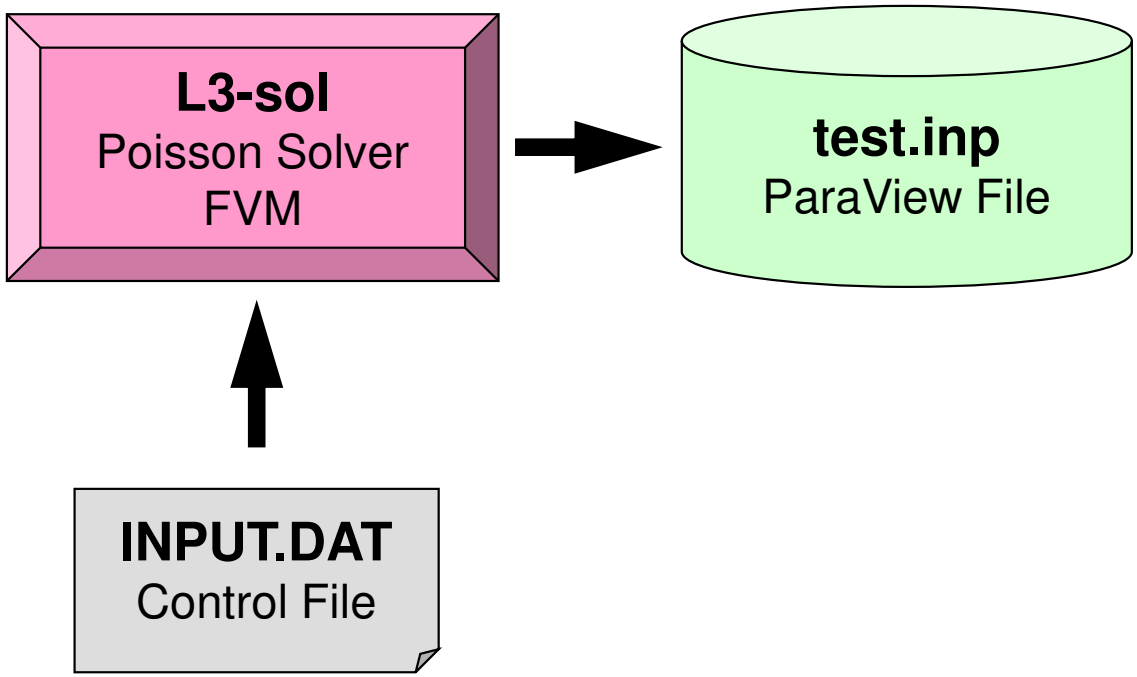
- Applying OpenMP to L2-sol
- Examples
- **Optimization + Exercise**

- Running the Code
- Further Optimization

Compile & Run

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

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

  L3-sol

>$ cd ../run

(modify INPUT.DAT, go1.sh)

>$ pjsub go1.sh
```

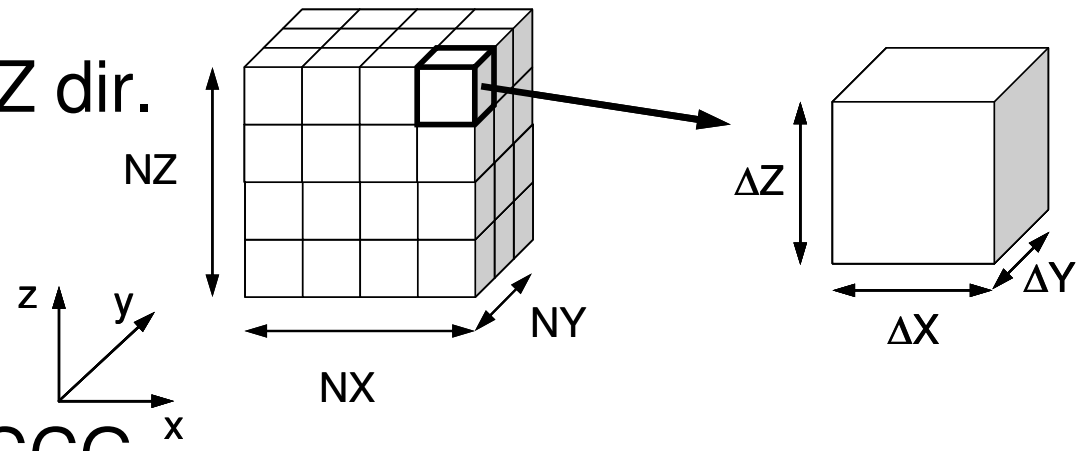
Running L3-sol



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



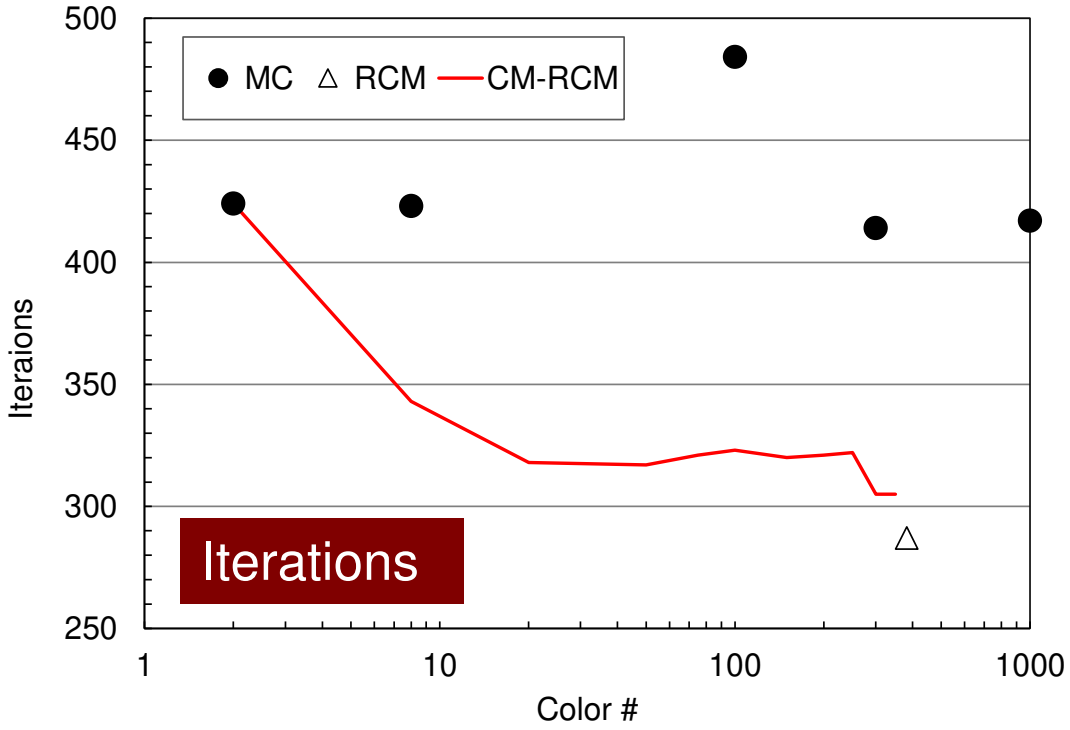
go1.sh

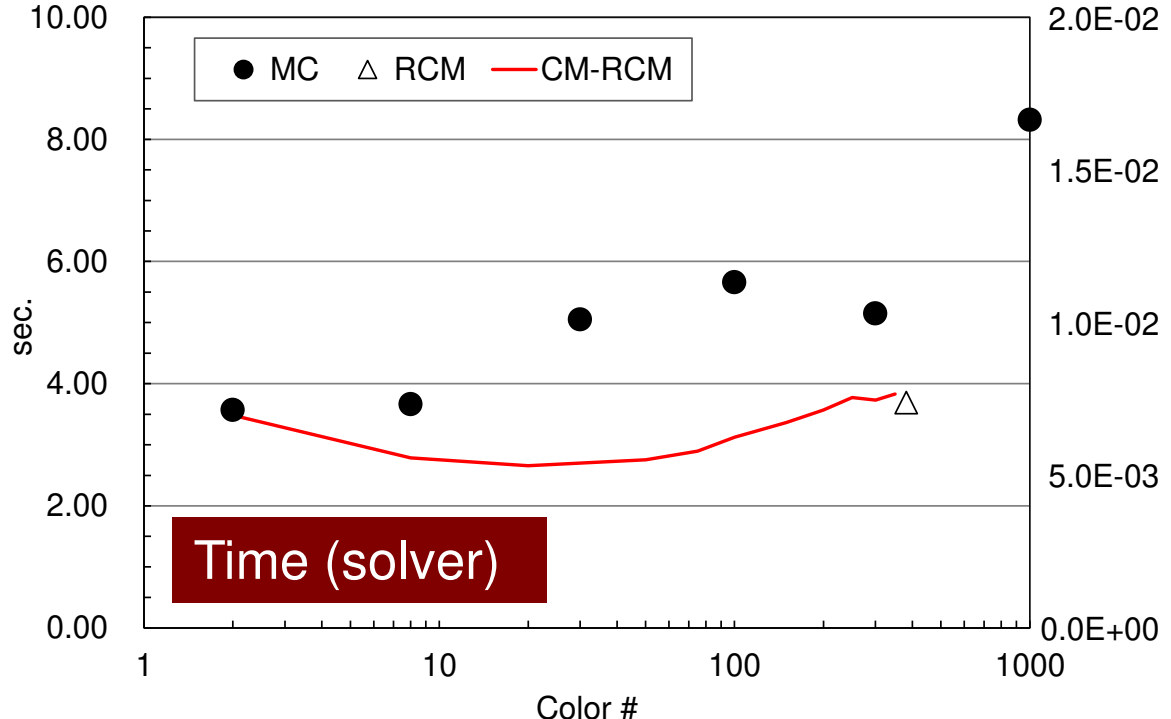
```
#!/bin/sh
#PJM -N "go1"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=12                (=PEsmpTOT)
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o test1.lst

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
```

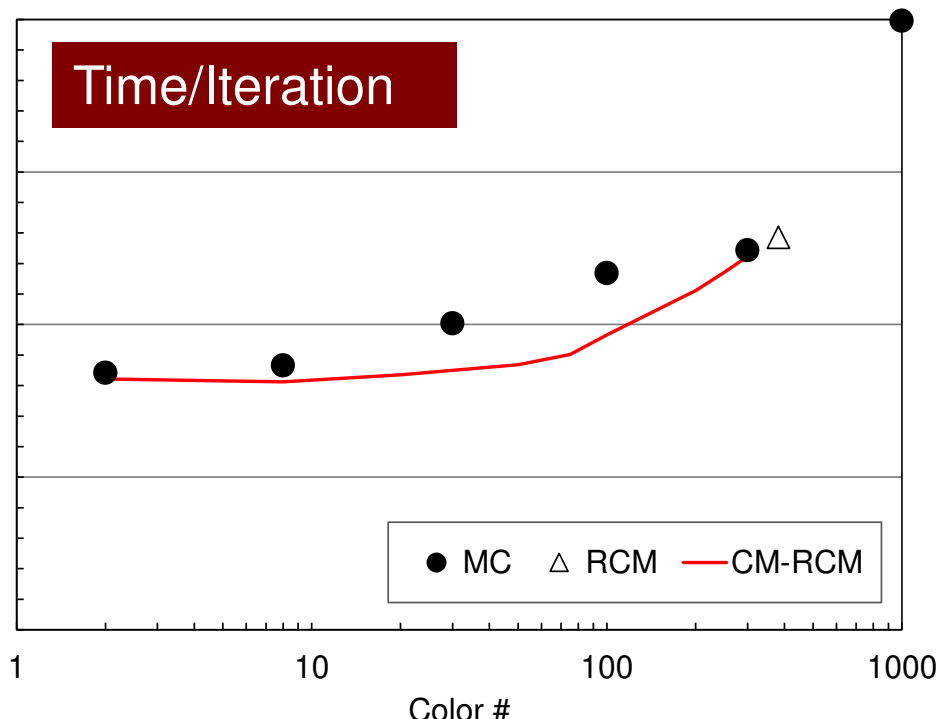
Odyssey

1-CMG/12-cores, 128^3

(●:MC, △:RCM, -:CM-RCM)







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

Forward Subst.: Current Impl. (F)

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

- 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 (F)

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

- Generation of threads occurs just once before starting forward substitutions.
- Loops with "**!omp do**" are parallelized.

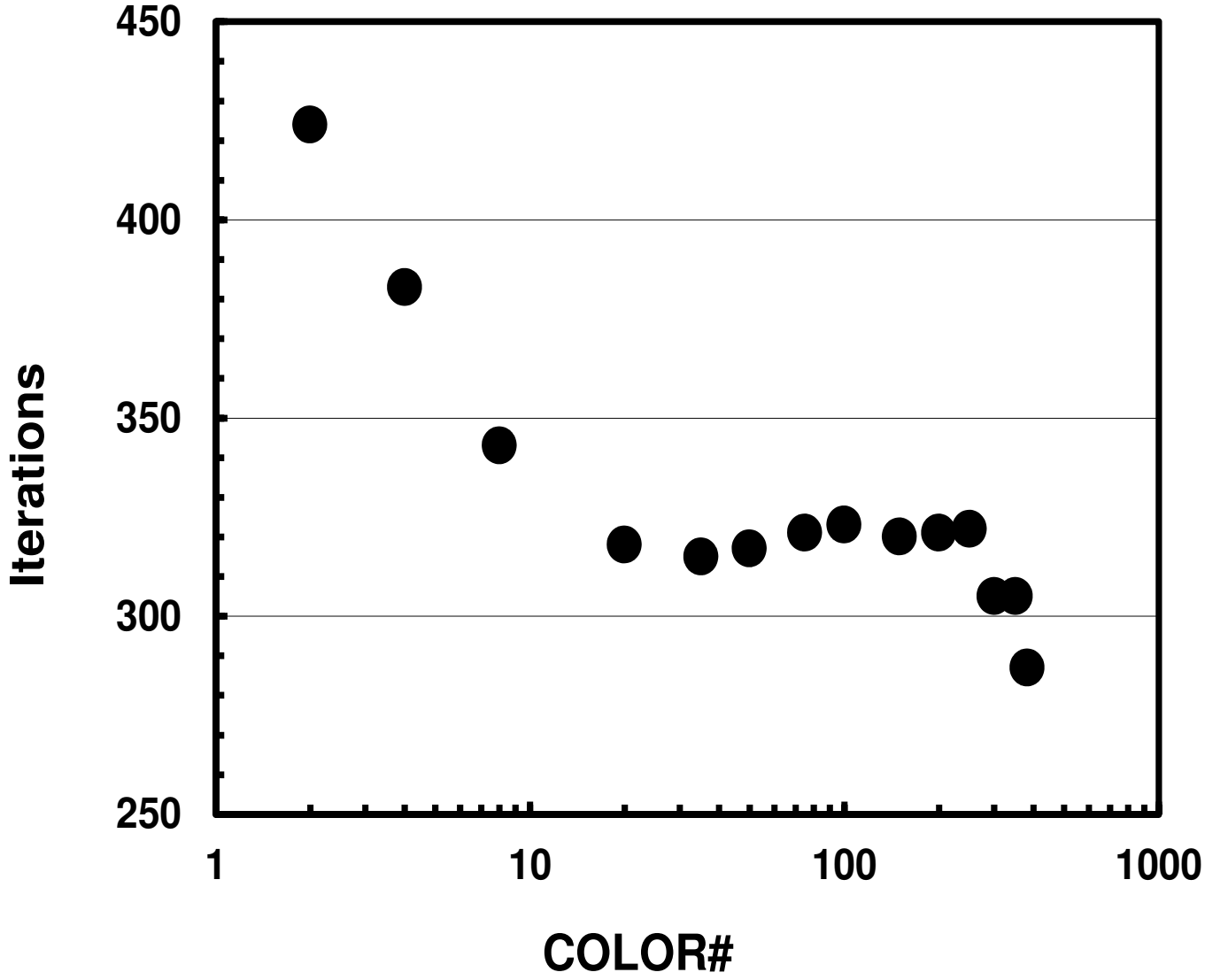
Programs (src0)

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

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

<modify "INPUT.DAT">
<modify "go0.sh">

% pjsub go0.sh
```

go0.sh

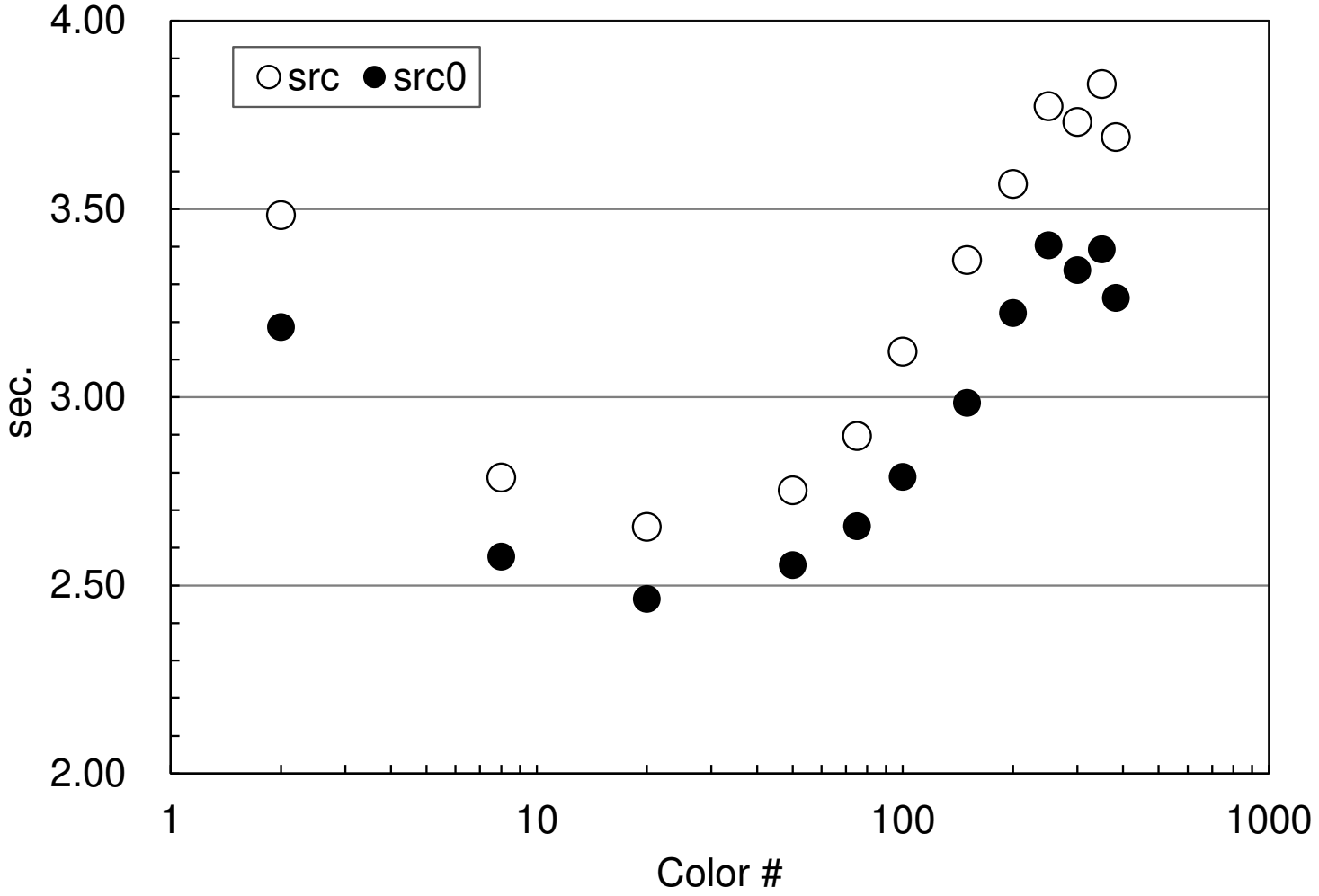
```
#!/bin/sh
#PJM -N "go0"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=12                (=PEsmpTOT)
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o test0.lst

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

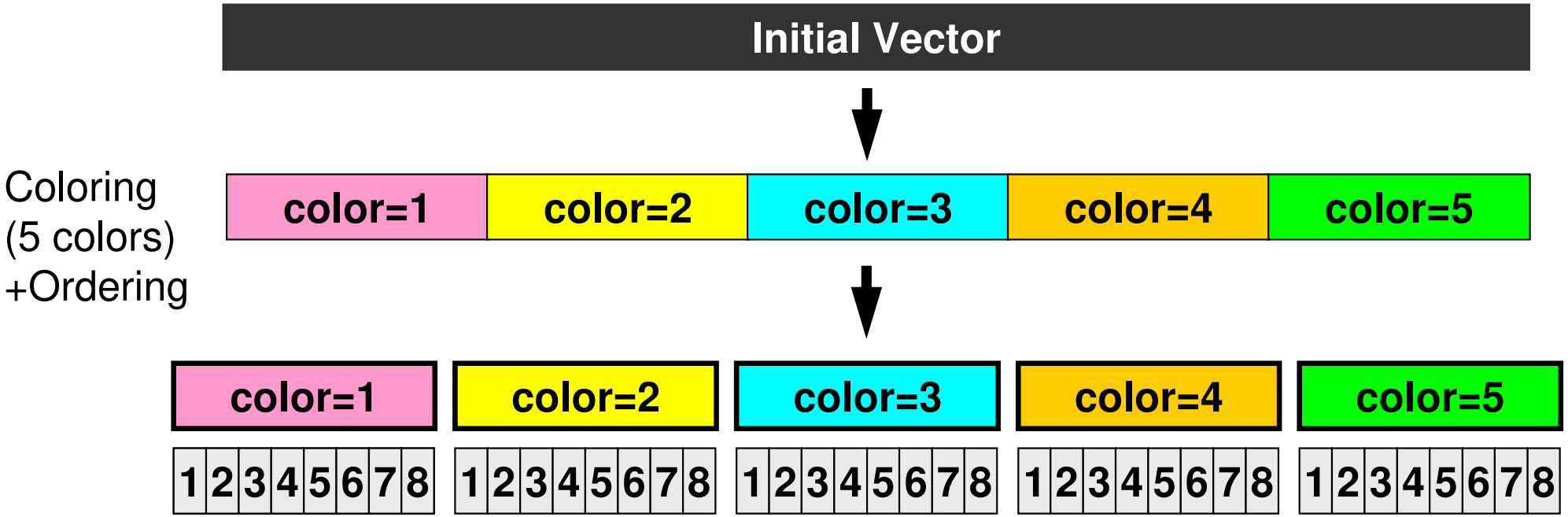
- Coloring
  - MC
  - RCM
  - CM-RCM
- Renumbering is according to color/level ID

- 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
```



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

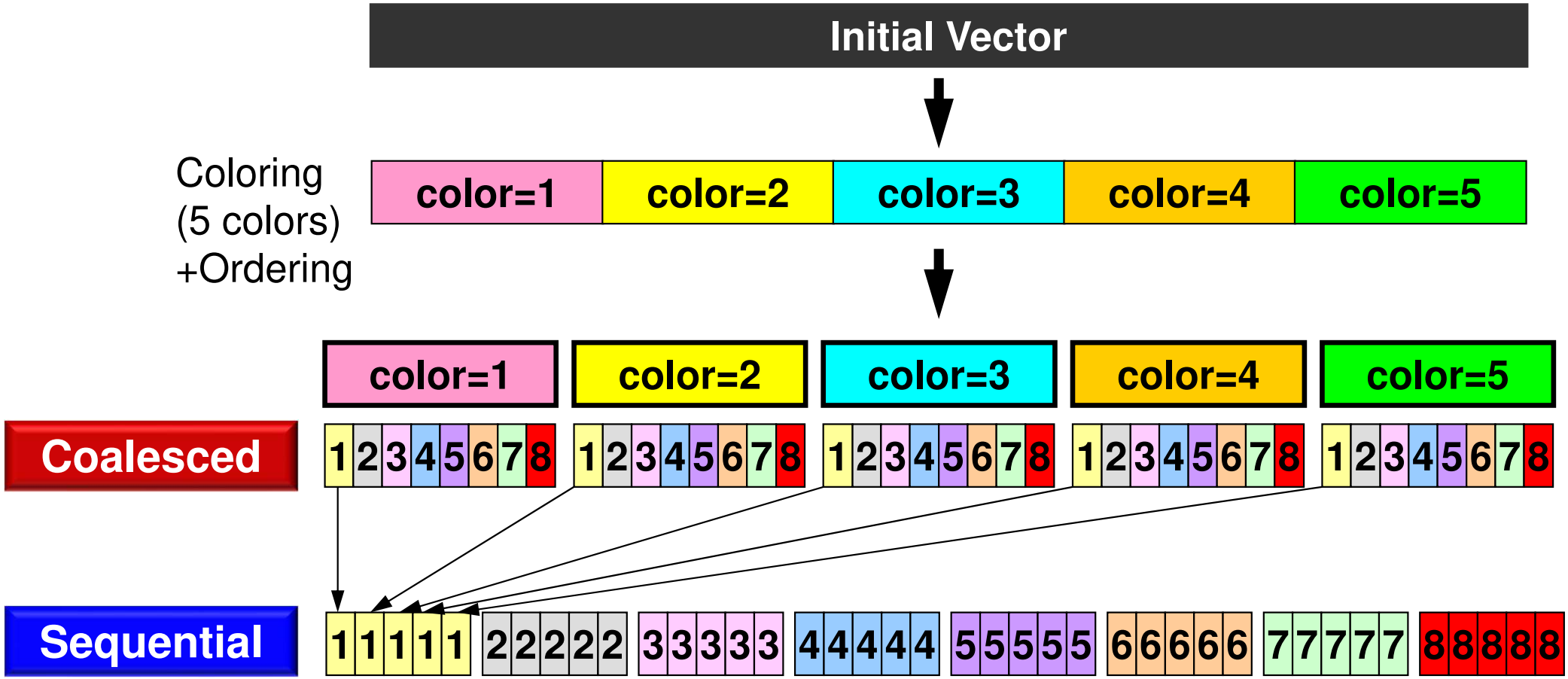
Sequential Reordering

- 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`**$\leqq$**`k`**$\leqq$**`indexL(icel)`**

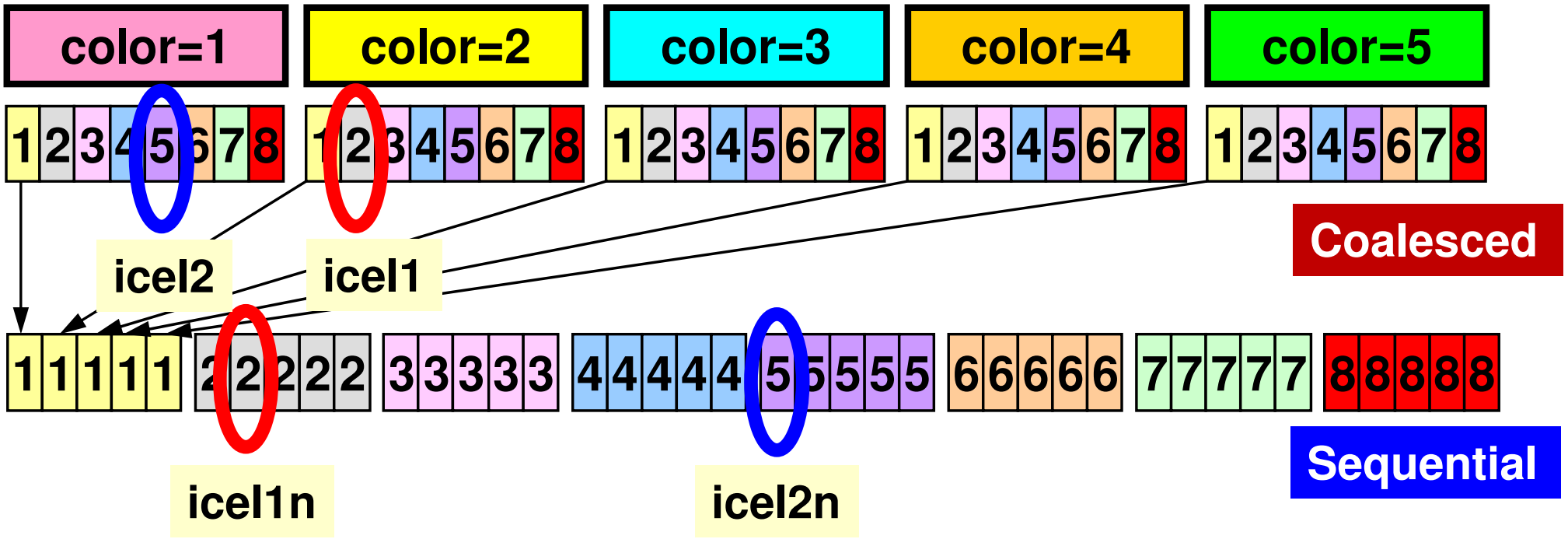
Sequential Reordering

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)+1≦k≦indexL[icel1+1]`**
- Sequential
  - **`icel1n < icel2n`**, but still **`icel2n= itemL(k)`**, where **`indexL(icel1n)+1≦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

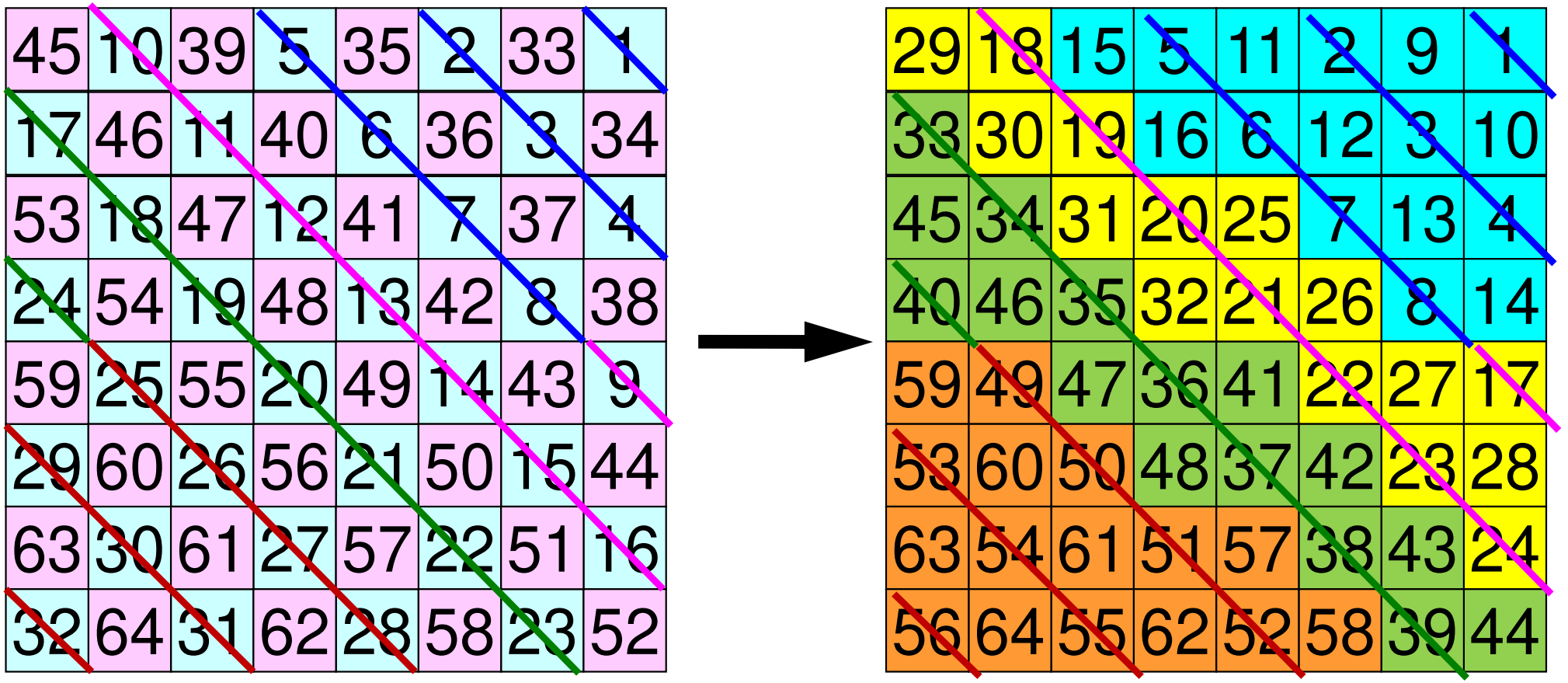
Sequential Reordering, 4-threads

Sequential Reordering

CM-RCM(2), 4-threads

1st-Color

#0 thread, #1, #2, #3



CM-RCM(2)

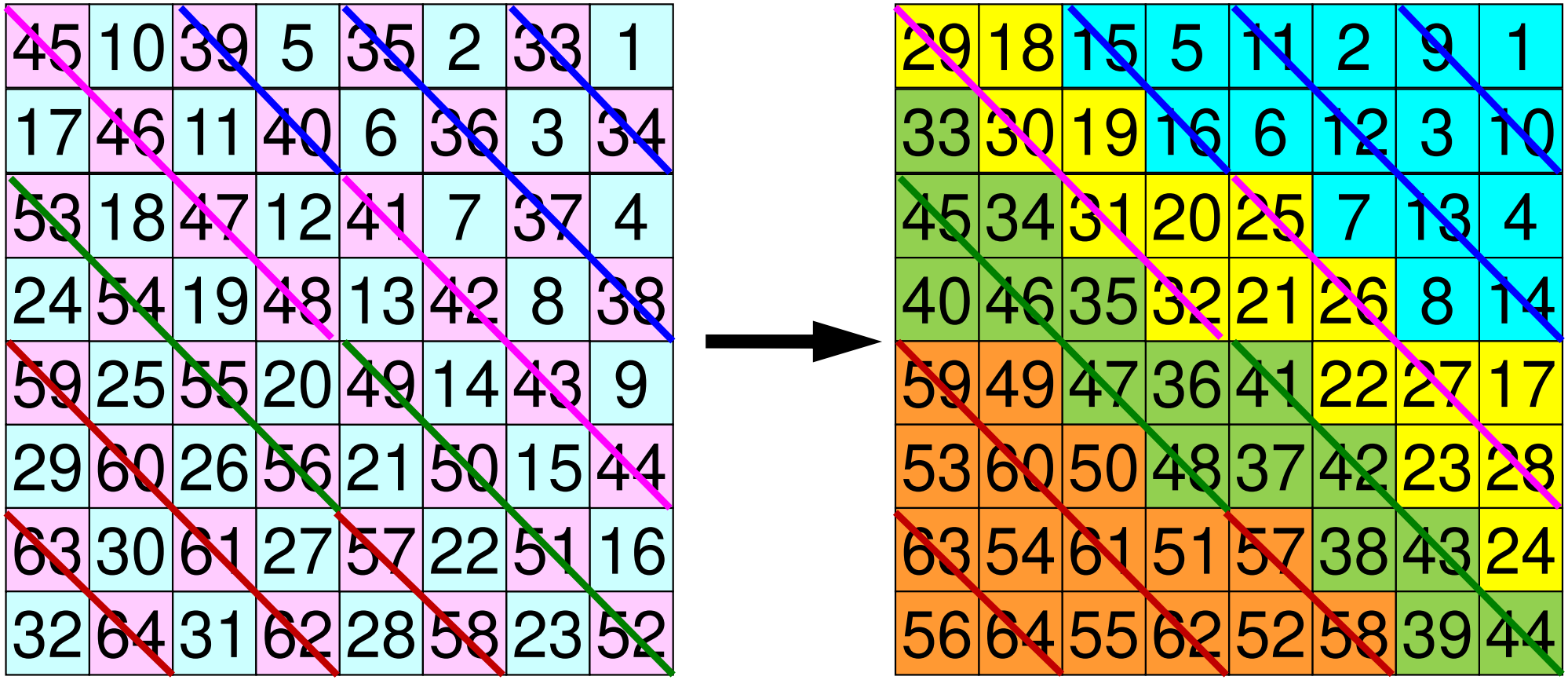
Sequential Reordering, 4-threads

Sequential Reordering

CM-RCM(2), 4-threads

2nd-Color

#0 thread, #1, #2, #3

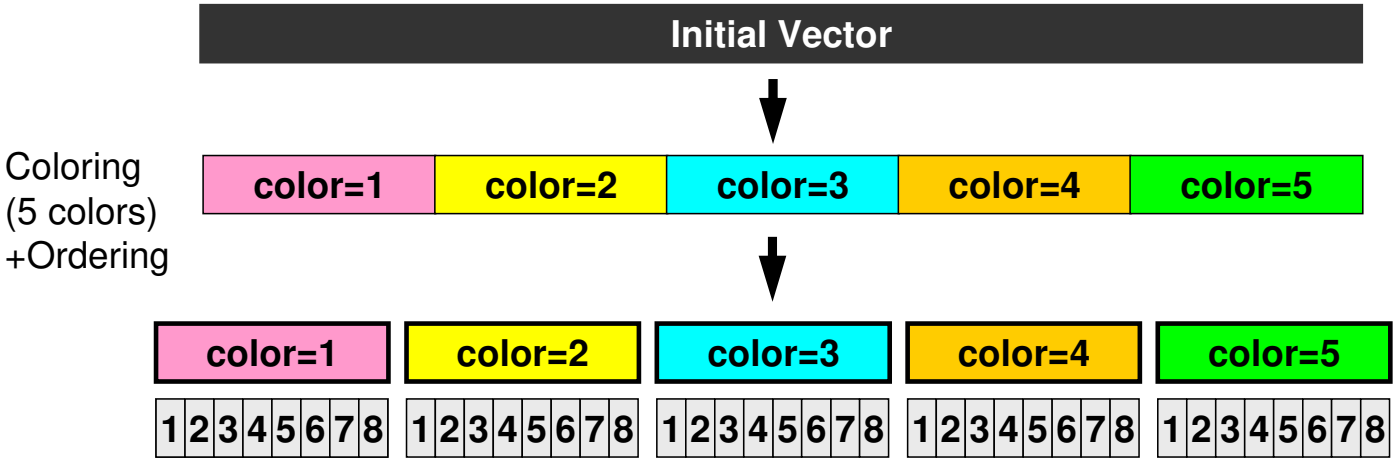


CM-RCM(2)

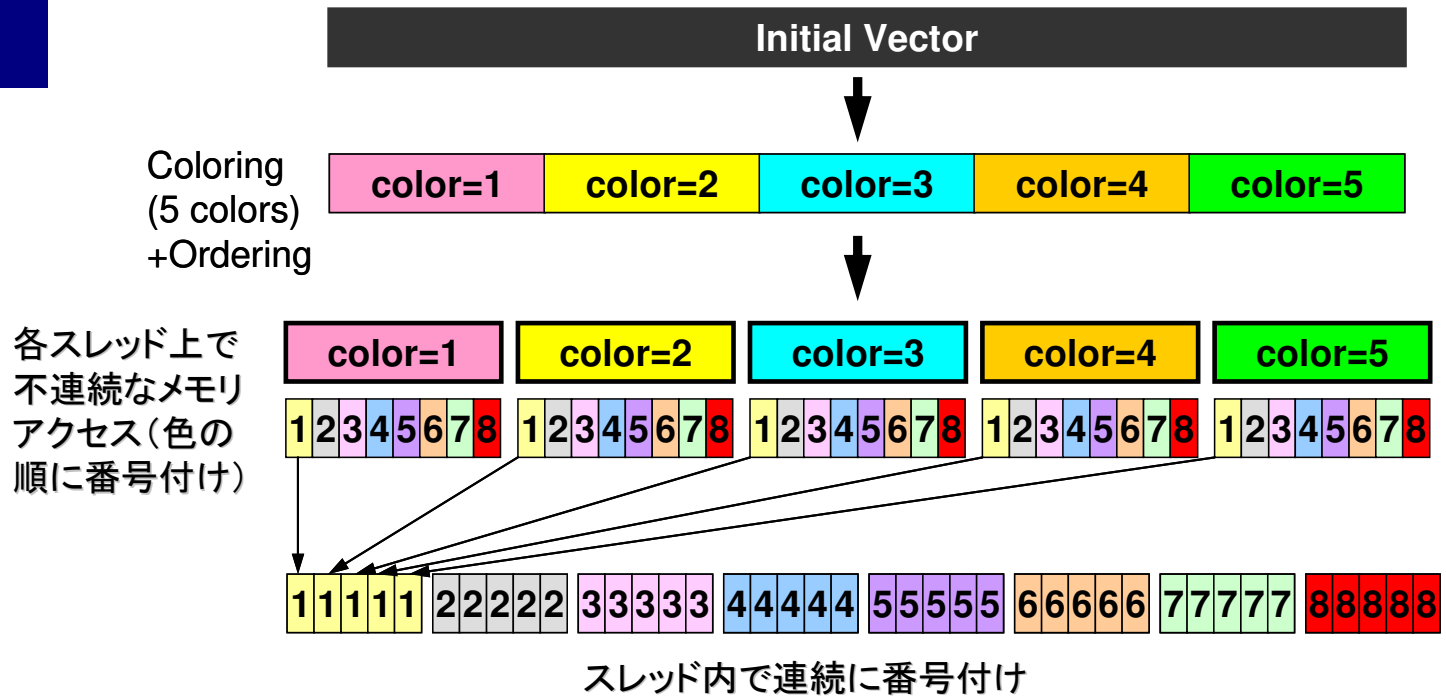
Sequential Reordering, 4-threads

Sequential Reordering

Coalesced
Good for GPU



Sequential



Programs (reorder0)

```
% cd /work/gt89/t89XXX/ompf/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

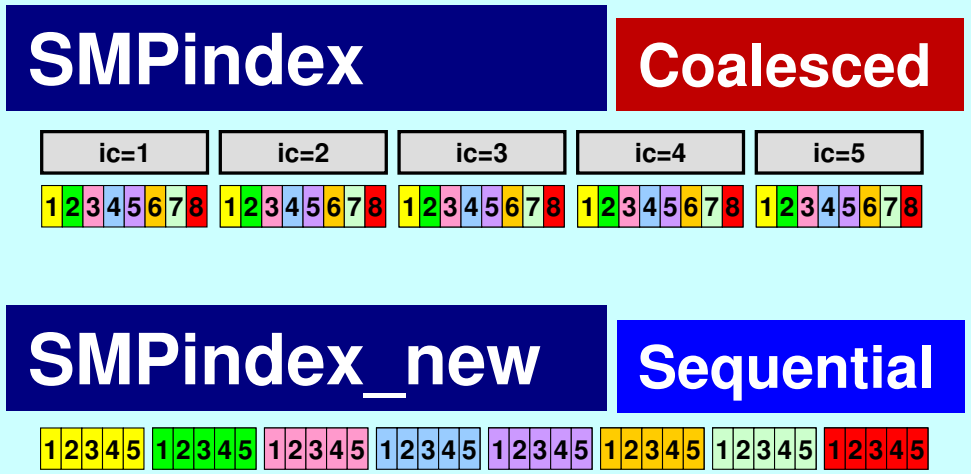
```
128 128 128                          NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00           DX/DY/DZ
1.0e-08                              EPSICC
12                                   PEsmpTOT
-10                                  NCOLORtot
0                                    NFLAG
0                       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

```
program MAIN

use STRUCT
use PCG
use solver_ICCG_mc
use solver_ICCG_mc_ft

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

call INPUT
call POINTER_INIT
call BOUNDARY_CELL
call CELL_METRICS
call POI_GEN

ISET= 0
allocate (WK(ICELTOT))

  if (METHOD.eq.0) then
    call solve_ICCG_mc                                          &
&        ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU,     &
&          D, BFORCE, PHI, AL, AU, NCOLORtot, PEsmpTOT,         &
&          SMPindex_new, EPSICCG, ITR, IER)
   else
    call solve_ICCG_mc_ft                                       &
&        ( ICELTOT, NPL, NPU, indexL, itemL, indexU, itemU,     &
&          D, BFORCE, PHI, AL, AU, NCOLORtot, PEsmpTOT,         &
&          SMPindex_new, EPSICCG, ITR, IER)
  endif

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

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

call OUTUCD

stop
end
```

```
allocate (SMPindex(0:PEsmpTOT*NCOLORtot))
SMPindex= 0
do ic= 1, NCOLORtot
  nn1= COLORindex(ic) - COLORindex(ic-1)
  num= nn1 / PEsmpTOT
  nr = nn1 - PEsmpTOT*num
  do ip= 1, PEsmpTOT
    if (ip.le.nr) then
      SMPindex((ic-1)*PEsmpTOT+ip)= num + 1
     else
      SMPindex((ic-1)*PEsmpTOT+ip)= num
    endif
  enddo
enddo

allocate (SMPindex_new(0:PEsmpTOT*NCOLORtot))
SMPindex_new(0)= 0
do ic= 1, NCOLORtot
  do ip= 1, PEsmpTOT
    j1= (ic-1)*PEsmpTOT + ip
    j0= j1 - 1
    SMPindex_new((ip-1)*NCOLORtot+ic)= SMPindex(j1)
    SMPindex(j1)= SMPindex(j0) + SMPindex(j1)
  enddo
enddo

do ip= 1, PEsmpTOT
  do ic= 1, NCOLORtot
    j1= (ip-1)*NCOLORtot + ic
    j0= j1 - 1
    SMPindex_new(j1)= SMPindex_new(j0) + SMPindex_new(j1)
  enddo
enddo
```

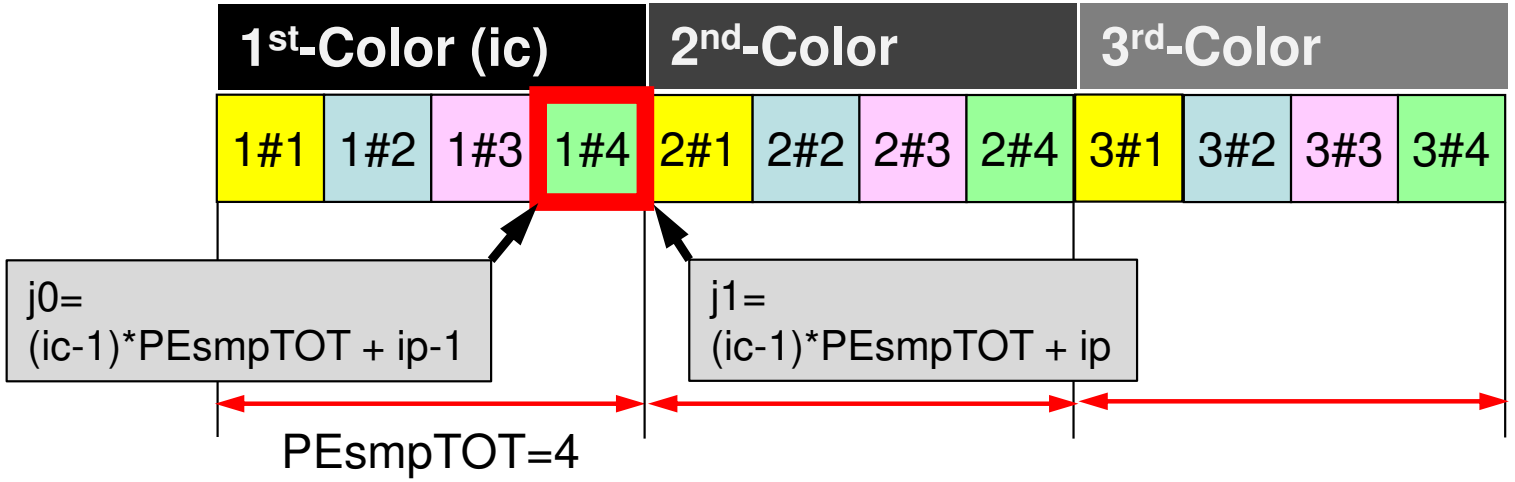


Sequential Reordering (2/5) poi_gen-1

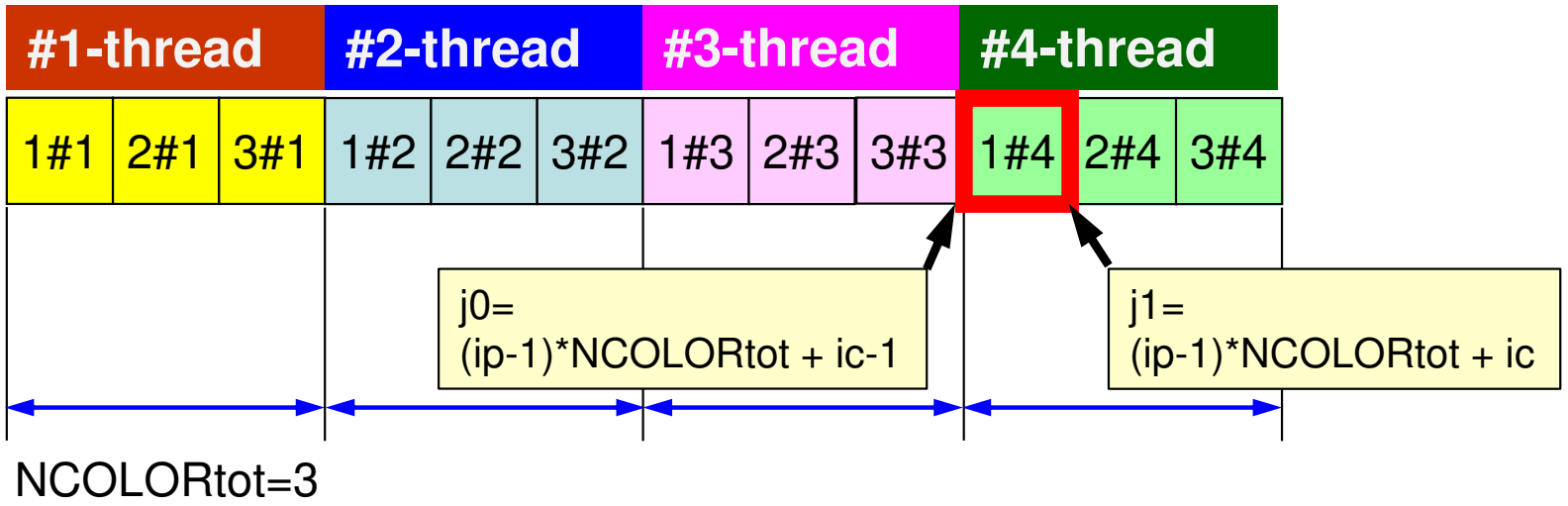
ic#ip

ic: 1~ NCOLORtot
ip: 1~ PEsmpTOT

SMPindex

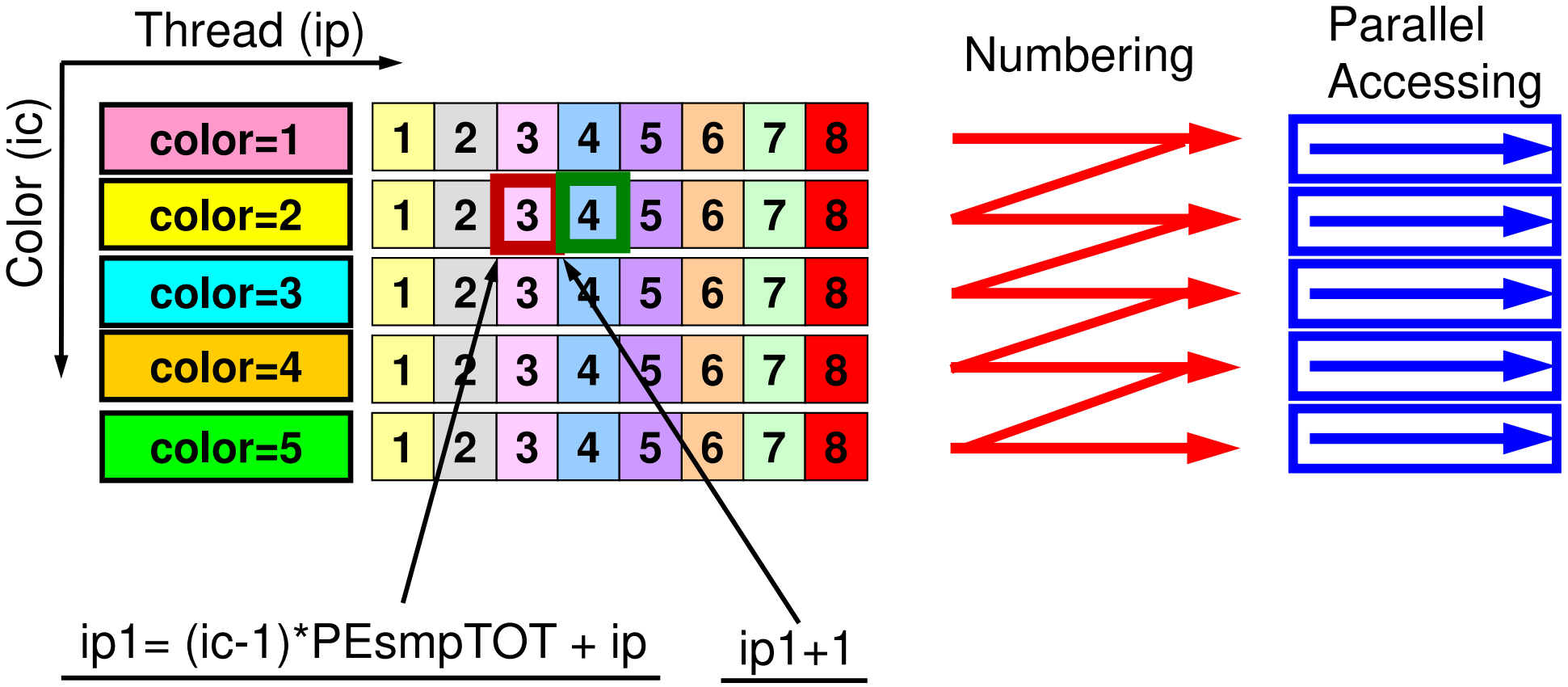


SMPindex_new



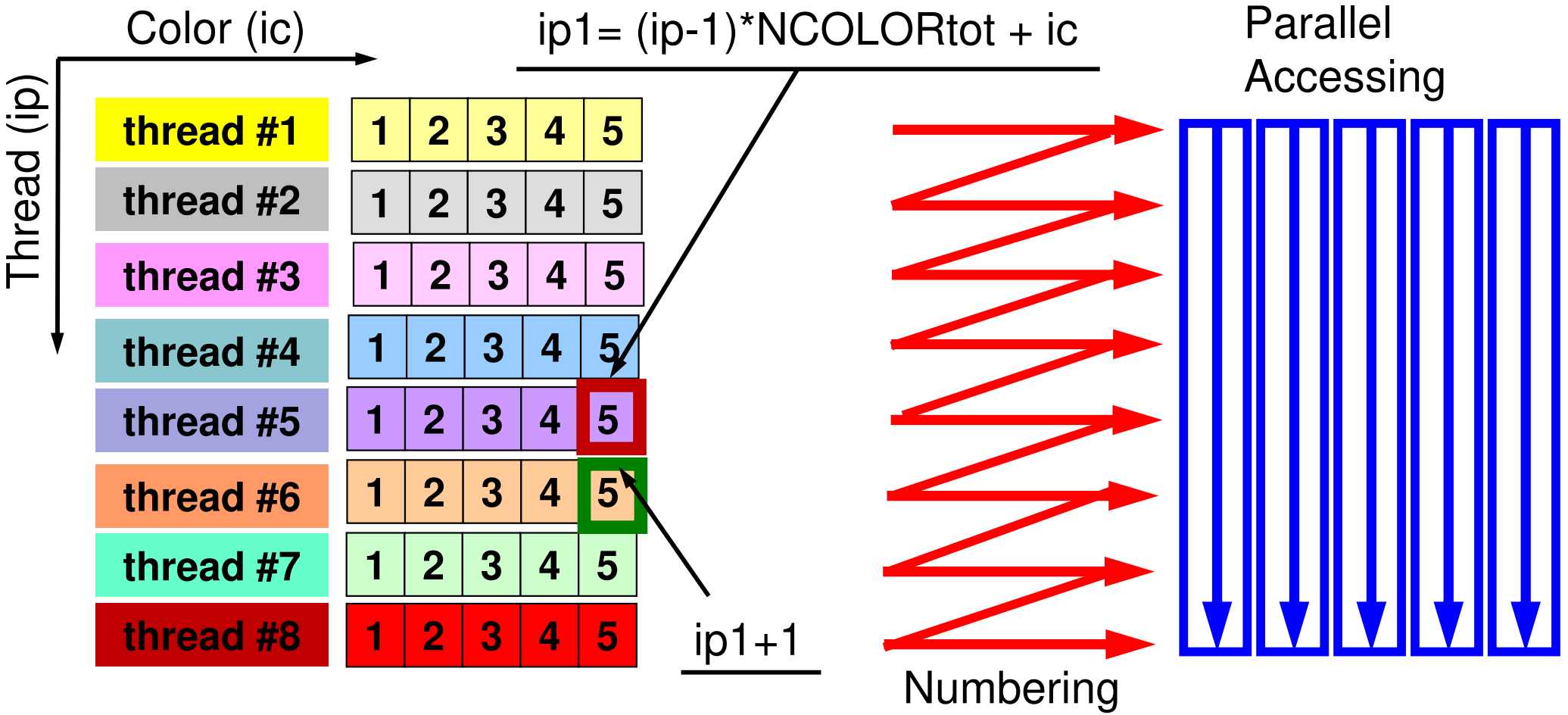
Coalesced

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



Sequential

```
!$omp parallel private(ip,ip1,i,WVAL,k)
      do ic= 1, NCOLORtot
!$omp do
        do ip= 1, PEsmpTOT
          ip1= (ip-1)*NCOLORtot + ic
        do i= SMPindex_new(ip1-1)+1, SMPindex_new(ip1) …
```



Sequential Reordering (3/5) poi_gen-2

```
do ip= 1, PEsmpTOT
     do ic= 1, NCOLORtot
       icNS= SMPindex_new((ip-1)*NCOLORtot + ic-1)
       ic01= SMPindex((ic-1)*PEsmpTOT + ip-1) + 1
       ic02= SMPindex((ic-1)*PEsmpTOT + ip  )
       icou= 0
       do k= ic01, ic02
         icel= NEWtoOLD(k)
         icou= icou + 1
         icelN= icNS + icou
         OLDtoNEWnew(icel )= icelN
         NEWtoOLDnew(icelN)= icel
       enddo
     enddo
     enddo
```

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

```
!$omp parallel do private (ip,icel,ic0,ik0)
     do ip  = 1, PEsmpTOT
     do icel= SMPindex_new((ip-1)*NCOLORtot)+1, SMPindex_new(ip*NCOLORtot)
       ic0 = NEWtoOLDnew(icel)
       ik0 = OLDtoNEW(ic0)
       indexL(icel)= INL(ik0)
       indexU(icel)= INU(ik0)
```

Sequential **Coalesced**

```
     enddo
     enddo

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

-Original: Initial ic0
-Coalesced ik0
-Sequential icel

Sequential Reordering (4/5) poi_gen-3

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

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

      if (NFLAG.eq.0) then
        itemL= 0
        itemU= 0
           AL= 0.d0
           AU= 0.d0
       else
!$omp parallel do private (ip,icel,k)
        do ip= 1, PEsmpTOT
          do icel= SMPindex_new((ip-1)*NCOLORtot+1),
     &             SMPindex_new(ip*NCOLORtot)
            do k= indexL(icel-1)+1, indexL(icel)
              itemL(k)= 0
                 AL(k)= 0.d0
            enddo
            do k= indexU(icel-1)+1, indexU(icel)
              itemU(k)= 0
                 AU(k)= 0.d0
            enddo
          enddo
        enddo
!$omp end parallel do
      endif
```

```
!$omp parallel do private (ip,icel,ic0,icN1,icN2,icN3,icN4, icN5,icN6)  &
!$omp&            private (coef,j,ii,jj,kk)                             &
!$omp&            private (ik0,icN10,icN20,icN30,icN40, icN50,icN60)
      do ip  = 1, PEsmpTOT
      do icel= SMPindex_new((ip-1)*NCOLORtot)+1, SMPindex_new(ip*NCOLORtot)
        ic0 = NEWtoOLDnew(icel)
        ik0 = OLDtoNEW(ic0)

        icN10= NEIBcell(ic0,1)
        icN20= NEIBcell(ic0,2)
        icN30= NEIBcell(ic0,3)
        icN40= NEIBcell(ic0,4)
        icN50= NEIBcell(ic0,5)
        icN60= NEIBcell(ic0,6)

        if (icN50.ne.0) then
          icN5= OLDtoNEW(icN50)
          coef= RDZ * ZAREA
          D(icel)= D(icel) - coef

          if (icN5.lt.ik0) then
            do j= 1, INL(ik0)
              if (IAL(j,ik0).eq.icN5) then
                itemL(j+indexL(icel-1))= OLDtoNEWnew(icN50)
                   AL(j+indexL(icel-1))= coef
                exit
              endif
            enddo
           else
            do j= 1, INU(ik0)
              if (IAU(j,ik0).eq.icN5) then
                itemU(j+indexU(icel-1))= OLDtoNEWnew(icN50)
                   AU(j+indexU(icel-1))= coef
                exit
              endif
            enddo
          endif
        endif
```

Sequential Reordering (5/5) poi_gen-4

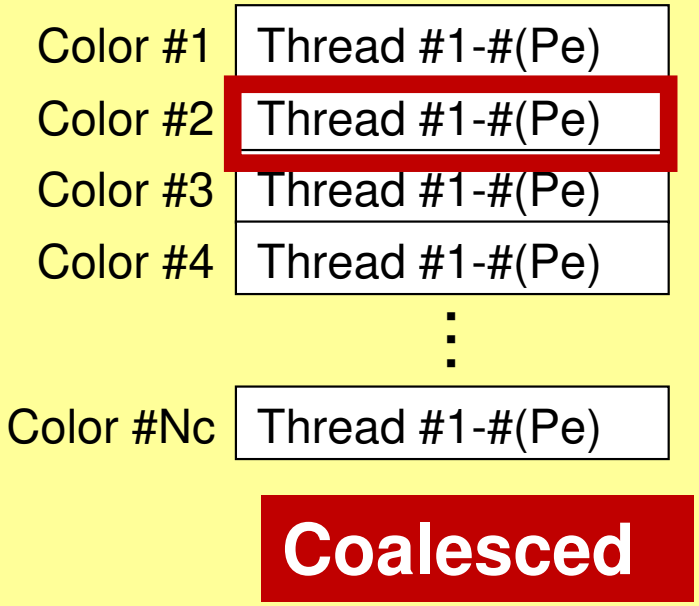
icel: Sequential
ic0: Original
ik0: Coalesced

icN50: Original
icN5 : Coalesced

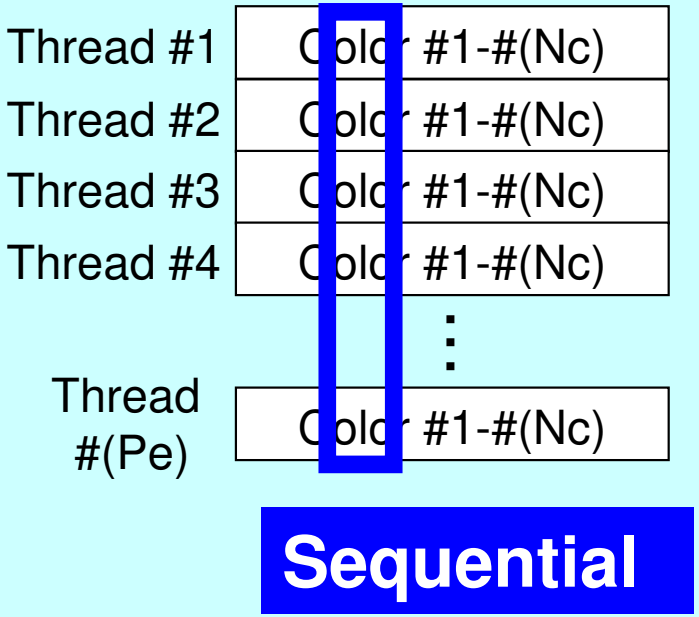
icN5>ik0: Upper (AU)
icN5<ik0: Lower (AL)

Forward Substitution

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




```
!$omp parallel private(ic,ip,ip1,i,WVAL,k)
      do ic= 1, NCOLORtot
!$omp do
        do ip= 1, PEsmpTOT
          ip1= (ip-1)*NCOLORtot + ic
        do i= SMPindex_new(ip1-1)+1, SMPindex_new(ip1)
          WVAL= W(i,Z)
          do k= indexLnew(i-1)+1, indexLnew(i)
            WVAL= WVAL -  ALnew(k) * W(itemLnew(k),Z)
          enddo
          W(i,Z)= WVAL * W(i,DD)
        enddo
        enddo
      enddo
!$omp end parallel
```



Mat-Vec

```
!$omp parallel do private(ip,i,VAL,k)
      do ip= 1, PEsmpTOT
        do i = SMPindexG(ip-1)+1, SMPindexG(ip)
          VAL= D(i)*W(i,P)
          do k= indexL(i-1)+1, indexL(i)
            VAL= VAL + AL(k)*W(itemL(k),P)
          enddo
          do k= indexU(i-1)+1, indexU(i)
            VAL= VAL + AU(k)*W(itemU(k),P)
          enddo
          W(i,Q)= VAL
        enddo
      enddo
!$omp end parallel do
```

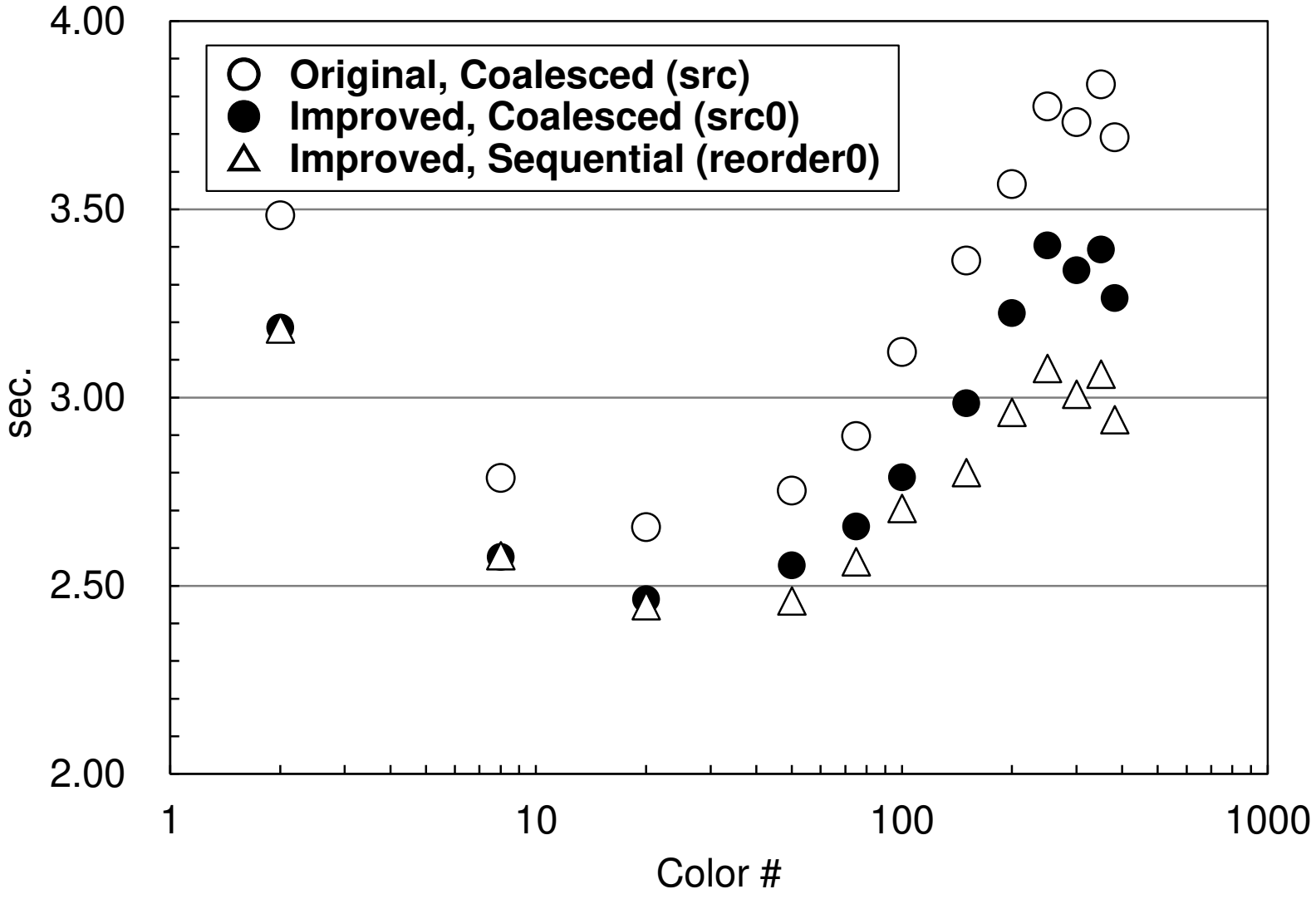
METHOD=0

```
!$omp parallel do private(ip,i,VAL,k)
      do ip= 1, PEsmpTOT
        do i= SMPindex_new((ip-1)*NCOLORtot)+1, SMPindex_new(ip*NCOLORtot)
          VAL= D(i)*W(i,P)
          do k= indexLnew(i-1)+1, indexLnew(i)
            VAL= VAL + ALnew(k)*W(itemLnew(k),P)
          enddo
          do k= indexUnew(i-1)+1, indexUnew(i)
            VAL= VAL + AUnew(k)*W(itemUnew(k),P)
          enddo
          W(i,Q)= VAL
        enddo
      enddo
!$omp end parallel do
```

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

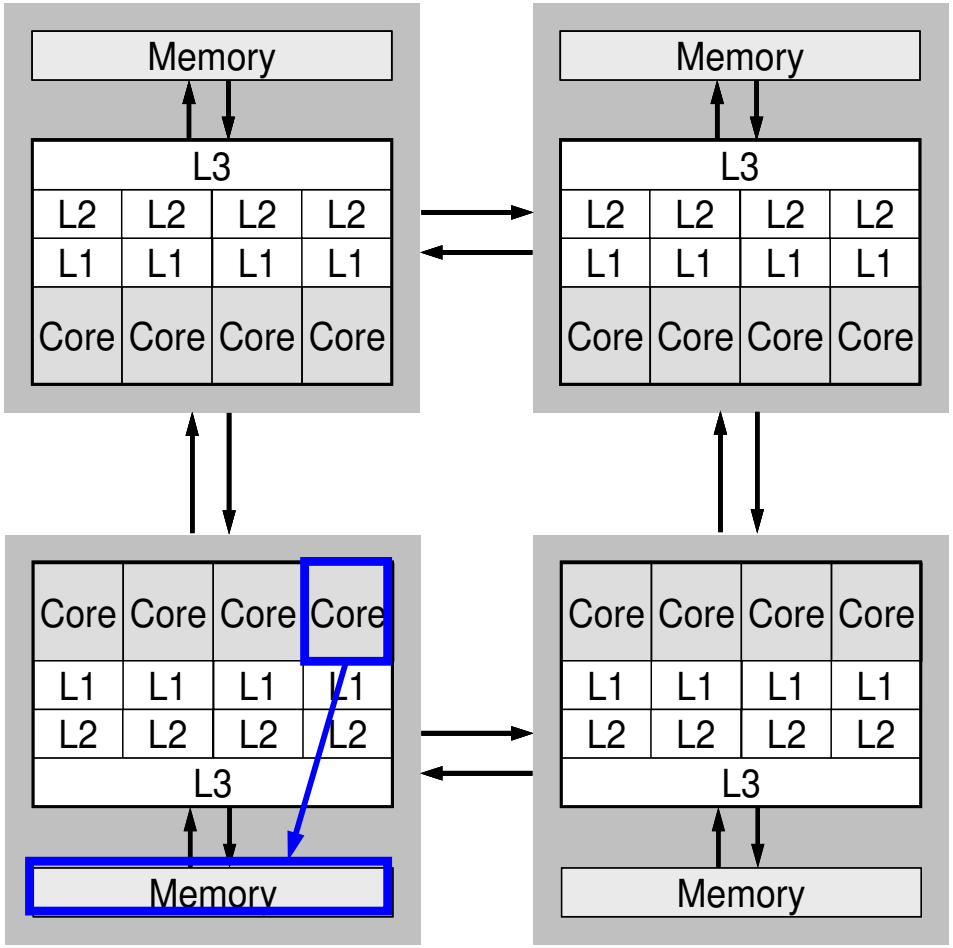
"Patterns for Parallel Programming" Mattson, T.G. et al.

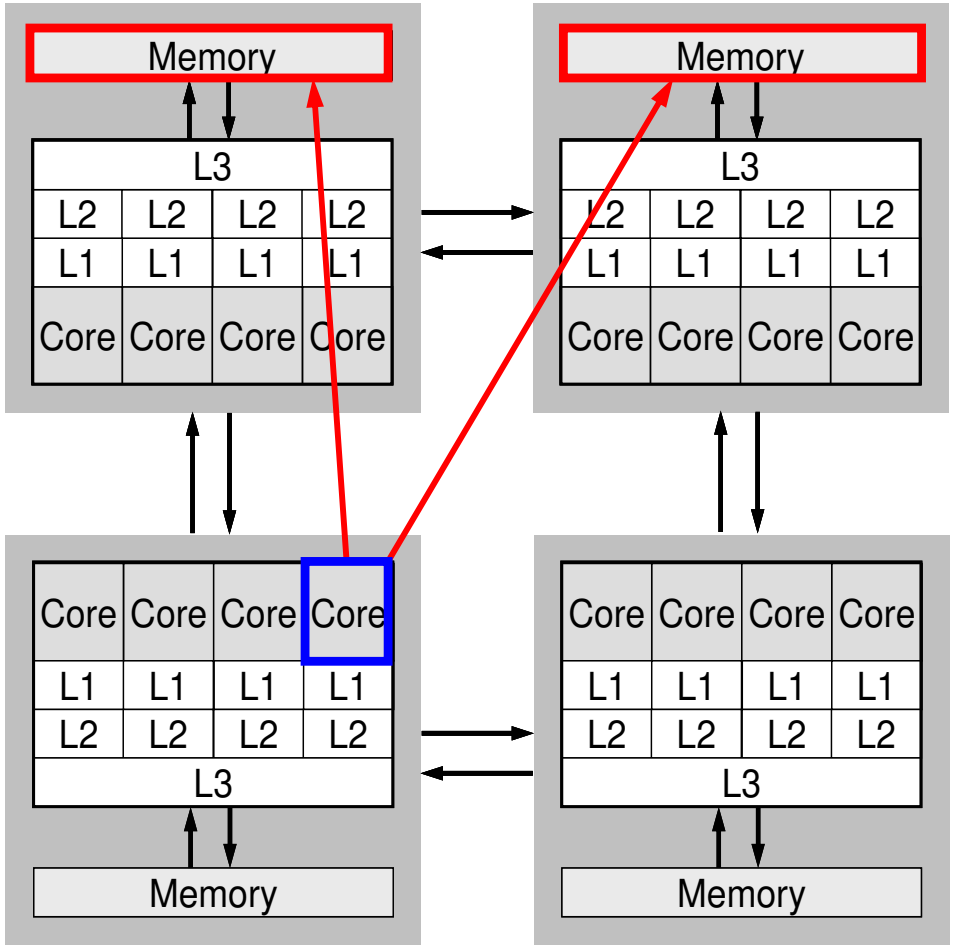
- To reduce memory traffic in the system, it is important to keep the data close to the PEs that will work with the data (e.g. NUMA control).
- On NUMA computers, this corresponds to making sure the pages of memory are allocated and "owned" by the PEs that will be working with the data contained in the 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-rso10
numactl -C 12-59 -m 4-7 ./L3-rso10
```

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

```
!C
!C-- ARRAY init.
      if (NFLAG.eq.0) then
        BFORCE= 0.d0
        PHI   = 0.d0
        D     = 0.d0
        OLDtoNEWnew= 0
        NEWtoOLDnew= 0
       else
!$omp parallel do private (ip,icel)
        do ip= 1, PEsmpTOT
          do icel= SMPindex_new((ip-1)*NCOLORtot+1),
     &             SMPindex_new(ip*NCOLORtot)
            BFORCE(icel)= 0.d0
            PHI   (icel)= 0.d0
            D(icel)     = 0.d0
            OLDtoNEWnew(icel)= 0
            NEWtoOLDnew(icel)= 0
          enddo
        enddo
!$omp end parallel do
      endif
```

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.eq.0) then
        do icel= 1, ICELTOT
          indexL(icel)= 0
          indexU(icel)= 0
        enddo
       else
!$omp parallel do private (ip,icel,k)
        do ip= 1, PEsmpTOT
          do icel= SMPindex_new((ip-1)*NCOLORtot+1),
     &             SMPindex_new(ip*NCOLORtot)
            indexL(icel)= 0
            indexU(icel)= 0
          enddo
        enddo
      endif
```

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 (3/3)

```
      if (NFLAG.eq.0) then
        itemL= 0
        itemU= 0
           AL= 0.d0
           AU= 0.d0
       else
!$omp parallel do private (ip,icel,k)
        do ip= 1, PEsmpTOT
          do icel= SMPindex_new((ip-1)*NCOLORtot+1),
     &             SMPindex_new(ip*NCOLORtot)
            do k= indexL(icel-1)+1, indexL(icel)
              itemL(k)= 0
                 AL(k)= 0.d0
            enddo
            do k= indexU(icel-1)+1, indexU(icel)
              itemU(k)= 0
                 AU(k)= 0.d0
            enddo
          enddo
        enddo
!$omp end parallel do
      endif
```

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.

Sequential Reordering (4/5) poi_gen-3

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

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

      if (NFLAG.eq.0) then
        itemL= 0
        itemU= 0
           AL= 0.d0
           AU= 0.d0
       else
!$omp parallel do private (ip,icel,k)
        do ip= 1, PEsmpTOT
          do icel= SMPindex_new((ip-1)*NCOLORtot+1),
     &             SMPindex_new(ip*NCOLORtot)
            do k= indexL(icel-1)+1, indexL(icel)
              itemL(k)= 0
                 AL(k)= 0.d0
            enddo
            do k= indexU(icel-1)+1, indexU(icel)
              itemU(k)= 0
                 AU(k)= 0.d0
            enddo
          enddo
        enddo
!$omp end parallel do
      endif
```

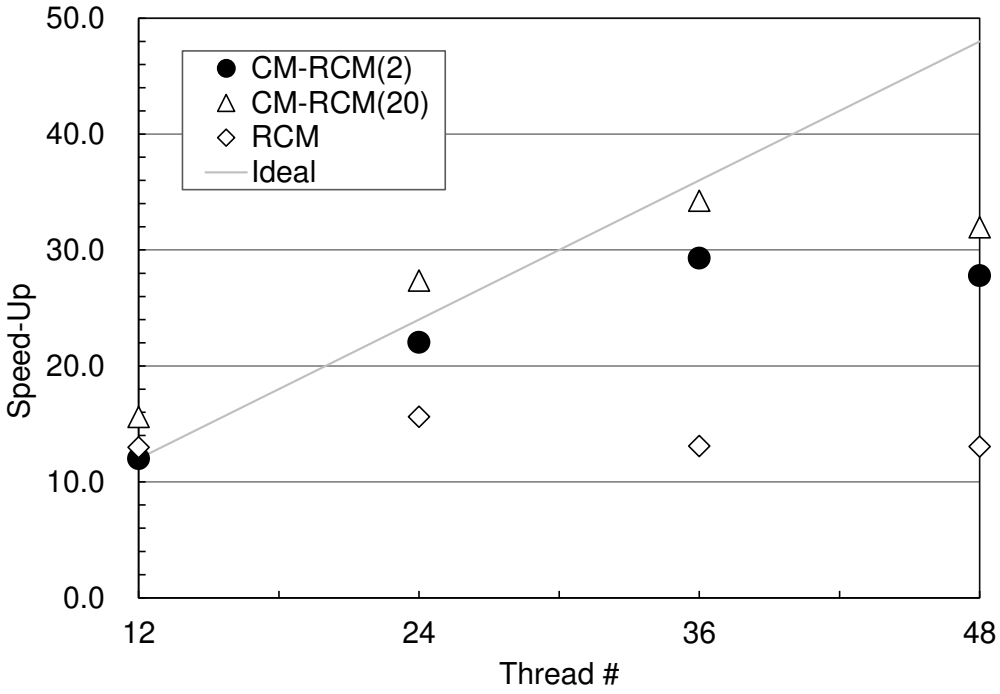
Pages are allocated at the local memory of the master thread

Pages are allocated at the local memory of each thread

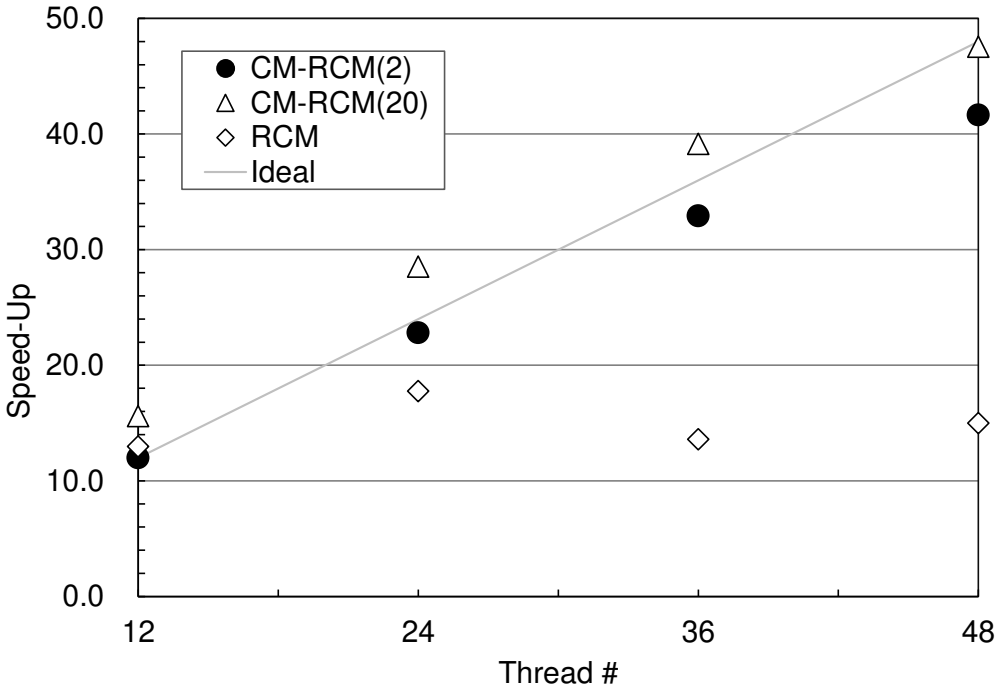
Results: reoder0, L3-rsol0, N=128^3, C

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

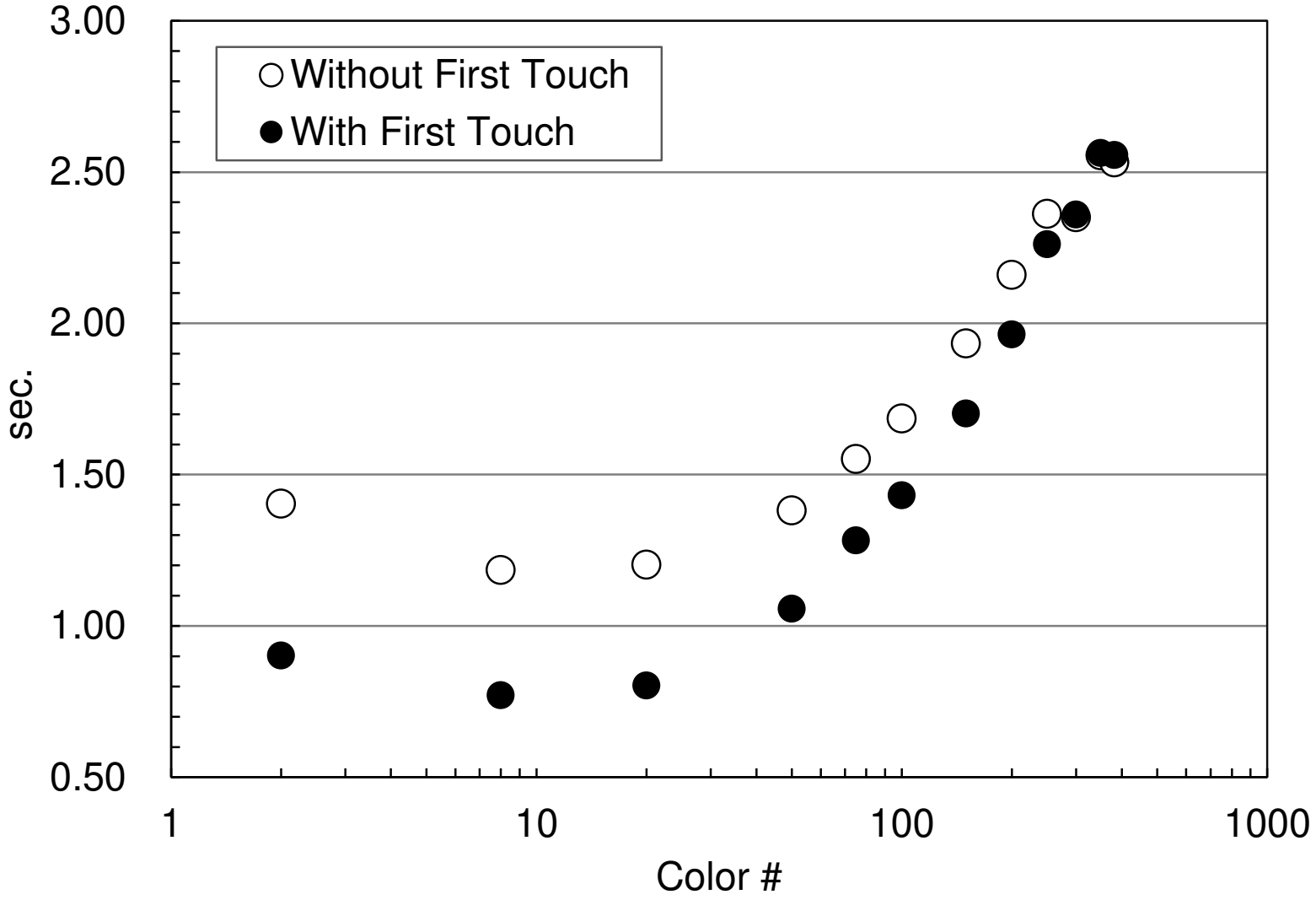
Without First-Touch



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.