Parallel Programming for Multicore Processors using OpenMP

Part III: Parallel Version + Exercise

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Programming for Parallel Computing (616-2057)
Seminar on Advanced Computing (616-4009)

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

Files on FX10

```
>$ cd <$O-TOP>

>$ cp /home/ss/aics60/C/multicore-c.tar .
>$ cp /home/ss/aics60/F/multicore-f.tar .

>$ tar xvf multicore-c.tar
>$ tar xvf multicore-f.tar

>$ cd multicore
```

Confirm the following directories:

L3 omp

<$O-L3>, <$O-stream>

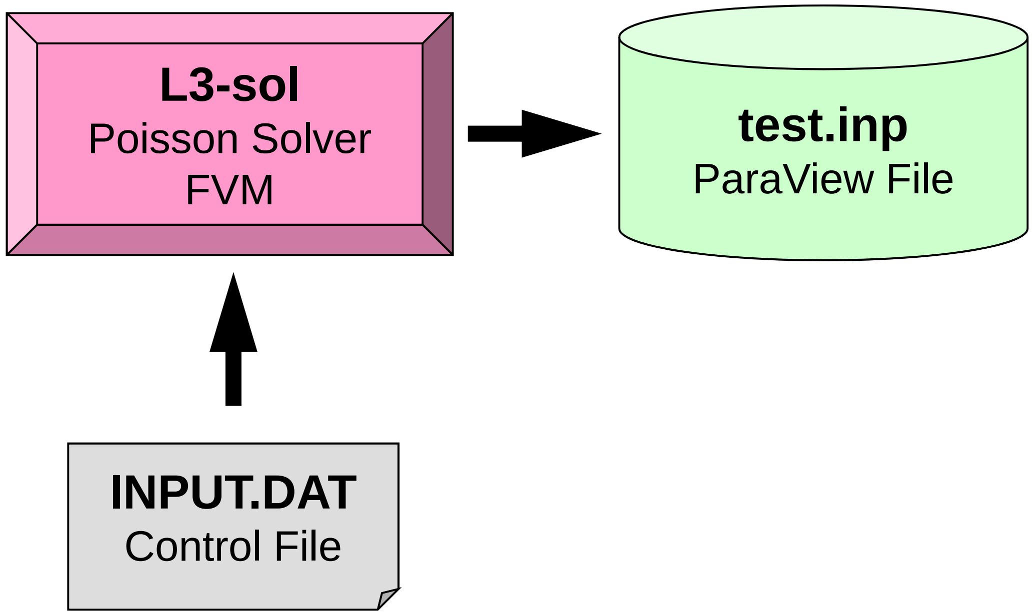
Files on FX10 (cont.)

- Location
  - `<$O-L3>/src`, `<$O-L3>/run`
- Compile/Run
  - Main Part
    - `cd <$O-L3>/src`
    - `make`
    - `<$O-L3>/run/L3-sol` (exec)
  - Control Data
    - `<$O-L3>/run/INPUT.DAT`
  - Batch Job Script
    - `<$O-L3>/run/go1.sh`

Running the Code

```
% cd <$O-L3>
% ls
    run   src  src0  reorder0

% cd src
% make
% cd ../run
% ls L3-sol
    L3-sol

% <modify “INPUT.DAT”>
% <modify “go1.sh”>

% pjsub go1.sh
```

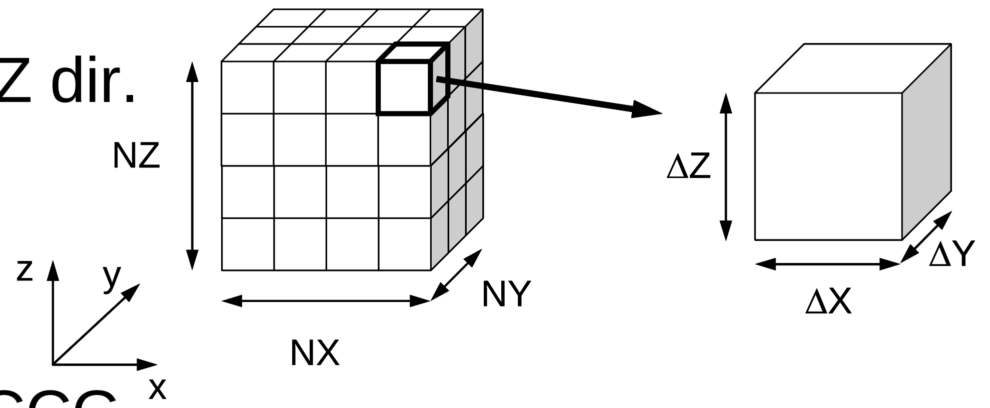
Running the Program



Control Data: INPUT.DAT

```
100 100 100                              NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00               DX/DY/DZ
1.0e-08                                  EPSICCG
16                                       PEsmpTOT
100                                      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
- **NCOLORtot**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM



go1.sh

```
#!/bin/sh
#PJM -L "node=1"
#PJM -L "elapse=00:10:00"
#PJM -L "rscgrp=lecture"
#PJM -g "gt71"
#PJM -j
#PJM -o "arcm.lst"

export OMP_NUM_THREADS=16     =PEsmpTOT
./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

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

Parallelize ICCG Method by OpenMP

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

Main Program (1/2)

```
      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)
```

Main Program (2/2)

```
      allocate (WK(ICELTOT))

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

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

      call OUTUCD

      stop
      end
```

Renumbering of “PHI” to original numbering

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)
```

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 (cont.)

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

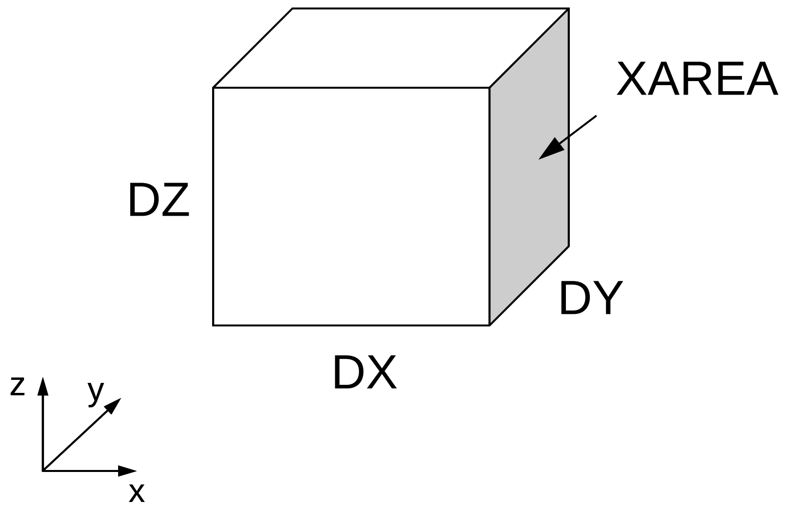
```
!C
!C***
!C*** INPUT
!C***
!C
!C     INPUT CONTROL DATA
!C
      subroutine INPUT
      use STRUCT
      use PCG
      implicit REAL*8 (A-H,O-Z)
      character*80 CNTFIL
!C
!C-- CNTL. file
      open  (11, file='INPUT.DAT', status='unknown')
        read (11,*) NX, NY, NZ
        read (11,*) DX, 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
16                                       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

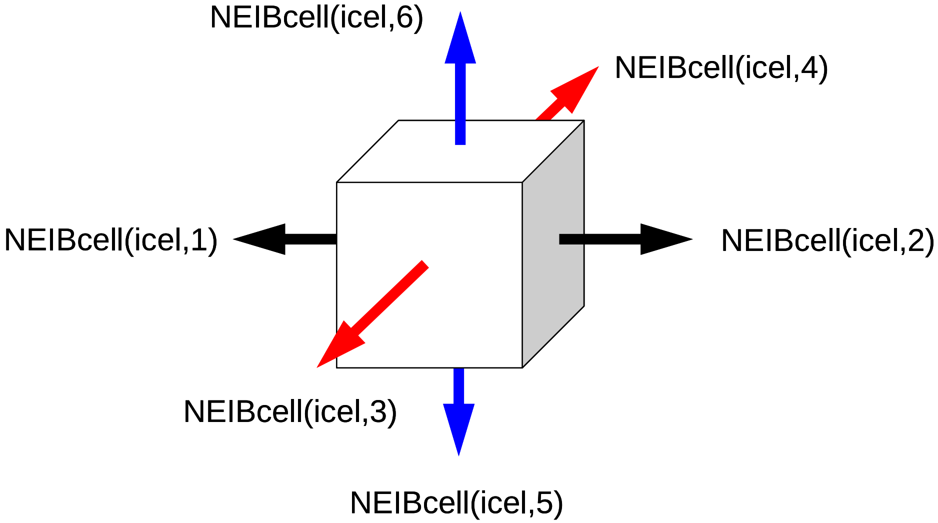
```
      program MAIN

      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
```

poi_gen (2/9)

```
!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===
```



Lower Triangular Part

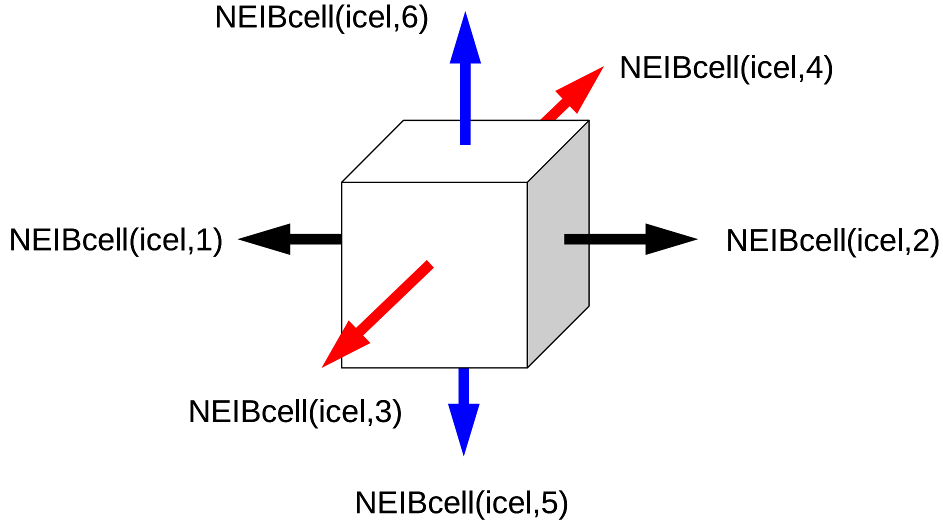
NEIBcell(icel,5)= icel – NX*NY

NEIBcell(icel,3)= icel – NX

NEIBcell(icel,1)= icel – 1

poi_gen (2/9)

```
!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===
```



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)

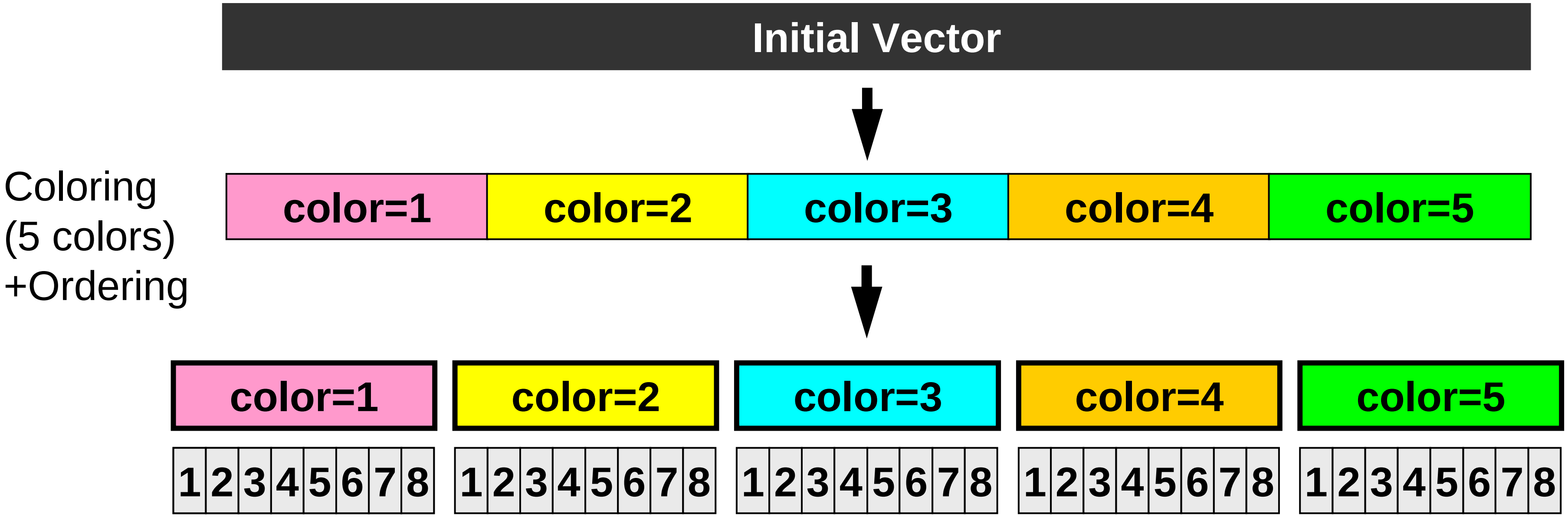
```
      allocate (SMPindex(0:PEsmpTOT*NCOLORtot))
      SMPindex= 0
      do ic= 1, NCOLORtot
        nn1= COLORindex(ic) - COLORindex(ic-1)
        num= nn1 / PEsmpTOT
        nr = nn1 - PEsmpTOT*num
        do ip= 1, PEsmpTOT
          if (ip.le.nr) then
            SMPindex((ic-1)*PEsmpTOT+ip)=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

poi_gen (4/9)

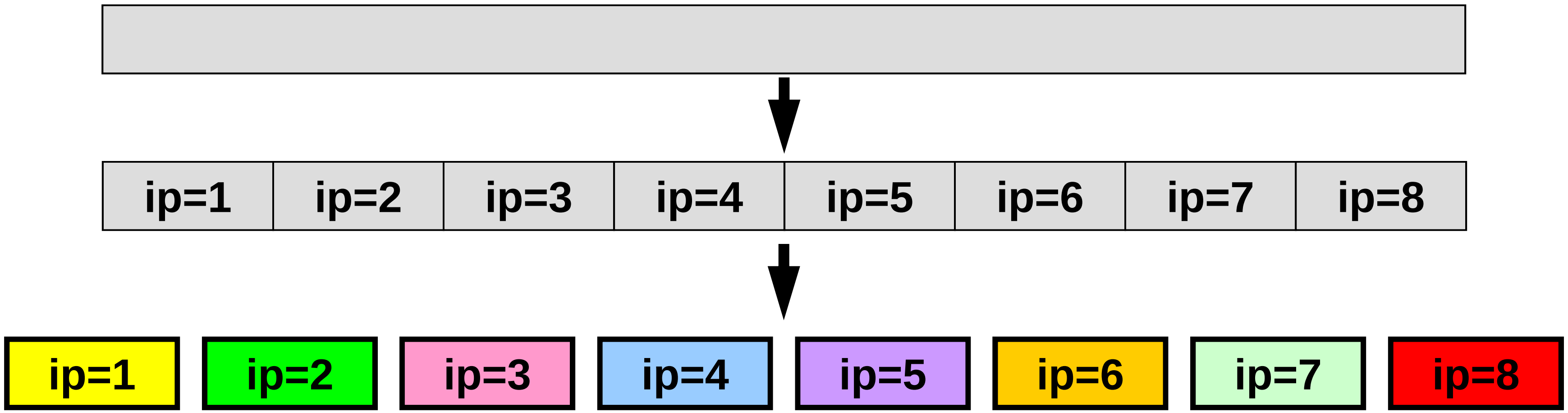
```
      allocate (SMPindex(0:PEsmpTOT*NCOLORtot))
      SMPindex= 0
      do ic= 1, NCOLORtot
        nn1= COLORindex(ic) - COLORindex(ic-1)
        num= nn1 / PEsmpTOT
        nr = nn1 - PEsmpTOT*num
        do ip= 1, PEsmpTOT
          if (ip.le.nr) then
            SMPindex((ic-1)*PEsmpTOT+ip)=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

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)

```
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
```

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
```

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

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

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

$$\frac{\phi_{neib(icel,1)} - \phi_{icel}}{\Delta x}\Delta y \Delta z + \frac{\phi_{neib(icel,2)} - \phi_{icel}}{\Delta x}\Delta y \Delta z + \frac{\phi_{neib(icel,3)} - \phi_{icel}}{\Delta y}\Delta z \Delta x + \frac{\phi_{neib(icel,4)} - \phi_{icel}}{\Delta y}\Delta z \Delta x + \frac{\phi_{neib(icel,5)} - \phi_{icel}}{\Delta z}\Delta x \Delta y + \frac{\phi_{neib(icel,6)} - \phi_{icel}}{\Delta z}\Delta x \Delta y = f_{icel}\Delta x \Delta y \Delta z$$

poi_gen (7/9)

```
      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
```

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

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

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

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

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

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

poi_gen (8/9)

```
        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
```

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

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

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

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

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

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

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,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(i,DD):	d_i
D(i):	a_{ii}
IAL(j,i):	k
AL(j,i):	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(i,DD):	d_i
D(i):	a_{ii}
IAL(j,i):	k
AL(j,i):	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 **$r^{(0)}= b-[A]x^{(0)}$**

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

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

```
      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===
```

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
      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===
```

SMPindex

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

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

Forward Substitution

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

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

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

<u>for</u> i= 1, 2, …

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

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

  <u>if</u> i=1

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

  <u>else</u>

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

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

  <u>endif</u>

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

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

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

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

  check convergence |r|

<u>end</u>

solve_ICCG_mc (6/6)

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

solve_ICCG_mc (6/6)

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

solve_ICCG_mc (6/6)

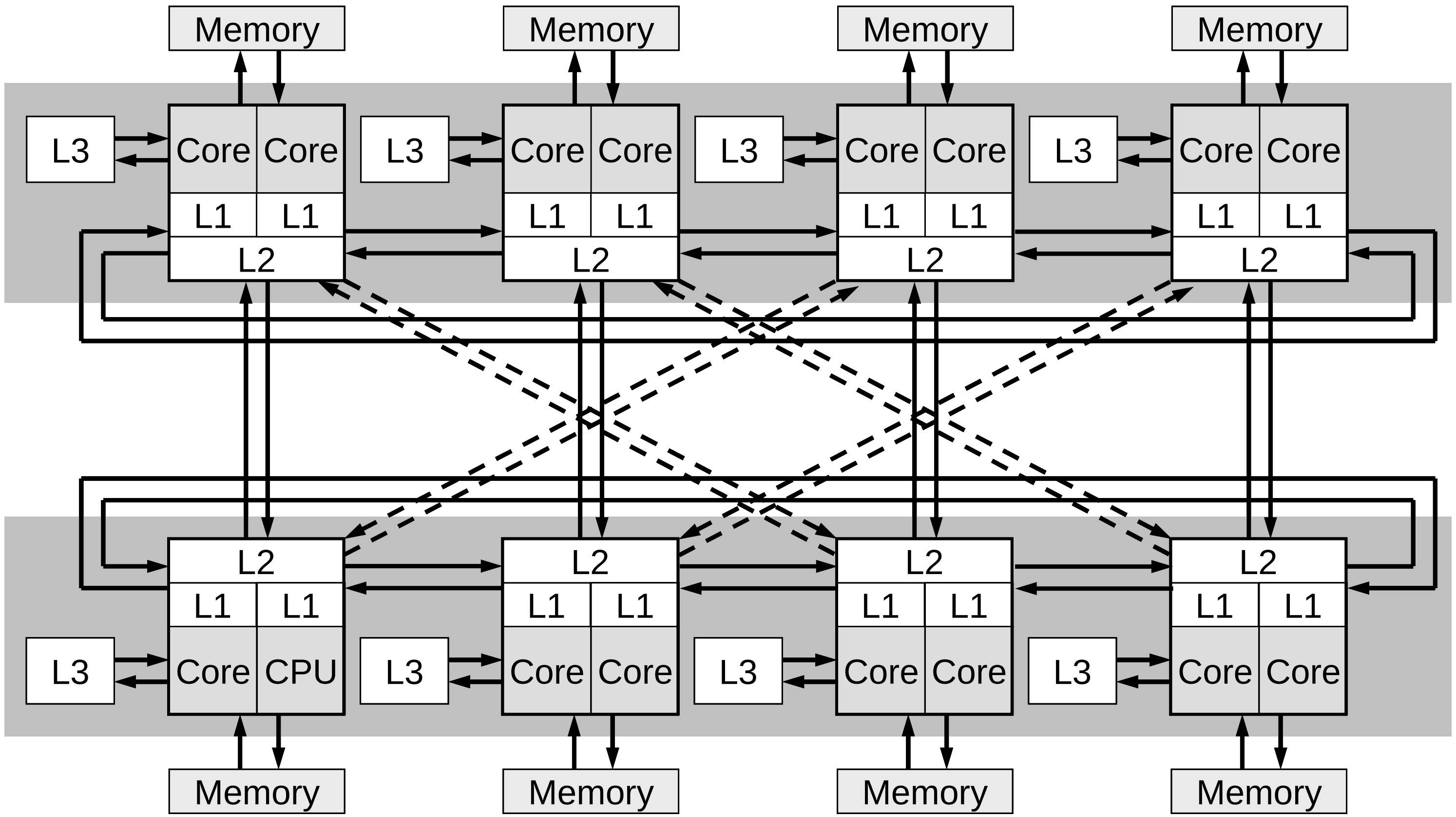
```
!C
!C +----------------------+
!C | ALPHA= RHO / {p}{q}  |
!C +----------------------+
!C===
      C1= 0.d0
!$omp parallel do private(ip,i) reduction(+:C1)
      do ip= 1, PEsmpTOT
      do i = SMPindexG(ip-1)+1, SMPindexG(ip)
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      enddo
!$omp end parallel 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 $r^{(0)}= b-[A]x^{(0)}$
<u>for</u> i= 1, 2, …
  solve $[M]z^{(i-1)}= r^{(i-1)}$
  $\rho_{i-1}= r^{(i-1)}\ z^{(i-1)}$
  <u>if</u> i=1
    $p^{(1)}= z^{(0)}$
  <u>else</u>
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i-1)}$
  <u>endif</u>
  $q^{(i)}= [A]p^{(i)}$
  $\alpha_i = \rho_{i-1}/p^{(i)}q^{(i)}$
  $x^{(i)}= x^{(i-1)} + \alpha_i p^{(i)}$
  $r^{(i)}= r^{(i-1)} - \alpha_i q^{(i)}$
  check convergence |r|
<u>end</u>

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

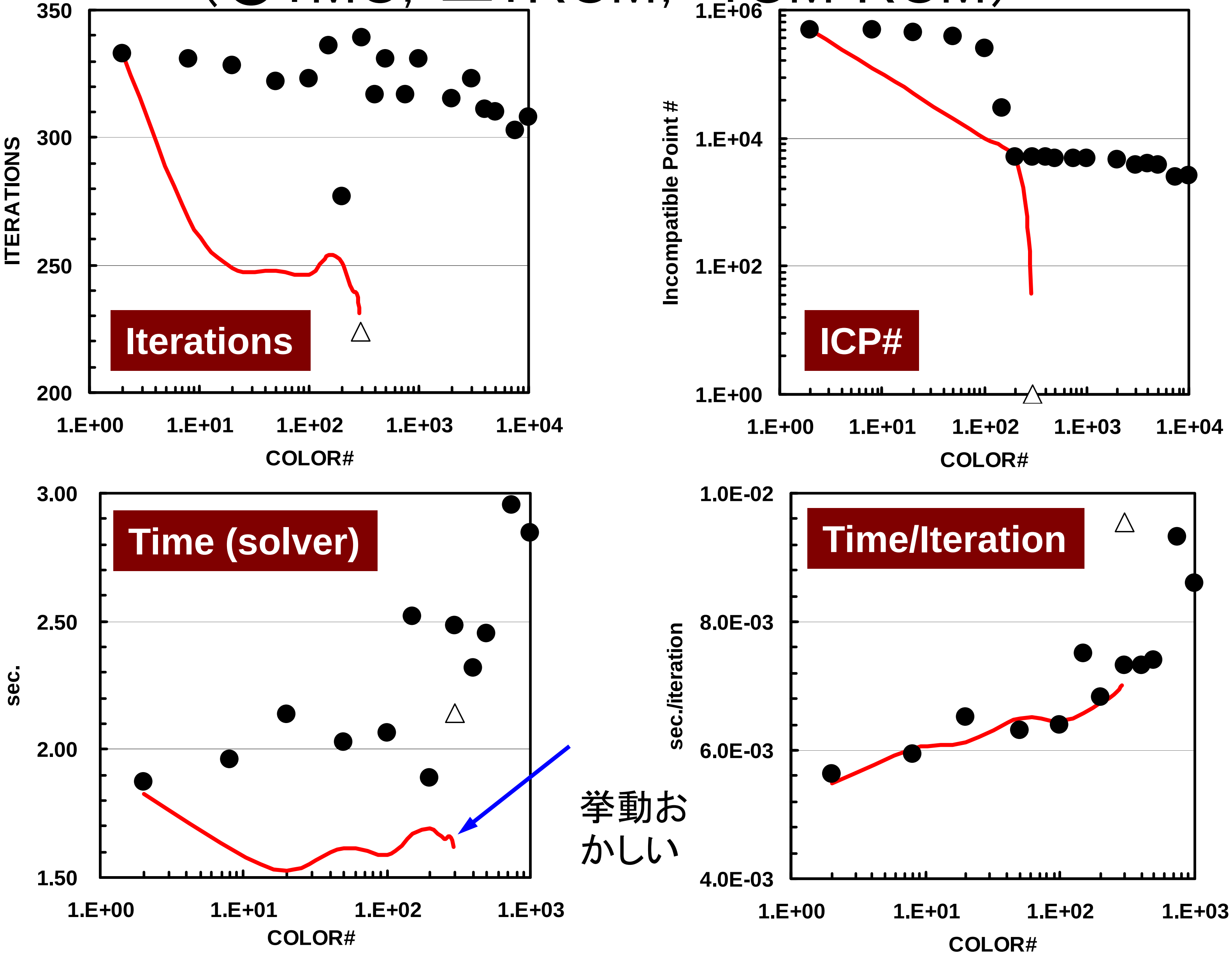
Results

- Hitachi SR11000/J2 1-node, 16-cores
- 100^3 Meshes



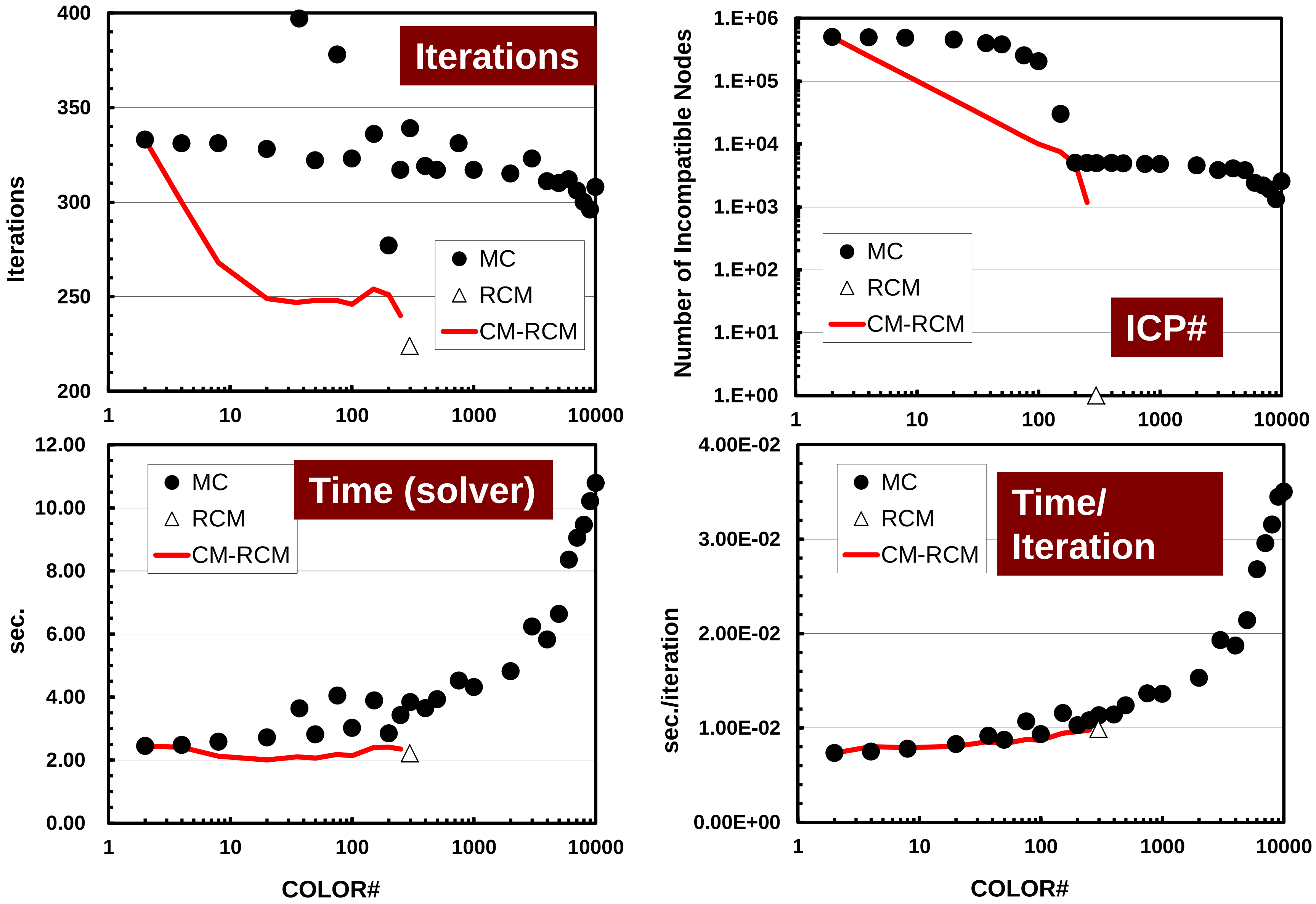
SR11000, 1-node/16-cores, 100^3

(●:MC, △:RCM, -:CM-RCM)



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

(●:MC, △:RCM, -:CM-RCM)



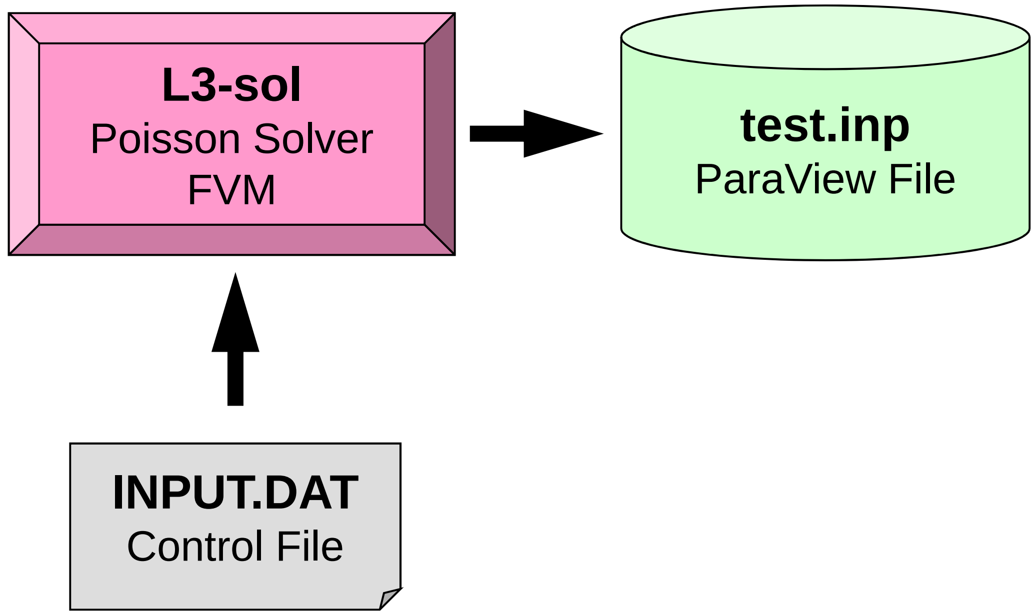
- Applying OpenMP to L2-sol
- Examples
- **Optimization + Exercise**

- Running the Code
- Further Optimization
- Profiler, Analyzing Compile Lists

Compile & Run

```
>$ cd <$O-L3>/src
>$ make
>$ ls ../run/L3-sol

  L3-sol

>$ cd ../run

>$ pjsub go1.sh
```

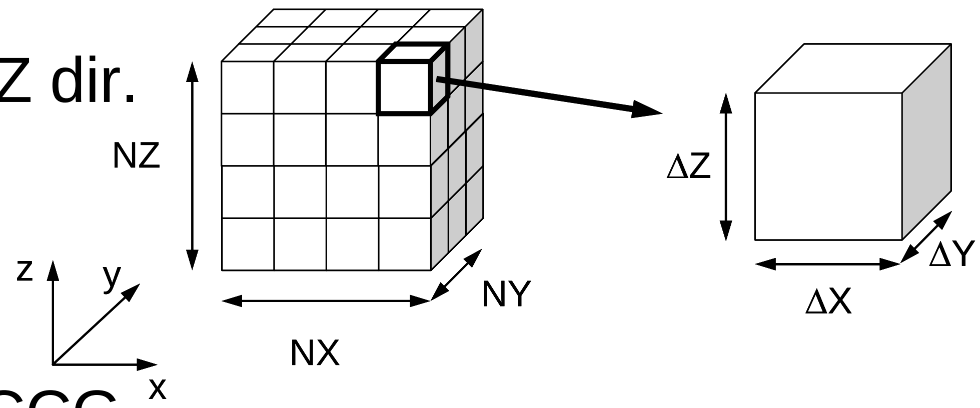
Running L3-sol



Control Data: INPUT.DAT

```
100 100 100                               NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00                DX/DY/DZ
1.0e-08                                   EPSICCG
16                                        PEsmpTOT
100                                       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
- **NCOLORtot**
  - Reordering Method + Initial Number of Colors/Levels
  - ≧2: MC, =0: CM, =-1: RCM, -2≧: CMRCM

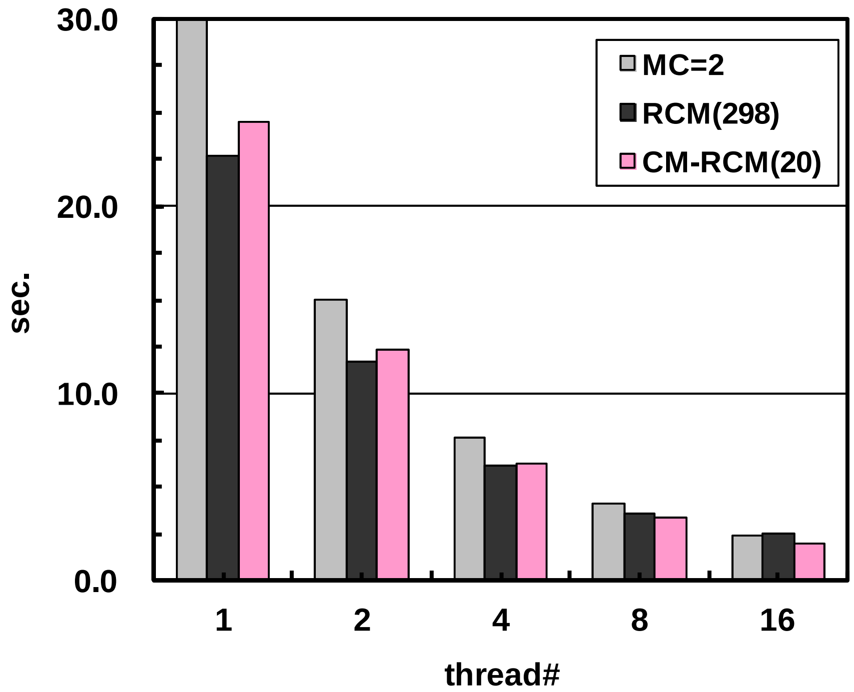


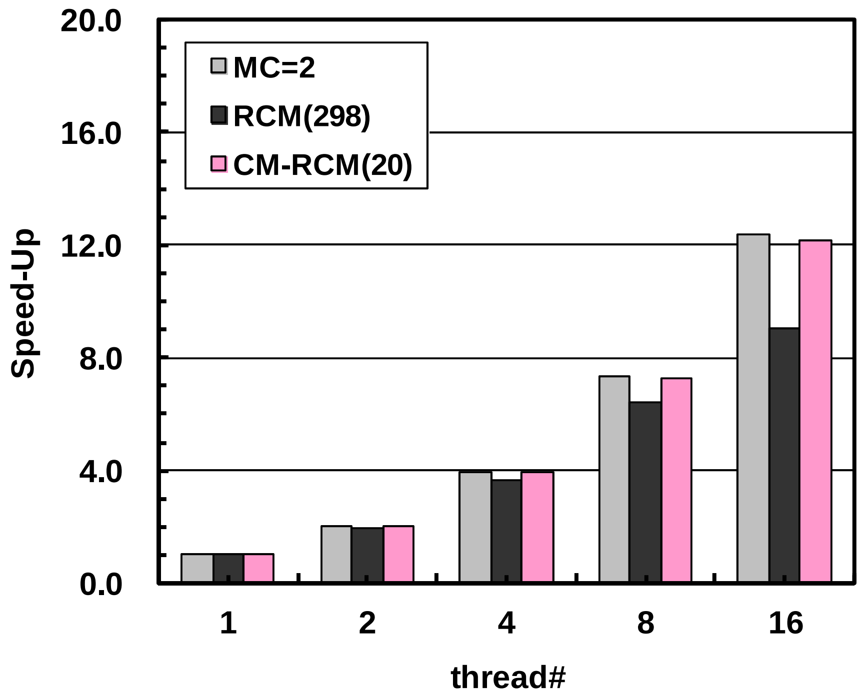
go1.sh

```
#!/bin/sh
#PJM -L "node=1"
#PJM -L "elapse=00:10:00"
#PJM -L "rscgrp=lecture"
#PJM -g "gt71"
#PJM -j
#PJM -o “test.lst“

export OMP_NUM_THREADS=16     =PEsmpTOT
./L3-sol
```

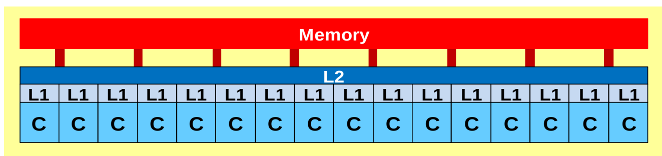
Results on FX10, 10^6 meshes

Iterations: MC(2): 333, RCM(298-levels): 224, CM-RCM(Nc=20): 249





16 threads
MC(2): 2.42 sec.
CM-RCM(20): 2.01 sec.



Exercise

- Various Configurations
  - Problem Size
  - Number of Threads
  - Number of Colors, Reordering Method (MC, RCM, CM-RCM)

- Running the Code
- **Further Optimization**
  - **OpenMP Statement**
  - Sequential Reordering
  - ELL
- Profiler, Analyzing Compile Lists

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 16) occurs.
  - In each color, this occurs
  - Some overhead
- Overhead increases, if number of color increases.

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 16) occurs.
  - In each color, this occurs
  - Some overhead
- Overhead increases, if number of color increases.

For. Subst.: Reduced Overhead (F)

```
!$omp parallel private(ip,ip1,i,WVAL,k)
      do ic= 1, NCOLORtot
!$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.

For. Subst.: Reduced Overhead (C)

```
#pragma omp parallel private (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 “**`!omp do`**” are parallelized.

Programs

```
% cd <$O-L3>
% ls
    run  reorder0  src  src0

% cd src0

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

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

% pjsub go0.sh
```

Results: L3-sol0 is better $N=128^3$

	L3-sol	L3-sol0
NCOLORtot= -20 CM-RCM (20) 318 Iterations	5.69 sec.	5.44 sec.
NCOLORtot= -1 RCM (382 levels) 287 Iterations	6.54 sec.	6.37 sec.

- Running the Code
- **Further Optimization**
  - OpenMP Statement
  - **Sequential Reordering**
  - **ELL**
- Profiler, Analyzing Compile Lists

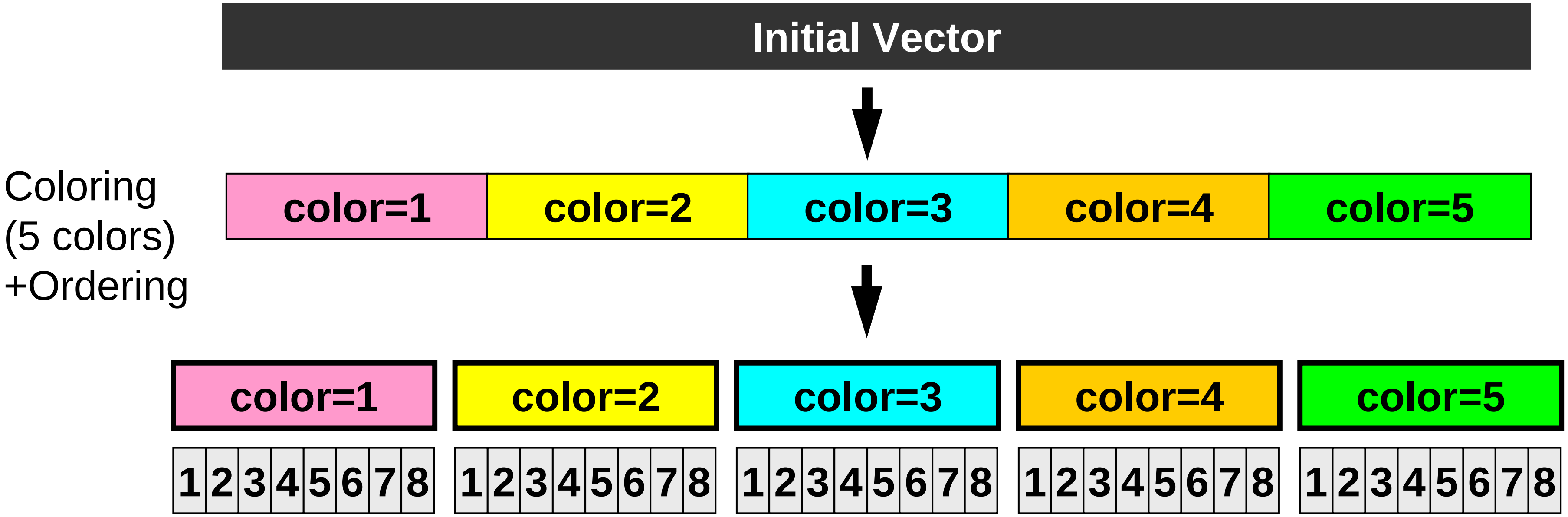
Problems in Reordering

- 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

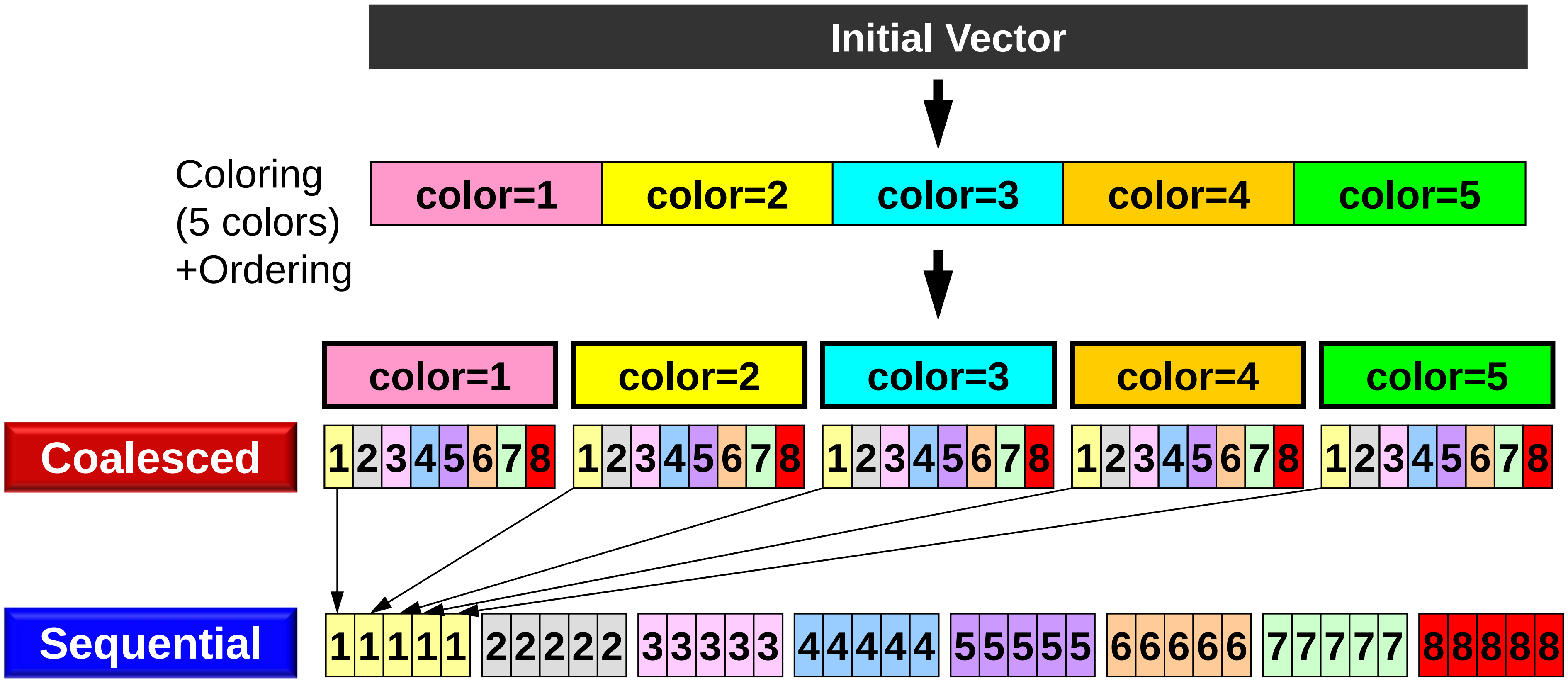
Sequential Reordering

- 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≦k≦indexL(icel)`**

Sequential Reordering

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



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)

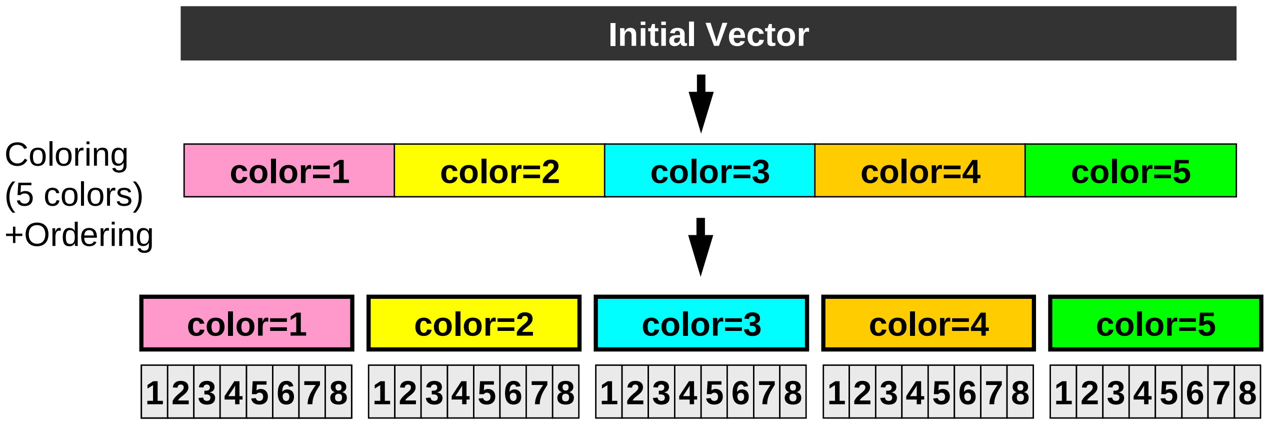
→

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

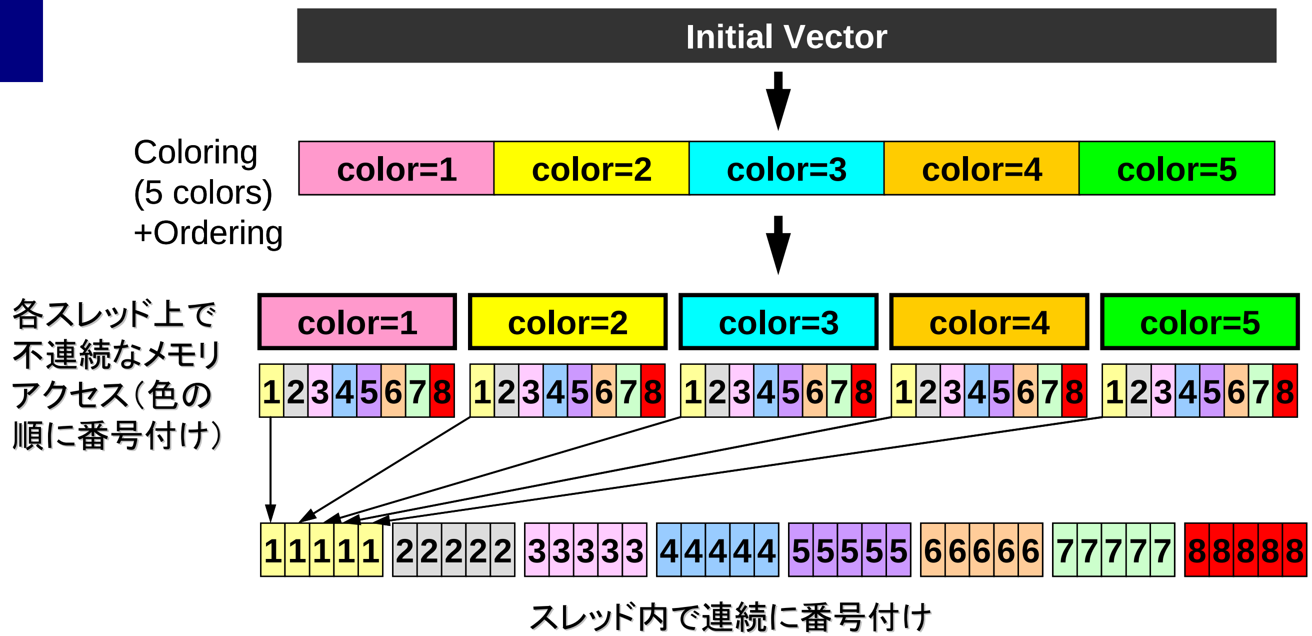
Sequential Reordering, 4-threads

Sequential Reordering

Coalesced
Good for GPU



Sequential



Files on FX10

- Location
  - `<$O-L3>/src`, `<$O-L3>/run`
- Compile/Run
  - Main Part
    - `cd <$O-L3>/reorder0`
    - `make`
    - `<$O-L3>/run/L3-rsol0` (exec)
  - Control Data
    - `<$O-L3>/run/INPUT.DAT`
  - Batch Job Script
    - `<$O-L3>/run/gor.sh`

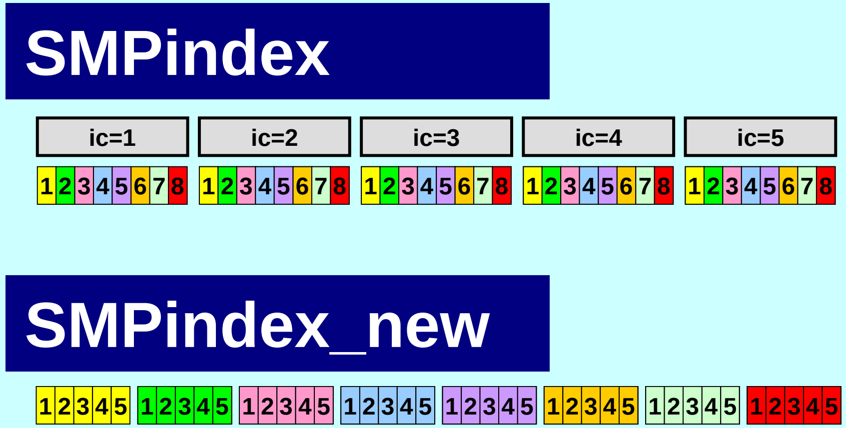
INPUT.DAT

```
100 100 100                          NX/NY/NZ
1.00e-00 1.00e-00 1.00e-00            DX/DY/DZ
1.0e-08                               EPSICC
16                                    PEsmpTOT
100                                   NCOLORtot
0                                     NFLAG
0                                     METHOD
```

- **PEsmpTOT**
  - Thread Number
- **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

```
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
```



Mat-Vec: METHOD=0

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

Original

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

New

Forward Substitution

```
!$omp parallel private(ip,ip1,i,WVAL,k)
      do ic= 1, NCOLORtot
!$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
```

Original

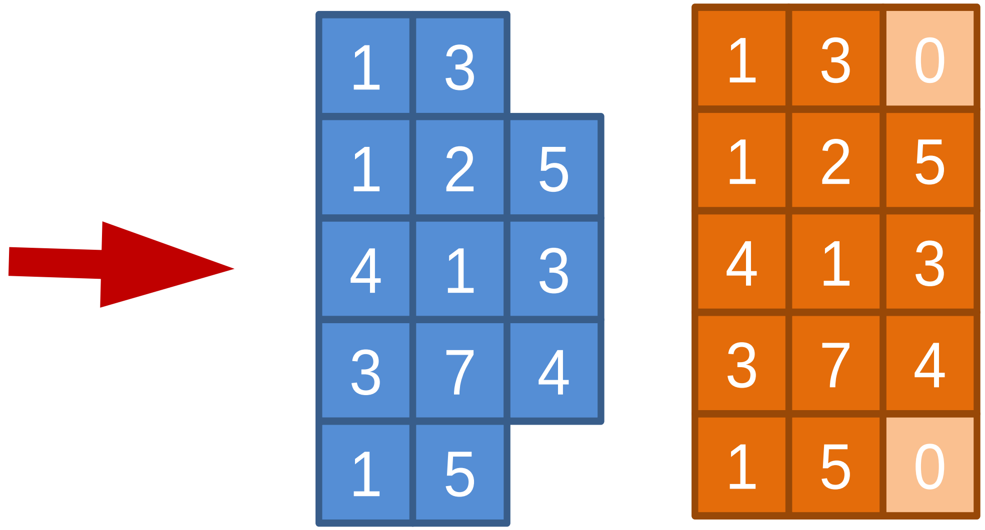
```
!$omp parallel private(ip,ip1,i,WVAL,k)
      do ic= 1, NCOLORtot
!$omp do
        do ip= 1, PEsmpTOT
          ip1= (ip-1)*NCOLORtot + ic
        do i= SMPindex(ip1-1)+1, SMPindex(ip1)
          WVAL= W(i,Z)
          do k= indexL(i-1)+1, indexL(i)
            WVAL= WVAL -  AL(k) * W(itemL(k),Z)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

New

Matrix Storage Format

ELL (Ellpack-Itpack): Fixed Loop Length, Good for Prefetching

$$\begin{bmatrix} 1 & 3 & 0 & 0 & 0 \\ 1 & 2 & 5 & 0 & 0 \\ 4 & 1 & 3 & 0 & 0 \\ 0 & 3 & 7 & 4 & 0 \\ 1 & 0 & 0 & 0 & 5 \end{bmatrix}$$

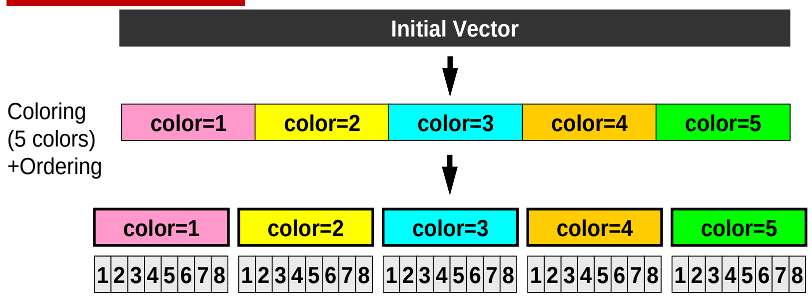


(a) CRS (b) ELL

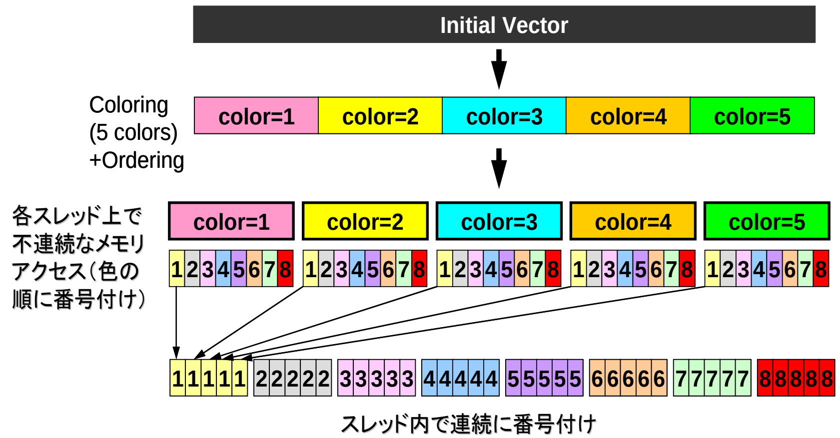
Cases: 128^3 meshes

		Coloring	Further Reordering	First Touch Data Placement	Matrix Storage Format
src0	Case-1	CM-RCM	Coalesced（図 4 (a)）	NO	CRS
reorder0	Case-2		Sequential（図 4 (b)）	YES	
ELL	Case-3				ELL

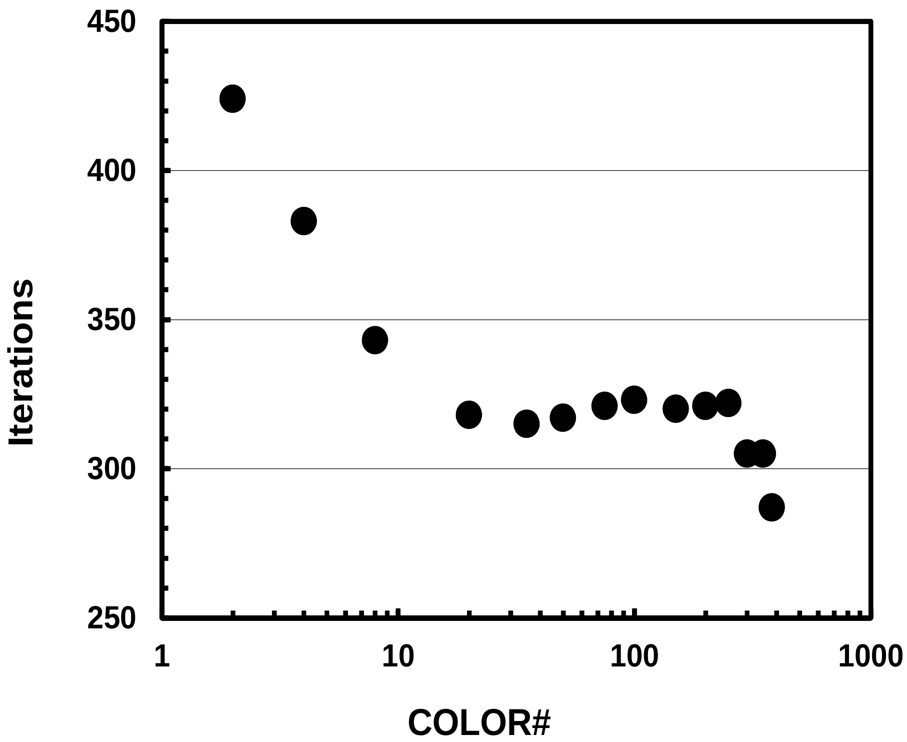
Coalesced



Sequential

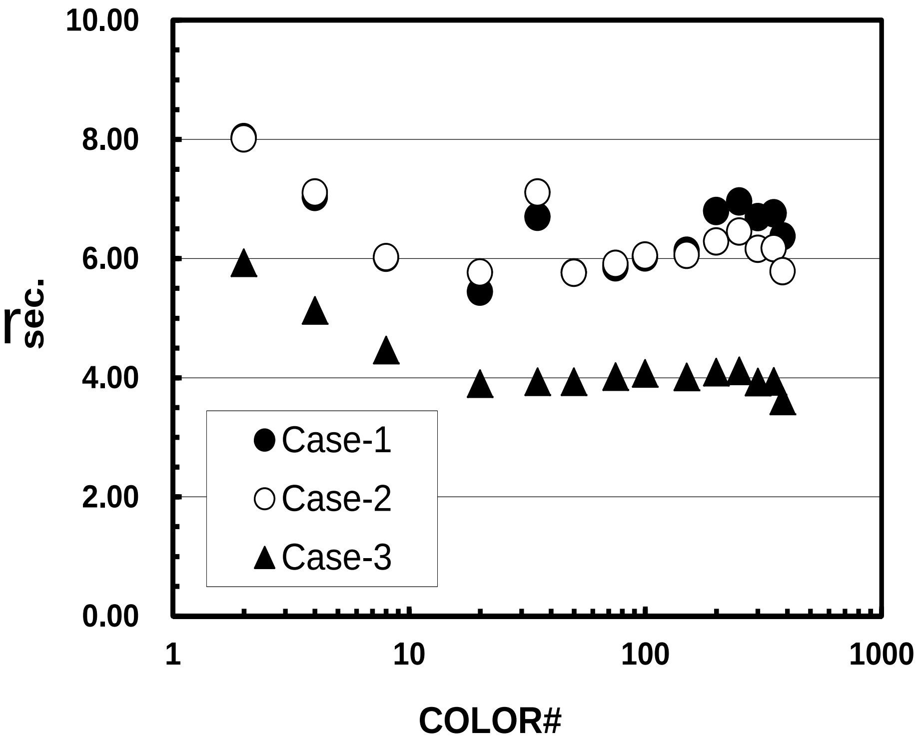


Color# ~ Iteration
CM-RCM



Results: FX10

- CASE-1(src0)⇒CASE-2(reorder0)
  - Slightly improved when number of colors are larger
  - Generally speaking, performance is getting worse if number of colors increases
    - In CASE-2, data on each thread is continuous, when computation proceeds to the next color.
  - First Touch: NO effect
- ELL: Big effect

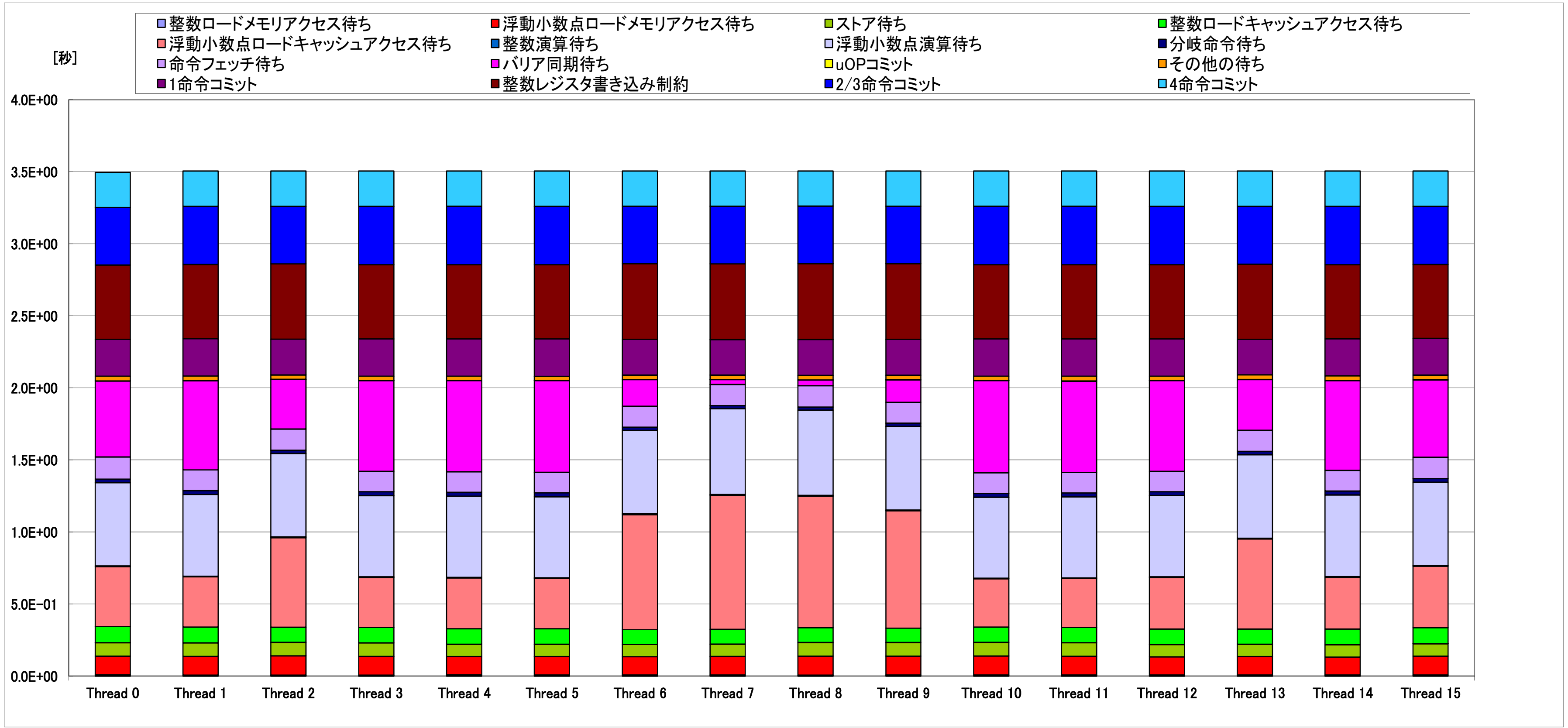


Case-1: src0
Case-2: reorder0
Case-3: reorder0 + ELL

Fujitsu FX10: CASE-1, CM-RCM(2)

L1-dem.-miss:25.6%, Mem. throughput:41.8GB/sec.

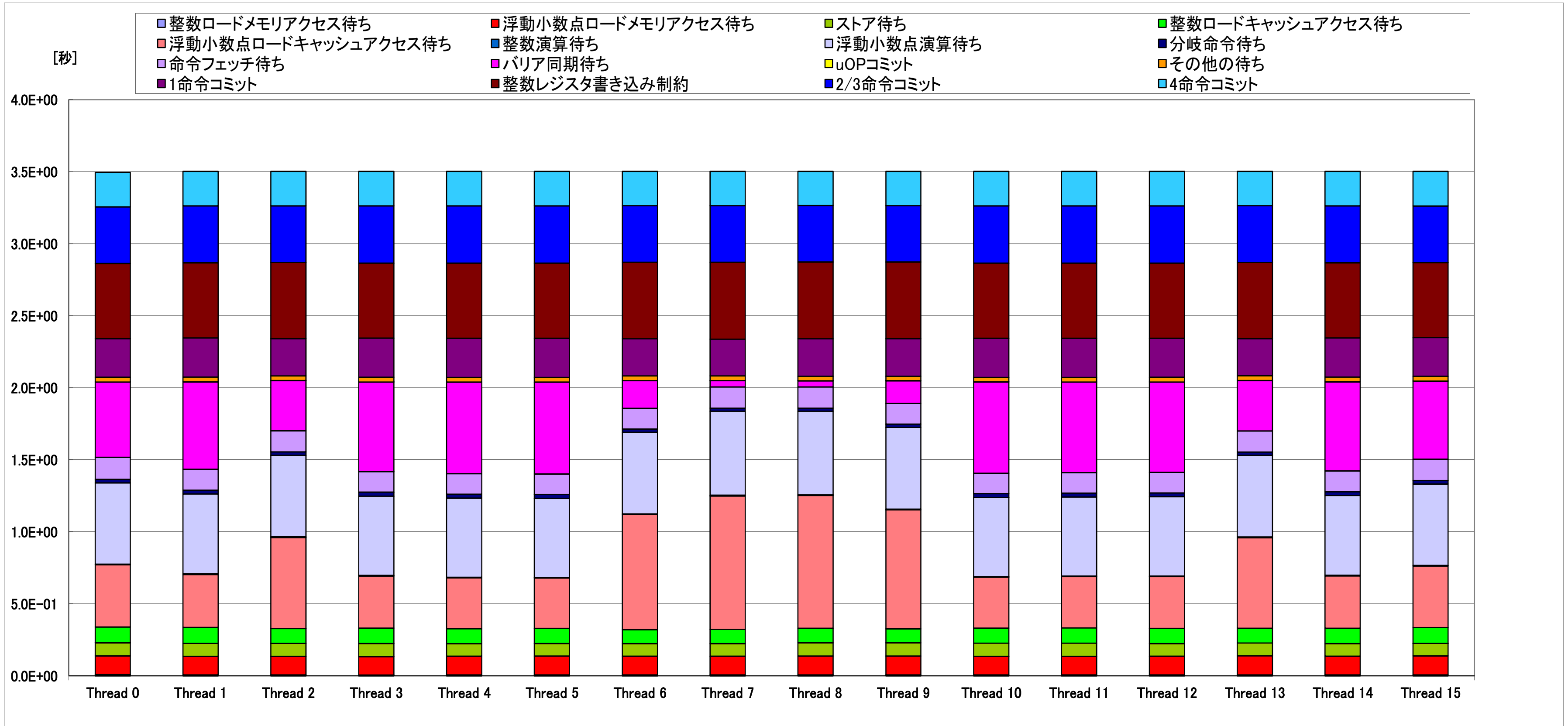
Forward/Backward Substitution



src0: CRS, Coalesced

Fujitsu FX10: CASE-2, CM-RCM(2)

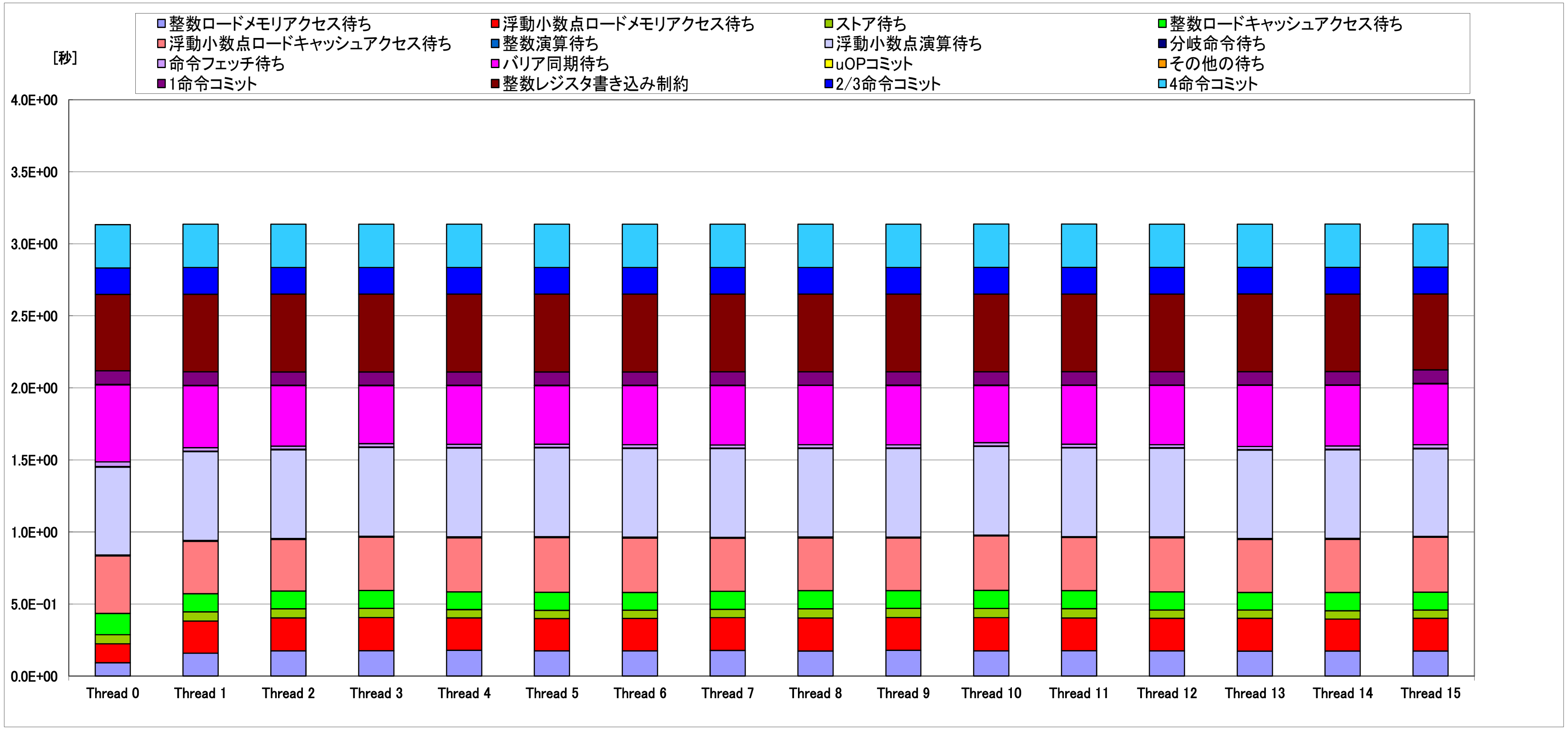
25.6%, 41.8GB/sec.



reorder0: CRS, Sequential

Fujitsu FX10: CASE-1, CM-RCM(382)

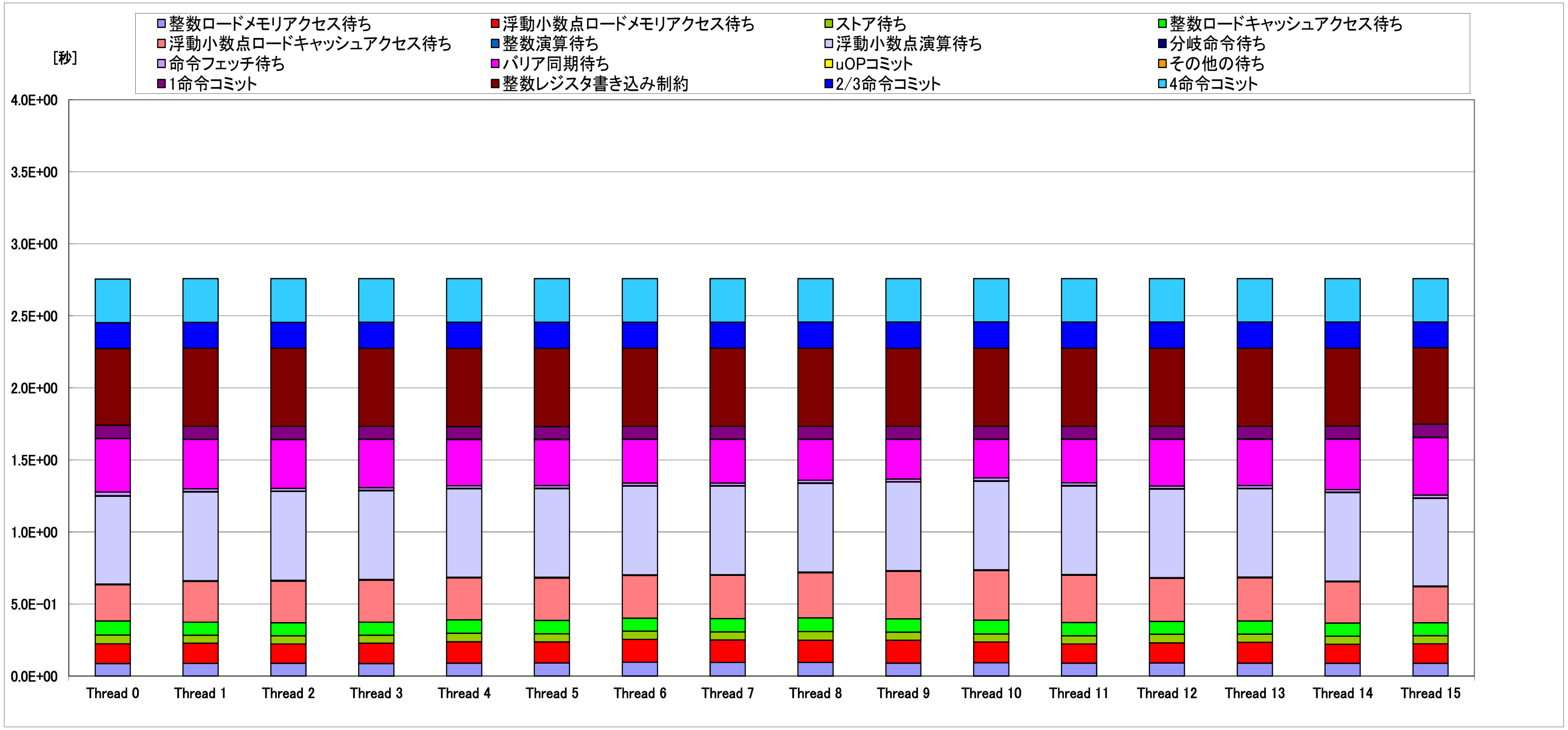
37.7%, 28.7GB/sec.



src0: CRS, Coalesced

Fujitsu FX10: CASE-2, CM-RCM(382)

29.3%, 32.6GB/sec.



reorder0: CRS, Sequential

Summary: Fujitsu FX10 Analysis by Profiler

Upper: L1 Demand Miss Rate
Lower: Memory Throughput

	src0 CASE-1 CRS+ Coalesced	reorder0 CASE-2 CRS+ Sequential	CASE-3 ELL+ Sequential
CM-RCM(2)	25.5 %	25.6 %	5.42 %
	41.8 GB/sec.	41.8 GB/sec.	64.0 GB/sec.
CM-RCM(382)	37.7 %	29.3 %	16.5 %
	28.7 GB/sec.	32.6 GB/sec.	52.2 GB/sec.

Summary: Fujitsu FX10 Analysis by Profiler

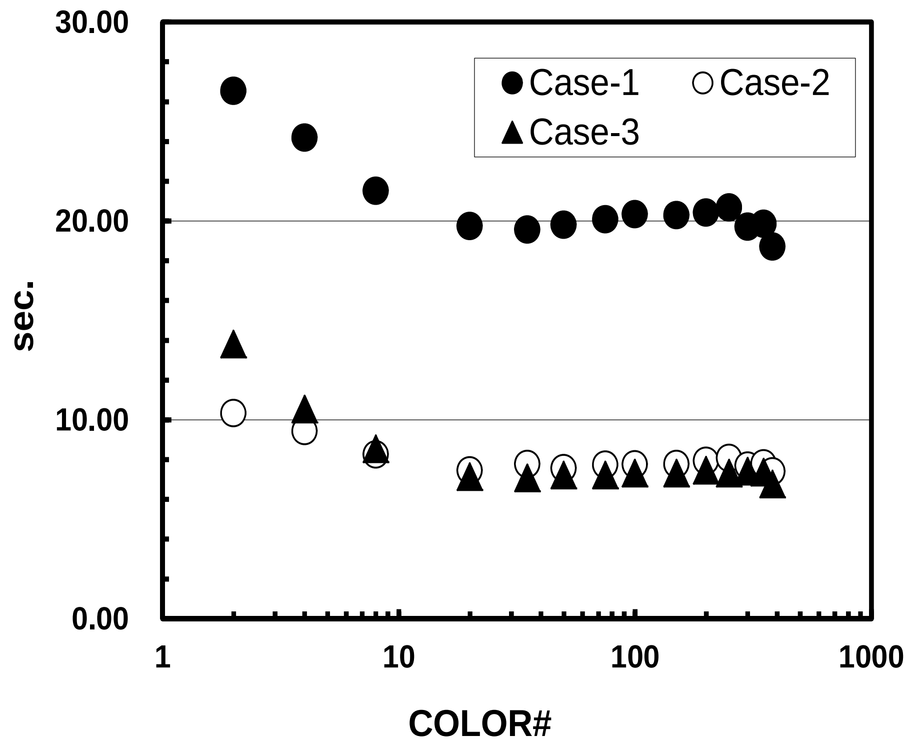
Upper: CM-RCM(20), Lower: CM-RCM(382)

	Instructions	SIMD（%）	Memory Access Throughput（%）
Case-2 CRS	1.83×10^{11} 1.83×10^{11}	7.17 6.90	50.2 44.5
Case-3 ELL	6.71×10^{10} 5.96×10^{10}	16.3 16.2	69.8 67.0

Case-1: src0
Case-2: reorder0
Case-3: reorder0 + ELL

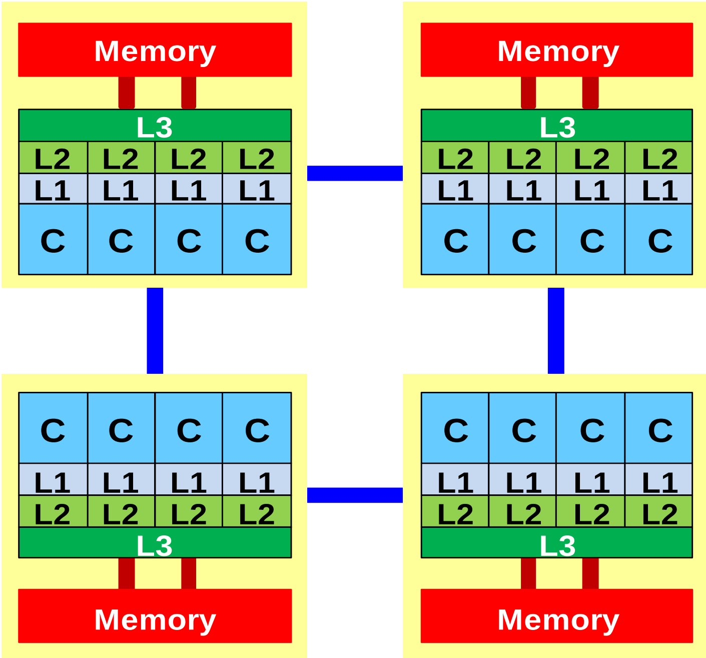
Results: Cray XE6

- CASE-1(src0)⇒ CASE-2(reorder0)
  - Significant Improvement
  - Optimization for NUMA Architecture
  - + First Touch
- CRS⇒ELL Improvement is not so large

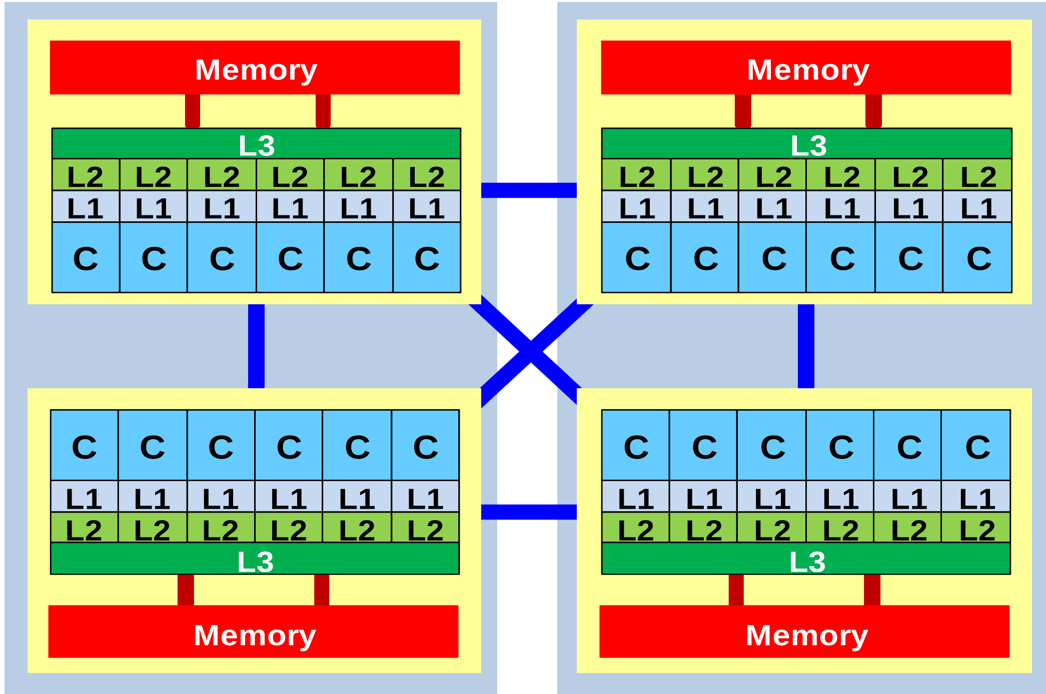


Case-1: src0
Case-2: reorder0
Case-3: reorder0 + ELL

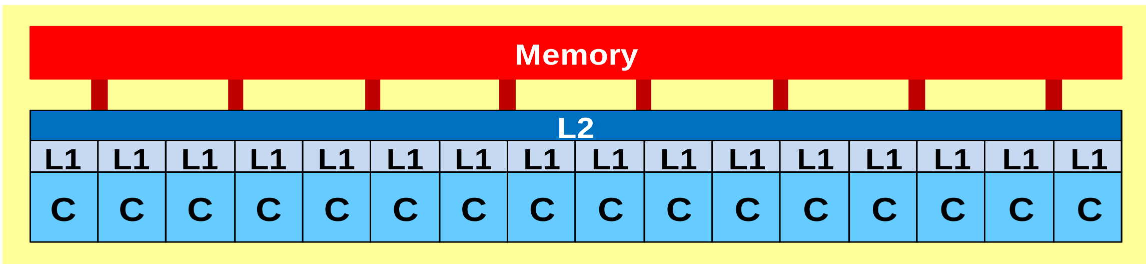
T2K/Tokyo



Cray XE6 (Hopper)



Fujitsu FX10 (Oakleaf-FX)



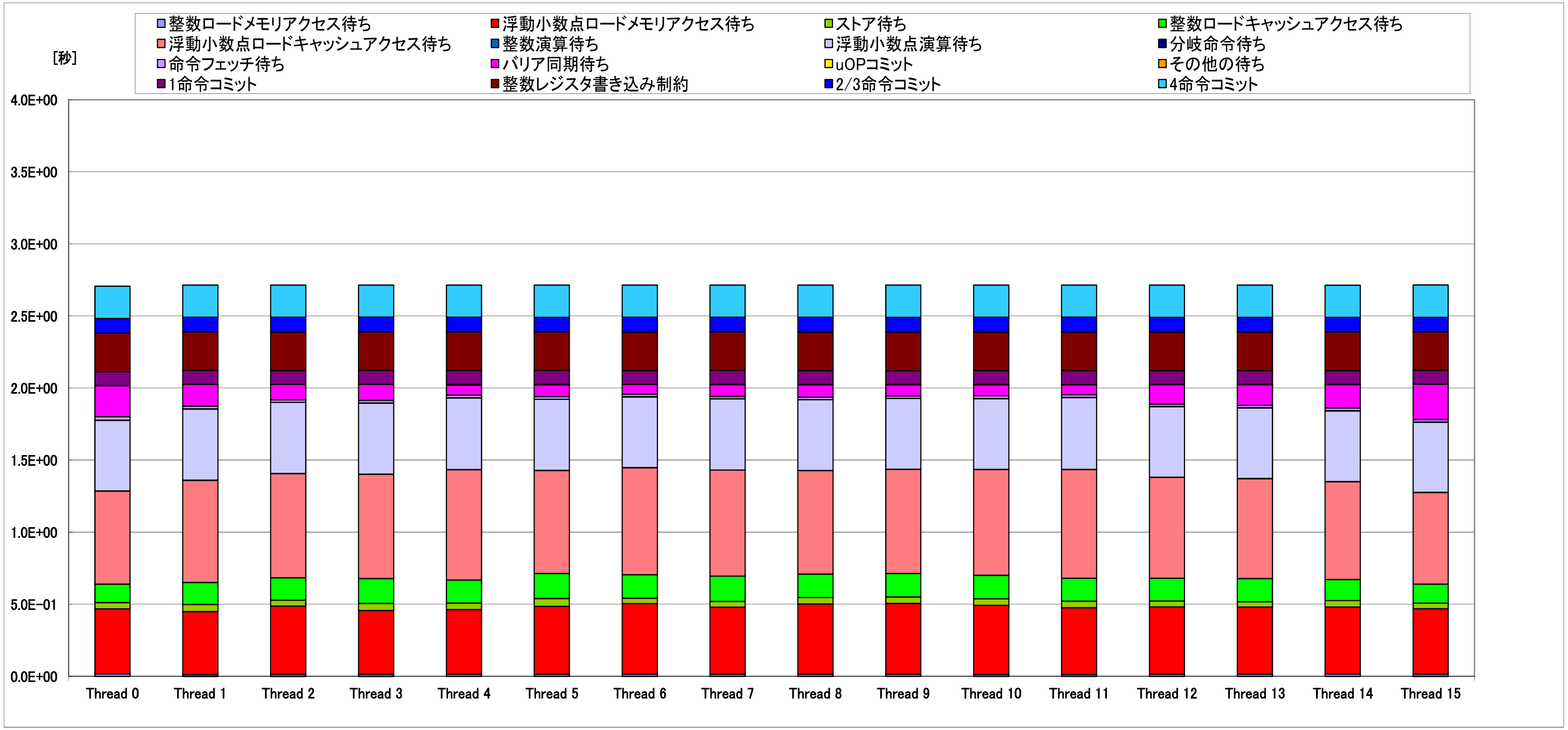
Summary

		CM-RCM(20)		CM-RCM(382) = RCM	
		Time (sec.)	Time/Iteration (sec.)	Time (sec.)	Time/Iteration (sec.)
Fujitsu FX10	Case-1	5.44	1.71×10^{-2}	6.37	2.22×10^{-2}
	Case-2	5.76	1.81×10^{-2}	5.78	2.02×10^{-2}
	Case-3	3.90	1.23×10^{-2}	3.61	1.26×10^{-2}
Cray XE6	Case-1	19.7	6.26×10^{-2}	18.7	6.52×10^{-2}
	Case-2	7.45	2.34×10^{-2}	7.40	2.58×10^{-2}
	Case-3	7.14	2.25×10^{-2}	6.77	2.36×10^{-2}

Case-1: src0
Case-2: reorder0
Case-3: reorder0 + ELL

Fujitsu FX10: CASE-3, CM-RCM(2)

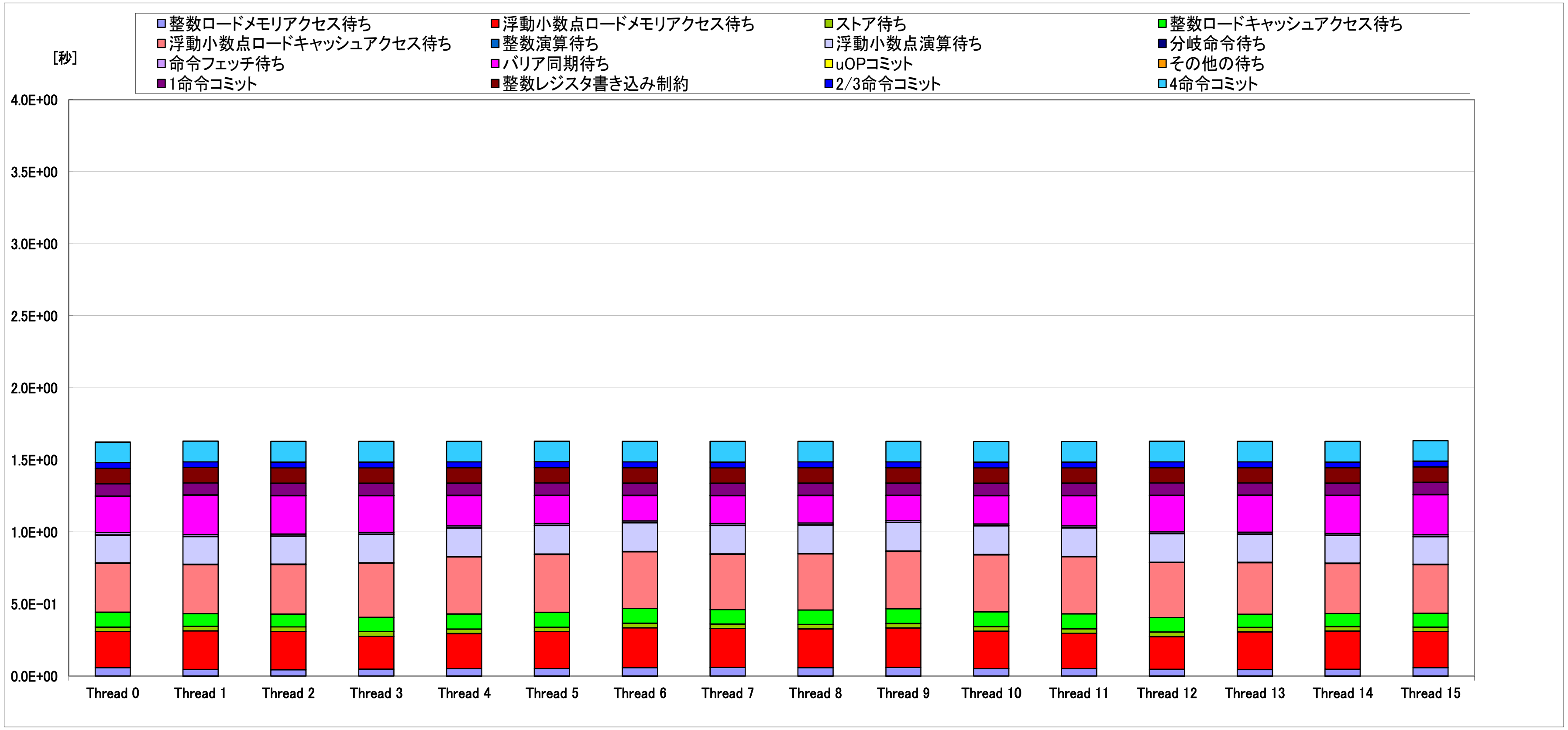
5.4%, 64.0GB/sec.



ELL, Sequential

Fujitsu FX10: CASE-3, CM-RCM(382)

16.5%, 52.2GB/sec.



ELL, Sequential

- Running the Code
- Further Optimization
- **Profiler, Analyzing Compile Lists**
  - **利用支援ポータル⇒ドキュメント閲覧⇒プログラム開発支援ツール⇒プロファイラ使用手引書⇒「3章：詳細プロファイラ」**
  - **Users Portal⇒Document⇒Programming Development Support Tool⇒Profiler User’s Guide⇒“Chap.3 Advanced Profiler”**

Compile & Run

Default

```
>$ cd <$O-L3>/src
>$ make
>$ ls ../run/L3-sol
   L3-sol
>$ cd ../run
>$ pjsub go1.sh
```

```
F90         = frtpx
F90OPTFLAGS= -Kfast,openmp -Qt
F90FLAGS =$(F90OPTFLAGS)
```

- -Qt
  - List of Messages by Compiler (Compile List)
  - *.lst
  - Fortran Only
- In C, "-Qt" is not avilable
  - Please use "-Nsrc"
  - Displayed on screen

Current version of C/C++ compiler can produce list of messages

Fortran/C/C++

-Nlst=p 標準の最適化情報（デフォルト）
-Nlst=t 詳細な最適化情報

Fortran ONLY

-Nlst=a 名前の属性情報
-Nlst=d 派生型の構成情報
-Nlst=i インクルードされたファイルのプログラムリストおよびインクルードファイル名一覧
-Nlst=m 自動並列化の状況を**OpenMP**指示文によって表現した原始プログラム出力
-Nlst=x 名前および文番号の相互参照情報

Info in *.lst

```
(line-no.)(nest)(optimize)
    1                   subroutine sub(a, b, n)
    2                   real*8 a(n), b(n)
                   <<< Loop-information Start >>>
                   <<<  [PARALLELIZATION]
                   <<<    Standard iteration count: 800
                   <<<  [OPTIMIZATION]
                   <<<    SIMD
                   <<<    SOFTWARE PIPELINING
                   <<< Loop-information  End >>>
    3   1  pp  8v         do i=1,n
    4   1  p   8v           a(i)=b(i)+b(i+1)+b(i+2)
    5   1  p   8v         enddo
    6                   end

Procedure information
  Lines      : 6
  Statements : 6
  Stack(byte): 64
  Prefetch num: 0
```

ネスト

行番号

統計情報

ループ単位の最適化情報
- ループ最適化情報
  （ループ融合、ループ交換等）
- SIMD化情報
- 並列化情報
- ソフトウェアパイプライニング
- プリフェッチ情報

ライン単位の最適化情報
- SIMD化情報
- 並列化情報
- ループアンローリング展開数
- インライン展開情報

SIMD Information

```
(line-no.)(nest)(optimize)
                         :
2                  real*8 a(n,n), b(n,n)
3    1              do j = 1 , n
               <<< Loop-information Start >>>
               <<<  [OPTIMIZATION]
               <<<    SIMD
               <<< Loop-information  End >>>
4    2     8v           do i = 1 , n
5    2     8v             a(i, j) = b(i, j)*2.0
6    2     8v           enddo
7    1              enddo
                         :
```

DOループのSIMD化情報
- v ：SIMD化された
- m ：SIMD化された部分とSIMD化されなかった部分を含む
- s ：SIMD化されなかった
- 空白 ：SIMD化対象でない

SIMD化された

実行文のSIMD化情報
- v ：SIMD化可能
- m ：SIMD化可能な部分とSIMD化不可能な部分を含む
- s ：SIMD化不可能

Automatic Parallelization

```
(line-no.)(nest)(optimize)
                         :
             <<< Loop-information Start >>>
             <<<  [PARALLELIZATION]
             <<<    Standard iteration count: 1778
             <<<  [OPTIMIZATION]
             <<<    SIMD
             <<< Loop-information  End >>>
17    1  pp  v      do i=1,n
18    1  p   v        a(i)=cnst
19    1  p   v      enddo
                         :
```

DOループの並列化情報

- pp：並列化された
- m ：並列化された部分と並列化されなかった部分を含む
- s ：並列化されなかった
- 空白：並列化対象でない

ループの繰返し数が
1778以上の時は並列実行
1778未満の時は逐次実行

実行文の並列化情報

- p ：並列化可能
- m：並列化可能な部分と並列化不可能な部分を含む
- s ：並列化不可能

solver_ICCG_mc.lst (src)

```
      1                !C
      1                !C +----------------+
      1                !C | {z}= [Minv]{r} |
      1                !C +----------------+
      1                !C===
      1
      1                !$omp parallel do private(ip,i)
      2   p                  do ip= 1, PEsmpTOT
                     <<< Loop-information Start >>>
                     <<<  [OPTIMIZATION]
                     <<<    SIMD
                     <<<    SOFTWARE PIPELINING
                     <<< Loop-information  End >>>
      3   p   8v             do i = SMPindexG(ip-1)+1, SMPindexG(ip)
      3   p   8v               W(i,Z)= W(i,R)
      3   p   8v             enddo
      2   p                  enddo
      1                !$omp end parallel do
      1
      1                      Stime= omp_get_wtime()
      1                      call fapp_start ("precond", 1, 1)
      2                      do ic= 1, NCOLORtot
      2                !$omp parallel do private(ip,ip1,i,WVAL,k)
      3   p                    do ip= 1, PEsmpTOT
      3   p                      ip1= (ic-1)*PEsmpTOT + ip
      4   p                    do i= SMPindex(ip1-1)+1, SMPindex(ip1)
      4   p                      WVAL= W(i,Z)
                     <<< Loop-information Start >>>
                     <<<  [OPTIMIZATION]
                     <<<    SIMD
                     <<<    SOFTWARE PIPELINING
                     <<< Loop-information  End >>>
      5   p   4v                 do k= indexL(i-1)+1, indexL(i)
      5   p   4v                   WVAL= WVAL -  AL(k) * W(itemL(k),Z)
      5   p   4v                 enddo
      4   p                      W(i,Z)= WVAL * W(i,DD)
      4   p                    enddo
      3   p                    enddo
      2                !$omp end parallel do
      2                      enddo
```

3.5 精密PA可視化機能 (Excel) (Precision PA Visibility Function)

(1/3): Inserting Call’s, Compile & Run

```
      call start_collection ("SpMV")
!$omp parallel do private(ip,i,VAL,k)
      do ip= 1, PEsmpTOT
        do i= SMPindex((ip-1)*NCOLORtot)+1, SMPindex(ip*NCOLORtot)
          VAL= D(i)*W(i,P)
          do k= 1, 3
            VAL= VAL + AL(k,i)*W(itemL(k,i),P)
          enddo
          do k= 1, 3
            VAL= VAL + AU(k,i)*W(itemU(k,i),P)
          enddo
          W(i,Q)= VAL
        enddo
      enddo
!$omp end parallel do
      call stop_collection ("SpMV")
```

3.5 精密PA可視化機能 (Excel) (Precision PA Visibility Function)

(2/3): Collecting Performance Data: 7X Exec's Directories: pa1~pa7, -Hpa=1~7

```
#!/bin/sh
#PJM -L "node=1"
#PJM -L "elapse=00:05:00"
#PJM -L "rscgrp=lecture"
#PJM -g  "gt71"
#PJM -j
#PJM -o "3.lst"
#PJM --mpi "proc=1"

export OMP_NUM_THREADS=16
fapp -C -d pa1 -Ihwm -Hpa=1 ./sol-r3k
```

3.5 精密PA可視化機能 (Excel) (Precision PA Visibility Function)

(3/3): Performance Analysis: Transformation + Excel

```
fapppx -A -d pa1 -o output_prof_1.csv -tcsv -Hpa
fapppx -A -d pa2 -o output_prof_2.csv -tcsv -Hpa
fapppx -A -d pa3 -o output_prof_3.csv -tcsv -Hpa
fapppx -A -d pa4 -o output_prof_4.csv -tcsv -Hpa
fapppx -A -d pa5 -o output_prof_5.csv -tcsv -Hpa
fapppx -A -d pa6 -o output_prof_6.csv -tcsv -Hpa
fapppx -A -d pa7 -o output_prof_7.csv -tcsv -Hpa
```

Summary

- Material: ICCG solver for sparse matrices derived from FVM applications (Finite Volume Method).
- Parallelization on a single node of Oakleaf-FX (FX10) using OpenMP
  - Data Placement
  - Reordering
- Effects of reordering

Future Directions

- Gap between performance of CPU & memory
  - BYTE/FLOP
- Multicore/Manycore
  - Intel Xeon/Phi
- 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