Introduction to Parallel Programming for Multicore/Manycore Clusters

Part A2: Introduction to OpenMP

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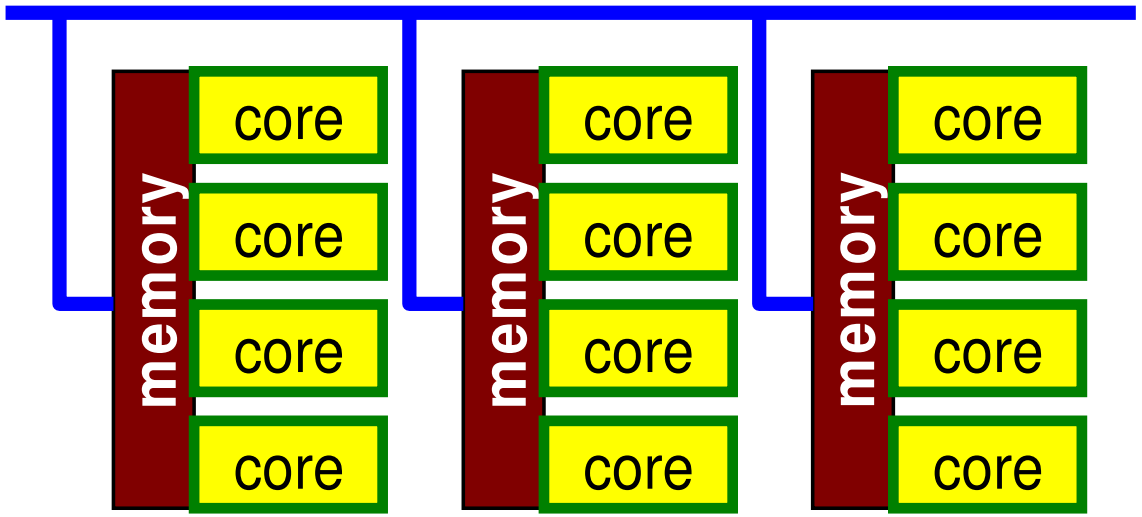
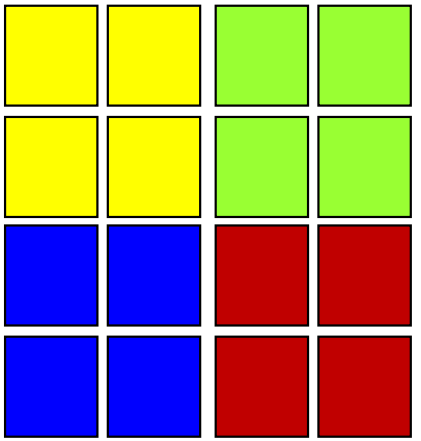
- OpenMP
- Login to Wisteria/BDEC-01
- Parallel Code by OpenMP (0): up to 12 cores
- Parallel Code by OpenMP (1): First Touch
- Parallel Code by OpenMP (2): +ELL
- Parallel Code by OpenMP (3): reduced omp-parallel
- Parallel Code by OpenMP (4): Further Optimization (Fortran only)

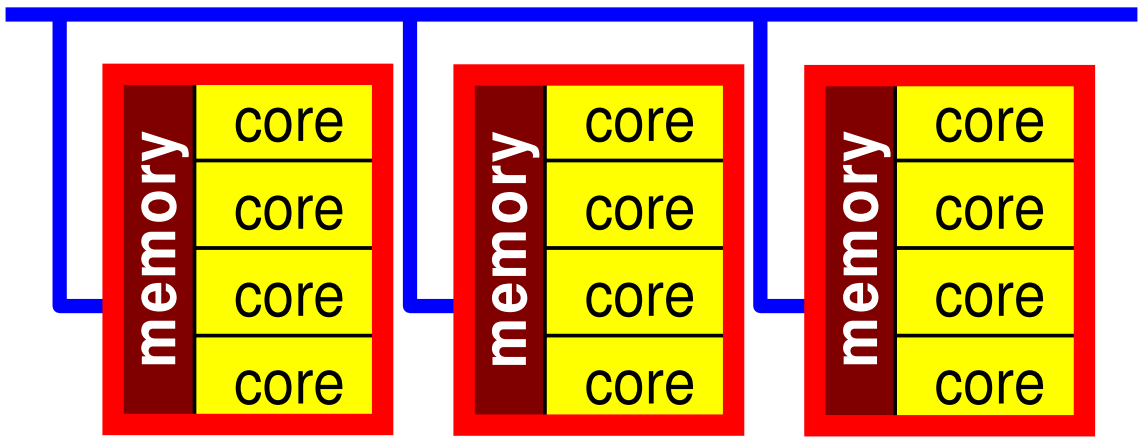
Flat MPI vs. Hybrid

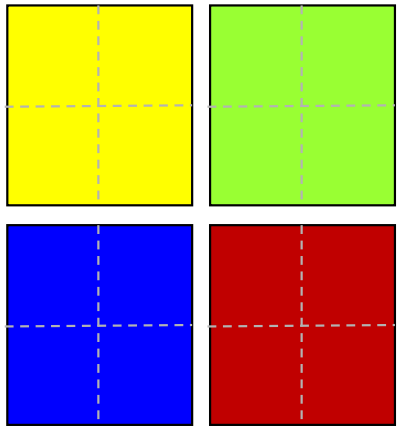
Flat-MPI：Each Core -> Independent



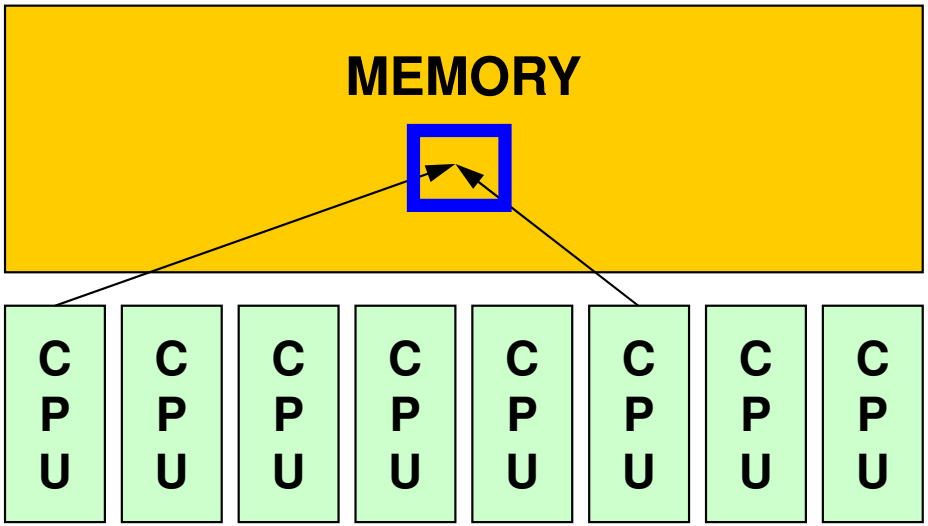


Hybrid：Hierarchal Structure





SMP



- SMP
  - Symmetric Multi Processors
  - Multiple CPU's (cores) share a single memory space

What is OpenMP ? (1/2)

http://www.openmp.org

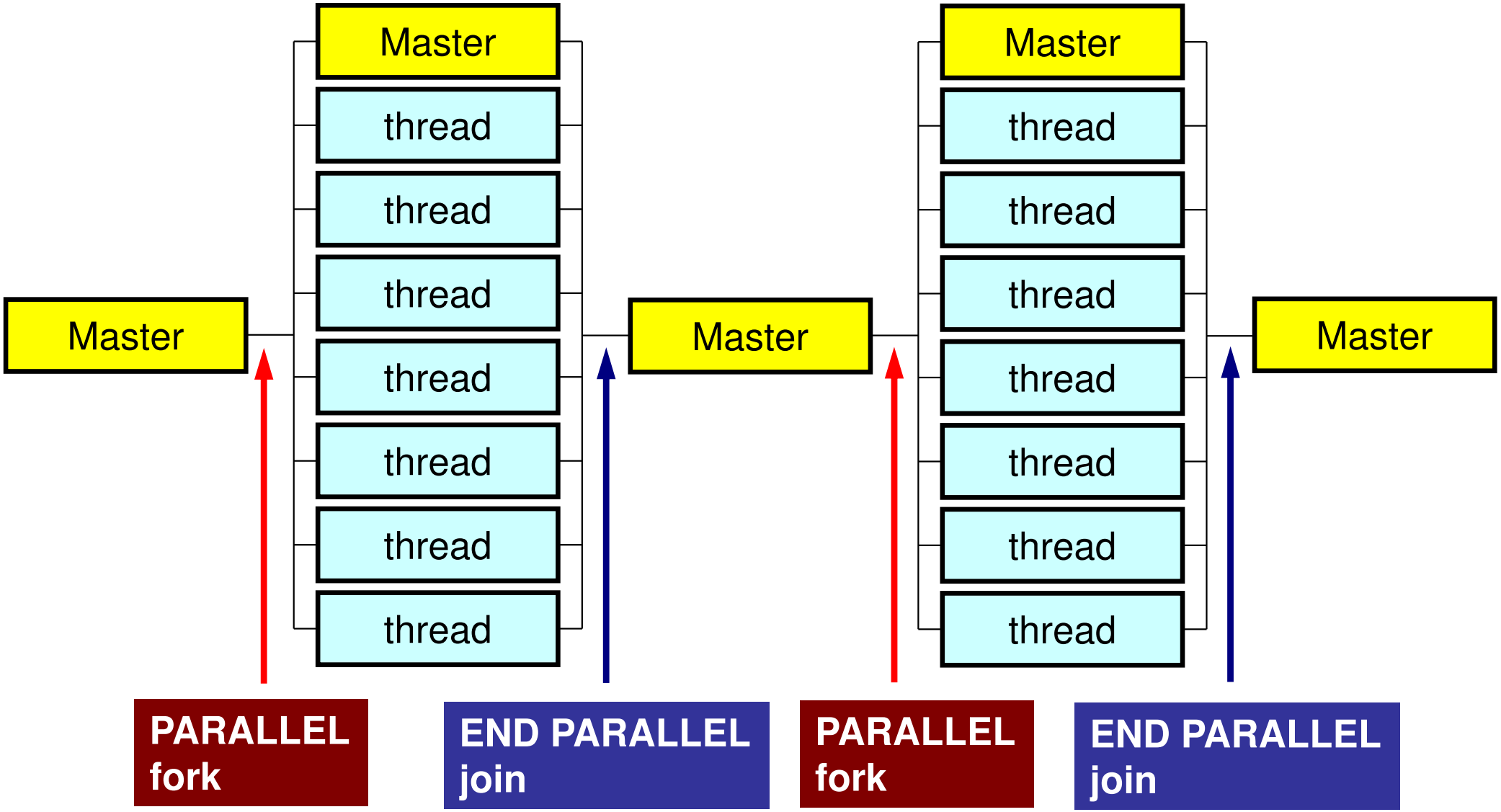
- An API (Application Programming Interface) for multi-platform shared-memory parallel programming in C/C++ and Fortran
  - Current version: 4.X (5.0 is already announced)
    - GPU, Accelerators: close to OpenACC
- Background
  - Merger of Cray and SGI in 1996
    - Separated later, … but both are now merged into HPE
  - ASCI project (US-DOE (Dept. of Energy)) started in 1995
    - Accelerated Strategic Computing Initiative (ASCI) -> Advanced Simulation and Computing Program (ASC)
      - The goal of ASCI is to simulate the results of new weapons designs as well as the effects of aging on existing and new designs, all in the absence of additional data from underground nuclear tests.
    - Development of Supercomputers & Software/Applications
      - SMP Clusters: Intel ASCI Red, IBM Power (Blue, White, Purple)/Blue Gene, SGI
      - Common API for SMP Clusters needed

What is OpenMP ? (2/2)

http://www.openmp.org

- C/C++ version and Fortran version have been separately developed until ver.2.5.
- Fork-Join Parallel Execution Model (Next Page)
  - Directives: Parallel, End Parallel
  - Serial Execution: Master Thread
  - Parallel Execution: Master Thread/Thread Team
- Users have to specify everything by directives.
  - Nothing happen, if there are no directives

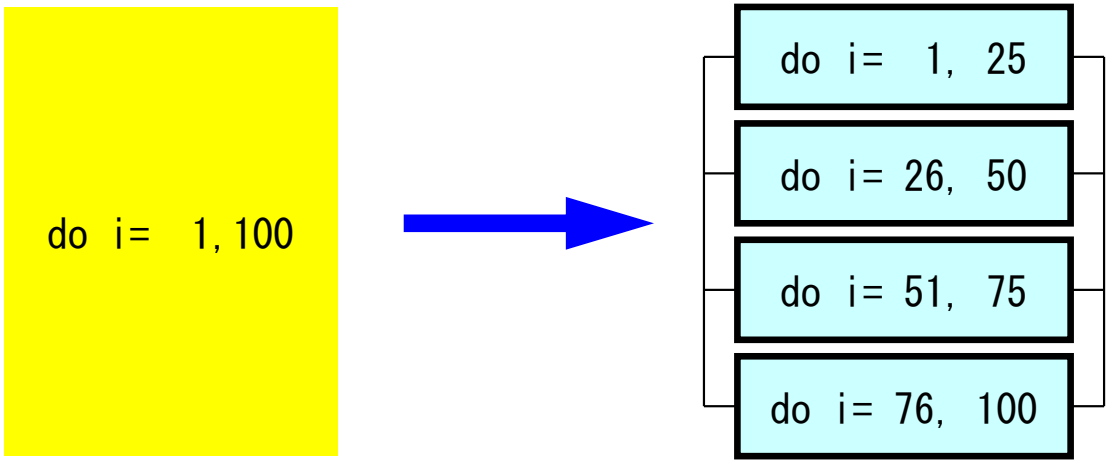
Fork-Join Parallel Execution Model



Number of Threads

- **OMP_NUM_THREADS**
  - How to change ?
    - bash(.bashrc) **export OMP_NUM_THREADS=8**
    - csh(.cshrc) **setenv OMP_NUM_THREADS 8**

- **OMP_NUM_THREADS=4**



Information about OpenMP

- OpenMP Architecture Review Board (ARB)
  - http://www.openmp.org
  - Spec. of OpenMP is available
- References
  - Chandra, R. et al.「Parallel Programming in OpenMP」（Morgan Kaufmann）
  - Quinn, M.J.「Parallel Programming in C with MPI and OpenMP」（McGrawHill）
  - Mattson, T.G. et al.「Patterns for Parallel Programming」（Addison Wesley）
  - 牛島「OpenMPによる並列プログラミングと数値計算法」（丸善）
  - Chapman, B. et al.「Using OpenMP」（MIT Press）
- Japanese Version of OpenMP 3.0 Spec. (Fujitsu etc.)
  - http://www.openmp.org/mp-documents/OpenMP30spec-ja.pdf

Features of OpenMP

- Directives
  - Loops right after the directives are parallelized.
  - If the compiler does not support OpenMP, directives are considered as just comments.

OpenMP/Directives Array Operations

Simple Substitution

```
!$omp parallel do
      do i= 1, N
        W(i,1)= 0.d0
        W(i,2)= 0.d0
      enddo
!$omp end parallel do
```

Dot Products

```
!$omp parallel do private(i)
!$omp&             reduction(+:RHO)
      do i= 1, N
        RHO= RHO + W(i,R)*W(i,Z)
      enddo
!$omp end parallel do
```

DAXPY

```
!$omp parallel do
      do i= 1, N
        Y(i)= ALPHA*X(i) + Y(i)
      enddo
!$omp end parallel do
```

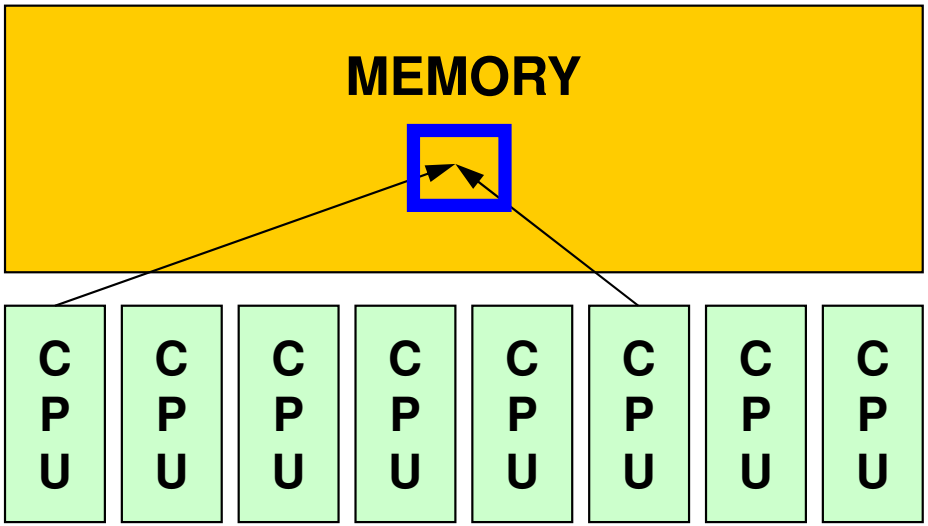
OpenMP/Direceives Matrix/Vector Products

```
!$omp parallel do private(i,k)
    do i= 1, N
      W(i,Q)= D(i)*W(i,P)
      do k= indexLU(i-1)+1, indexLU(i)
        W(i,Q)= W(i,Q) + AMAT(k)*W(itemLU(k),P)
      enddo
    enddo
!$omp end parallel do
```

Features of OpenMP

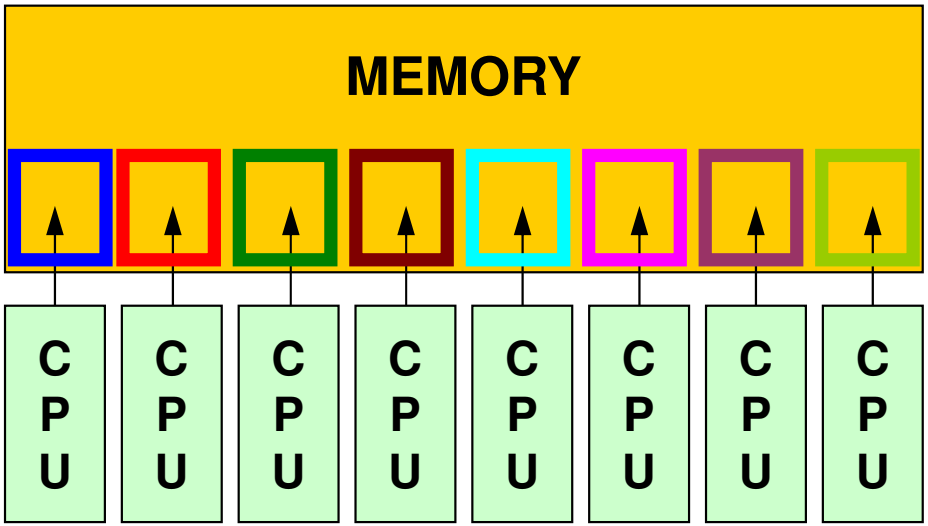
- Directives
  - Loops right after the directives are parallelized.
  - If the compiler does not support OpenMP, directives are considered as just comments.
- Nothing happen without explicit directives
  - Different from “automatic parallelization/vectorization”
  - Something wrong may happen by un-proper way of usage
  - Data configuration, ordering etc. are done under users’ responsibility
- “Threads” are created according to the number of cores on the node
  - Thread: “Process” in MPI
  - Generally, “# threads = # cores”: Xeon Phi supports 4 threads per core (Hyper Multithreading)

Memory Contention: メモリ競合



- During a complicated process, multiple threads may simultaneously try to update the data in same address on the memory.
  - e.g.: Multiple cores update a single component of an array.
  - This situation is possible.
  - Answers may change compared to serial cases with a single core (thread).

Memory Contention (cont.)



- In this lecture, any such case does not happen by reordering etc.
  - In OpenMP, users are responsible for such issues (e.g. proper data configuration, reordering etc.)
- Data Dependency
- Performance per core reduces as number of used cores (thread #) increases (Memory Saturation)

Features of OpenMP (cont.)

- “!omp parallel do”-”!omp end parallel do”
- Global (Shared) Variables, Private Variables
  - Default: Global (Shared)
  - Dot Products: reduction

```
!$omp parallel do private(i)
!$omp&             reduction(+:RHO)
      do i= 1, N
        RHO= RHO + W(i,R)*W(i,Z)
      enddo
!$omp end parallel do
```

W(:,:), R, Z
global (shared)

FORTRAN & C

```
use omp_lib
...
!$omp parallel do shared(n,x,y) private(i)
      do i= 1, n
        x(i)= x(i) + y(i)
      enddo
!$ omp end parallel do
```

```
#include <omp.h>
...
{
  #pragma omp parallel for default(none) shared(n,x,y) private(i)

    for (i=0; i<n; i++)
        x[i] += y[i];
}
```

In this class ...

- There are many capabilities of OpenMP.
- In this class, only several functions are shown for parallelization of PCG/ICCG solver.

First things to be done

- use omp_lib Fortran
- #include <omp.h> C

OpenMP Directives (Fortran)

```
sentinel directive_name [clause[[,] clause]…]
```

- NO distinctions between upper and lower cases.
- sentinel
  - Fortran: !OMP, COMP, *$OMP
    - !$OMP only for free format
  - Continuation Lines (Same rule as that of Fortran compiler is applied)
    - Example for **`!$OMP PARALLEL DO SHARED(A,B,C)`**

```
!$OMP PARALLEL DO
!$OMP+SHARED (A,B,C)
```

```
!$OMP PARALLEL DO &
!$OMP SHARED (A,B,C)
```

OpenMP Directives (C)

```
#pragma omp directive_name [clause[[,] clause]…]
```

- “＼” for continuation lines
- Only lower case (except names of variables)

```
#pragma omp parallel for shared (a,b,c)
```

PARALLEL DO/for

```
!$OMP PARALLEL DO[clause[[,] clause] … ]
   (do_loop)
!$OMP END PARALLEL DO
```

```
#pragma parallel for [clause[[,] clause] … ]
   (for_loop)
```

- Parallerize DO/for Loops
- Examples of “clause”
  - private(list)
  - shared(list)
  - default(private|shared|none)
  - reduction({operation|intrinsic}: list)

REDUCTION

```
REDUCTION ({operator|intrinsic}: list)
```

```
reduction ({operator|intrinsic}: list)
```

- Similar to “MPI_Reduce”
- Operator
  - +, *, -, .AND., .OR., .EQV., .NEQV.
- Intrinsic
  - MAX, MIN, IAND, IOR, IEQR

Example-1: A Simple Loop

```
!$OMP PARALLEL DO
      do i= 1, N
        B(i)= (A(i) + B(i)) * 0.50
      enddo
!$OMP END PARALLEL DO
```

- Default status of loop variables (“i” in this case) is private. Therefore, explicit declaration is not needed.
- “END PARALLEL DO” is not required
  - In C, there are no definitions of “end parallel do”

Example-1: REDUCTION

```
!$OMP PARALLEL DO DEFAULT(PRIVATE) REDUCTION(+:A,B)
      do i= 1, N
        call WORK (Alocal, Blocal)
        A= A + Alocal
        B= B + Blocal
      enddo
!$OMP END PARALLEL DO
```

- “END PARALLEL DO” is not required

Functions in OpenMP

functions	description
int omp_get_num_threads (void)	Thread #
int omp_get_thread_num (void)	Thread ID
double omp_get_wtime (void)	Timer
void omp_set_num_threads (int num_threads) call omp_set_num_threads (num_threads)	Specifying Thread #

OpenMP for Dot Products

```
      VAL= 0.d0
      do i= 1, N
        VAL= VAL + W(i,R) * W(i,Z)
      enddo
```

OpenMP for Dot Products

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      VAL= 0.d0
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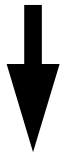
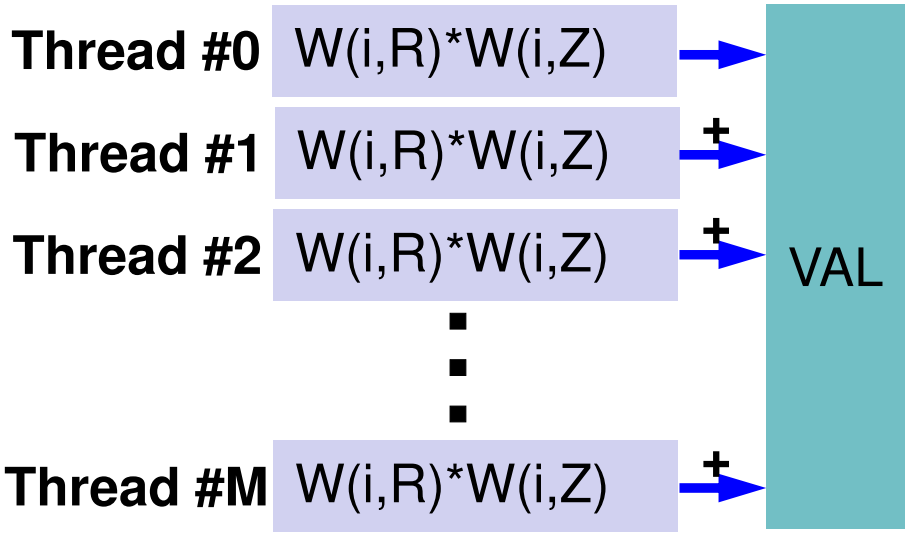


```
      VAL= 0.d0
!$OMP PARALLEL DO PRIVATE(i) REDUCTION(+:VAL)
      do i= 1, N
        VAL= VAL + W(i,R) * W(i,Z)
      enddo
!$OMP END PARALLEL DO
```

Directives are just inserted.



OpenMP for Dot Products

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      do i= 1, N
        VAL= VAL + W(i,R) * W(i,Z)
      enddo
!$OMP END PARALLEL DO
```

Directives are just inserted.

```
      VAL= 0.d0
!$OMP PARALLEL DO PRIVATE(ip,i) REDUCTION(+:VAL)
      do ip= 1, PEsmpTOT
        do i= index(ip-1)+1, index(ip)
          VAL= VAL + W(i,R) * W(i,Z)
        enddo
      enddo
!$OMP END PARALLEL DO
```

Multiple Loop
`PEsmpTOT`: Number of threads

Additional array **`INDEX(:)`** is needed.
Efficiency is not necessarily good, but users can specify thread for each component of data.

OpenMP for Dot Products

```
      VAL= 0.d0
!$OMP PARALLEL DO PRIVATE(ip,i) REDUCTION(+:VAL)
      do ip= 1, PEsmpTOT
        do i= index(ip-1)+1, index(ip)
          VAL= VAL + W(i,R) * W(i,Z)
        enddo
      enddo
!$OMP END PARALLEL DO
```

Multiple Loop
PEsmpTOT: Number of threads

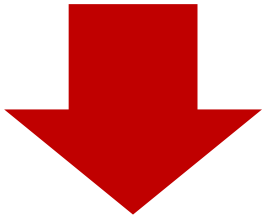
Additional array **INDEX(:)** is needed.
Efficiency is not necessarily good, but users can specify thread for each component of data.

e.g.: N=100, PEsmpTOT=4

INDEX(0)= 0
INDEX(1)= 25
INDEX(2)= 50
INDEX(3)= 75
INDEX(4)= 100

Matrix-Vector Multiply

```
      do i= 1, N
        W(i,Q)= D(i)*W(i,P)
        do k= indexLU(i-1)+1, indexLU(i)
          W(i,Q)= W(i,Q) + AMAT(k)*W(itemLU(k),P)
        enddo
      enddo
```



```
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```

Matrix-Vector Multiply

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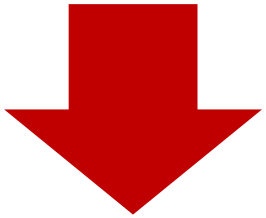
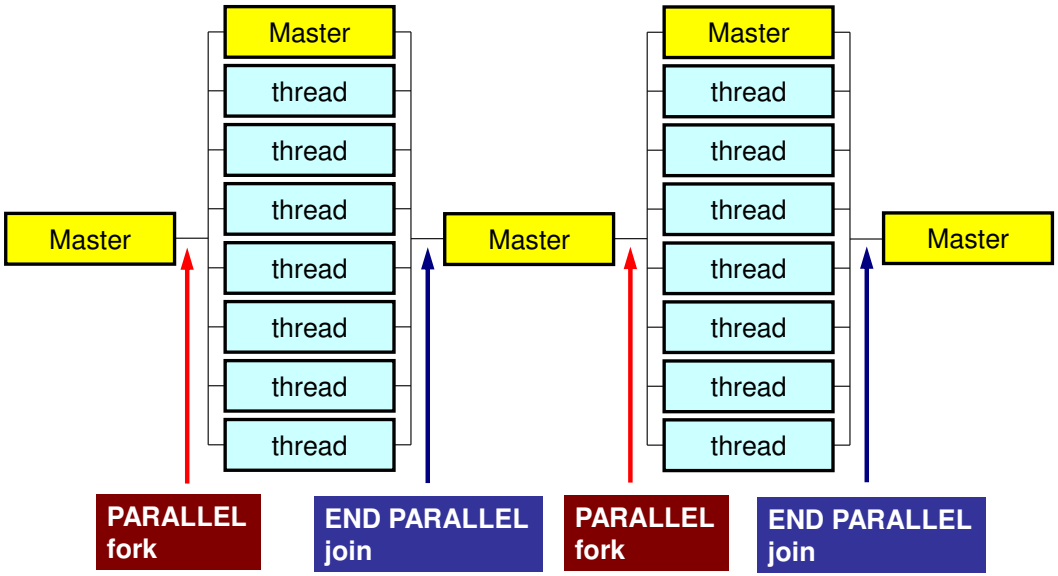


```
!$omp parallel do private(ip,i,k)
      do ip= 1, PEsmpTOT
      do i= index(ip-1)+1, index(ip)
        W(i,Q)= D(i)*W(i,P)
        do k= indexLU(i-1)+1, indexLU(i)
          W(i,Q)= W(i,Q) + AMAT(k)*W(itemLU(k),P)
        enddo
      enddo
      enddo
!$omp end parallel do
```

omp parallel (do)

- “omp parallel-omp end parallel” = “fork-join”
- If you have many loops, these “fork-join’s” cause overheads
- omp parallel + omp do/omp for




```
#pragma omp parallel ...

#pragma omp for {

...
#pragma omp for {
```

```
!$omp parallel ...

!$omp do
   do i= 1, N
...
!$omp do
   do i= 1, N
...
!$omp end parallel   required
```

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Target for Parallelization

- “Parallelization” of the FVM code
- Just inserting OpenMP directives
  - “poi_gen.f/c”(poi_gen),
  - “solver_PCG.f/c” (solve_PCG)

Preconditioned Conjugate Gradient Method（PCG）

```
Compute r(0)= b-[A]x(0)
for i= 1, 2, …
    solve [M]z(i-1)= r(i-1)
    ρi-1= r(i-1) z(i-1)
    if i=1
      p(1)= z(0)
     else
      βi-1= ρi-1/ρi-2
      p(i)= z(i-1) + βi-1 p(i-1)
    endif
    q(i)= [A]p(i)
    αi  = ρi-1/p(i)q(i)
    x(i)= x(i-1) + αip(i)
    r(i)= r(i-1) - αiq(i)
    check convergence |r|
end
```

Solving the following equation:

$$\{z\}=[M]^{-1}\{r\}$$

"Approximate Inverse Matrix"

$$[M]^{-1}\approx[A]^{-1},\quad [M]\approx[A]$$

Ultimate Preconditioning: Inverse Matrix

$$[M]^{-1}=[A]^{-1},\quad [M]=[A]$$

Diagonal Scaling: Simple but weak

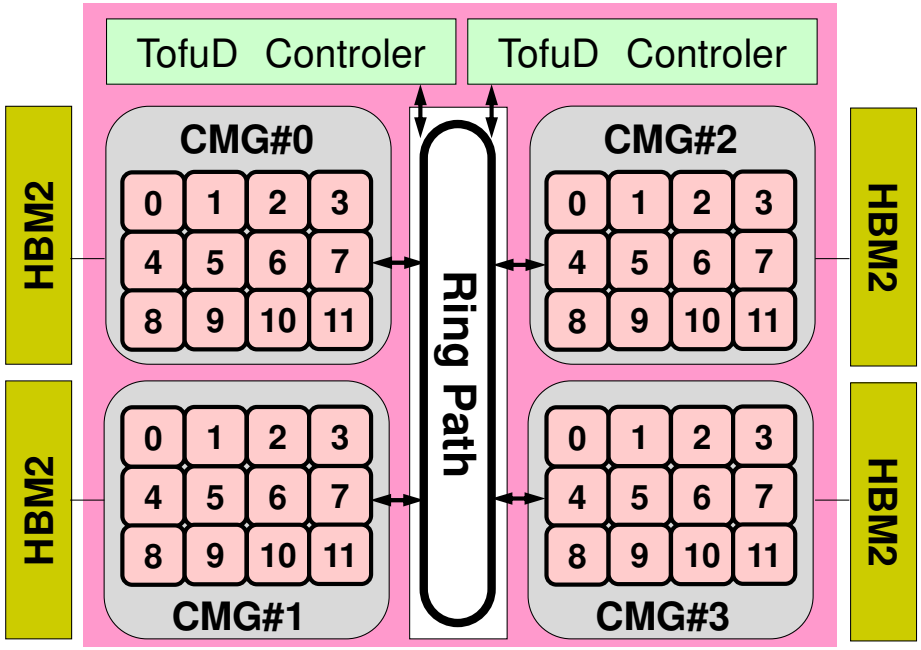
$$[M]^{-1}=[D]^{-1},\quad [M]=[D]$$

Diagonal Scaling, Point-Jacobi

$$[M]=\begin{bmatrix} D_1 & 0 & \dots & 0 & 0 \\ 0 & D_2 & & 0 & 0 \\ \dots & & \dots & & \dots \\ 0 & 0 & & D_{N-1} & 0 \\ 0 & 0 & \dots & 0 & D_N \end{bmatrix}$$

- **`solve [M]z(i-1)= r(i-1)`** is very easy.
- Provides fast convergence for simple problems.

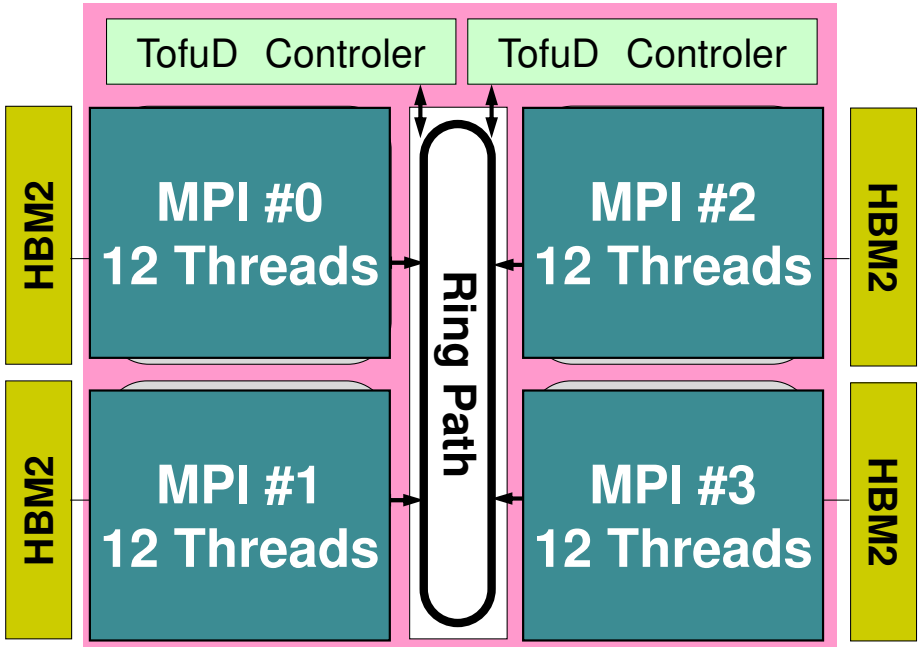
A64FX Processor on Odyssey



Name	A64FX
Processor # (Core #)	1 (48+ 2or4 Assistant Cores)
Frequency	2.2 GHz
Peak Performance	3.3792 TFLOPS
Memory Size	32 GiB
Memory Bandwidth	1,024 GB/s
L1 Cache	64 KiB/core (Inst/Data)
L2 Cache	8 MiB/CMG

- 4 CMG's (Core Memory Group), 12 cores/CMG
  - 48 Cores/Node (Processor)
  - 2.2GHz × 32DP × 48= 3379.2 GFLOPS= 3.3792 TFLOPS
- NUMA Architecture (Non-Uniform Memory Access)
  - Each core of a CMG can access to the memory on other CMG's
  - Utilization of the local memory is more efficient

A64FX Processor on Odyssey



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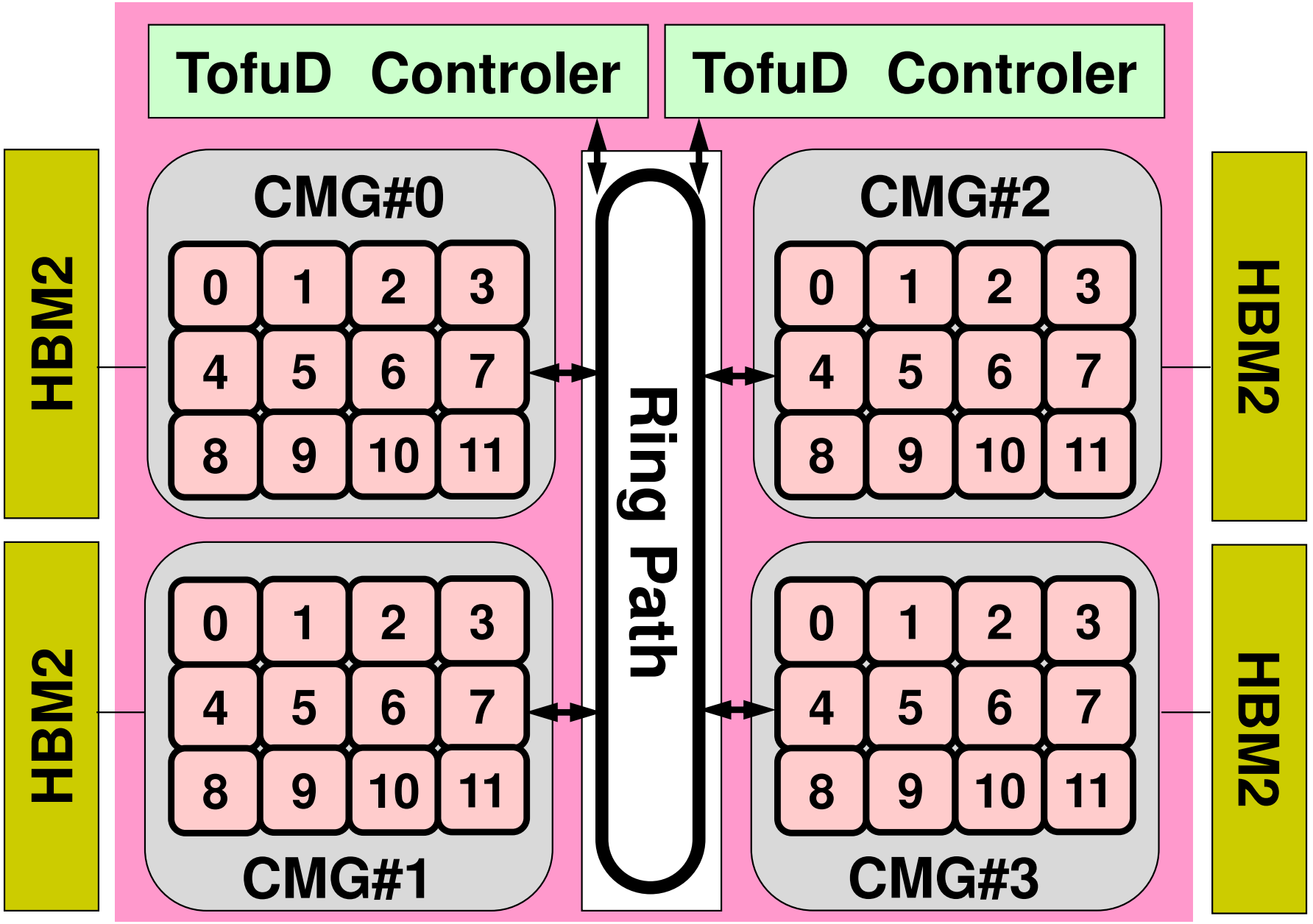
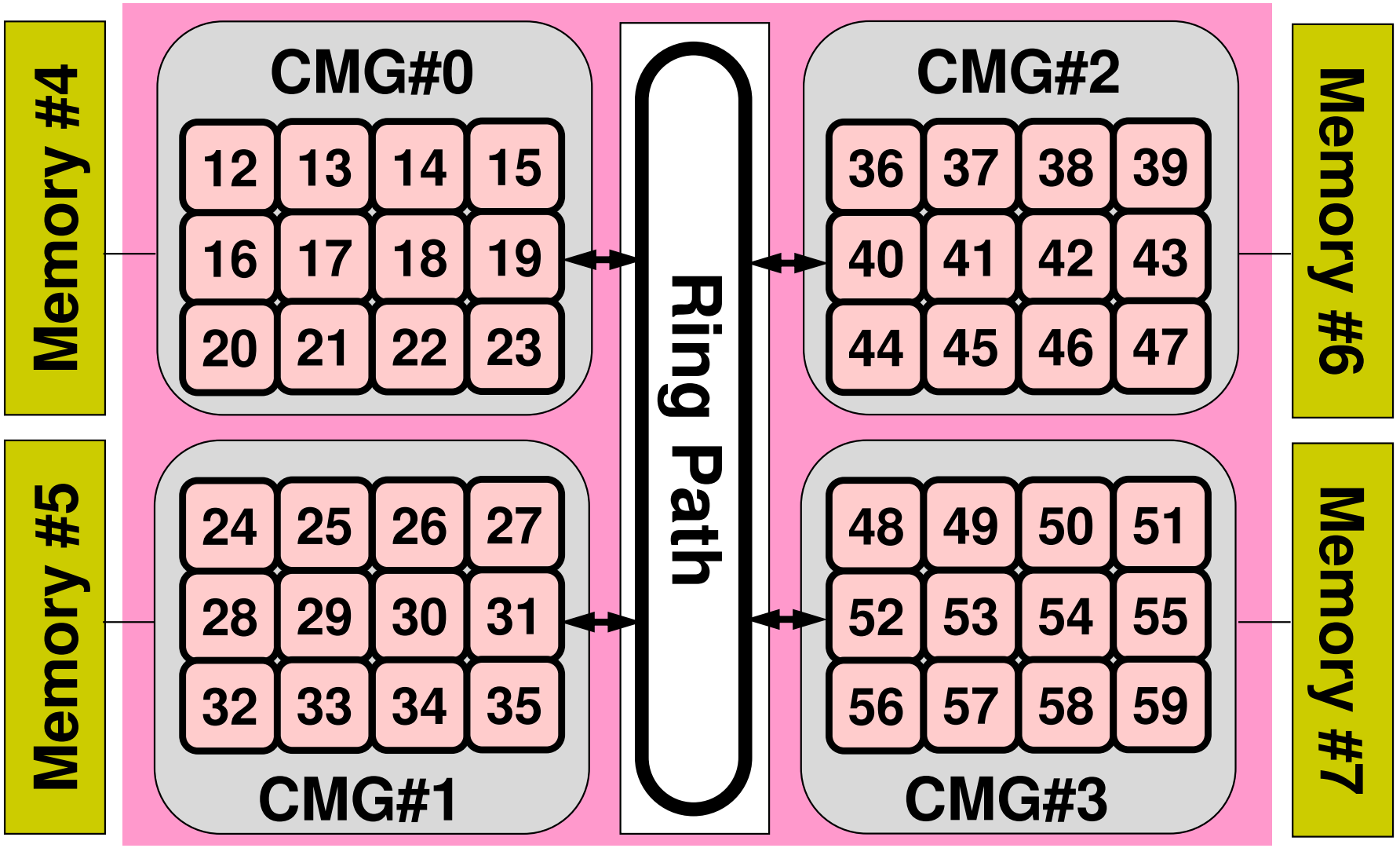
A64FX：CMG（Core Memory Group）



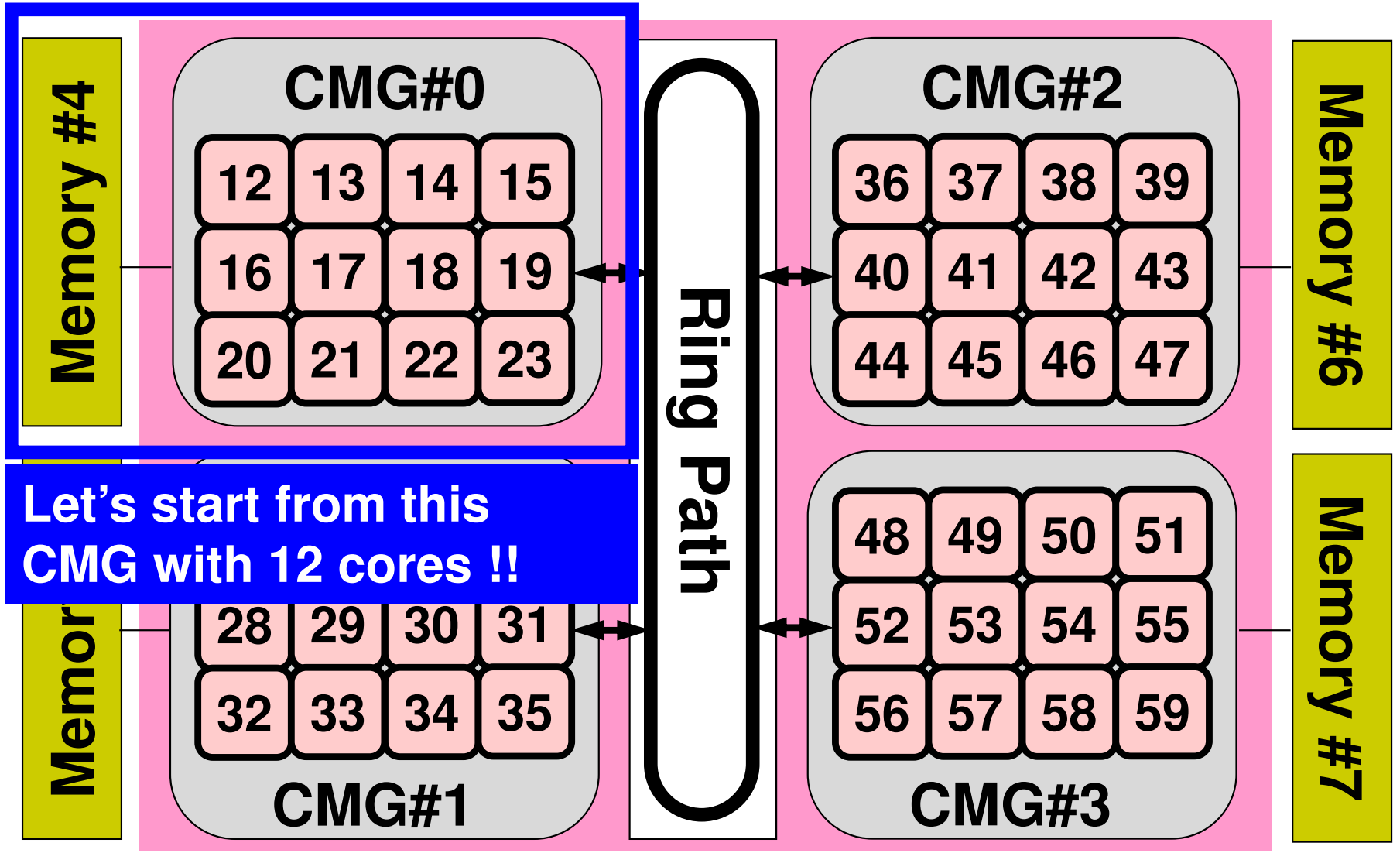
ID of CMGs, Cores, Memory's (1/2)

CMG:#0-#3, Core:#12-59, Memory:#4-#7



ID of CMGs, Cores, Memory's (1/2)

CMG:#0-#3, Core:#12-59, Memory:#4-#7



Files on Wisteria/BDEC-01 (Odyssey)

```
>$ cd /work/gt89/t89XYZ
>$ cp /work/gt00/z30088/ompw.tar .

>$ tar xvf ompw.tar

>$ cd ompw          <$O-ompw>
```

Please make sure that following directories are created

```
run src-c0 src-c1 src-c2 src-c3 src-c3b src-f0 src-f1 src-f2 src-f3 src-f4
```

```
>$ module load fj
>$ make -f makef
>$ ls run/solf0
   solf0
>$ cd run

<modify "INPUT.DAT", "f12.sh">

>$ pjsub f12.sh
```

Please type this at every login !

<$O-ompw>/makef

parallel computing by OpenMP

```
default:
        (cd src-f0 ; make )
        (cd src-f1 ; make )
        (cd src-f2 ; make )
        (cd src-f3 ; make )
        (cd src-f4 ; make )
clean:
        (cd src-f0 ; make clean)
        (cd src-f1 ; make clean)
        (cd src-f2 ; make clean)
        (cd src-f3 ; make clean)
        (cd src-f4 ; make clean)
```

<$O-ompw>/src-f0/Makefile

parallel computing by OpenMP

```
F90   = frtpx
F90OPTFLAGS= -Kfast,openmp

F90FLAGS =$(F90OPTFLAGS)

.SUFFIXES:
.SUFFIXES: .o .f .f90 .c
#
.f90.o:; $(F90) -c $(F90FLAGS)  $(F90OPTFLAG) $<
.f.o:; $(F90) -c $(F90FLAGS)  $(F90OPTFLAG) $<
#
OBJS = ¥
solver_PCG.o struct.o pcg.o ¥
boundary_cell.o cell_metrics.o ¥
input.o main.o poi_gen.o pointer_init.o outucd.o

TARGET = ../run/solf0

all: $(TARGET)

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

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

C-Compiler：2-modes

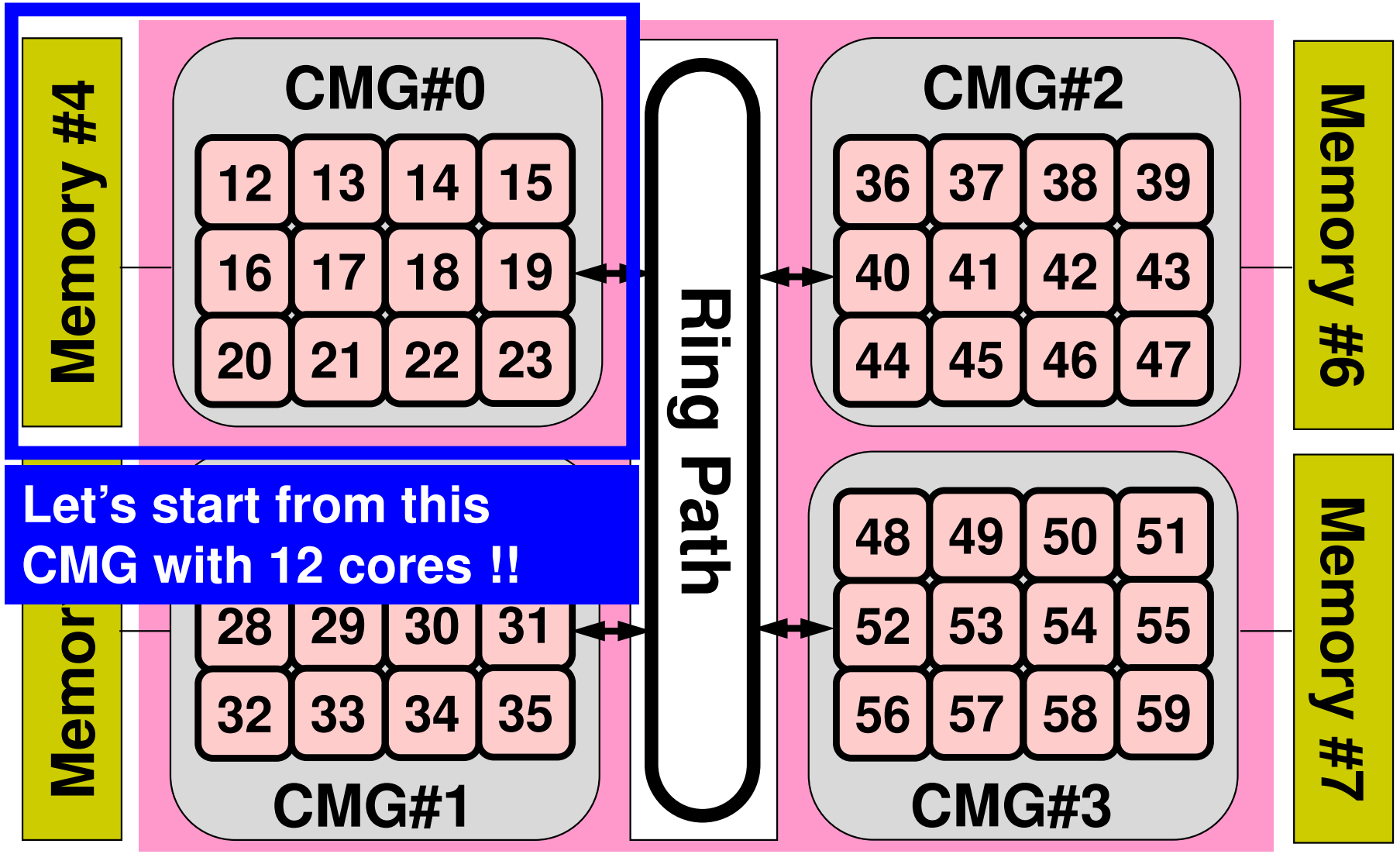
trad (-Nnoclang) （default）	• Based on Fujitsu's compiler developed for K and PRIMEHPC FX100 or older • Compatible with Fujitsu's Traditional Compilers • C89/C99/C11，OpenMP 3.1/OpenMP 4.5 (partially) • Default (-Nnoclang) • Generally slow for the materials in this class • make –f make-org (make-o)
clang (-Nclang)	• Based on Clang/LLVM Compilers (Open Source) • Suitable for using Most Updated Capability's, and for using OSS (Open Source Software) • C89/C99/C11，OpenMP 4.5/OpenMP 5.0 (partially) • Generally faster than "trad" modes, difference between "trad" and "clang" is smaller for optimized codes • In this class, default is "clang" mode • make –f makec (Makefile)

Running Job

- Batch Jobs
  - Only batch jobs are allowed.
  - Interactive executions of jobs are not allowed.
- How to run
  - writing job script
  - submitting job
  - checking job status
  - checking results
- Utilization of computational resources
  - 1-node (48 cores) is occupied by each job.
  - Your node is not shared by other jobs.

ID of CMGs, Cores, Memory's (1/2)

CMG:#0-#3, Core:#12-59, Memory:#4-#7



Job Script (1/3) : f12.sh

- /work/gt89/t89XXX/ompw/run/f12.sh
- Scheduling + Shell Script

```
#!/bin/sh
#PJM -N "f12"                    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 # (1-48, ~12 for a while)
#PJM -L elapse=00:15:00          Elapsed Computation Time
#PJM -g gt89                     Group Name (Wallet)
#PJM -j
#PJM -e err                      Standard Error
#PJM -o f12.lst                  Standard Output

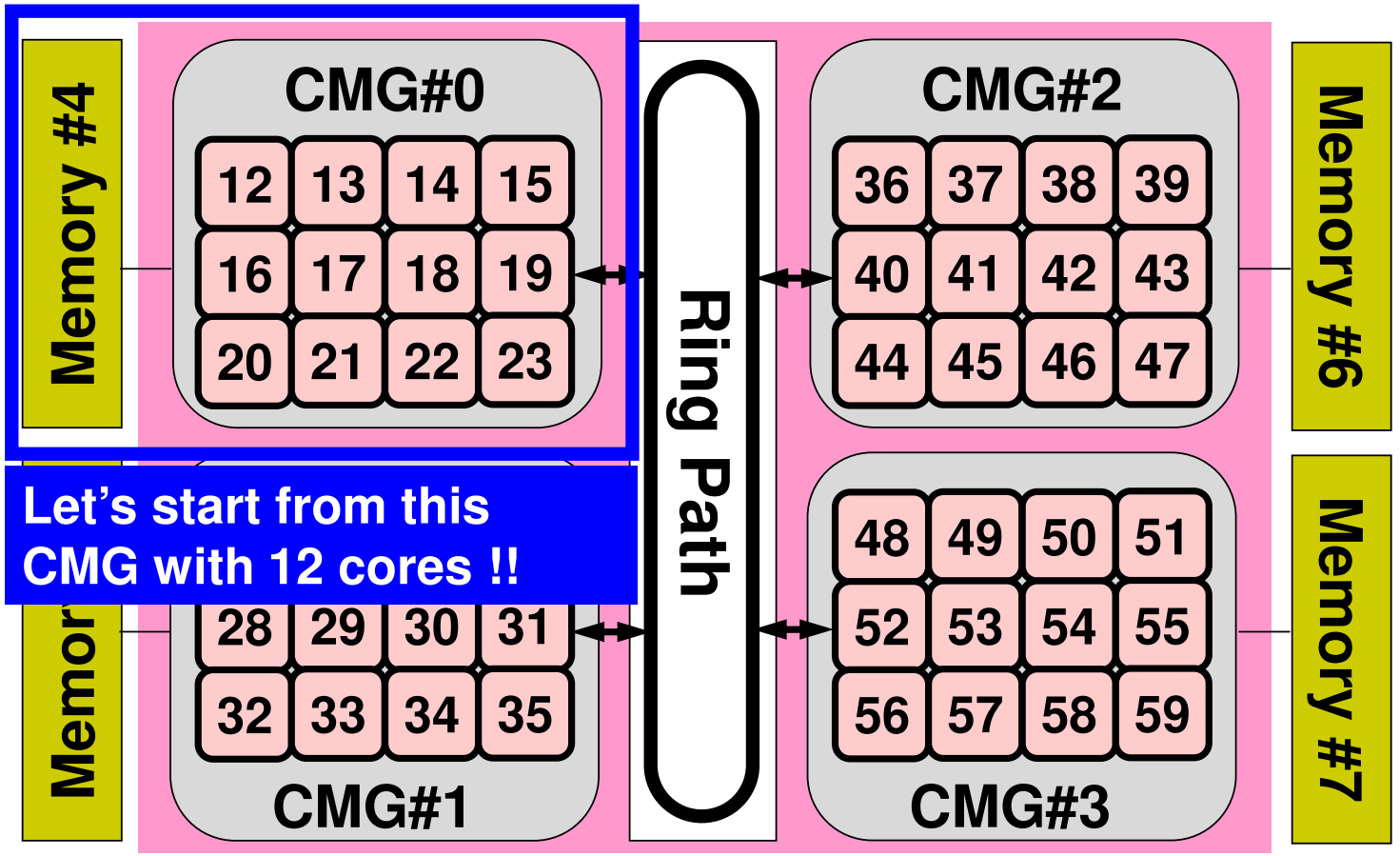
module load fj
export OMP_NUM_THREADS=12        Thread #(--omp thread=XX)
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl ./solf0
numactl -C 12-23 -m 4 ./solf0
```

Job Script (2/3) : f12.sh

- **`/work/gt89/t89XXX/ompw/run/f12.sh`**
- **`numactl:`** utilization of local resources as much as possible

```
numactl ./solf0
numactl -C 12-23 -m 4 ./solf0
```



Job Script (3/3) : f12.sh

```
export XOS_MMM_L_PAGING_POLICY=
demand:demand:demand
```

Parameters	Values (Underline: Default)	Description
XOS_MMM_L_PAGING_POLICY	[demand | prepage] [demand | prepage] [demand | prepage]	Paging policy (page allocation trigger) of each memory unit ✓ demand: Demand Paging Method ✓ prepage: Prepaging Method 3 Items are defined ✓ 1st Item: .bss area of static data (.data area of static data is always "prepage") ✓ 2nd Item: Stack Area, Thread Stack Area ✓ 3rd Item: Area for Dynamic Memory Allocation If a value other than the specified value (demand/prepage), the configuration is considered as "prepage:demand:prepage" **"demand:demand:demand" is recommended for using multiple CMG's**

Running Jobs

```
>$ cd /work/gt89/t89XYZ
>$ cd ompw/run
>$ pjsub f12.sh

>$ cat f12.lst
```

INPUT.DAT

```
128 128 128                          NX NY NZ
1.00e-0  1.00e-00 1.00e-00           DX/DY/DZ
1.0e-08                              EPSICCG
```

Output (1/2)

```
[t00XYZ@wisteria01 run]$ cat f12.lst
   128   128   128
     1    8.958216E+00
   101    8.313496E+00
   201    2.090443E+00
   301    3.811029E-01
   401    3.769653E-02
   501    9.429978E-04
   601    4.940783E-05
   701    1.888611E-06
   801    2.243179E-08
   826    9.818026E-09
     5.275418E+00 sec. (solver)
##ANSWER   2097152    1.459831E+04

   128   128   128
     1    8.958216E+00
   101    8.313496E+00
   201    2.090443E+00
   301    3.811029E-01
   401    3.769653E-02
   501    9.429978E-04
   601    4.940783E-05
   701    1.888611E-06
   801    2.243179E-08
   826    9.818026E-09
     5.270398E+00 sec. (solver)
##ANSWER   2097152    1.459831E+04
```

Output (2/2): 5-times

```
[t00XYZ@wisteria01 run]$ grep "(sol" f12.lst

    5.275418E+00 sec. (solver)
    5.270398E+00 sec. (solver)
    5.270445E+00 sec. (solver)
    5.271554E+00 sec. (solver)
    5.270543E+00 sec. (solver)

    5.272427E+00 sec. (solver)
    5.272081E+00 sec. (solver)
    5.270522E+00 sec. (solver)
    5.271067E+00 sec. (solver)
    5.271237E+00 sec. (solver)
```

```
numactl ./solf0
```

```
numactl -C 12-23 -m 4 ./solf0
```

Available Resource Groups (Queue's)

- Following 2 resource groups are available
- Up to 12 nodes are available, while you need a single node in this class
  - **`lecture-o`**
    - 12 nodes (576 cores), 15 min., valid until the end of Sep. 2022
    - Shared by all "educational" users
  - **`lecture9-o`**
    - 12 nodes (576 cores), 15 min., active during class time
    - More jobs (compared to **`lecture-o`**) can be processed up on availability.

Submitting & Checking Jobs

• Submitting Jobs	`pjsub SCRIPT NAME`
• Checking status of jobs	`pjstat`
• Deleting/aborting	`pjdel JOB ID`
• Checking status of queues	`pjstat --rsc`
• Detailed info. of queues	`pjstat --rsc -x`
• Number of running jobs	`pjstat -a`
• History of Submission	`pjstat -H`
• Limitation of submission	`pjstat --limit`

```
[t00470@wisteria01 run]$ pjsub f2_48.sh
[INFO] PJM 0000 pjsub Job 15713 submitted.

[t00470@wisteria01 run]$ pjsub f3_48.sh
[INFO] PJM 0000 pjsub Job 15714 submitted.

[t00470@wisteria01 run]$ pjstat
Wisteria/BDEC-01 scheduled stop time: 2021/05/28(Fri) 09:00:00 (Remain:  4days 1:25:56)

JOB_ID       JOB_NAME   STATUS  PROJECT    RSCGROUP          START_DATE        ELAPSE       TOKEN            NODE  GPU
15713        f2_48      RUNNING gt00       lecture-o         05/24 07:34:03    00:00:02         -               1    -
15714        f3_48      QUEUED  gt00       lecture-o         --/-- --:--:--    00:00:00         -               1    -

[t00470@wisteria01 run]$ pjstat
Wisteria/BDEC-01 scheduled stop time: 2021/05/28(Fri) 09:00:00 (Remain:  4days 1:25:56)

JOB_ID       JOB_NAME   STATUS  PROJECT    RSCGROUP          START_DATE        ELAPSE       TOKEN            NODE  GPU
15713        f2_48      RUNNING gt00       lecture-o         05/24 07:34:03    00:00:02         -               1    -
15714        f3_48      RUNNING gt00       lecture-o         (05/24 07:34)     00:00:00         -               1    -

[t00XYZ@wisteria01 ~]$ pjdel 15714
[INFO] PJM 0100 pjdel Accepted Job 15714

[t00XYZ@wisteria01 ~]$ pjstat
Wisteria/BDEC-01 scheduled stop time: 2021/05/28(Fri) 09:00:00 (Remain:  4days 1:25:56)

JOB_ID       JOB_NAME   STATUS  PROJECT    RSCGROUP          START_DATE        ELAPSE       TOKEN            NODE  GPU
15713        f2_48      RUNNING gt00       lecture-o         05/24 07:34:03    00:00:02         -               1    -

[t00XYZ@wisteria01 ~]$ pjstat
Wisteria/BDEC-01 scheduled stop time: 2021/05/28(Fri) 09:00:00 (Remain:  4days 1:21:45)

No unfinished job found.
```

```
[t00XYZ@wisteria01 ~]$ pjstat --rsc
SYSTEM: Odyssey
RSCGRP                  STATUS                  NODE
lecture-o               [ENABLE,START]            96
lecture0-o              [DISABLE,STOP]         2x12x16

[t00XYZ@wisteria01 ~]$ pjstat --rsc -x
SYSTEM: Odyssey
RSCGRP                  STATUS           MIN_NODE MAX_NODE MAX_ELAPSE REMAIN_ELAPSE MEM(GiB) PROJECT
lecture-o               [ENABLE,START]          1       12   00:15:00      00:15:00       28 gt00
lecture0-o              [DISABLE,STOP]          1       12   00:15:00      --:--:--       28 gt00

[t00XYZ@wisteria01 ~]$ pjstat --limit
SYSTEM: Odyssey
PROJECT        ACCEPT         RUN  BULK_ACCEPT    BULK_RUN          NODE
gt80          0/  128     0/   16      0/    8     0/   16       0/ 2304

SYSTEM: Aquarius
PROJECT        ACCEPT         RUN  BULK_ACCEPT    BULK_RUN           GPU
gt80          0/    4     0/    2      0/    0     0/    0       0/   64
```

poi_gen (1/2): Main Part

Be carefule with “private” !!

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

        VOL0= VOLCEL(icel)

        icou= 0
        if (icN5.ne.0) then
          coef   =RDZ * ZAREA
          D(icel)= D(icel) - coef
                   icou= icou + 1
                   k   = icou + indexLU(icel-1)
          itemLU(k)= icN5
            AMAT(k)= coef
        endif
(…)
        ii= XYZ(icel,1)
        jj= XYZ(icel,2)
        kk= XYZ(icel,3)

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

      enddo
```

poi_gen (2/2): Boundary Conditions

Be carefule with “private” !!

```
!$omp parallel do private (ib,icel,coef)
      do ib= 1, ZmaxCELtot
        icel= ZmaxCEL(ib)
        coef= 2.d0 * RDZ * ZAREA
        D(icel)= D(icel) - coef
      enddo
```

solve_PCG (1/5)

parallel computing by OpenMP

```
 module solver_PCG
      contains
!C
!C*** solve_PCG
!C
      subroutine solve_PCG                                              &
     &         ( N, NPLU, indexLU, itemLU, D, B, X, AMAT, EPS, ITR, IER)

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

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

      integer, dimension(0:N)   :: indexLU
      integer, dimension(NPLU)  ::  itemLU

      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_PCG (2/5)

```
!$omp parallel do private(i)
      do i= 1, N
        X(i)   = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,DD)= 1.d0/D(i)
      enddo

!$omp parallel do private(i,VAL,k)
      do i= 1, N
        VAL= D(i)*X(i)
        do k= indexLU(i-1)+1, indexLU(i)
          VAL= VAL + AMAT(k)*X(itemLU(k))
        enddo
        W(i,R)= B(i) - VAL
      enddo

      BNRM2= 0.0D0
!$omp parallel do private(i) reduction(+:BNRM2)
      do i= 1, N
        BNRM2 = BNRM2 + B(i)  **2
      enddo
```

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_PCG (3/5)

```
      ITR= N
      Stime= omp_get_wtime()

      do L= 1, ITR

!$omp parallel do private(i)
      do i= 1, N
        W(i,Z)= W(i,R)*W(i,DD)
      enddo

      RHO= 0.d0
!$omp parallel do private(i) reduction(+:RHO)
      do i= 1, N
        RHO= RHO + W(i,R)*W(i,Z)
      enddo

      if ( L.eq.1 ) then
!$omp parallel do private(i)
        do i= 1, N
          W(i,P)= W(i,Z)
        enddo
       else
        BETA= RHO / RHO1
!$omp parallel do private(i)
        do i= 1, N
          W(i,P)= W(i,Z) + BETA*W(i,P)
        enddo
      endif
```

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_PCG (4/5)

```
!$omp parallel do private(i,VAL,k)
      do i= 1, N
        VAL= D(i)*W(i,P)
        do k= indexLU(i-1)+1, indexLU(i)
          VAL= VAL + AMAT(k)*W(itemLU(k),P)
        enddo
        W(i,Q)= VAL
      enddo
      C1= 0.d0
!$omp parallel do private(i) reduction(+:C1)
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo
      ALPHA= RHO / C1

!$omp parallel do private(i)
      do i= 1, N
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo

      DNRM2= 0.d0
!$omp parallel do private(i) reduction(+:DNRM2)
      do i= 1, N
        DNRM2= DNRM2 + W(i,R)**2
      enddo

      ERR = dsqrt(DNRM2/BNRM2)...
```

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_PCG (5/5)

```
      Stime = omp_get_wtime()

      do L= 1, ITR
...
        if (ERR .lt. EPS) then
          IER = 0
          goto 900
         else
          RHO1 = RHO
        endif

      enddo
      IER = 1
  900 continue
      Etime= omp_get_wtime()

      write (*,'(i5,2(1pe16.6))') L, ERR
      write (*,'(1pe16.6, a)') Etime-Stime, ' sec. (solver)'

      ITR= L
      deallocate (W)

      return
      end
```

Elapsed Time= Etime - Stime

f01,f02,f04,f06,f08,f12.sh

- /work/gt89/t89XXX/ompw/run/fYZ.sh
- Scheduling + Shell Script

```
#!/bin/sh
#PJM -N "fYZ"                    Job Name (not required)
#PJM -L rscgrp=lecture0-o        Name of Queue (Resource Group)
#PJM -L node=1                   Node # (=1)
#PJM --omp thread=YZ             Thread # (1-48, ~12 for a while)
#PJM -L elapse=00:15:00          Elapsed Computation Time
#PJM -g gt89                     Group Name (Wallet)
#PJM -j
#PJM -e err                      Standard Error
#PJM -o fYZ.lst                  Standard Output

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

numactl ./solf0
numactl -C 12-23 -m 4 ./solf0
```

Time for PCG: Etime-Stime：Fortran

NX=NY=NZ=128

5 measurements, best result

Efficiency decreases as core# increases: decreasing of memory performance

Large
大

Granularity：粒度
Problem Size/Thread

Small
小

Thread #	sec	Speed-up	Parallel Efficiency (%)
1	50.27	1.00	100.00
2	25.24	1.99	99.60
4	12.98	3.87	96.86
6	9.24	5.44	90.73
8	7.27	6.92	86.50
12	5.09	9.88	82.30

Parallel Efficiency(%)= 100*(Speed-Up)/Thread#

f04.sh

```
#!/bin/sh
#PJM   -N      "f04"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=4
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f04.lst

module load   fj
export OMP_NUM_THREADS=4
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
```

f08.sh

```
#!/bin/sh
#PJM   -N      "f08"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=8
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f08.lst

module load   fj
export OMP_NUM_THREADS=8
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
```

Multiple CMG's Time for PCG: Etime-Stime：Fortran

NX=NY=NZ=128

5 measurements, best result

Large
大

Granularity：粒度
Problem Size/Thread

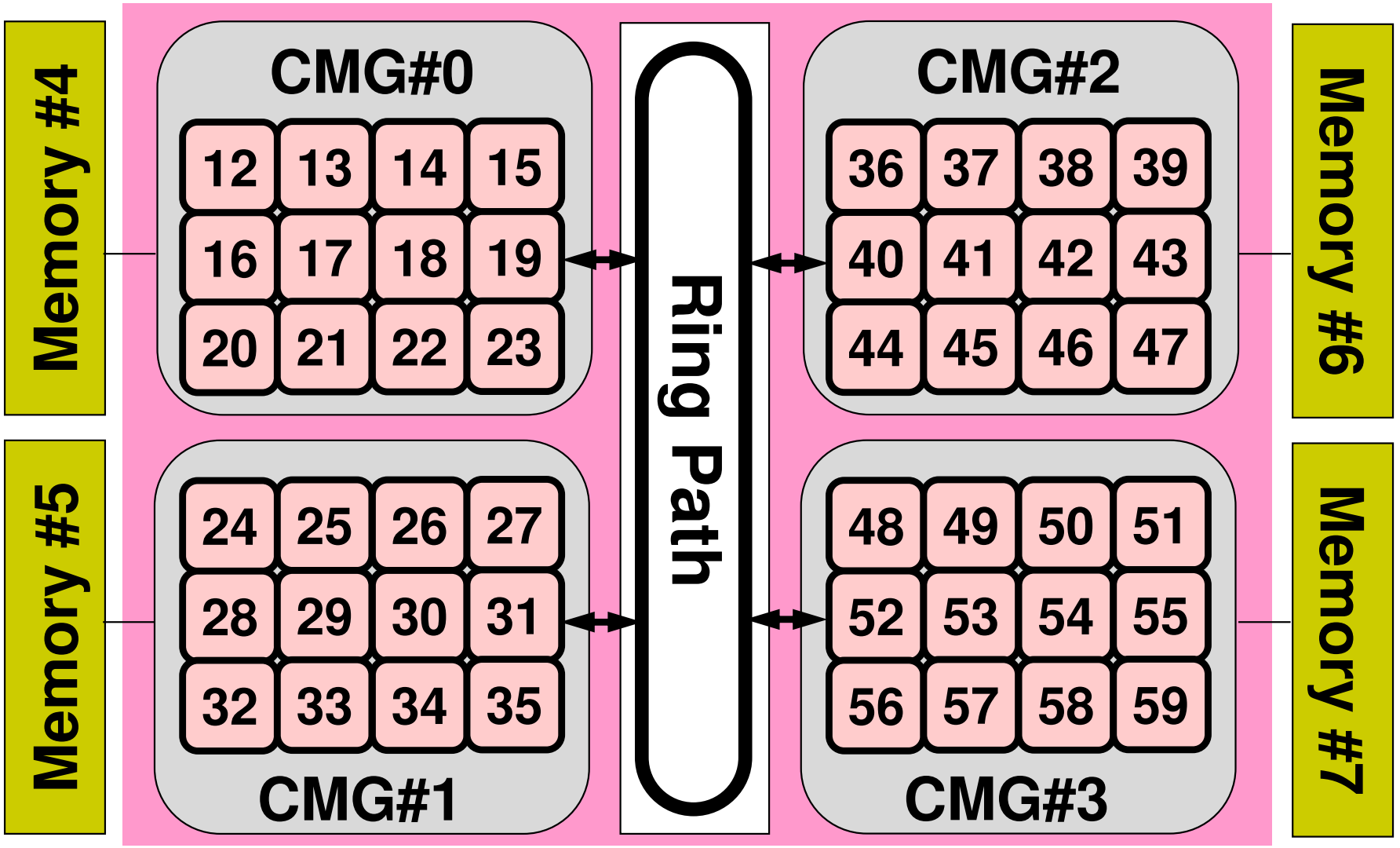
Small
小

Thread #	sec	Speed-up	Parallel Efficiency (%)
12	5.09	12.00	100.00
24	2.79	21.88	91.18
36	1.99	30.75	85.41
48	1.70	35.97	74.95

Parallel Efficiency(%)= 100*(Speed-Up)/Thread#

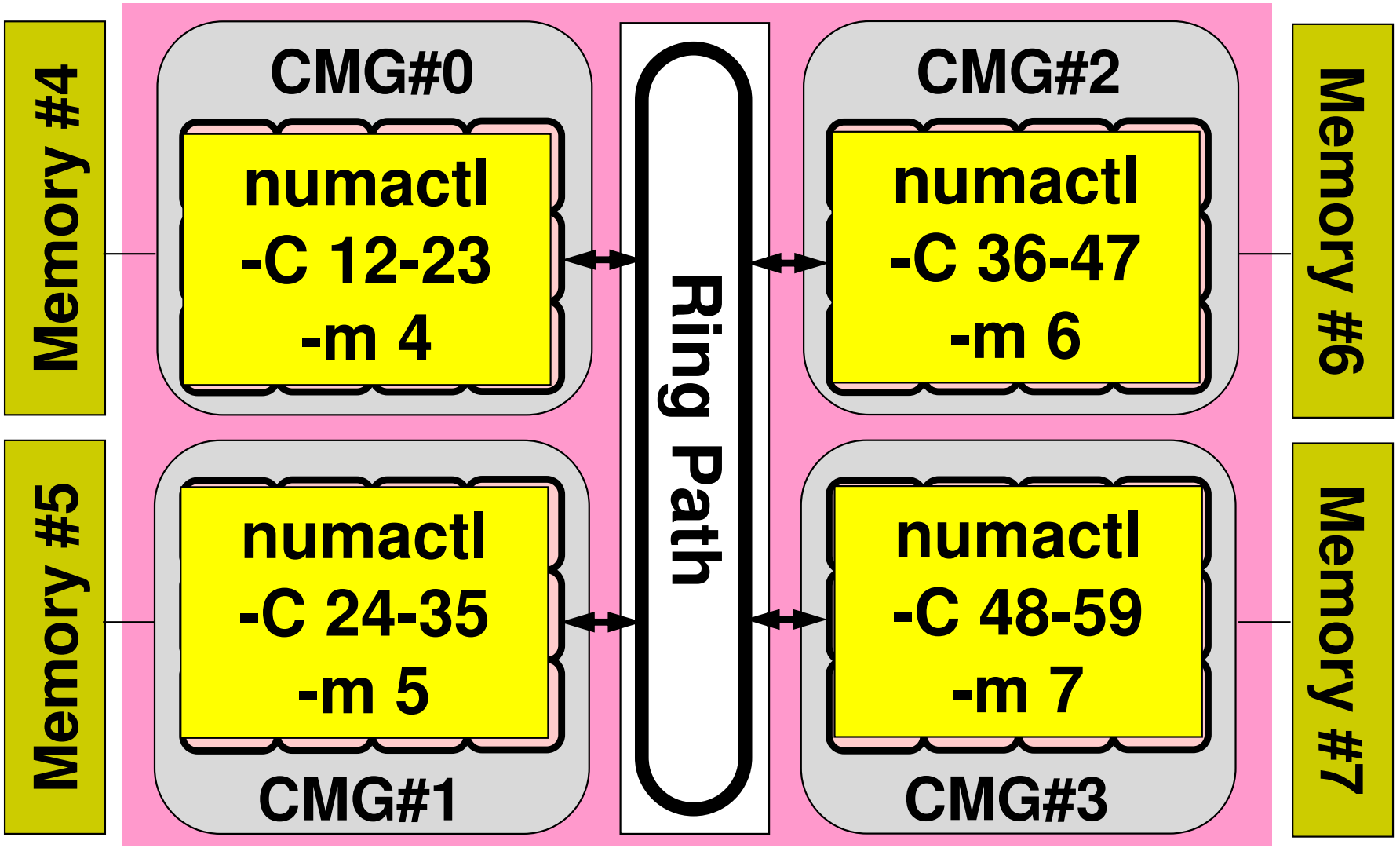
ID of CMGs, Cores, Memory's (1/2)

CMG:#0-#3, Core:#12-59, Memory:#4-#7



ID of CMGs, Cores, Memory's (2/2)

CMG:#0-#3, Core:#12-59, Memory:#4-#7

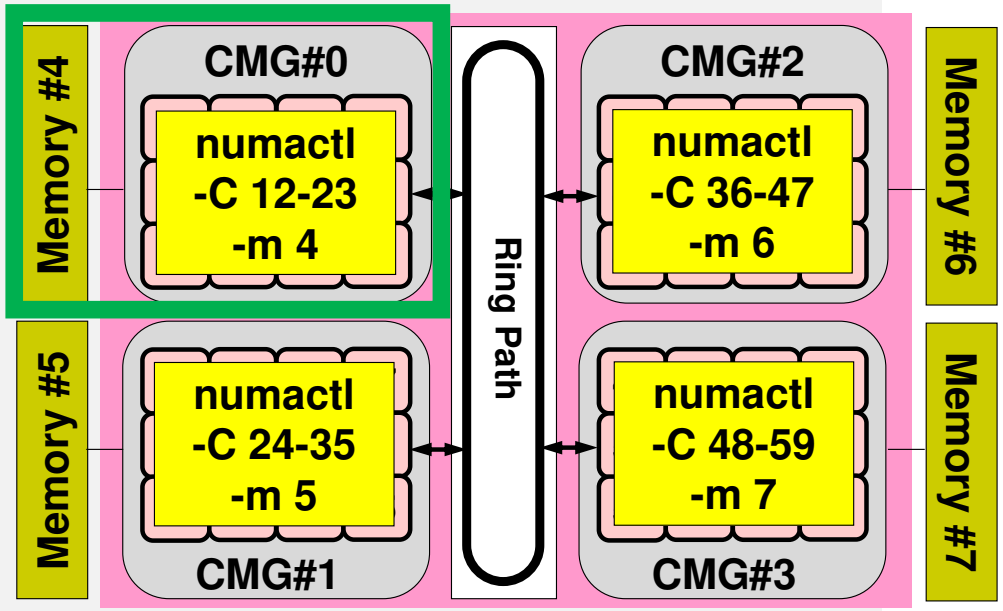


f0_12.sh

```
#!/bin/sh
#PJM   -N      "f0_12"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=12
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f0_12.lst

module load   fj
export OMP_NUM_THREADS=12
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
numactl       -C     12-23  -m     4       ./solf0
```

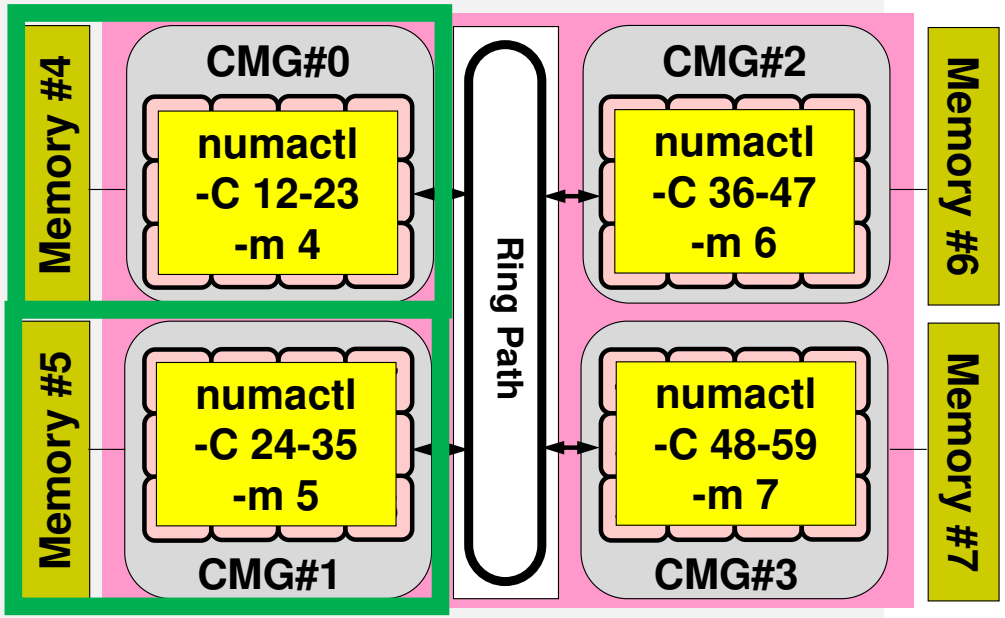


f0_24.sh

```
#!/bin/sh
#PJM   -N      "f0_24"
#PJM   -L      rscgrp=lectur9-o
#PJM   -L      node=1
#PJM   --omp   thread=24
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f0_24.lst

module load   fj
export OMP_NUM_THREADS=24
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       -C     12-35  -m     4-5    ./solf0
numactl       -C     12-35  -m     4-5    ./solf0
numactl       -C     12-35  -m     4-5    ./solf0
numactl       -C     12-35  -m     4-5    ./solf0
numactl       -C     12-35  -m     4-5    ./solf0
```

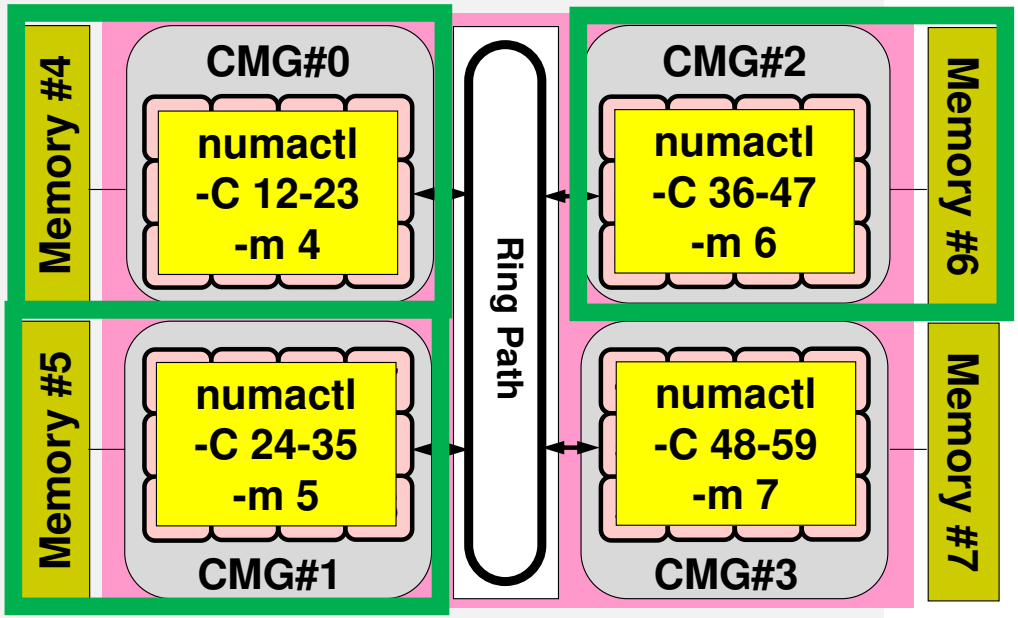


f0_36.sh

```
#!/bin/sh
#PJM   -N      "f0_36"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=36
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f0_36.lst

module load   fj
export OMP_NUM_THREADS=36
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       -C     12-47  -m     4-6    ./solf0
numactl       -C     12-47  -m     4-6    ./solf0
numactl       -C     12-47  -m     4-6    ./solf0
numactl       -C     12-47  -m     4-6    ./solf0
numactl       -C     12-47  -m     4-6    ./solf0
```

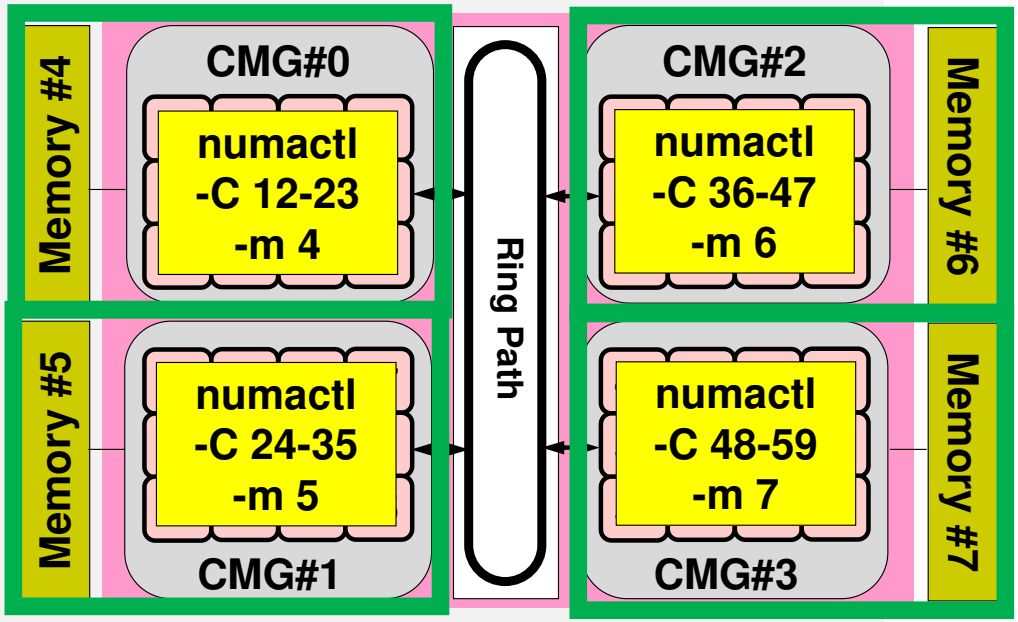


f0_48.sh

```
#!/bin/sh
#PJM   -N      "f0_48"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=48
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f0_48.lst

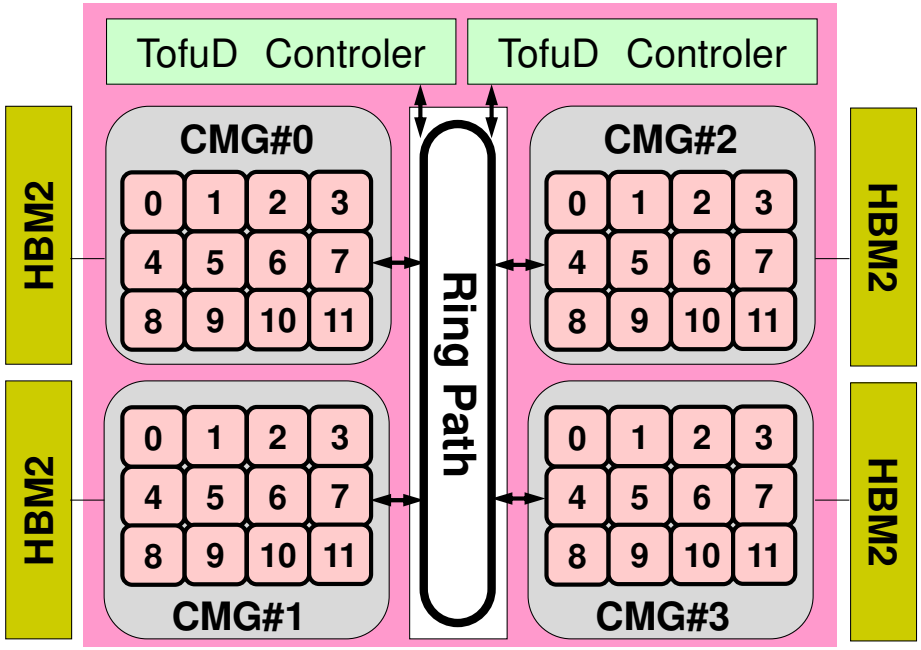
module load   fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       ./solf0
numactl       -C     12-59  -m     4-7    ./solf0
numactl       -C     12-59  -m     4-7    ./solf0
numactl       -C     12-59  -m     4-7    ./solf0
numactl       -C     12-59  -m     4-7    ./solf0
numactl       -C     12-59  -m     4-7    ./solf0
```



- OpenMP
- Login to Wisteria/BDEC-01
- Parallel Code by OpenMP (0): up to 12 cores
- **Parallel Code by OpenMP (1): First Touch**
- Parallel Code by OpenMP (2): +ELL
- Parallel Code by OpenMP (3): reduced omp-parallel
- Parallel Code by OpenMP (4): Further Optimization (Fortran only)

A64FX Processor on Odyssey



Name	A64FX
Processor # (Core #)	1 (48+ 2or4 Assistant Cores)
Frequency	2.2 GHz
Peak Performance	3.3792 TFLOPS
Memory Size	32 GiB
Memory Bandwidth	1,024 GB/s
L1 Cache	64 KiB/core (Inst/Data)
L2 Cache	8 MiB/CMG

- 4 CMG's (Core Memory Group), 12 cores/CMG
  - 48 Cores/Node (Processor)
  - 2.2GHz × 32DP × 48= 3379.2 GFLOPS= 3.3792 TFLOPS
- NUMA Architecture (Non-Uniform Memory Access)
  - Each core of a CMG can access to the memory on other CMG's
  - Utilization of the local memory is more efficient

First Touch Data Placement

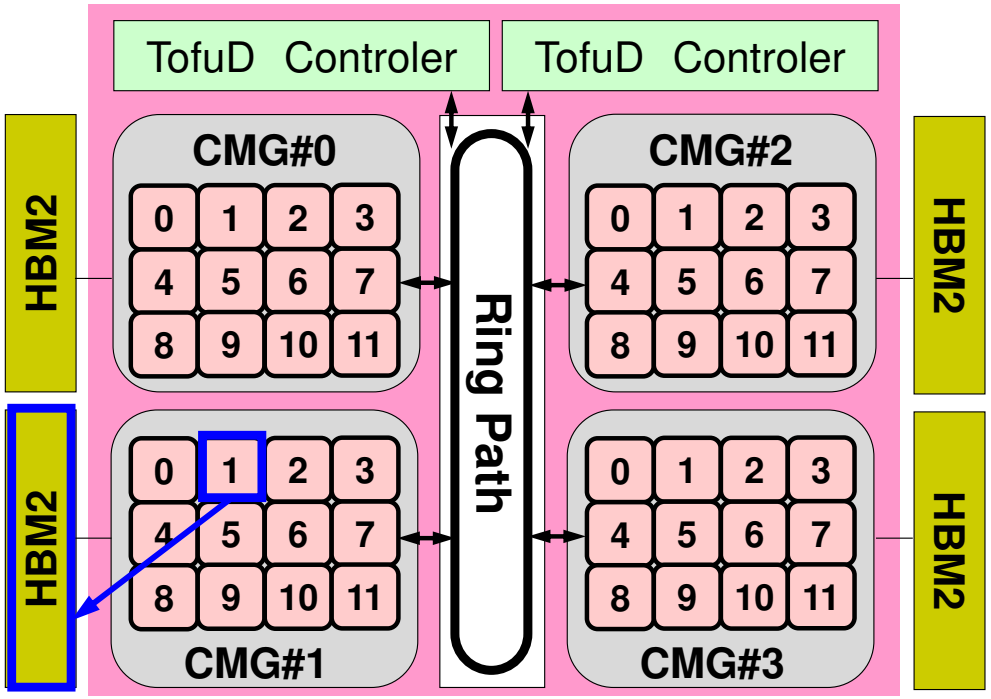
"Patterns for Parallel Programming" Mattson, T.G. et al.

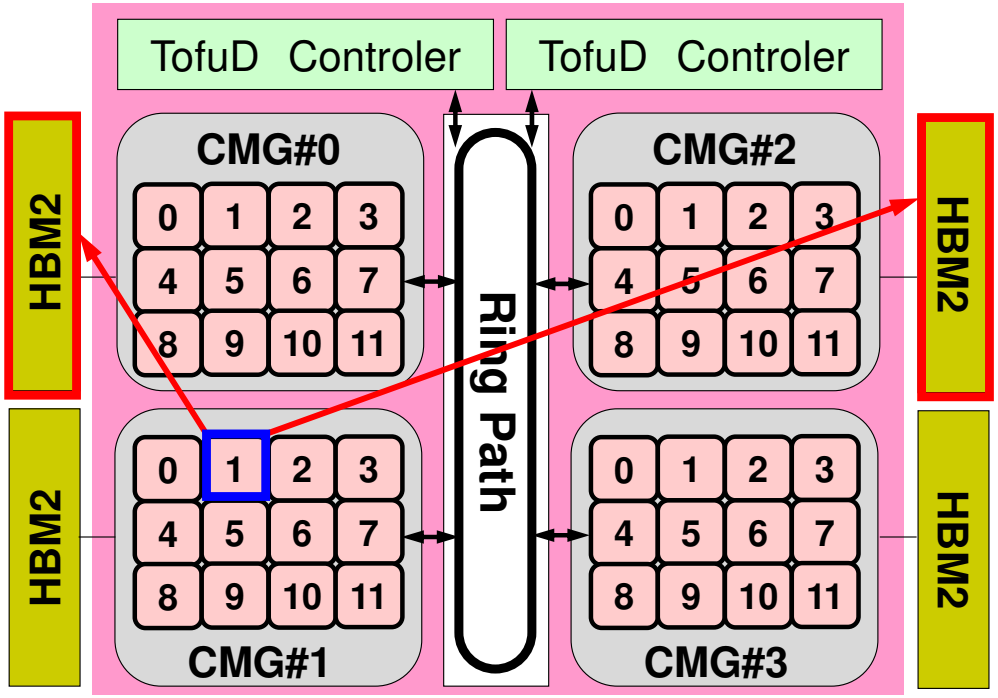
- To reduce memory traffic in the system, it is important to keep the data close to the PEs that will work with the data (e.g. NUMA control).
- On NUMA computers, this corresponds to making sure the pages of memory are allocated and "owned" by the PEs that will be working with the data contained in the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

Program by “First-Touch”: src-f1 Original Program in src-f0

```
>$ cd /work/gt89/t89XYZ/ompw
>$ cd run

<modify “INPUT.DAT”, “f1_XY.sh”> (XY:12,24,36,48)

>$ pjsub f1_XY.sh
```

```
[XYZ@wisteria01 run]$ cd ../src-f0
[XYZ@wisteria01 src-f0]$ diff poi_gen.f ../src-f1/poi_gen.f
25,29c25,31
<         PHI    = 0.d0
<         BFORCE= 0.d0
<           D    = 0.d0
<
<         INLU= 0
---
>  !$omp parallel do private (icel)
>         do icel= 1, ICELTOT
>           PHI    (icel)= 0.d0
>           BFORCE(icel)= 0.d0
>           D      (icel)= 0.d0
>           INLU   (icel)= 0
>         enddo
```

src-f0

src-f1

```
71,72c73,75
<         indexLU= 0
<
<         do icel= 1, ICELTOT
<           indexLU(icel)= INLU(icel)
<         enddo
---
>         indexLU(0)= 0
>
> !$omp parallel do private (icel)
>         do icel= 1, ICELTOT
>           indexLU(icel)= INLU(icel)
>         enddo

85,86c88,94
<         itemLU= 0
<           AMAT= 0.d0
---
> !$omp parallel do private (icel,k)
>         do icel= 1, ICELTOT
>         do k= indexLU(icel-1)+1, indexLU(icel)
>           itemLU(k)= 0
>           AMAT   (k)= 0.d0
>         enddo
>         enddo
```

src-f0

src-f1

src-f0

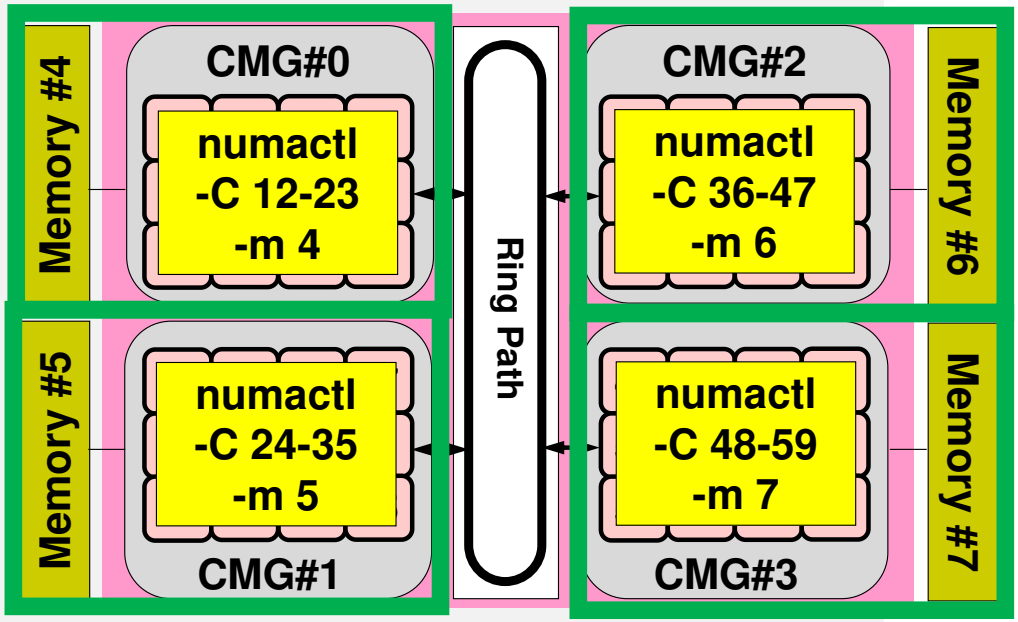
src-f1

f1_48.sh

```
#!/bin/sh
#PJM   -N      "f1_48"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=48
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f1_48.lst

module load   fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf1
numactl       ./solf1
numactl       ./solf1
numactl       ./solf1
numactl       ./solf1
numactl       -C     12-59  -m     4-7    ./solf1
numactl       -C     12-59  -m     4-7    ./solf1
numactl       -C     12-59  -m     4-7    ./solf1
numactl       -C     12-59  -m     4-7    ./solf1
numactl       -C     12-59  -m     4-7    ./solf1
```



Multiple CMG's
Time for PCG: Etime-Stime : Fortran

NX=NY=NZ=128, Best Case for 5 Measurements
based on src-f0 with 12-threads

	Thread #	sec	Speed-up	Parallel Efficiency (%)
src-f0	12	5.09	12.00	100.00
	24	2.79	21.88	91.18
	36	1.99	30.75	85.41
	48	1.70	35.97	74.95
src-f1	12	5.27	-	-
	24	2.70	22.61	94.20
	36	1.87	32.65	90.69
	48	1.52	40.09	83.51

Multiple CMG's Time for PCG: Etime-Stime : C(clang)

NX=NY=NZ=128, Best Case for 5 Measurements based on src-c0 with 12-threads

	Thread #	sec	Speed-up	Parallel Efficiency (%)
src-c0	12	5.03	12.00	100.00
	24	2.69	22.42	93.41
	36	1.91	31.57	87.69
	48	1.57	38.51	80.23
src-c1	12	5.22	-	-
	24	2.70	22.39	93.29
	36	1.85	32.66	90.71
	48	1.17	51.70	107.7

Cache is well-utilized, because the problem size is small

Multiple CMG's Time for PCG: Etime-Stime

NX=NY=NZ=128, Best Case for 5 Measurements

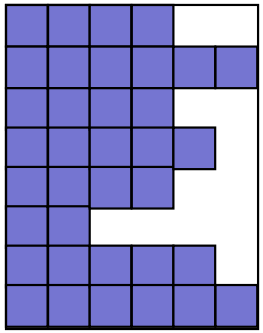
	Language	12	24	36	48
Original	Fortran	5.09	2.79	1.99	1.70
	C (clang)	5.03	2.69	1.91	1.57
	C (trad)	7.75	4.19	2.90	2.36
First-Touch	Fortran	5.27	2.70	1.87	1.52
	C (clang)	5.22	2.70	1.85	1.17
	C (trad)	7.85	4.05	2.79	1.72 (112.6 %)

- OpenMP
- Login to Wisteria/BDEC-01
- Parallel Code by OpenMP (0): up to 12 cores
- Parallel Code by OpenMP (1): First Touch
- **Parallel Code by OpenMP (2): +ELL**
- Parallel Code by OpenMP (3): reduced omp-parallel
- Parallel Code by OpenMP (4): Further Optimization (Fortran only)

Storage of Sparse Matrices

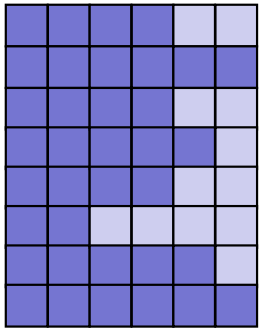
CRS（Compressed Row Storage）

```
do i= 1, N
  W(i,Q)= D(i)*W(i,P)
  do k= indexLU(i-1)+1, indexLU(i)
    W(i,Q)= W(i,Q) + AMAT(k)*W(itemLU(k),P)
  enddo
enddo
```



ELL (ELLPACK/ITPACK)

```
do i= 1, N
  W(i,Q)= D(i)*W(i,P)
  do j= 1, 6
    W(i,Q)= W(i,Q) + AMAT(j,i)*W(itemLU(j,i),P)
  enddo
enddo
```

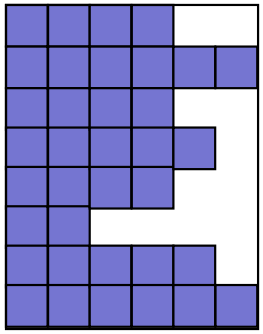


- CRS: Compressed Row Storage
  - Only non-zero off-diag's: saving memory, low performance
- ELL：ELLPACK/ITPACK
  - Fixed # of non-zero off-diag's, 0 padding needed
  - More expensive, better memory performance due to prefetch

Storage of Sparse Matrices

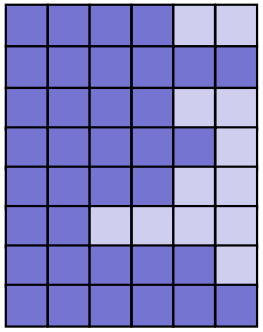
CRS (Compressed Row Storage)

```
do i= 1, N
  W(i,Q)= D(i)*W(i,P)
  do k= indexLU(i-1)+1, indexLU(i)
    W(i,Q)= W(i,Q) + AMAT(k)*W(itemLU(k),P)
  enddo
enddo
```



ELL (ELLPACK/ITPACK)

```
do i= 1, N
  W(i,Q)= D(i)*W(i,P)
  do j= 1, 6
    W(i,Q)= W(i,Q) + AMAT(j,i)*W(itemLU(j,i),P)
  enddo
enddo
```



ELL (ELLPACK/ITPACK) This is a little bit slow

```
do i= 1, N
  W(i,Q)= D(i)*W(i,P)
  do j= 1, 6
    W(i,Q)= W(i,Q) + AMAT(6*(i-1)+k)*W(itemLU(6*(i-1)+j),P)
  enddo
enddo
```

poi_gen (1/2): Private

```
!C
!C-- INTERIOR & NEUMANN BOUNDARY CELLs

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

      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)

        VOL0= VOLCEL(icel)

        icou= 0
        if (icN5.ne.0) then
          coef= RDZ * ZAREA
          D(icel)= D(icel) - coef
                   icou      = icou + 1
          itemLU (icou,icel)= icN5
             AMAT(icou,icel)= coef
         endif

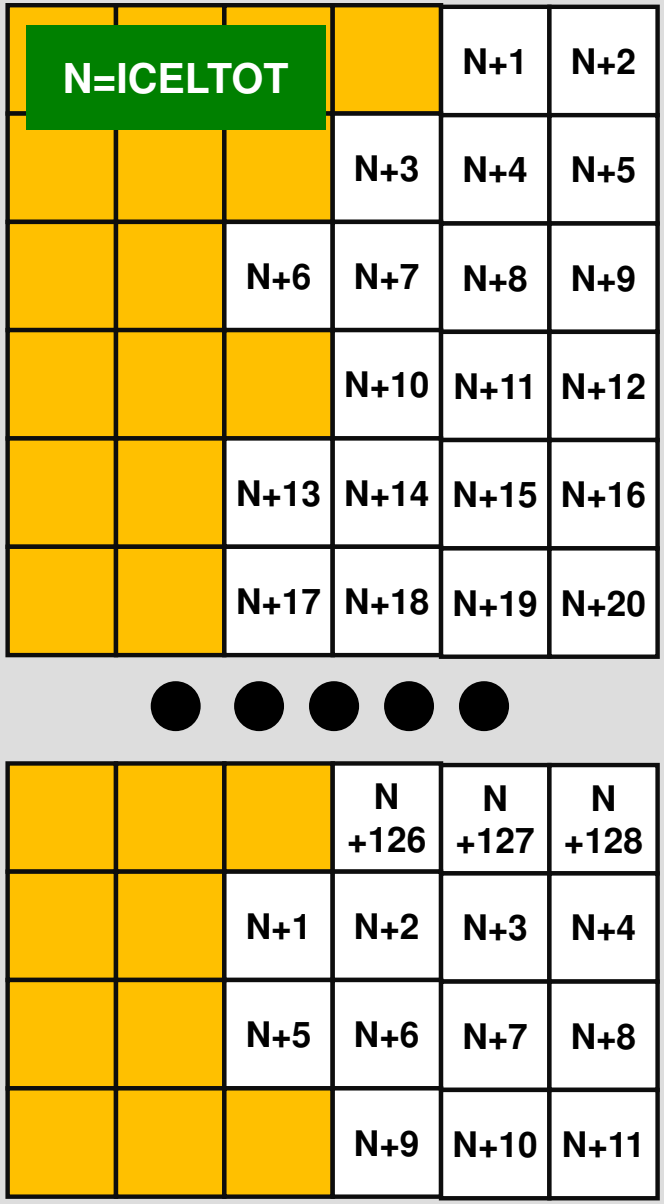
        if (icN3.ne.0) then
          coef= RDY * YAREA
          D(icel)= D(icel) - coef
                   icou      = icou + 1
          itemLU (icou,icel)= icN3
             AMAT(icou,icel)= coef
        endif
(...)
      enddo
```

poi_gen (2/2):Padding

```
      N2= 128 (pcg.f)


!C
!C-- PADDING
!C

       icou= 0
       do icel= 1, ICELTOT
         do k = 1, 6
           if (itemLU(k,icel).eq.0) then
             icou= icou + 1
             itemLU(k,icel)= icou + ICELTOT
             if (icou.eq.N2) icou= 0
           endif
         enddo
       enddo
!C===
```



solve_PCG (1/2)

```
!C
!C +------+
!C | INIT |
!C +------+
!C===

      allocate (W(N+N2,4))

!$omp parallel do private(i)
      do i= 1, N
        X(i)  = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,DD)= 1.d0/D(i)
      enddo

!$omp parallel do private(i)
      do i= N+1, N+N2
        X(i)  = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,DD)= 1.d0/D(i)
      enddo
```

solve_PCG (2/2)

```
!C
!C +-------------+
!C | {q}= [A]{p} |
!C +-------------+
!C===

!$omp parallel do private(i,VAL,k)
      do i= 1, N
        VAL= D(i)*W(i,P)
        do k= 1, 6
          VAL= VAL + AMAT(k,i)*W(itemLU(k,i),P)
        enddo
        W(i,Q)= VAL
      enddo
!C===
```

Program by “ELL”: src-c2

```
>$ cd /work/gt89/t89XYZ/ompw
>$ cd run

<modify “INPUT.DAT”, “f2_48.sh”>

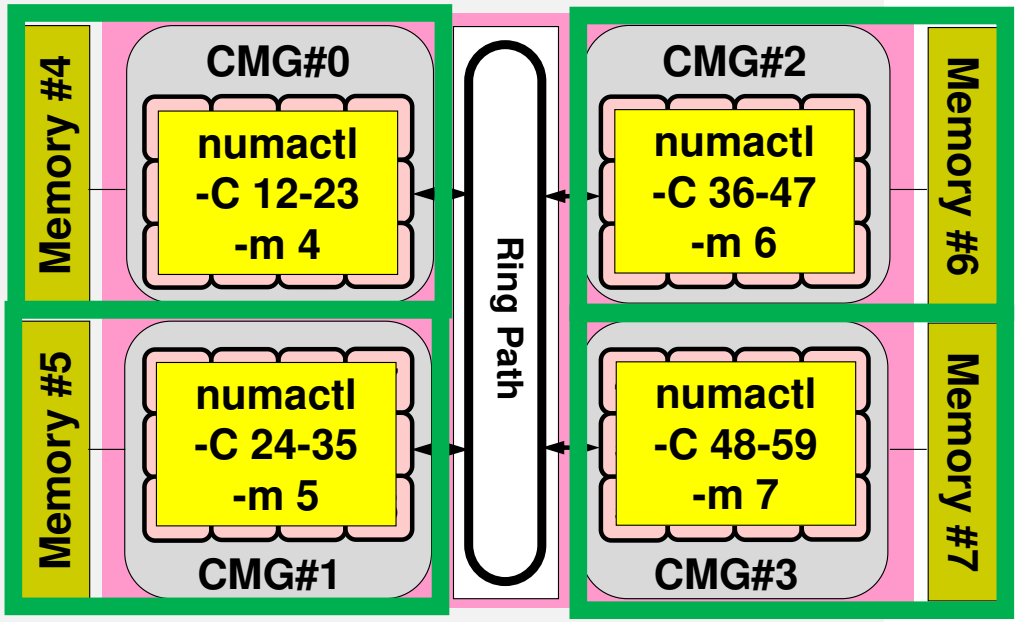
>$ pjsub f2_48.sh
```

f2_48.sh

```
#!/bin/sh
#PJM   -N      "f2_48"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=48
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f2_48.lst

module load   fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf2
numactl       ./solf2
numactl       ./solf2
numactl       ./solf2
numactl       ./solf2
numactl       -C     12-59  -m     4-7    ./solf2
numactl       -C     12-59  -m     4-7    ./solf2
numactl       -C     12-59  -m     4-7    ./solf2
numactl       -C     12-59  -m     4-7    ./solf2
numactl       -C     12-59  -m     4-7    ./solf2
```



Results (1/2): Fortran

```
[t00XYZ@wisteria01 run]$ cat f12.lst
    1    8.958216E+00
  101    8.313496E+00
  201    2.090443E+00
  301    3.811029E-01
  401    3.769653E-02
  501    9.429978E-04
  601    4.940783E-05
  701    1.888611E-06
  801    2.243179E-08
  826    9.818026E-09
    5.275418E+00 sec. (solver)

##ANSWER   2097152    1.459831E+04


    1    8.958216E+00
  101    8.313496E+00
  201    2.090443E+00
  301    3.811029E-01
  401    3.769653E-02
  501    9.429978E-04
  601    4.940783E-05
  701    1.888611E-06
  801    2.243179E-08
  826    9.818026E-09
    5.270398E+00 sec. (solver)

##ANSWER   2097152    1.459831E+04
```

Results (1/2): Best for 5 Mesurements

```
[XYZ@wisteria01 run]$ grep "(sol" f1_48.lst
   1.480524E+00 sec.  (solver)
   1.501454E+00 sec.  (solver)
   1.441297E+00 sec.  (solver)
   1.483405E+00 sec.  (solver)
   1.481864E+00 sec.  (solver)

   1.475129E+00 sec.  (solver)
   1.483695E+00 sec.  (solver)
   1.485036E+00 sec.  (solver)
   1.502549E+00 sec.  (solver)
   1.487192E+00 sec.  (solver)
```

```
numactl ./solf1
```

```
numactl -C 12-59 -m 4-7 ./solf1
```

```
[XYZ@wisteria01 run]$ grep "(sol" f2_48.lst
   7.713702E-01 sec.  (solver)
   7.568300E-01 sec.  (solver)
   7.328739E-01 sec.  (solver)
   7.826090E-01 sec.  (solver)
   7.884219E-01 sec.  (solver)

   7.546160E-01 sec.  (solver)
   7.937970E-01 sec.  (solver)
   7.403760E-01 sec.  (solver)
   7.745121E-01 sec.  (solver)
   7.862871E-01 sec.  (solver)
```

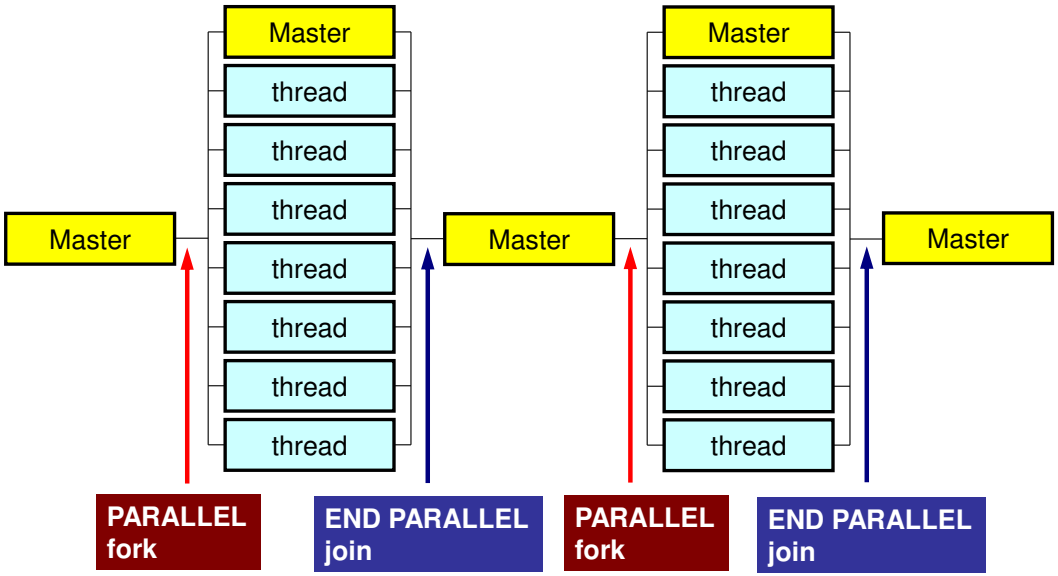
```
numactl ./solf2
```

```
numactl -C 12-59 -m 4-7 ./solf2
```

- OpenMP
- Login to Wisteria/BDEC-01
- Parallel Code by OpenMP (0): up to 12 cores
- Parallel Code by OpenMP (1): First Touch
- Parallel Code by OpenMP (2): +ELL
- **Parallel Code by OpenMP (3): reduced omp-parallel**
- **Parallel Code by OpenMP (4): Further Optimization (Fortran only)**

omp parallel (do)

- “omp parallel-omp end parallel” = “fork-join”
- If you have many loops, these “fork-join’s” cause overheads
- omp parallel + omp do/omp for




```
#pragma omp parallel ...

#pragma omp for {

...
#pragma omp for {
```

```
!$omp parallel ...

!$omp do
   do i= 1, N
...
!$omp do
   do i= 1, N
...
!$omp end parallel   required
```

!$omp parallel do: Fork-Join

```
!$omp parallel do private(i,VAL,k)
      do i= 1, N
        VAL= D(i)*W(i,P)
        do k= indexLU(i-1)+1, indexLU(i)
          VAL= VAL + AMAT(k)*W(itemLU(k),P)
        enddo
        W(i,Q)= VAL
      enddo

      C1= 0.d0
!$omp parallel do private(i) reduction(+:C1)
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo

      ALPHA= RHO / C1

!$omp parallel do private(i)
      do i= 1, N
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo

      DNRM2= 0.d0
!$omp parallel do private(i) reduction(+:DNRM2)
      do i= 1, N
        DNRM2= DNRM2 + W(i,R)**2
      enddo

      ERR = dsqrt(DNRM2/BNRM2)...
```

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

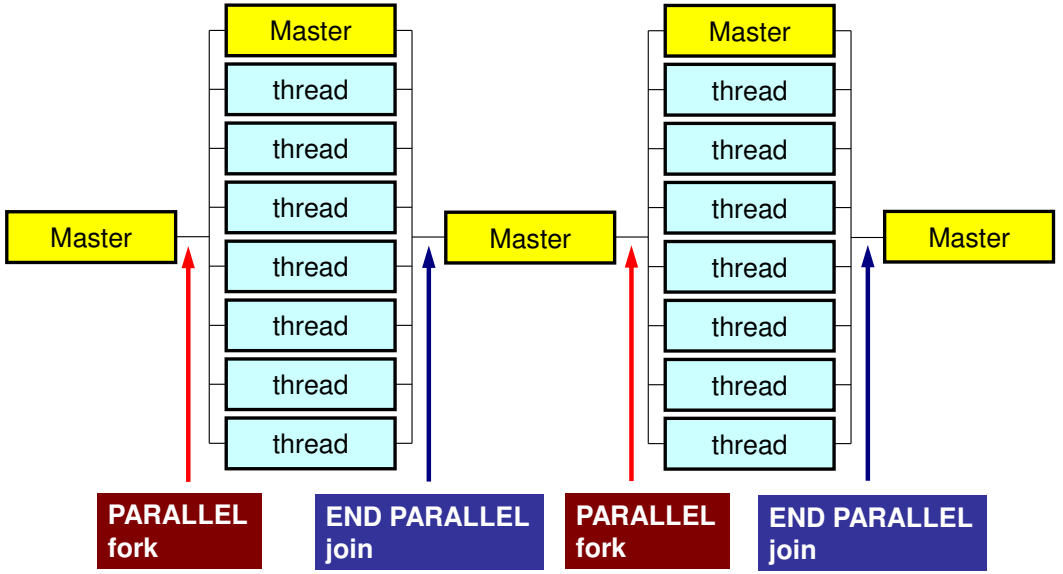
for i= 1, 2, …

- 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

Strategy for Further Optimization

- src-c3, src-f3
  - Only 1 omp-parallel in each iteration
- src-f4 (Fortran Only)
  - Only 1 !$omp parallel during PCG
  - NO !$omp do
  - Operations for reduction in dot-product's are NOT parallelized



Further Optimization

src-f3

```
      do L= 1, ITR
!$omp parallel private (i,k,VAL)
(…)
!$omp end parallel
      enddo

900 continue

      ITR= L


      deallocate (W)

      return
      end
```

src-f4

```
!$omp parallel private (…)
      do L= 1, ITR

(…)


      enddo

900 continue

      ITR= L
!$omp end parallel

      deallocate (W)

      return
      end
```

src_f3 (1/2)

```
      ITR= N
      Stime= omp_get_wtime()

      do L= 1, ITR
!$omp parallel private(i,k,VAL)

!$omp do
      do i= 1, N
        W(i,Z)= W(i,R)*W(i,DD)
      enddo

      RHO= 0.d0
!$omp do reduction(+:RHO)
      do i= 1, N
        RHO= RHO + W(i,R)*W(i,Z)
      enddo

      if ( L.eq.1 ) then
!$omp do
        do i= 1, N
          W(i,P)= W(i,Z)
        enddo
       else
        BETA= RHO / RHO1
!$omp do
        do i= 1, N
          W(i,P)= W(i,Z) + BETA*W(i,P)
        enddo
      endif
```

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

src_f3 (2/2)

```
!$omp do
      do i= 1, N
        VAL= D(i)*W(i,P)
        do k= indexLU(i-1)+1, indexLU(i)
          VAL= VAL + AMAT(k)*W(itemLU(k),P)
        enddo
        W(i,Q)= VAL
      enddo

      C1= 0.d0
!$omp do reduction(+:C1)
      do i= 1, N
        C1= C1 + W(i,P)*W(i,Q)
      enddo

      ALPHA= RHO / C1

!$omp do
      do i= 1, N
        X(i)   = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo

      DNRM2= 0.d0
!$omp do reduction(+:DNRM2)
      do i= 1, N
        DNRM2= DNRM2 + W(i,R)**2
      enddo

!$omp end parallel
      ERR = dsqrt(DNRM2/BNRM2)...
```

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

Program for “src-f3”

```
>$ cd /work/gt89/t89XYZ/ompw
>$ cd run

<modify “INPUT.DAT”, “f3_48.sh”>

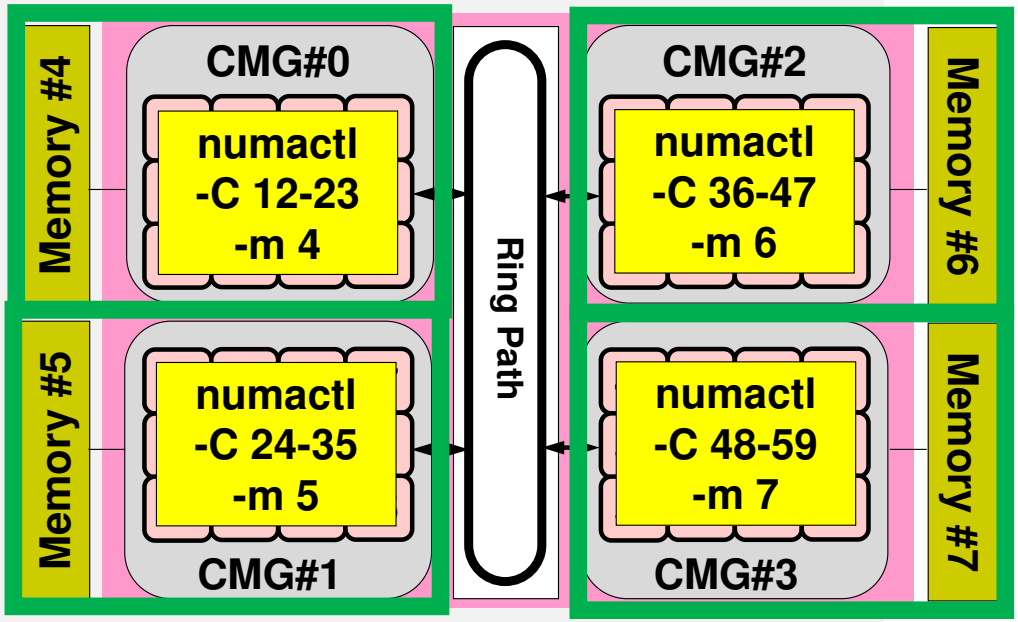
>$ pjsub f3_48.sh
```

f3_48.sh

```
#!/bin/sh
#PJM   -N      "f3_48"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=48
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f3_48.lst

module load   fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf3
numactl       ./solf3
numactl       ./solf3
numactl       ./solf3
numactl       ./solf3
numactl       -C     12-59  -m     4-7    ./solf3
numactl       -C     12-59  -m     4-7    ./solf3
numactl       -C     12-59  -m     4-7    ./solf3
numactl       -C     12-59  -m     4-7    ./solf3
numactl       -C     12-59  -m     4-7    ./solf3
```



C Language : trad

```
>$ cd /work/gt89/t89XYZ/ompw
>$ cd run

<modify “INPUT.DAT”, “c48org.sh”>

>$ pjsub c48org.sh
```

c48org.sh

```
#!/bin/sh
#PJM -N "cx48"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --omp thread=48
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o c48org_160.lst

module load fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl ./solc0org
numactl ./solc0org
numactl ./solc0org
numactl ./solc0org
numactl ./solc0org
…
```

Time for PCG, N=128^3, 48 Threads N= 2,097,152

	Fortran	C (clang)	C (trad)
src0	1.671	1.564	2.354
src1 (First Touch)	1.480	1.122	1.720
src2 (+ ELL)	0.747	0.809	1.127
src3 (+ reduced “omp-parallel”)	0.707	0.834	0.854

Time for PCG, N=160^3, 48 Threads N= 4,096,000

	Fortran	C (clang)	C (trad)
src0	3.610	3.484	4.067
src1 (First Touch)	2.993	2.228	3.425
src2 (+ ELL)	1.534	1.690	2.340
src3 (+ reduced “omp-parallel”)	1.556	1.693	1.742

Time for PCG, N=200^3, 48 Threads N= 8,000,000

	Fortran	C (clang)	C (trad)
src0	7.666	8.321	9.397
src1 (First Touch)	6.952	5.102	8.008
src2 (+ ELL)	3.421	3.910	5.381
src3 (+ reduced “omp-parallel”)	3.440	3.920	3.824

Time for PCG, N=256^3, 48 Threads N= 16,777,216

	Fortran	C (clang)	C (trad)
src0	34.308	24.772	25.547
src1 (First Touch)	32.202	22.172	23.814
src2 (+ ELL)	8.916	10.761	14.566
src3 (+ reduced “omp-parallel”)	8.915	10.764	10.415

src_f4 (1/5)

parallel computing by OpenMP

```
 module solver_PCG
      contains
!C
!C*** solve_PCG
!C
      subroutine solve_PCG                                              &
     &         ( N, NPLU, indexLU, itemLU, D, B, X, AMAT, EPS, ITR, IER)

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

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

      integer, dimension(0:N)   :: indexLU
      integer, dimension(NPLU)  ::  itemLU

      real(kind=8), dimension(:,:), allocatable :: W
      integer(kind=4), dimension(:  ), allocatable :: SMPindex

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

       real(kind=8), dimension(:)  , allocatable :: W_RHO, W_C1, W_DNRM2
```

src_f4 (2/5)

```
      allocate (W(N+N2,4))

!$omp parallel do private(i)
      do i= 1, N
        X(i)  = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,DD)= 1.d0/D(i)
      enddo
!$omp parallel do private(i)
      do i= N+1, N+N2
        X(i)  = 0.d0
        W(i,2)= 0.0D0
        W(i,3)= 0.0D0
        W(i,DD)= 1.d0/D(i)
      enddo

!$omp parallel
      PEsmpTOT= omp_get_num_threads()    PEsmpTOT: Total Number of Threads
!$omp end parallel

      allocate (SMPindex(0:PEsmpTOT))    SMPindex(0:PEsmpTOT): Element# for each thread
      SMPindex(0)= 0
      m = N/PEsmpTOT
      nr= N - PEsmpTOT*m
      do ip= 1, PEsmpTOT
        SMPindex(ip)= m
        if (ip.le.nr) SMPindex(ip)= m+1
      enddo
      do ip= 1, PEsmpTOT
        SMPindex(ip)= SMPindex(ip)+SMPindex(ip-1)
      enddo

      allocate (W_RHO(PEsmpTOT), W_C1(PEsmpTOT), W_DNRM2(PEsmpTOT))     内積用
```

src_f4 (3/5)

```
!$omp parallel do private(i,VAL,k)
      do i= 1, N
        VAL= D(i)*X(i)
        do k= 1, 6
          VAL= VAL + AMAT(k,i)*X(itemLU(k,i))
        enddo
        W(i,R)= B(i) - VAL
      enddo

      BNRM2= 0.0D0
!$omp parallel do private(i) reduction(+:BNRM2)
      do i= 1, N
        BNRM2 = BNRM2 + B(i)  **2
      enddo
```

src_f4 (4/5)

```
      ITR= N
      Stime= omp_get_wtime()

!$omp parallel private(L,ip,ip1,ip2,i,k,VAL)
!$omp&         private(RHO,BETA,RHO1,C1,ALPHA,DNRM2)
      do L= 1, ITR

      ip = omp_get_thread_num()+1
      ip1= SMPindex(ip-1)+1
      ip2= SMPindex(ip)
!$omp simd
      do i= ip1, ip2
        W(i,Z)= W(i,R)*W(i,DD)
      enddo

      W_RHO(ip)= 0.0d0
!$omp simd
      do i= ip1, ip2
        W_RHO(ip)= W_RHO(ip) + W(i,R)*W(i,Z)
      enddo
!$omp barrier
      RHO= 0.d0
!$omp simd
      do i = 1, PEsmpTOT
        RHO= RHO + W_RHO(i)
      enddo

      if ( L.eq.1 ) then
!$omp simd
        do i= ip1, ip2
          W(i,P)= W(i,Z)
        enddo
       else
        BETA= RHO / RHO1
!$omp simd
        do i= ip1, ip2
          W(i,P)= W(i,Z) + BETA*W(i,P)
        enddo
      endif
!$omp barrier
```

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

src_f4 (5/5)

```
      do i= ip1, ip2
        VAL= D(i)*W(i,P)
        do k= 1, 6
          VAL= VAL + AMAT(k,i)*W(itemLU(k,i),P)
        enddo
        W(i,Q)= VAL
      enddo

      W_C1(ip)= 0.0d0
!$omp simd
      do i= ip1, ip2
        W_C1(ip)= W_C1(ip) + W(i,P)*W(i,Q)
      enddo
!$omp barrier
      C1= 0.d0
!$omp simd
      do i = 1, PEsmpTOT
        C1= C1 + W_C1(i)
      enddo
      ALPHA= RHO / C1

!$omp simd
      do i= ip1, ip2
        X(i)  = X(i)   + ALPHA * W(i,P)
        W(i,R)= W(i,R) - ALPHA * W(i,Q)
      enddo

      W_DNRM2(ip)= 0.0d0
!$omp simd
      do i= ip1, ip2
        W_DNRM2(ip)= W_DNRM2(ip) + W(i,R)**2
      enddo
!$omp barrier
      DNRM2= 0.d0
!$omp simd
      do i = 1, PEsmpTOT
        DNRM2= DNRM2 + W_DNRM2(i)
      enddo
      ERR = dsqrt(DNRM2/BNRM2)...
```

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

Program for “src4”

```
>$ cd /work/gt89/t89XYZ/ompw
>$ cd run

<modify “INPUT.DAT”, “f4_48.sh”>

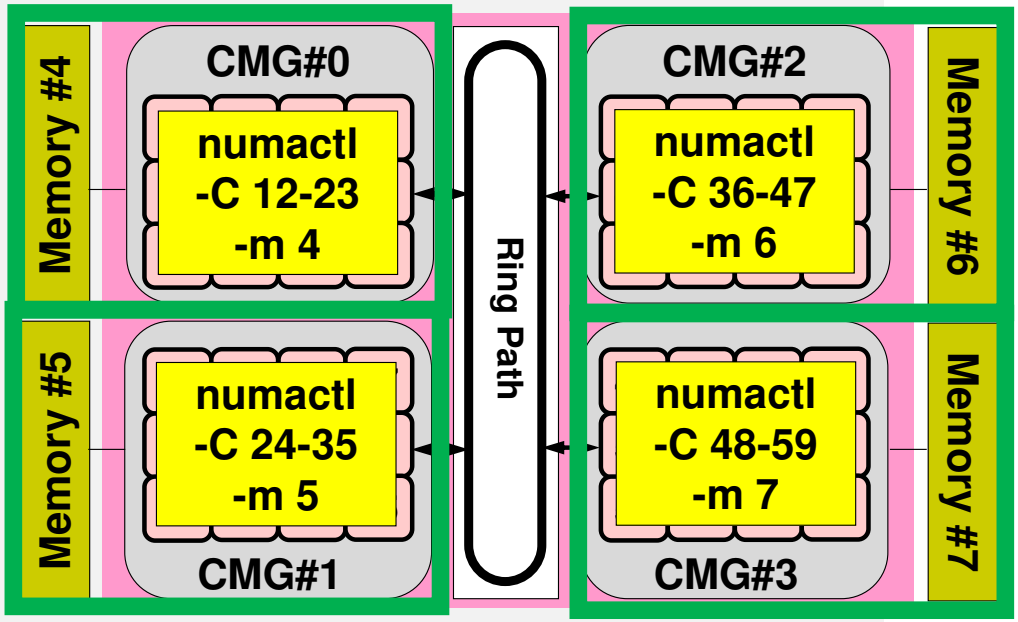
>$ pjsub f4_48.sh
```

f4_48.sh

```
#!/bin/sh
#PJM   -N      "f4_48"
#PJM   -L      rscgrp=lecture9-o
#PJM   -L      node=1
#PJM   --omp   thread=48
#PJM   -L      elapse=00:15:00
#PJM   -g      gt89
#PJM   -j
#PJM   -e      err
#PJM   -o      f4_48.lst

module load   fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

numactl       ./solf4
numactl       ./solf4
numactl       ./solf4
numactl       ./solf4
numactl       ./solf4
numactl       -C     12-59  -m     4-7    ./solf4
numactl       -C     12-59  -m     4-7    ./solf4
numactl       -C     12-59  -m     4-7    ./solf4
numactl       -C     12-59  -m     4-7    ./solf4
numactl       -C     12-59  -m     4-7    ./solf4
```



Time for PCG：N=128^3, 48 Threads
N= 2,097,152

	Fortran	C (clang)	C (trad)
src0	1.671	1.564	2.354
src1 (First Touch)	1.480	1.122	1.720
src2 (+ ELL)	0.747	0.809	1.127
src3 (+ reduced “omp-parallel”)	0.707	0.834	0.854
src3b （+ clang loop unroll_count）	-	0.764	-
src4 (+ No OMP-DO/Reduction)	0.676	-	-

src_c3b (5/5)

src-c3

```
#pragma omp for

for(i=0; i<N; i++) {
    VAL = D[i] * W[P][i];
    for(j=0; j<6; j++) {
        VAL += AMAT[6*i+j]*W[P][itemLU[6*i+j]];
    }
    W[Q][i] = VAL;
}
```

src-c3b: clang only

```
#pragma omp for
#pragma clang loop unroll_count(8)

for(i=0; i<N; i++) {
    VAL = D[i] * W[P][i];
    for(j=0; j<6; j++) {
        VAL += AMAT[6*i+j]*W[P][itemLU[6*i+j]];
    }
    W[Q][i] = VAL;
}
```

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

for i= 1, 2, …

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

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

  if i=1

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

  else

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

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

  endif

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

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

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

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

  check convergence $|r|$

end

Time for PCG：N=160³, 48 Threads N= 4,096,000

	Fortran	C (clang)	C (trad)
src0	3.610	3.484	4.067
src1 (First Touch)	2.993	2.228	3.425
src2 (+ ELL)	1.534	1.690	2.340
src3 (+ reduced “omp-parallel”)	1.556	1.693	1.742
src3b （+ clang loop unroll_count）	-	1.586	-
src4 (+ No OMP-DO/Reduction)	1.435	-	-

Time for PCG：N=200³, 48 Threads
N= 8,000,000

	Fortran	C (clang)	C (trad)
src0	7.666	8.321	9.397
src1 (First Touch)	6.952	5.102	8.008
src2 (+ ELL)	3.421	3.910	5.381
src3 (+ reduced “omp-parallel”)	3.440	3.920	3.824
src3b （+ clang loop unroll_count）	-	3.624	-
src4 (+ No OMP-DO/Reduction)	3.276	-	-

Time for PCG：N=256^3，48 Threads
N= 16,777,216

	Fortran	C (clang)	C (trad)
src0	34.308	24.772	25.547
src1 (First Touch)	32.202	22.172	23.814
src2 (+ ELL)	8.916	10.761	14.566
src3 (+ reduced “omp-parallel”)	8.915	10.764	10.415
src3b （+ clang loop unroll_count）	-	10.003	-
src4 (+ No OMP-DO/Reduction)	8.620	-	-

Exercises

- Problem size (NX, NY, NZ)
- Thread # (OMP_NUM_THREADS: 1-48)
- Various Types of Implementation
- Profiling

Performance Evaluation: Profiler

- Specify the measuring unit in the program (multiple settings are possible)
- 17 runs needed for each case
- Performance of Computation & Memory, Power Consumption
- Excel Macro File
  - https://www.dropbox.com/s/kat9ny5aoxp7cqm/cpu_pa_report.xlsm?dl=0

Profiling (1/4)

Specifying the measuring unit in the program, No additional options for compiling: solver_PCG.c/f

```
#include "fj_tool/fapp.h"

        fapp_start ("CG",1,0);
        Stime = omp_get_wtime();

for(L=0; L<(*ITR); L++) {
...
        if(ERR < EPS) {
           *IER = 0;
           goto N900;
        } else {
           RHO1 = RHO;
        }
}

        *IER = 1;
N900:
        Etime = omp_get_wtime();
        fapp_stop ("CG",1,0);

        return 0;
}
```

```
      call fapp_start ("CG",1,0)
      Stime = omp_get_wtime()

      do L= 1, ITR
...
        if (ERR .lt. EPS) then
          IER = 0
          goto 900
         else
          RHO1 = RHO
        endif

      enddo
      IER = 1
  900 continue
      Etime= omp_get_wtime()
      call fapp_stop ("CG",1,0)

      return
      end
```

Profiling (2/4)
Running on Wisteria/BDEC-01 (Odyssey)

```
>$ cd /work/gt89/t89XYZ/ompw
>$ cd run

<modify “fapp.sh”, “data.sh”>

>$ pjsub fapp.sh

(after finishing)

>$ pjsbu data.sh

>$ ls pa*.csv
   pa1.csv … pa17.csv
```

Profiling (3/4)

Each Directory (e.g. repo01 etc.) should be empty before running the code

fapp.sh

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

module load fj
export OMP_NUM_THREADS=48
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand

fapp -C -d ./repo01 -Hevent=pa1 ./solf2
fapp -C -d ./repo02 -Hevent=pa2 ./solf2
fapp -C -d ./repo03 -Hevent=pa3 ./solf2
fapp -C -d ./repo04 -Hevent=pa4 ./solf2
fapp -C -d ./repo05 -Hevent=pa5 ./solf2
fapp -C -d ./repo06 -Hevent=pa6 ./solf2
fapp -C -d ./repo07 -Hevent=pa7 ./solf2
fapp -C -d ./repo08 -Hevent=pa8 ./solf2
fapp -C -d ./repo09 -Hevent=pa9 ./solf2
fapp -C -d ./repo10 -Hevent=pa10 ./solf2
fapp -C -d ./repo11 -Hevent=pa11 ./solf2
fapp -C -d ./repo12 -Hevent=pa12 ./solf2
fapp -C -d ./repo13 -Hevent=pa13 ./solf2
fapp -C -d ./repo14 -Hevent=pa14 ./solf2
fapp -C -d ./repo15 -Hevent=pa15 ./solf2
fapp -C -d ./repo16 -Hevent=pa16 ./solf2
fapp -C -d ./repo17 -Hevent=pa17 ./solf2
```

data.sh

```
#!/bin/sh
#PJM -N "data"
#PJM -L rscgrp=lecture9-o
#PJM -L node=1
#PJM --mpi proc=1
#PJM -L elapse=00:15:00
#PJM -g gt89
#PJM -j
#PJM -e err
#PJM -o data.lst

module load fj
module load fjmpi

fapp -A -d./repo01 -Icpupa,mpi -tcsv -o pa1.csv
fapp -A -d./repo02 -Icpupa,mpi -tcsv -o pa2.csv
fapp -A -d./repo03 -Icpupa,mpi -tcsv -o pa3.csv
fapp -A -d./repo04 -Icpupa,mpi -tcsv -o pa4.csv
fapp -A -d./repo05 -Icpupa,mpi -tcsv -o pa5.csv
fapp -A -d./repo06 -Icpupa,mpi -tcsv -o pa6.csv
fapp -A -d./repo07 -Icpupa,mpi -tcsv -o pa7.csv
fapp -A -d./repo08 -Icpupa,mpi -tcsv -o pa8.csv
fapp -A -d./repo09 -Icpupa,mpi -tcsv -o pa9.csv
fapp -A -d./repo10 -Icpupa,mpi -tcsv -o pa10.csv
fapp -A -d./repo11 -Icpupa,mpi -tcsv -o pa11.csv
fapp -A -d./repo12 -Icpupa,mpi -tcsv -o pa12.csv
fapp -A -d./repo13 -Icpupa,mpi -tcsv -o pa13.csv
fapp -A -d./repo14 -Icpupa,mpi -tcsv -o pa14.csv
fapp -A -d./repo15 -Icpupa,mpi -tcsv -o pa15.csv
fapp -A -d./repo16 -Icpupa,mpi -tcsv -o pa16.csv
fapp -A -d./repo17 -Icpupa,mpi -tcsv -o pa17.csv
```

Profiling (4/4): Operations on PC

- Copying all “pa*.csv”’s to your PC

```
>$ scp t00XYZ@wisteria.cc.u-tokyo.ac.jp:/work/gt00/t00XYZ/ompw/run/pa*.csv .
```

- All “pa*.csv”’s and Macro for Excel should be in the same directory
- “Double Click” the Excel Macro
  - Just follow instructions
  - Please select “CG”, not “All”

Time for PCG: N=160^3, 48 Threads

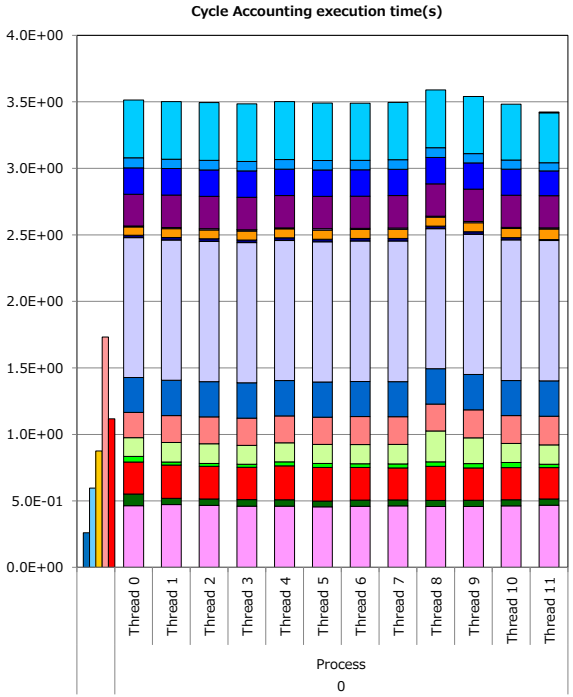
N= 4,096,000, for Each Node, Fortran

Optimization – Busy Memory – More Watt

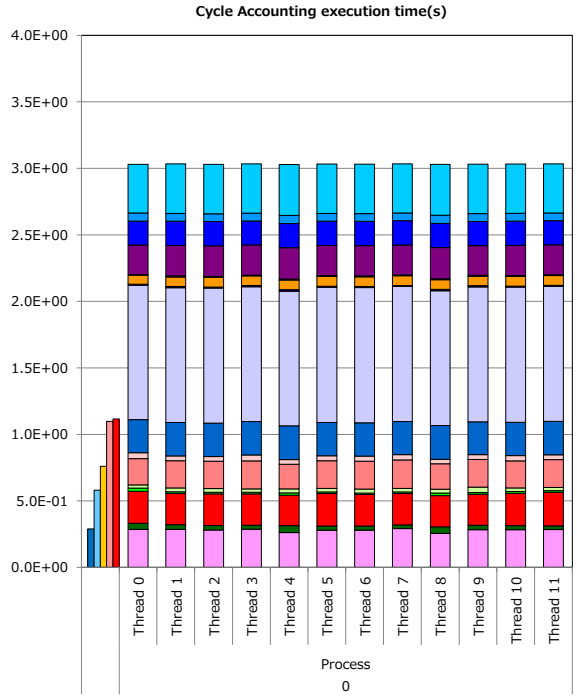
	Time (sec.)	Peak Perf. Ratio (%)	SIMD Ratio (%)	Memory Throughput (%)	Instruction		Power (W)	
					Effective	Load/ Store	Core L2 Memory	Node
solf0	3.69	1.59	20.0	30.3	3.39×10^{11}	8.27×10^{10}	81.6 10.9 20.2	112.
solf1 (First Touch)	2.98	1.97	28.8	37.5	2.35×10^{11}	5.33×10^{10}	92.1 10.8 33.3	136.
solf2 (+ ELL)	1.58	3.73	49.7	70.0	1.19×10^{11}	4.17×10^{10}	104. 15.0 51.7	170.
solf3 (+ reduced “omp-parallel”)	1.58	3.72	48.4	69.8	1.22×10^{11}	4.10×10^{10}	101. 14.9 51.0	167.
solf4 (+ further optimization)	1.45	4.06	55.1	75.8	1.10×10^{11}	3.78×10^{10}	102. 15.8 56.5	174.

PCG, N=160³, 48 Threads Fortran, Each CMG

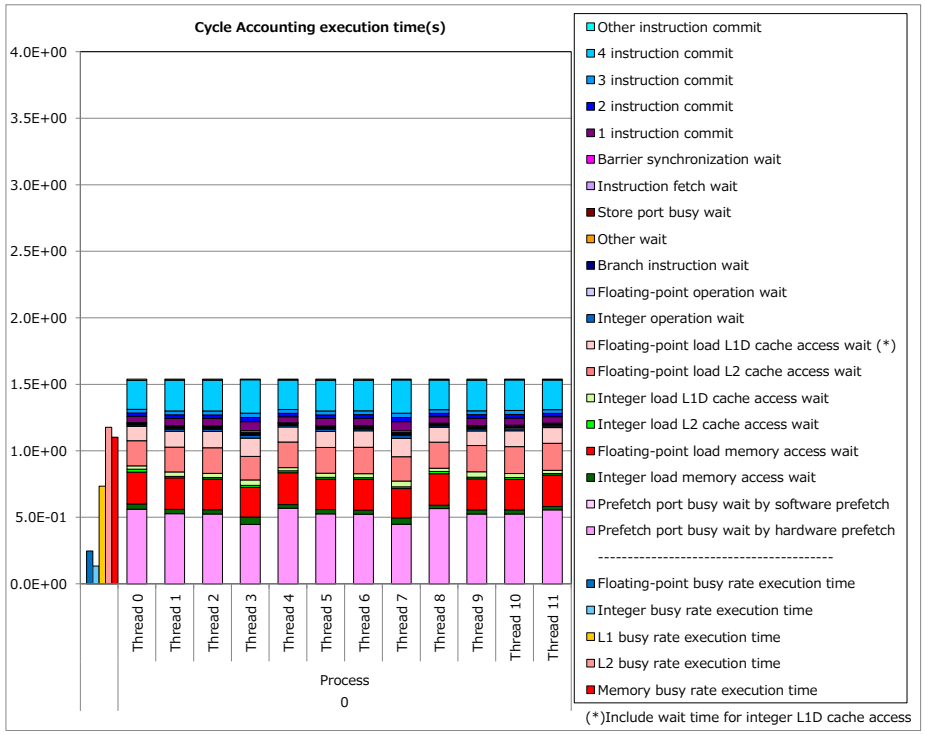
src0:Initial



src1:First Touch



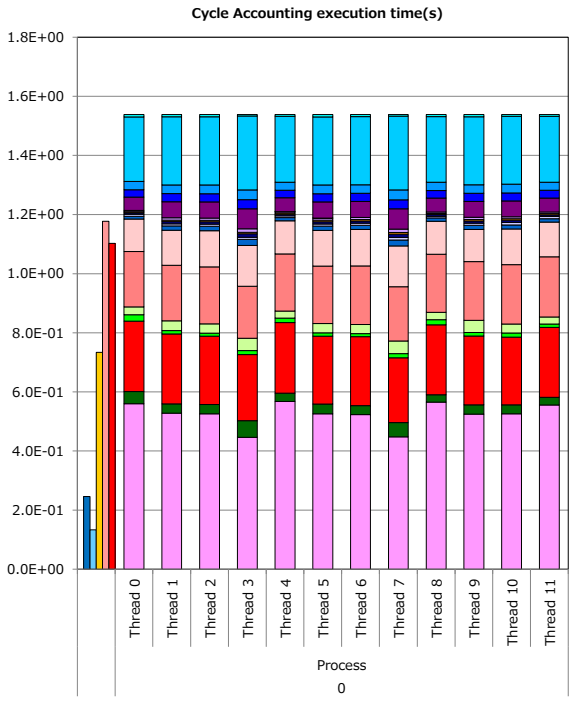
src2: +ELL



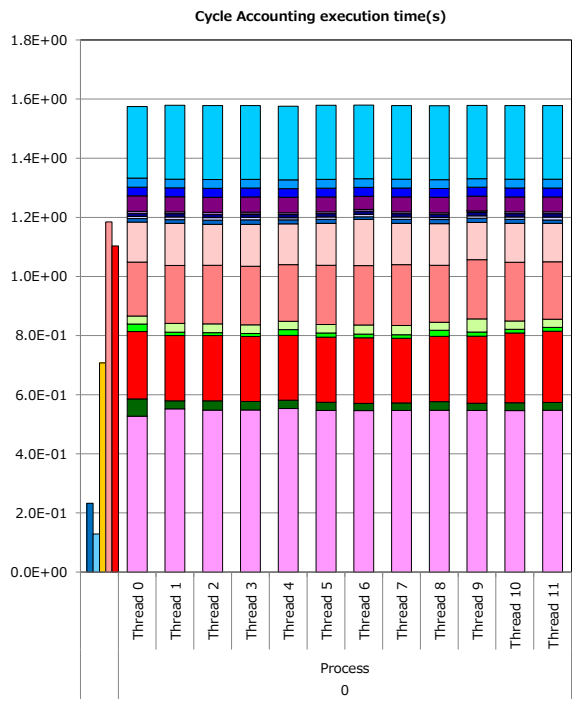
Prefetch Port Busy Wait (H/W)
Integer Load L1D Cache Access Wait
Floating-Point Operation Wait
Instruction Commit

PCG, N=160³, 48 Threads Fortran, Each CMG

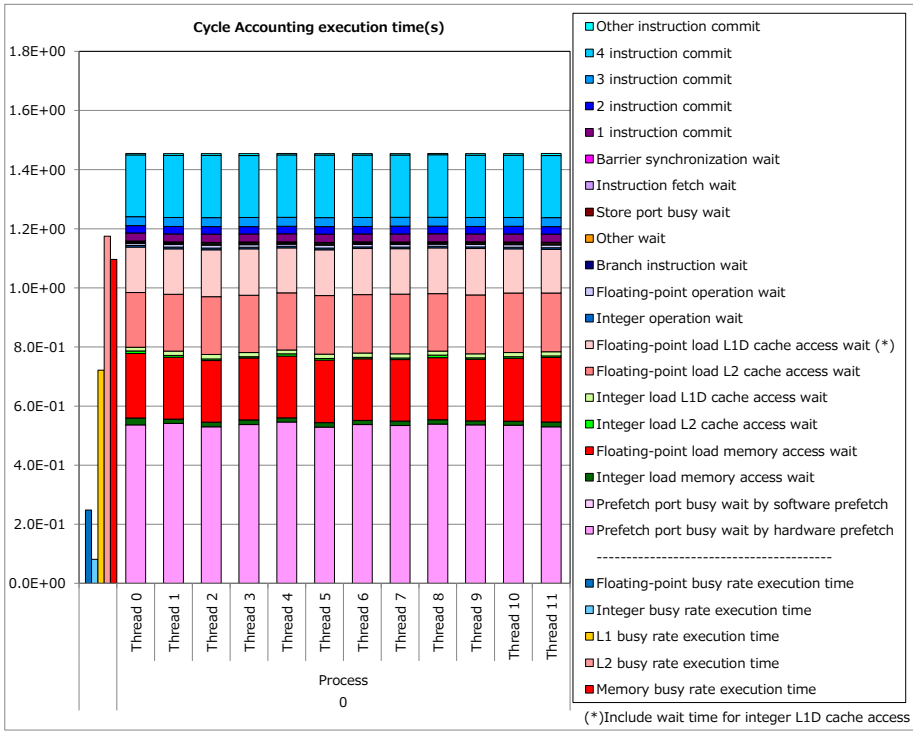
src2:+ELL



src3



src4



- **Prefetch Port Busy Wait (H/W)**
- **Floating-Point Load Memory Access Wait**
- **Floating-Point Load L2D Cache Access Wait**
- **Floating-Point Load L1D Cache Access Wait**
- **Instruction Commit**

Time for PCG: N=160³, 48 Threads

N= 4,096,000, for Each Node, C (clang)

Optimization – Busy Memory – More Watt

	Time (sec.)	Peak Perf. Ratio (%)	SIMD Ratio (%)	Memory Throughput (%)	Instruction		Power (W)	
					Effective	Load/ Store	Core L2 Memory	Node
solc0	3.53	0.90	2.95	31.7	4.83×10^{11}	1.65×10^{11}	103. 12.9 17.9	134.
solc1 (First Touch)	2.42	1.34	4.82	46.2	2.97×10^{11}	1.10×10^{11}	107. 11.9 33.8	153.
solc2 (+ ELL)	1.73	1.88	8.21	63.8	1.74×10^{11}	8.92×10^{10}	104. 13.9 44.8	163.
solc3 (+ reduced “omp-parallel”)	1.75	1.86	8.51	62.9	1.68×10^{11}	8.88×10^{10}	108. 14.2 45.0	167.
solc3b （+ clang loop unroll_count）	1.62	2.00	10.4	67.8	1.37×10^{11}	8.22×10^{10}	109. 14.6 44.4	168.

Time for PCG: N=160^3, 48 Threads

N= 4,096,000, for Each Node, C (trad)

Optimization – Busy Memory – More Watt

	Time (sec.)	Peak Perf. Ratio (%)	SIMD Ratio (%)	Memory Throughput (%)	Instruction		Power (W)	
					Effective	Load/ Store	Core L2 Memory	Node
solc0org	4.14	2.66	27.3	27.1	3.78×10^{11}	7.40×10^{10}	91.3 11.3 18.4	121.
solc1org (First Touch)	3.52	3.13	37.4	31.8	2.75×10^{11}	6.14×10^{10}	90. 9.86 28.4	128.
solc2org (+ ELL)	2.34	4.70	58.1	47.1	1.63×10^{11}	4.77×10^{10}	95.1 11.7 37.6	144.
solc3org (+ reduced “omp-parallel”)	1.70	3.46	47.1	64.8	1.17×10^{11}	4.14×10^{10}	96.7 13.9 48.7	159.