

# **3D Parallel FEM (IV)**

## **(OpenMP + MPI) Hybrid Parallel Programming Model**

Kengo Nakajima  
Information Technology Center

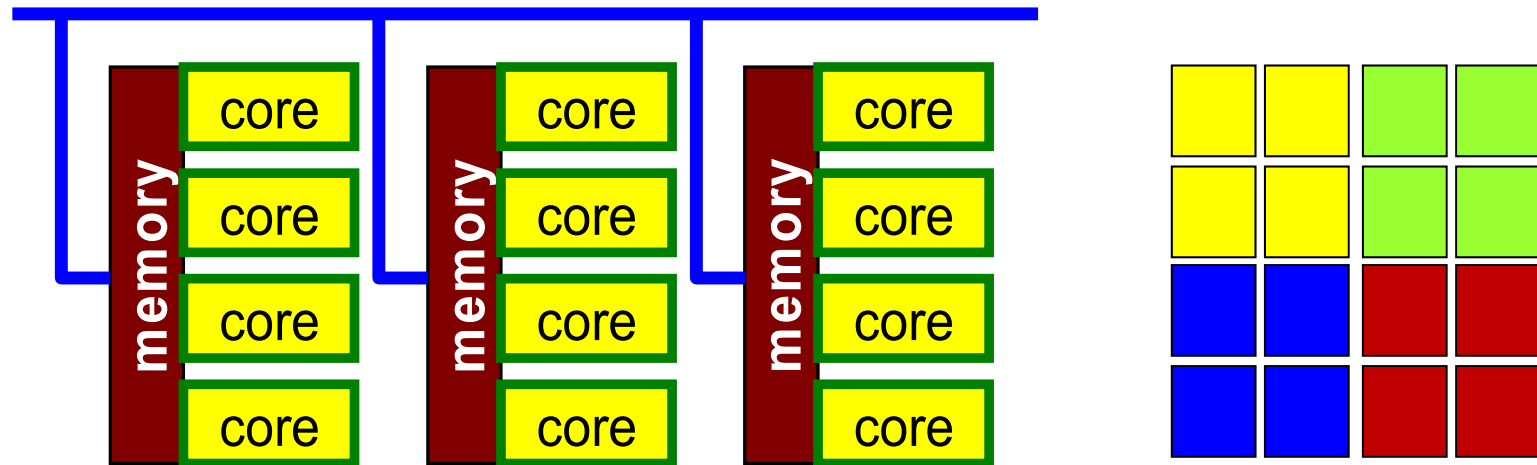
Technical & Scientific Computing II (4820-1028)  
Seminar on Computer Science II (4810-1205)

# Hybrid Parallel Programming Model

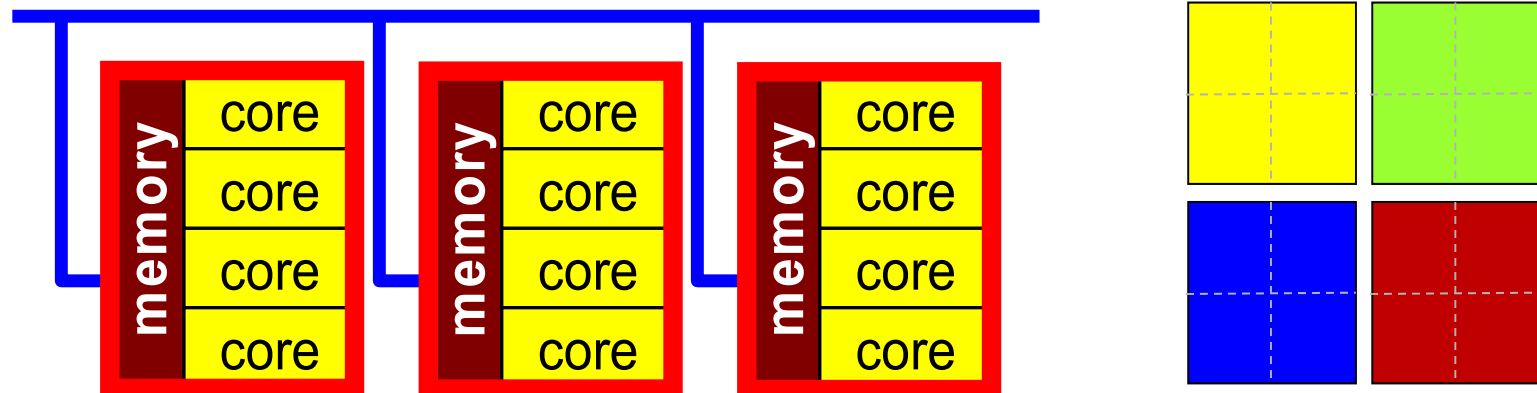
- Message Passing (e.g. MPI) + Multi Threading (e.g. OpenMP, CUDA, OpenCL, OpenACC etc.)
- In K computer and FX10, hybrid parallel programming is recommended
  - MPI + Automatic Parallelization by Fujitsu's Compiler
  - Personally, I do not like to call this "hybrid" !!!
- Expectations for Hybrid
  - Number of MPI processes (and sub-domains) to be reduced
  - $O(10^8-10^9)$ -way MPI might not scale in Exascale Systems
  - Easily extended to Heterogeneous Architectures
    - CPU+GPU, CPU+Manycores (e.g. Intel MIC/Xeon Phi)
    - MPI+X: OpenMP, OpenACC, CUDA, OpenCL

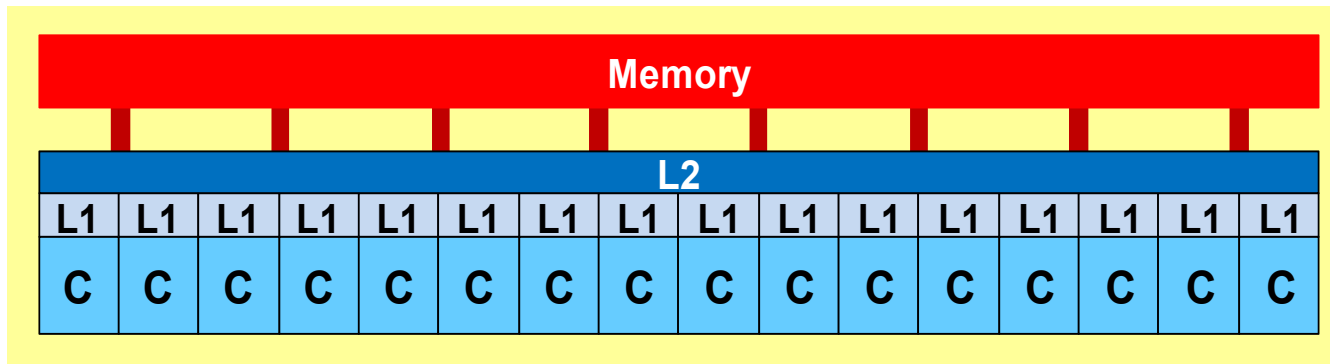
# Flat MPI vs. Hybrid

## Flat-MPI: Each Core -> Independent

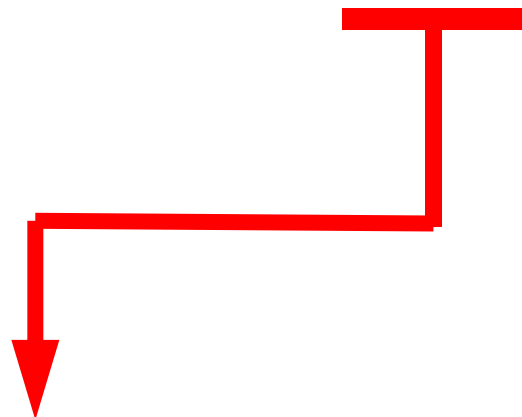


## Hybrid: Hierarchical Structure

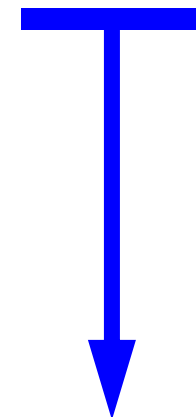




**HB M x N**



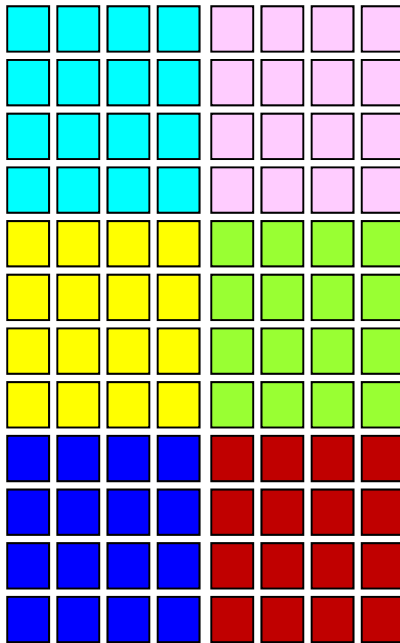
Number of OpenMP threads  
per a single MPI process



Number of MPI process  
per a single node

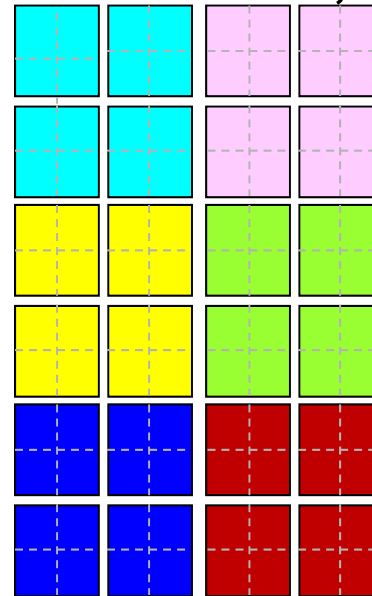
# Size (and number) of local data changes according to parallel programming model

example: 6 nodes, 96 cores



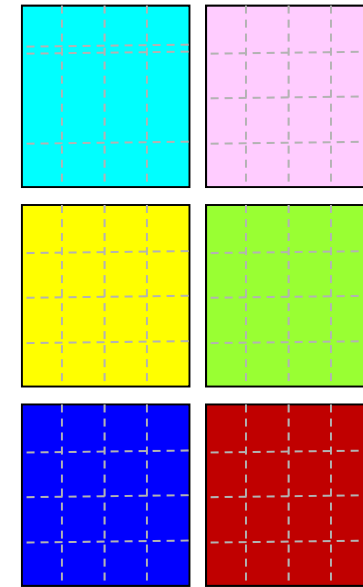
**Flat MPI**

128	192	64
8	12	1
pcube		



**HB 4x4**

128	192	64
4	6	1
pcube		



**HB 16x1**

128	192	64
2	3	1
pcube		

# Batch Script (1/2)

## Env. Var.: OMP\_NUM\_THREADS

### Flat MPI

```
#PJM -L "node=6"  
#PJM -L "elapse=00:05:00"  
#PJM -j  
#PJM -L "rscgrp=lecture5"  
#PJM -g "gt95"  
#PJM -o "test.lst"  
#PJM --mpi "proc=96"  
  
mpiexec ./sol  
  
rm wk.*
```

### Hybrid 16 × 1

```
#!/bin/sh  
#PJM -L "node=6"  
#PJM -L "elapse=00:05:00"  
#PJM -j  
#PJM -L "rscgrp=lecture5"  
#PJM -g "gt95"  
#PJM -o "test.lst"  
#PJM --mpi "proc=6"  
  
export OMP_NUM_THREADS=16  
mpiexec ./sol  
  
rm wk.*
```

# Batch Script (2/2)

## Env. Var.: OMP\_NUM\_THREADS

### Hybrid 4 × 4

```
#!/bin/sh
#PJM -L "node=6"
#PJM -L "elapse=00:05:00"
#PJM -j
#PJM -L "rscgrp=lecture5"
#PJM -g "gt95"
#PJM -o "test.lst"
#PJM --mpi "proc=24"

export OMP_NUM_THREADS=4
mpiexec ./sol

rm wk.*
```

### Hybrid 8 × 2

```
#!/bin/sh
#PJM -L "node=6"
#PJM -L "elapse=00:05:00"
#PJM -j
#PJM -L "rscgrp=lecture5"
#PJM -g "gt95"
#PJM -o "test.lst"
#PJM --mpi "proc=12"

export OMP_NUM_THREADS=8
mpiexec ./sol

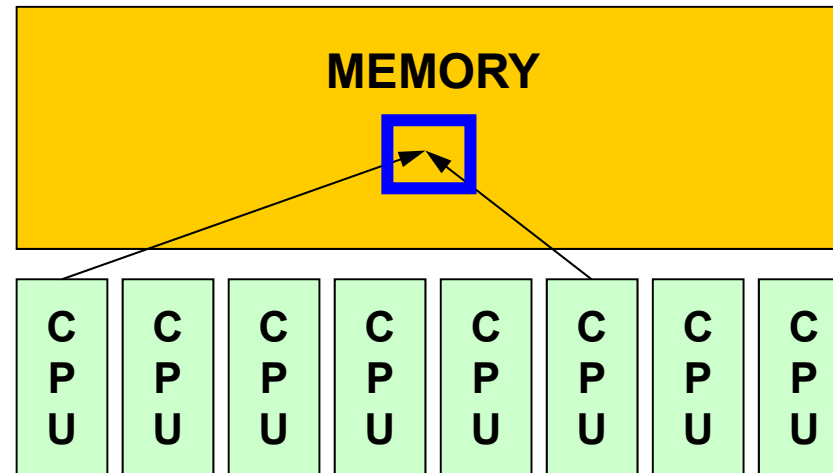
rm wk.*
```

# Background

- Multicore/Manycore Processors
  - Low power consumption, Various types of programming models
- OpenMP
  - Directive based, (seems to be) easy
  - Many books
- Data Dependency (no classes this year)
  - Conflict of reading from/writing to memory
  - Appropriate reordering of data is needed for “consistent” parallel computing
  - NO detailed information in OpenMP books: very complicated
- OpenMP/MPI Hybrid Parallel Programming Model for Multicore/Manycore Clusters



# SMP



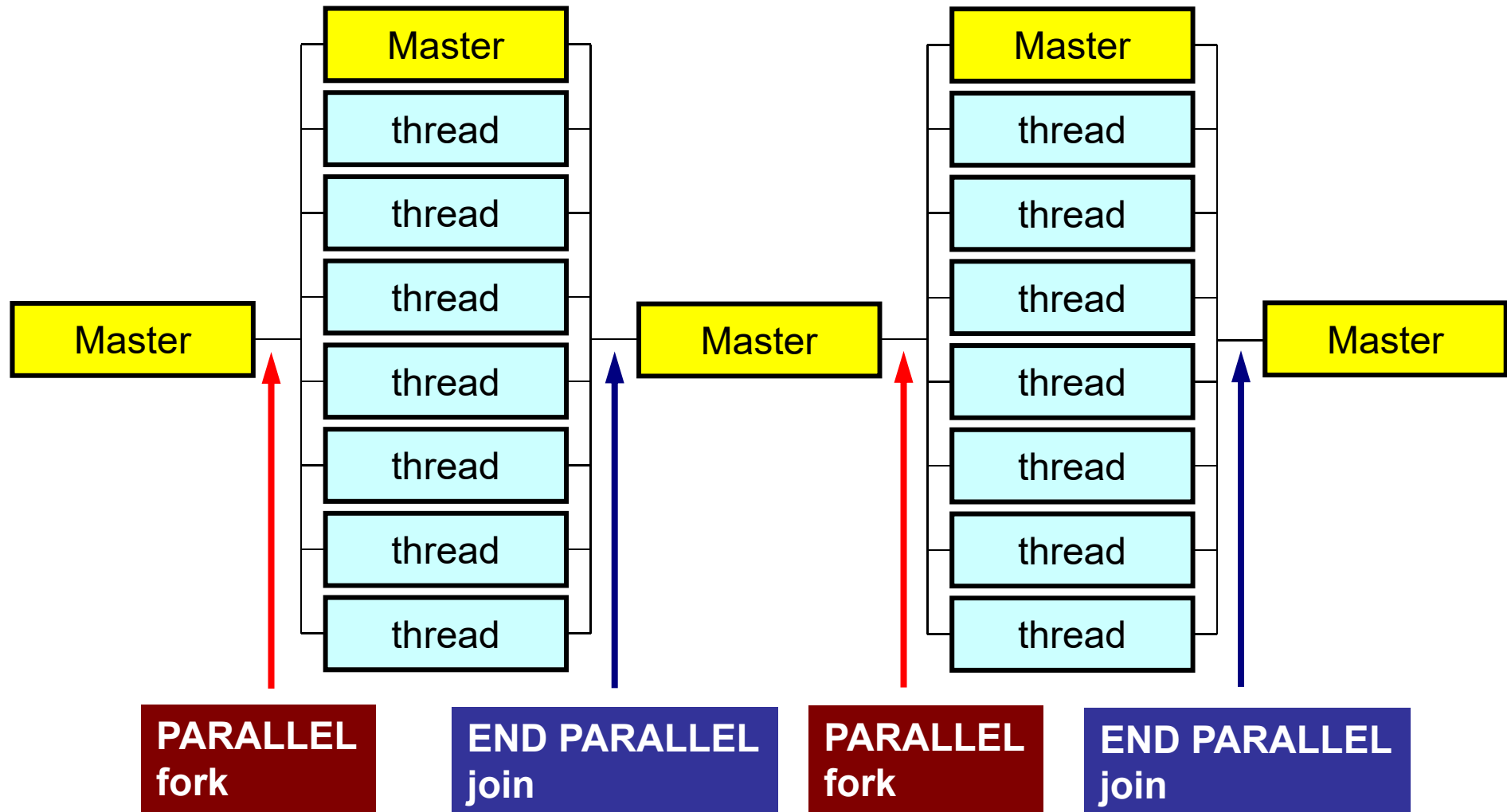
- SMP
  - Symmetric Multi Processors
  - Multiple CPU's (cores) share a single memory space

# What is OpenMP ?

<http://www.openmp.org>

- An API for multi-platform shared-memory parallel programming in C/C++ and Fortran
  - Current version: 4.0
- Background
  - Merger of Cray and SGI in 1996
  - ASCI project (DOE) started
- C/C++ version and Fortran version have been separately developed until ver.2.5.
- Fork-Join Parallel Execution Model
- 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
```

# Information about OpenMP

- OpenMP Architecture Review Board (ARB)
  - <http://www.openmp.org>
- 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

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

### DAXPY

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

### Dot Products

```
!$omp parallel do private(iS, iE, i)
!$omp&                reduction(+:RHO)
  do ip= 1, PEsmptOT
    iS= STACKmcG(ip-1) + 1
    iE= STACKmcG(ip )
    do i= iS, iE
      RHO= RHO + W(i, R)*W(i, Z)
    enddo
  enddo
!$omp end parallel do
```

# OpenMP/Direceives Matrix/Vector Products

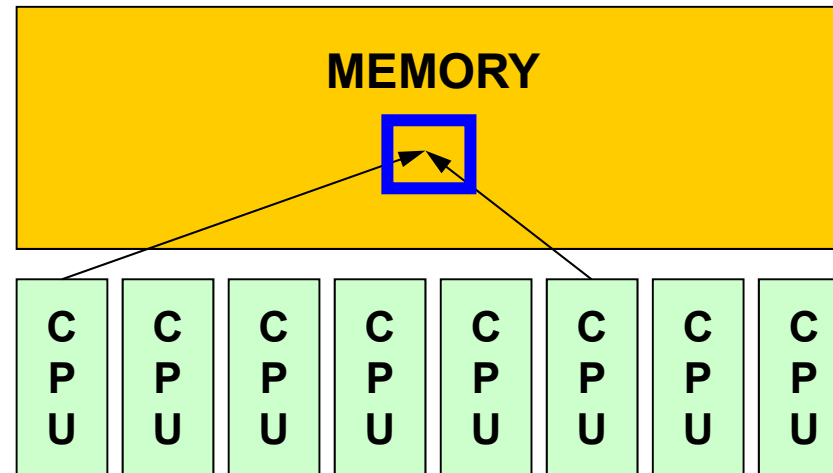
```
!$omp parallel do private(ip, iS, iE, i, j)
  do ip= 1, PEsmptOT
    iS= STACKmcG(ip-1) + 1
    iE= STACKmcG(ip )
    do i= iS, iE
      W(i, Q)= D(i)*W(i, P)
      do j= 1, INL(i)
        W(i, Q)= W(i, Q) + W(IAL(j, i), P)
      enddo
      do j= 1, INU(i)
        W(i, Q)= W(i, Q) + W(IAU(j, i), P)
      enddo
    enddo
  enddo
!$omp end parallel do
```



# Features of OpenMP

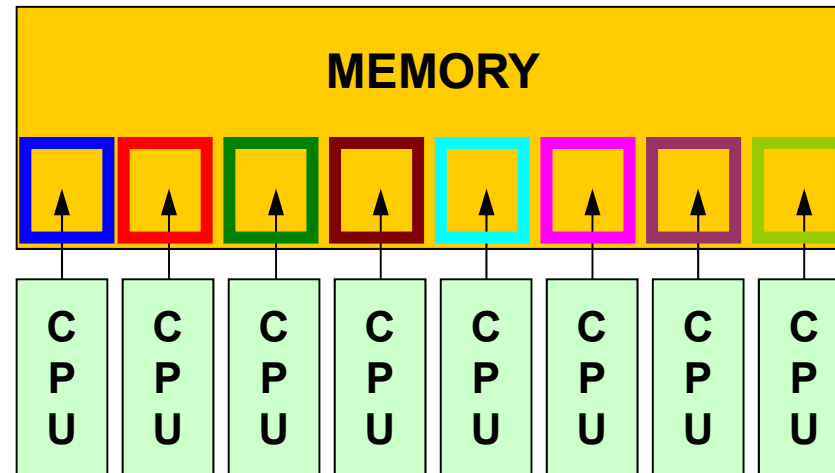
- Directives
  - Loops right after the directives are parallelized.
  - If the compiler does not support OpenMP, directives are considered as just comments.
- **Nothing happen without explicit directives**
  - Different from “automatic parallelization/vectorization”
  - Something wrong may happen by 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, no such case does not happen by reordering etc.
  - In OpenMP, users are responsible for such issues (e.g. proper data configuration, reordering etc.)
- Generally speaking, performance per core reduces as number of used cores (thread number) increases.
  - Memory access performance: STREAM

# Features of OpenMP (cont.)

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

```
!$omp parallel do private(iS, iE, i)
!$omp&                reduction(+:RHO)
  do ip= 1, PEsmptOT
    iS= STACKmcG(ip-1) + 1
    iE= STACKmcG(ip )
    do i= iS, iE
      RHO= RHO + W(i, R)*W(i, Z)
    enddo
  enddo
!$omp end parallel do
```

W(:, :), R, Z, PEsmptOT  
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 parallel FEM.

# First things to be done (after OpenMP 3.0)

- 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, C\$OMP, \*\$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

```
!$OMP PARALLEL DO[clause[[,] clause] ... ]  
    (do_loop)  
!$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|instinsic} : list )
```

```
reduction ( {operator|instinsic} : 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 which can be used with OpenMP

<b>Name</b>	<b>Functions</b>
int omp_get_num_threads (void)	Total Thread #
int omp_get_thread_num (void)	Thread ID
double omp_get_wtime (void)	= MPI_Wtime
void omp_set_num_threads (int num_threads) call omp_set_num_threads (num_threads)	Setting 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

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



```
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

```

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

```



```

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.



```

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

```

NOT good for GPU's

# Matrix-Vector Multiply

```
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
```

# Matrix-Vector Multiply

```

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

```

# Matrix-Vector Multiply: Other Approach

This is rather better for GPU and (very) many-core architectures: simpler structure of loops

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

# omp parallel (do)

- Each “omp parallel-omp end parallel” pair starts & stops threads: fork-join
- If you have many loops, these operations on threads could be overhead
- omp parallel + omp do/omp for

```
!$omp parallel ...
```

```
!$omp do  
    do i= 1, N
```

```
...
```

```
!$omp do  
    do i= 1, N
```

```
...
```

```
!$omp end parallel 必須
```

```
#pragma omp parallel ...
```

```
#pragma omp for {
```

```
...
```

```
#pragma omp for {
```

# Exercise !!

- Apply multi-threading by OpenMP on parallel FEM code using MPI
  - CG Solver (solver\_CG, solver\_SR)
  - Matrix Assembling (mat\_ass\_main, mat\_ass\_bc)
- Hybrid parallel programming model
- Evaluate the effects of
  - Problem size, parallel programming model, thread #

# Makefile (Fortran, C)

```

F90      = mpifrtpx
F90LINKER = $(F90)
LIB_DIR  =
INC_DIR  =
OPTFLAGS = -Kfast,openmp
FFLAGS  = $(OPTFLAGS)
FLIBS   =
F90LFLAGS=
#
TARGET = ../run/sol1
default: $(TARGET)
OBJS =¥
pfem_util.o ¥
...
pfem_finalize.o output_ucd.o

$(TARGET): $(OBJS)
            $(F90LINKER) $(OPTFLAGS)
-o $(TARGET) $(OBJS) $(F90LFLAGS)
clean:
    /bin/rm -f *.o $(TARGET)
*~ *.mod
.f.o:
    $(F90) $(FFLAGS)
$(INC_DIR) -c $*.f
.f90.o:
    $(F90) $(FFLAGS)
$(INC_DIR) -c $*.f90
.SUFFIXES: .f90 .f

```

```

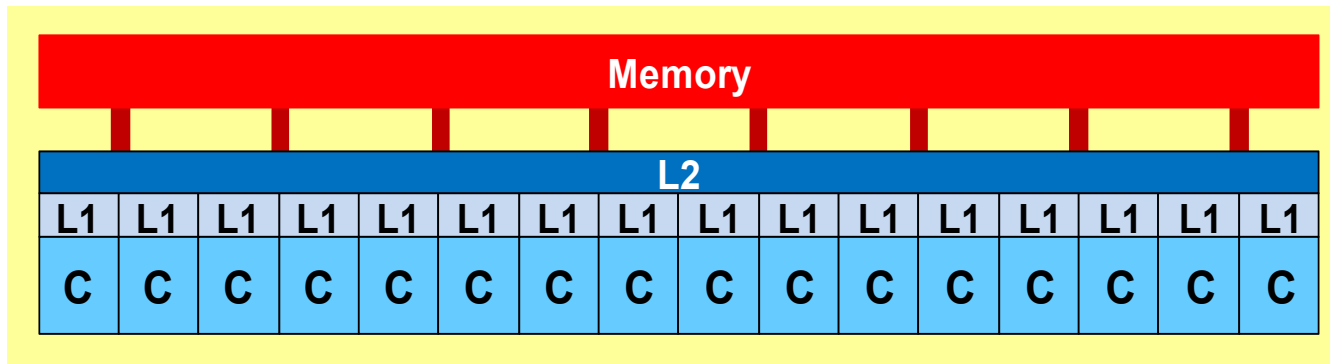
CC      = mpifccpx
LIB_DIR=
INC_DIR=
OPTFLAGS= -Kfast,openmp
LIBS =
LFLAGS=
#
TARGET = ../run/sol1
default: $(TARGET)
OBJS =¥
    test1.o¥
...
    util.o

$(TARGET): $(OBJS)
            $(CC) $(OPTFLAGS) -o $@
$(OBJS) $(LFLAGS)
.c.o:
    $(CC) $(OPTFLAGS) -c

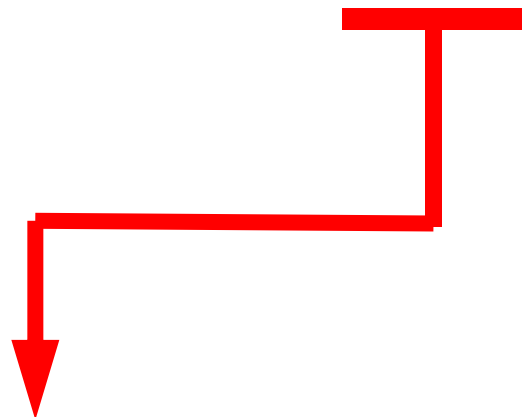
$*.c
clean:
    /bin/rm -f *.o $(TARGET)
*~ *.mod

```

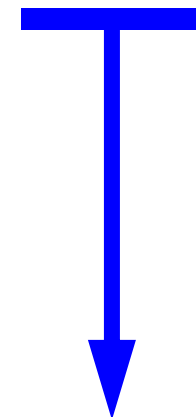




**HB M x N**



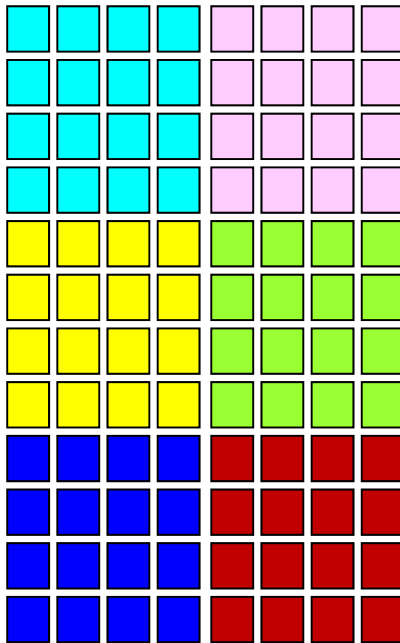
Number of OpenMP threads  
per a single MPI process



Number of MPI process  
per a single node

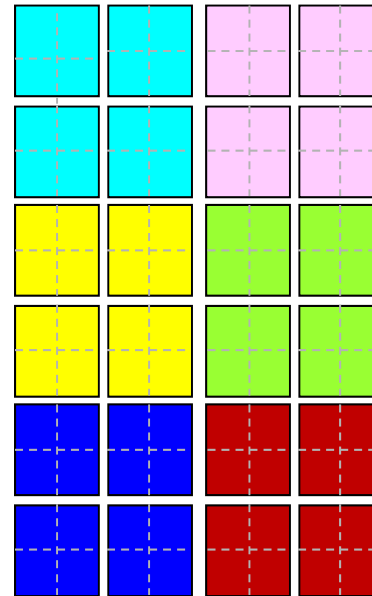
# Distributed Local Meshes for Flat MPI, HB 4x4, and HB 16x1

example: 6 nodes, 96 cores



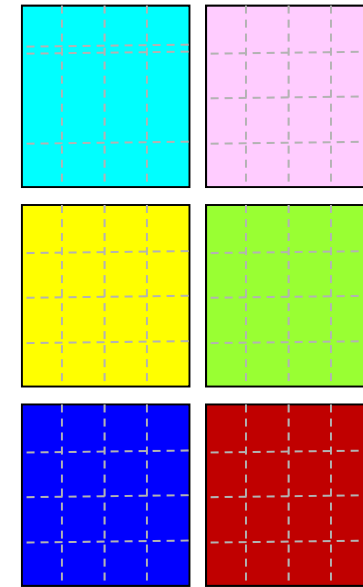
**Flat MPI**

128	192	64
8	12	1
pcube		



**HB 4x4**

128	192	64
4	6	1
pcube		



**HB 16x1**

128	192	64
2	3	1
pcube		

# go0.sh (1/2): OMP\_NUM\_THREADS

## Flat MPI (go.sh)

```
#PJM -L "node=6"  
#PJM -L "elapse=00:05:00"  
#PJM -j  
#PJM -L "rscgrp=lecture5"  
#PJM -g "gt95"  
#PJM -o "test.lst"  
#PJM --mpi "proc=96"  
  
mpiexec ./sol  
  
rm wk.*
```

## Hybrid 16 × 1

```
#!/bin/sh  
#PJM -L "node=6"  
#PJM -L "elapse=00:05:00"  
#PJM -j  
#PJM -L "rscgrp=lecture5"  
#PJM -g "gt95"  
#PJM -o "test.lst"  
#PJM --mpi "proc=6"  
  
export OMP_NUM_THREADS=16  
mpiexec ./sol1  
  
rm wk.*
```

# go0.sh (2/2): OMP\_NUM\_THREADS

## Hybrid 4 × 4

```
#!/bin/sh
#PJM -L "node=6"
#PJM -L "elapse=00:05:00"
#PJM -j
#PJM -L "rscgrp=lecture5"
#PJM -g "gt95"
#PJM -o "test.lst"
#PJM --mpi "proc=24"

export OMP_NUM_THREADS=4
mpiexec ./sol1

rm wk.*
```

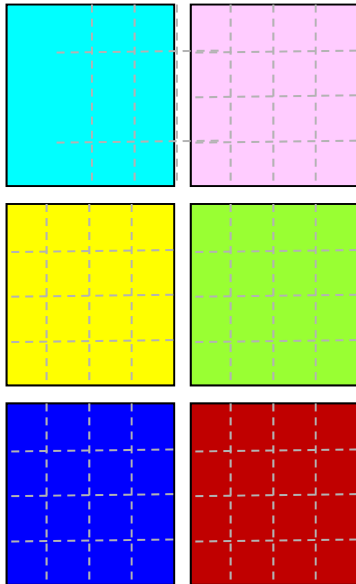
## Hybrid 8 × 2

```
#!/bin/sh
#PJM -L "node=6"
#PJM -L "elapse=00:05:00"
#PJM -j
#PJM -L "rscgrp=lecture5"
#PJM -g "gt95"
#PJM -o "test.lst"
#PJM --mpi "proc=12"

export OMP_NUM_THREADS=8
mpiexec ./sol1

rm wk.*
```

# Example: HB 16 × 1



**HB 16x1**

```
128 192 64
  2   3   1
pcube
```

## go0.sh

```
#!/bin/sh
#PJM -L "node=6"
#PJM -L "elapse=00:05:00"
#PJM -j
#PJM -L "rscgrp=lecture5"
#PJM -g "gt95"
#PJM -o "test.lst"
#PJM --mpi "proc=6"

export OMP_NUM_THREADS=16
mpixec ./sol1

rm wk.*
```

# How to apply multi-threading

- CG Solver
  - Just insert OpenMP directives
  - ILU/IC preconditioning is much more difficult
- MAT\_ASS (mat\_ass\_main, mat\_ass\_bc)
  - Data Dependency
    - Avoid to accumulate contributions of multiple elements to a single node simultaneously (in parallel)
      - results may be changed
      - deadlock may occur
    - Coloring
      - Elements in a same color do not share a node
      - Parallel operations are possible for elements in each color
      - In this case, we need only 8 colors for 3D problems (4 colors for 2D problems)
      - Coloring part is very expensive: parallelization is difficult

# FORTRAN (solver\_CG)

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

```
DNRM20= 0. d0
!$omp parallel do private(i) reduction (+:DNRM20)
do i= 1, N
  DNRM20= DNRM20 + WW (i, R)**2
enddo
```

```
!$omp parallel do private(j, k, i, WVAL)
do j= 1, N
  WVAL= D (j)*WW (j, P)
  do k= index(j-1)+1, index(j)
    i= item(k)
    WVAL= WVAL + AMAT (k)*WW (i, P)
  enddo
  WW (j, Q)= WVAL
enddo
```

# C (solver\_CG)

```
#pragma omp parallel for private (i)
for (i=0; i<N; i++) {
    X [i] += ALPHA *WW[P] [i];
    WW[R] [i] += -ALPHA *WW[Q] [i];
}
```

```
DNRM20= 0. e0;
#pragma omp parallel for private (i) reduction (+:DNRM20)
for (i=0; i<N; i++) {
    DNRM20+=WW[R] [i]*WW[R] [i];
}
```

```
#pragma omp parallel for private (j, i, k, WVAL)
for ( j=0; j<N; j++) {
    WVAL= D[j] * WW[P] [j];
    for (k=indexLU[j]; k<indexLU[j+1]; k++) {
        i=itemLU[k];
        WVAL+= AMAT[k] * WW[P] [i];
    }
    WW[Q] [j]=WVAL;
```



# solver\_SR (send)

```

do neib= 1, NEIBPETOT
  istart= EXPORT_INDEX(neib-1)
  inum  = EXPORT_INDEX(neib ) - istart
!$omp parallel do private(k, ii)
  do k= istart+1, istart+inum
    ii  = EXPORT_ITEM(k)
    WS(k)= X(ii)
  enddo

  call MPI_Isend (WS(istart+1), inum, MPI_DOUBLE_PRECISION,      &
&                NEIBPE(neib), 0, MPI_COMM_WORLD, req1(neib),  &
&                ierr)
enddo

```

```

for( neib=1;neib<=NEIBPETOT;neib++) {
  istart=EXPORT_INDEX[neib-1];
  inum  =EXPORT_INDEX[neib]-istart;
#pragma omp parallel for private (k, ii)
  for( k=istart;k<istart+inum;k++) {
    ii= EXPORT_ITEM[k];
    WS[k]= X[ii-1];
  }
  MPI_Isend(&WS[istart], inum, MPI_DOUBLE,
            NEIBPE[neib-1], 0, MPI_COMM_WORLD, &req1[neib-1]);
}

```

# Results (1/2)

$512 \times 384 \times 256 = 50,331,648$  nodes

12 nodes, 192 cores

$64^3 = 262,144$  nodes/core

512 384 256  
 ndx ndy ndz  
 pcube

	ndx,ndy,ndz (#MPI proc.)	Iter's	sec.	
Flat MPI	8 6 4 (192)	1240	73.9	
HB 1 × 16	8 6 4 (192)	1240	73.6	-Kopenmpでコンパイル, OMP_NUM_THREADS=1
HB 2 × 8	4 6 4 ( 96)	1240	78.8	
HB 4 × 4	4 3 4 ( 48)	1240	80.3	
HB 8 × 2	4 3 2 ( 24)	1240	81.1	
HB 16 × 1	2 3 2 ( 12)	1240	81.9	

# Results (2/2)

$512 \times 384 \times 256 = 50,331,648$  nodes

12 nodes, 192 cores

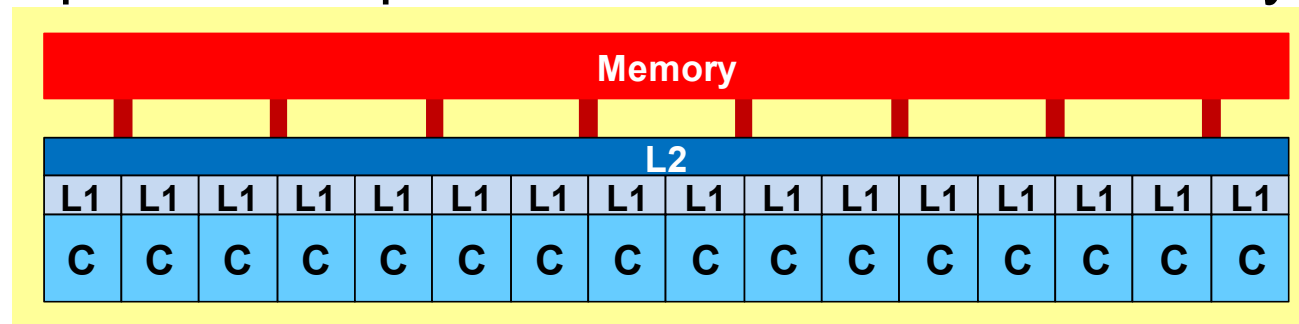
$64^3 = 262,144$  nodes/core

512	384	256
2	3	2
pcube		

OMP_NUM_THREADS	sec.	Speed-Up
1	1056.2	1.00
2	592.5	1.78
4	289.8	3.64
8	148.1	7.13
12	103.6	10.19
16	81.9	12.90
Flat MPI, 1 proc./node	1082.4	-

# Flat MPI vs. Hybrid

- Depends on applications, problem size, HW etc.
- Flat MPI is generally better for sparse linear solvers, if number of computing nodes is not so large.
  - Memory contention
- Hybrid becomes better, if number of computing nodes is larger.
  - Fewer number of MPI processes.
- Flat MPI is not realistic for Intel Xeon Phi/MIC with 240 threads/node
  - MPI process requires certain amount of memory.

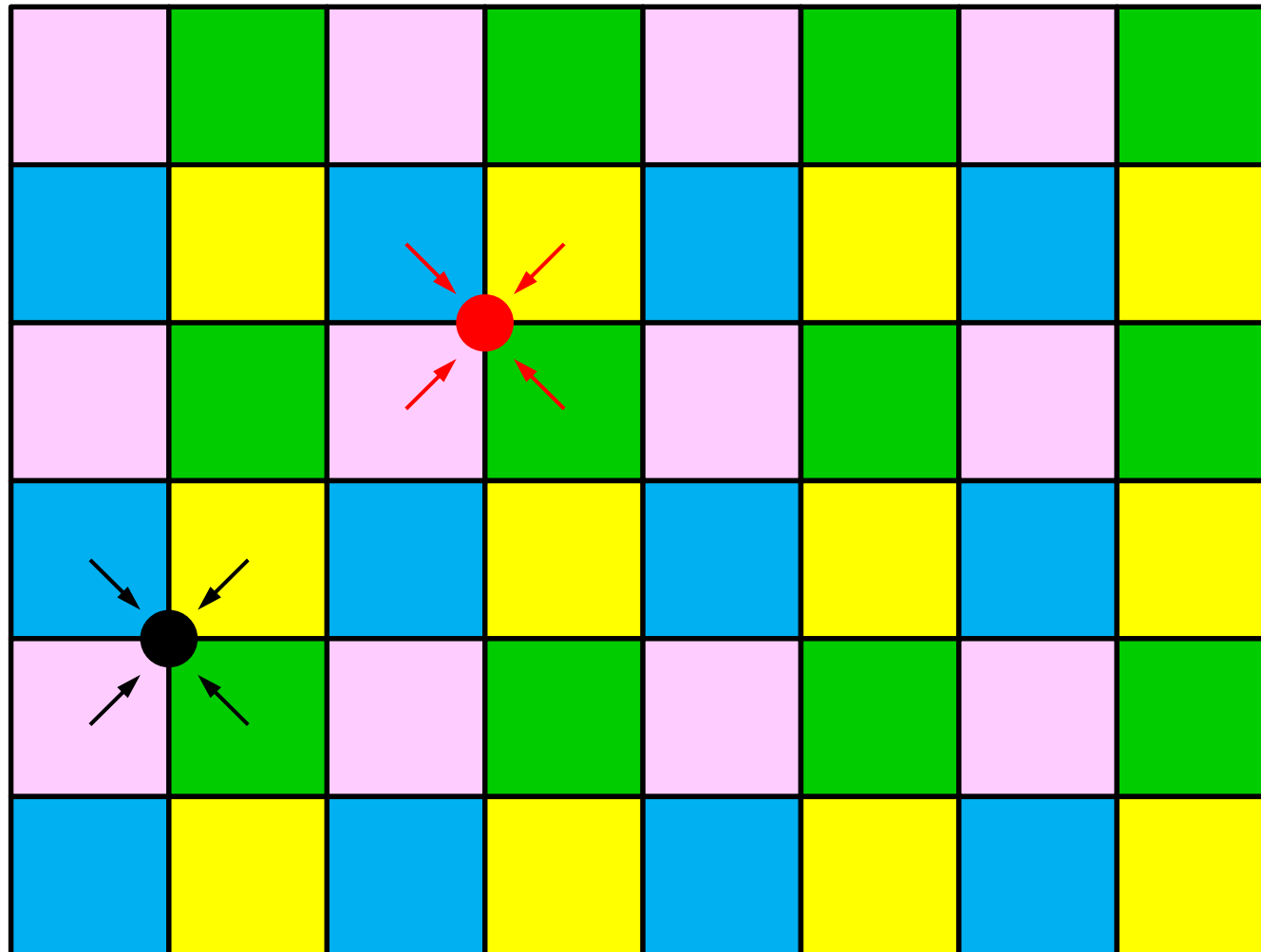


# How to apply multi-threading

- CG Solver
  - Just insert OpenMP directives
  - ILU/IC preconditioning is much more difficult
- MAT\_ASS (mat\_ass\_main, mat\_ass\_bc)
  - Data Dependency
  - Avoid to accumulate contributions of multiple elements to a single node simultaneously (in parallel)
    - results may be changed
    - deadlock may occur
  - Coloring
    - Elements in a same color do not share a node
    - Parallel operations are possible for elements in each color
    - In this case, we need only 8 colors for 3D problems (4 colors for 2D problems)
    - Coloring part is very expensive: parallelization is difficult

# Multi-Threading: Mat\_Ass

Parallel operations are possible for elements in same color (they are independent)



# Coloring (1/2)

```

allocate (ELMCOLORindex(0:NP))      Number of elements in each color
allocate (ELMCOLORitem (ICELTOT))   Element ID renumbered according to "color"
if (allocated (IWKX)) deallocate (IWKX)
allocate (IWKX(0:NP,3))

```

```

IWKX= 0
icou= 0
do icol= 1, NP
  do i= 1, NP
    IWKX(i,1)= 0
  enddo
  do icel= 1, ICELTOT
    if (IWKX(icel,2).eq.0) then
      in1= ICELNOD(icel,1)
      in2= ICELNOD(icel,2)
      in3= ICELNOD(icel,3)
      in4= ICELNOD(icel,4)
      in5= ICELNOD(icel,5)
      in6= ICELNOD(icel,6)
      in7= ICELNOD(icel,7)
      in8= ICELNOD(icel,8)

      ip1= IWKX(in1,1)
      ip2= IWKX(in2,1)
      ip3= IWKX(in3,1)
      ip4= IWKX(in4,1)
      ip5= IWKX(in5,1)
      ip6= IWKX(in6,1)
      ip7= IWKX(in7,1)
      ip8= IWKX(in8,1)
    end if
  enddo
enddo

```

# Coloring (2/2)

```

isum= ip1 + ip2 + ip3 + ip4 + ip5 + ip6 + ip7 + ip8
if (isum.eq.0) then      None of the nodes is accessed in same color
  icou= icou + 1
  IWKX(icol,3)= icou    (Current) number of elements in each color
  IWKX(icol,2)= icol
  ELMCOLORitem(icou)= icel  ID of icou-th element= icel

  IWKX(in1,1)= 1        These nodes on the same elements can not be
  IWKX(in2,1)= 1        accessed in same color
  IWKX(in3,1)= 1
  IWKX(in4,1)= 1
  IWKX(in5,1)= 1
  IWKX(in6,1)= 1
  IWKX(in7,1)= 1
  IWKX(in8,1)= 1
  if (icou.eq.ICELTOT) goto 100  until all elements are colored
endif
endif
enddo
enddo

100 continue
ELMCOLORtot= icol      Number of Colors
IWKX(0,3)= 0
IWKX(ELMCOLORtot,3)= ICELTOT

do icol= 0, ELMCOLORtot
  ELMCOLORindex(icol)= IWKX(icol,3)
enddo

```



# Multi-Threaded Matrix Assembling Procedure

```

do icol= 1, ELMCOLORTot
!$omp parallel do private (icel0, icel)                                &
!$omp& private (in1, in2, in3, in4, in5, in6, in7, in8)                &
!$omp& private (nodLOCAL, ie, je, ip, jp, kk, iiS, iiE, k)            &
!$omp& private (DETJ, PNx, PNY, PNz, QVC, QV0, COEFij, coef, SHi)     &
!$omp& private (PNXi, PNYi, PNzi, PNxj, PNYj, PNzj, ipn, jpn, kpn)    &
!$omp& private (X1, X2, X3, X4, X5, X6, X7, X8)                       &
!$omp& private (Y1, Y2, Y3, Y4, Y5, Y6, Y7, Y8)                       &
!$omp& private (Z1, Z2, Z3, Z4, Z5, Z6, Z7, Z8, CONDO)                &
do icel0= ELMCOLORindex(icol-1)+1, ELMCOLORindex(icol)
icel= ELMCOLORitem(icel0)
in1= ICELNOD(icel, 1)
in2= ICELNOD(icel, 2)
in3= ICELNOD(icel, 3)
in4= ICELNOD(icel, 4)
in5= ICELNOD(icel, 5)
in6= ICELNOD(icel, 6)
in7= ICELNOD(icel, 7)
in8= ICELNOD(icel, 8)

```

...