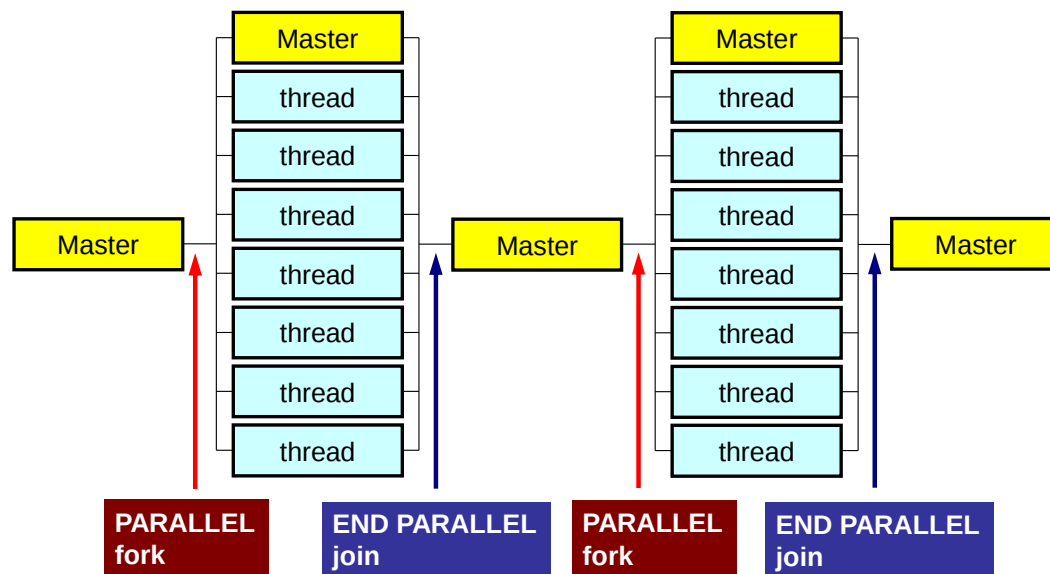


3D Parallel FEM (V) (OpenMP + MPI) Hybrid Parallel Programming Model Further Optimization

C Language

Kengo Nakajima
RIKEN R-CCS

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**

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

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

```
...
```

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

```
...
```

```
!$omp end parallel essential
```

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

```
#pragma omp for {
```

```
...
```

```
#pragma omp for {
```

```
...
```

```
}
```

SOLVER_CG (0/5): Additional Array

Mod.A: src3

```
#pragma omp parallel for {
for (i=0; i<N; i++) {
    (...)
} }
```



```
#pragma omp parallel {

ip=omp_get_thread_num();
for (i=SMPindex[ip];
     i<SMPindex[ip+1];
     i++) {
    (...)
}
}
```

PEsmpTOT: Total Number of Threads

```
#pragma omp parallel
{
    #pragma omp master
    {PEsmpTOT= omp_get_num_threads();}
}

ERROR= 0;

COMPtime=0.0;
COMMtime=0.0;

WW=(KREAL**) allocate_matrix(sizeof(KREAL), 4, NP);

allocate_vector (KREAL) WS[NP], WR[NP]
allocate_vector (KREAL) W_RH00[PEsmpTOT], W_C10[PEsmpTOT],
                    W_BNRM20[PEsmpTOT],
                    W_DNRM20[PEsmpTOT]
allocate_vector (KINT) SMPindex[PEsmpTOT+1]

nth= N/PEsmpTOT; nr = N - nth*PEsmpTOT;

for (ip=1; ip<PEsmpTOT+1; ip++) {
    SMPindex[ip]= nth;
    if (ip <= nr) SMPindex[ip]=nth+1;
}
for (ip=1; ip<PEsmpTOT+1; ip++) {
    SMPindex[ip]= SMPindex[ip-1] + SMPindex[ip];
}
```

SOLVER_CG (1/5)

Original: src2

```

/**
+-----+
| {z}= [Minv]{r} |
+-----+
**/
#pragma omp parallel for private (i)
for (i=0; i<N; i++) {
    WW[Z][i]= WW[DD][i]*WW[R][i];
}
/**
+-----+
| {RHO}= {r} {z} |
+-----+
**/
RH00= 0. e0;

#pragma omp parallel for private (i) reduction (+:RH00)
for (i=0; i<N; i++) {
    RH00+= WW[R][i]*WW[Z][i];
}

MPI_Allreduce (&RH00, &RHO, ...);

```

Mod.A: src3

```

/**
+-----+
| {z}= [Minv]{r} |
+-----+
**/
#pragma omp parallel private (ip,i,RH00)
{
    ip= omp_get_thread_num();
    for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
        WW[Z][i]= WW[DD][i]*WW[R][i];
    }
}
/**
+-----+
| {RHO}= {r} {z} |
+-----+
**/
W_RH00[ip]=0. 0;
for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
    W_RH00[ip]+= WW[R][i]*WW[Z][i];
}
}
/** END PARALLEL **/

RH00= 0. 0;
for (ip0=0; ip0<PEsmpTOT; ip0++) {
    RH00+= W_RH00[ip0];
}

MPI_Allreduce (&RH00, &RHO, ...);

```

NOT parallel

SOLVER_CG (2/5)

Original: src2

```

/**
+-----+
| {p} = {z} if      ITER=1 |
| BETA= RHO / RH01  otherwise |
+-----+
**/
if( ITER == 1 ) {
#pragma omp parallel for private (i)
    for (i=0; i<N; i++) {
        WW[P][i]=WW[Z][i];
    }
} else {
    BETA= RHO / RH01;
#pragma omp parallel for private (i)
    for (i=0; i<N; i++) {
        WW[P][i]=WW[Z][i] + BETA*WW[P][i];
    }
}

```

Mod.A: src3

```

**
+-----+
| {p} = {z} if      ITER=1 |
| BETA= RHO / RH01  otherwise |
+-----+
**/
#pragma omp parallel private (ip,i)
{
    ip= omp_get_thread_num();
    if( ITER == 1 ) {
        for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
            WW[P][i]=WW[Z][i];
        }
    } else {
        BETA= RHO / RH01;
        for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
            WW[P][i]=WW[Z][i] + BETA*WW[P][i];
        }
    }
}
}
/** END PARALLEL **/

```

SOLVER_CG (3/5)

Original: src2

```

/**
+-----+
| {q} = [A] {p} |
+-----+
**/

SOLVER_SEND_RECV (...);

#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;
}

```

Mod.A: src3

```

/**
+-----+
| {q} = [A] {p} |
+-----+
**/

SOLVER_SEND_RECV (...);

#pragma omp parallel private (ip, j, i, k, WVAL)
{
    ip= omp_get_thread_num();
    for (j=SMPindex[ip]; j<SMPindex[ip+1]; 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;
    }
}

```

“#pragma omp parallel” is still active (fork)

SOLVER_CG (4/5)

Original: src2

```

/**
+-----+
| ALPHA= RHO / {p} {q} |
+-----+
**/
C10= 0. e0;
#pragma omp parallel for private (i) reduction (+:C10)
for (i=0; i<N; i++) {
    C10+=WW[P][i]*WW[Q][i];
}
MPI_Allreduce (&C10, &C1, ...);

ALPHA= RHO / C1;

```

Mod.A: src3

```

/**
+-----+
| ALPHA= RHO / {p} {q} |
+-----+
**/
W_C10[ip]=0.0;
for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
    W_C10[ip]+= WW[P][i]*WW[Q][i];
}
}
/** END PARALLEL **/

C10= 0.0;
for (ip0=0; ip0<PEsmpTOT; ip0++) {
    C10+= W_C10[ip0];
}

MPI_Allreduce (&C10, &C1, ...);
ALPHA= RHO / C1;

```

NOT parallel

SOLVER_CG (5/5)

Original: src2

```

**
+-----+
| {x} = {x} + ALPHA*{p} |
| {r} = {r} - ALPHA*{q} |
+-----+
**/
#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];
}

MPI_Allreduce (&DNRM20, &DNRM2, ...);
RESID = sqrt(DNRM2/BNRM2);

```

Mod.A: src3

```

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

    W_DNRM20[ip] = 0.0;
    for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
        W_DNRM20[ip] += WW[R][i] * WW[R][i];
    }
}
/** END PARALLEL **/

DNRM20 = 0. e0;
for (ip0=0; ip0<PEsmpTOT; ip0++) {
    DNRM20 += W_DNRM20[ip0];
}

MPI_Allreduce (&DNRM20, &DNRM2, ...);
RESID = sqrt(DNRM2/BNRM2);

```

NOT parallel

Mod.A & B (1/5)

Mod.B: src4

```

/**
+-----+
| {z}= [Minv]{r} |
+-----+
**/
#pragma omp parallel private (ip,i,RH00)
{
    ip= omp_get_thread_num();
    for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
        WW[Z][i]= WW[DD][i]*WW[R][i];
    }
}

/**
+-----+
| {RH0}= {r} {z} |
+-----+
**/
W_RH00[ip]=0.0;
for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
    W_RH00[ip]+= WW[R][i]*WW[Z][i];
}
#pragma omp barrier
#pragma omp master
{
    RH00= 0.0;
    for (ip0=0; ip0<PEsmpTOT; ip0++) {
        RH00+= W_RH00[ip0];
    }
    MPI_Allreduce (&RH00, &RH0, ...);
}

```

Only Master Thread

“#pragma omp parallel” is still active (fork)

Mod.A: src3

```

/**
+-----+
| {z}= [Minv]{r} |
+-----+
**/
#pragma omp parallel private (ip,i,RH00)
{
    ip= omp_get_thread_num();
    for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
        WW[Z][i]= WW[DD][i]*WW[R][i];
    }
}

/**
+-----+
| {RH0}= {r} {z} |
+-----+
**/
W_RH00[ip]=0.0;
for (i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
    W_RH00[ip]+= WW[R][i]*WW[Z][i];
}
}
/** END PARALLEL **/

RH00= 0.0;
for (ip0=0; ip0<PEsmpTOT; ip0++) {
    RH00+= W_RH00[ip0];
}

MPI_Allreduce (&RH00, &RH0, ...);

```

NOT parallel

Mod.A & B (2/5)

Mod.B: src4

```

/**
+-----+
| {p} = {z} if      ITER=1 |
| BETA= RHO / RH01 otherwise |
+-----+
**/
#pragma omp barrier
if( ITER == 1 ) {
    for(i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
        WW[P][i]=WW[Z][i];
    }
} else {
    BETA= RHO / RH01;
    for(i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
        WW[P][i]=WW[Z][i] + BETA*WW[P][i];
    }
}
}
/** END PARALLEL **/

```

Mod.A: src3

```

**
+-----+
| {p} = {z} if      ITER=1 |
| BETA= RHO / RH01 otherwise |
+-----+
**/
#pragma omp parallel private (ip,i)
{
    ip= omp_get_thread_num();
    if( ITER == 1 ) {
        for(i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
            WW[P][i]=WW[Z][i];
        }
    } else {
        BETA= RHO / RH01;
        for(i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
            WW[P][i]=WW[Z][i] + BETA*WW[P][i];
        }
    }
}
}
/** END PARALLEL **/

```

Mod.A & B (3/5)

Mod.B: src4

```

/**
+-----+
| {q}= [A] {p} |
+-----+
**/

SOLVER_SEND_RECV (...);

#pragma omp parallel private (ip, j, i, k, WVAL)
{
    ip= omp_get_thread_num();
    for (j=SMPindex[ip]; j<SMPindex[ip+1]; 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;
    }
}

```

Mod.A: src3

```

/**
+-----+
| {q}= [A] {p} |
+-----+
**/

SOLVER_SEND_RECV (...);

#pragma omp parallel private (ip, j, i, k, WVAL)
{
    ip= omp_get_thread_num();
    for (j=SMPindex[ip]; j<SMPindex[ip+1]; 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;
    }
}

```

“#pragma omp parallel” is still active (fork)

Mod.A & B (4/5)

Mod.B: src4

```

/**
+-----+
| ALPHA= RHO / {p} {q} |
+-----+
**/
W_C10[ip]=0.0;
for(i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
    W_C10[ip] += WW[P][i]*WW[Q][i];
}
#pragma omp barrier

#pragma omp master
{
    C10= 0.0;
    for(ip0=0; ip0<PEsmpTOT; ip0++) {
        C10 += W_C10[ip0];
    }

    MPI_Allreduce (&C10, &C1, ...);
}

#pragma omp barrier
ALPHA= RHO / C1;

```

Only Master Thread

“#pragma omp parallel” is still active (fork)

Mod.A: src3

```

/**
+-----+
| ALPHA= RHO / {p} {q} |
+-----+
**/
W_C10[ip]=0.0;
for(i=SMPindex[ip]; i<SMPindex[ip+1]; i++) {
    W_C10[ip] += WW[P][i]*WW[Q][i];
}
}
/** END PARALLEL **/

C10= 0.0;
for(ip0=0; ip0<PEsmpTOT; ip0++) {
    C10 += W_C10[ip0];
}

MPI_Allreduce (&C10, &C1, ...);
ALPHA= RHO / C1;

```

NOT parallel

Mod.A & B (5/5)

Mod.B: src4

```

/**
+-----+
| {x}= {x} + ALPHA*{p} |
| {r}= {r} - ALPHA*{q} |
+-----+
**/

for(i=SMPindex[ip];i<SMPindex[ip+1];i++) {
    X[i] += ALPHA *WW[P][i];
    WW[R][i] += -ALPHA *WW[Q][i];
}

W_DNRM20[ip]=0.0;
for(i=SMPindex[ip];i<SMPindex[ip+1];i++) {
    W_DNRM20[ip] += WW[R][i]*WW[R][i];
}

}
/** END PARALLEL **/

DNRM20= 0. e0;
for(ip0=0;ip0<PEsmpTOT;ip0++) {
    DNRM20 += W_DNRM20[ip0];
}

MPI_Allreduce (&DNRM20, &DNRM2, ...);
RESID= sqrt(DNRM2/BNRM2);

```

NOT parallel

Mod.A: src3

```

/**
+-----+
| {x}= {x} + ALPHA*{p} |
| {r}= {r} - ALPHA*{q} |
+-----+
**/

#pragma omp parallel private (ip,i)
{
    ip= omp_get_thread_num();
    for(i=SMPindex[ip];i<SMPindex[ip+1];i++) {
        X[i] += ALPHA *WW[P][i];
        WW[R][i] += -ALPHA *WW[Q][i];
    }

    W_DNRM20[ip]=0.0;
    for(i=SMPindex[ip];i<SMPindex[ip+1];i++) {
        W_DNRM20[ip] += WW[R][i]*WW[R][i];
    }
}

}
/** END PARALLEL **/

DNRM20= 0. e0;
for(ip0=0;ip0<PEsmpTOT;ip0++) {
    DNRM20 += W_DNRM20[ip0];
}

MPI_Allreduce (&DNRM20, &DNRM2, ...);
RESID= sqrt(DNRM2/BNRM2);

```

NOT parallel

Features of Each Implementation

- Original
 - All loops are *!\$omp parallel do/#pragma omp parallel for*
- Mod.A
 - *!\$omp parallel/#pragma omp parallel* blocks: 4 blocks
 - NO *!\$omp do/#pragma omp for*
- Mod.B
 - *!\$omp parallel/#pragma omp parallel* blocks: 2 blocks
 - Before/After SEND-RECV
 - Could be a Single Block
 - NO *!\$omp do/#pragma omp for*
 - Overhead of *!\$omp master/#pragma omp master*
 - Overhead of *!\$omp barrier/#pragma omp barrier*
- Mod.A and Mod.B are better if thread# is larger

OpenMP (Mod.A, Mod.B) (F·C)

```
>$ cd /work/gt36/t36XXX/pFEM/pfem3d/src3
```

Mod.A: src3

```
>$ module load fj
```

```
>$ make
```

```
>$ cd ../run
```

```
>$ ls sol3  
sol3
```

```
>$ cd /work/gt36/t36XXX/pFEM/pfem3d/src4
```

Mod.B: src4

```
>$ module load fj
```

```
>$ make
```

```
>$ cd ../run
```

```
>$ ls sol4  
sol4
```

y12.sh

```
#!/bin/sh
#PJM -N "hb-12"
#PJM -L rscgrp=lecture5-o
#PJM -L node=12
#PJM --mpi proc=48
#PJM --omp thread=12
#PJM -L elapse=00:15:00
#PJM -g gt55
#PJM -j
#PJM -e err
#PJM -o y12.lst
```

```
module load fj
module load fjmpi
```

```
export OMP_NUM_THREADS=12
export XOS_MMM_L_PAGING_POLICY=demand:demand:demand
```

```
mpiexec ./sol2
mpiexec ./sol3
mpiexec ./sol4
mpiexec numactl -l ./sol2
mpiexec numactl -l ./sol3
mpiexec numactl -l ./sol4
```

Time for PCG Solver

$N=256 \times 256 \times 192$, 12-nodes

