Introduction to Parallel Programming for Multicore/Manycore Clusters

Part II-2: Parallel FVM using OpenMP

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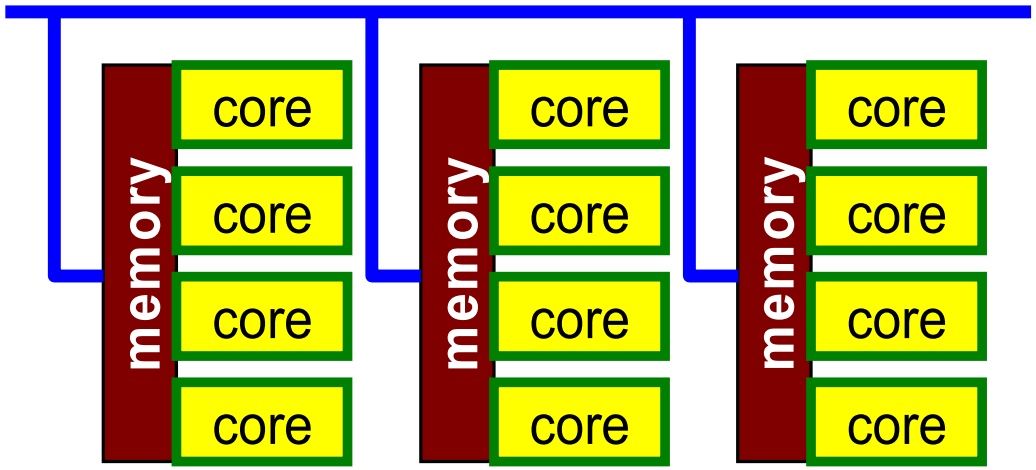
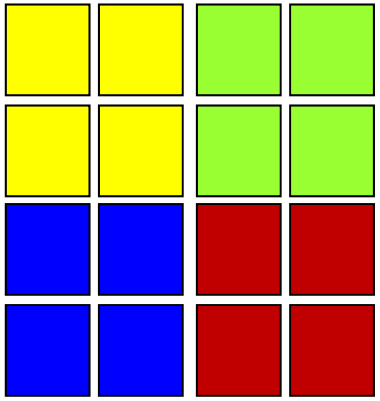
- OpenMP
- Parallel Version of the Code by OpenMP
- STREAM

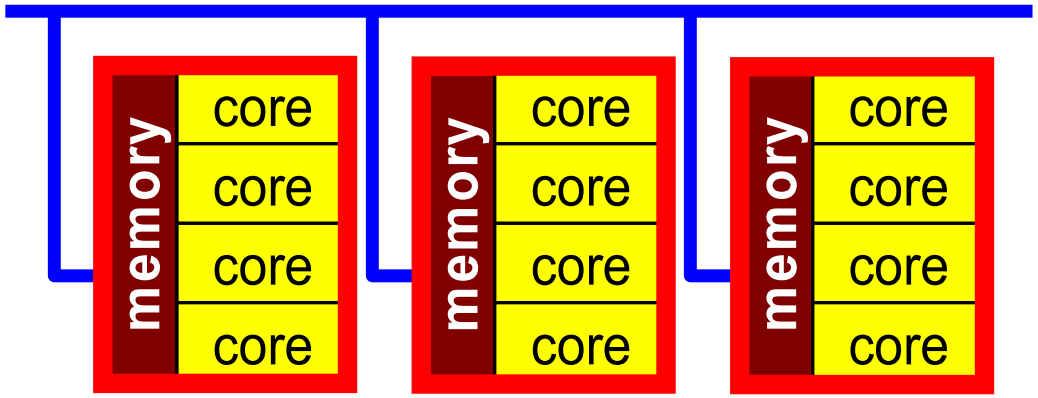
Flat MPI vs. Hybrid

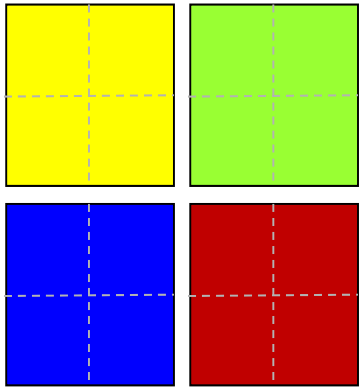
Flat-MPI：Each Core -> Independent

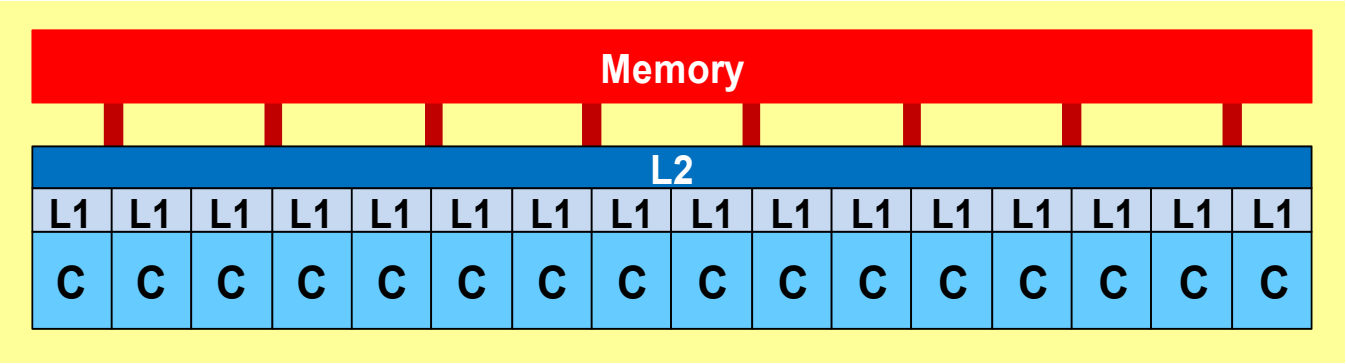




Hybrid：Hierarchal Structure







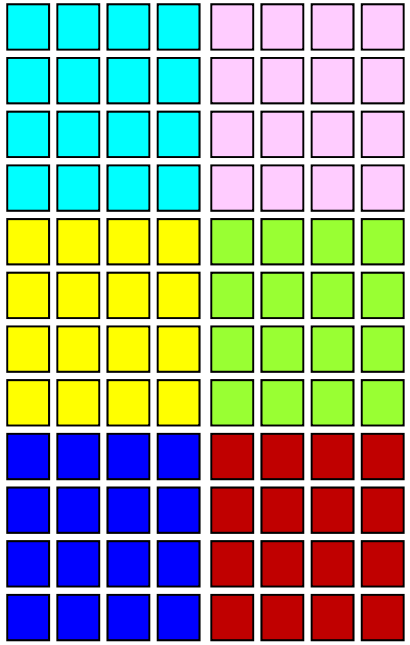
HB M x N

Number of OpenMP threads per a single MPI process

Number of MPI process per a single node

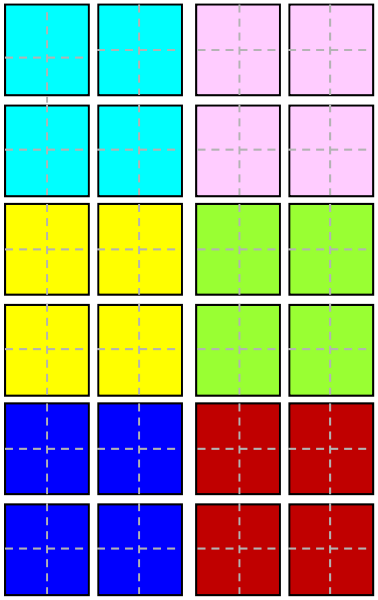
Size of data for each MPI process varies according to HB MxN

example: 6 nodes, 96 cores



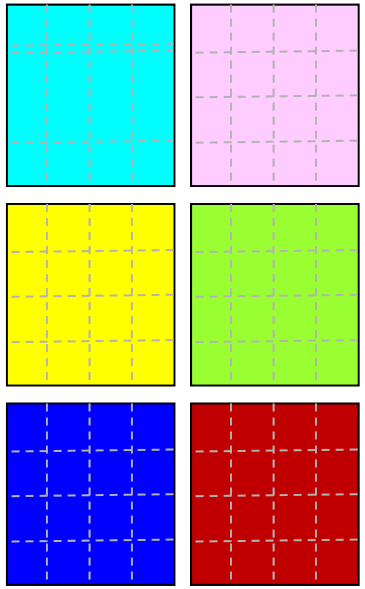
Flat MPI

```
128  192  64
  8   12   1
pcube
```



HB 4x4

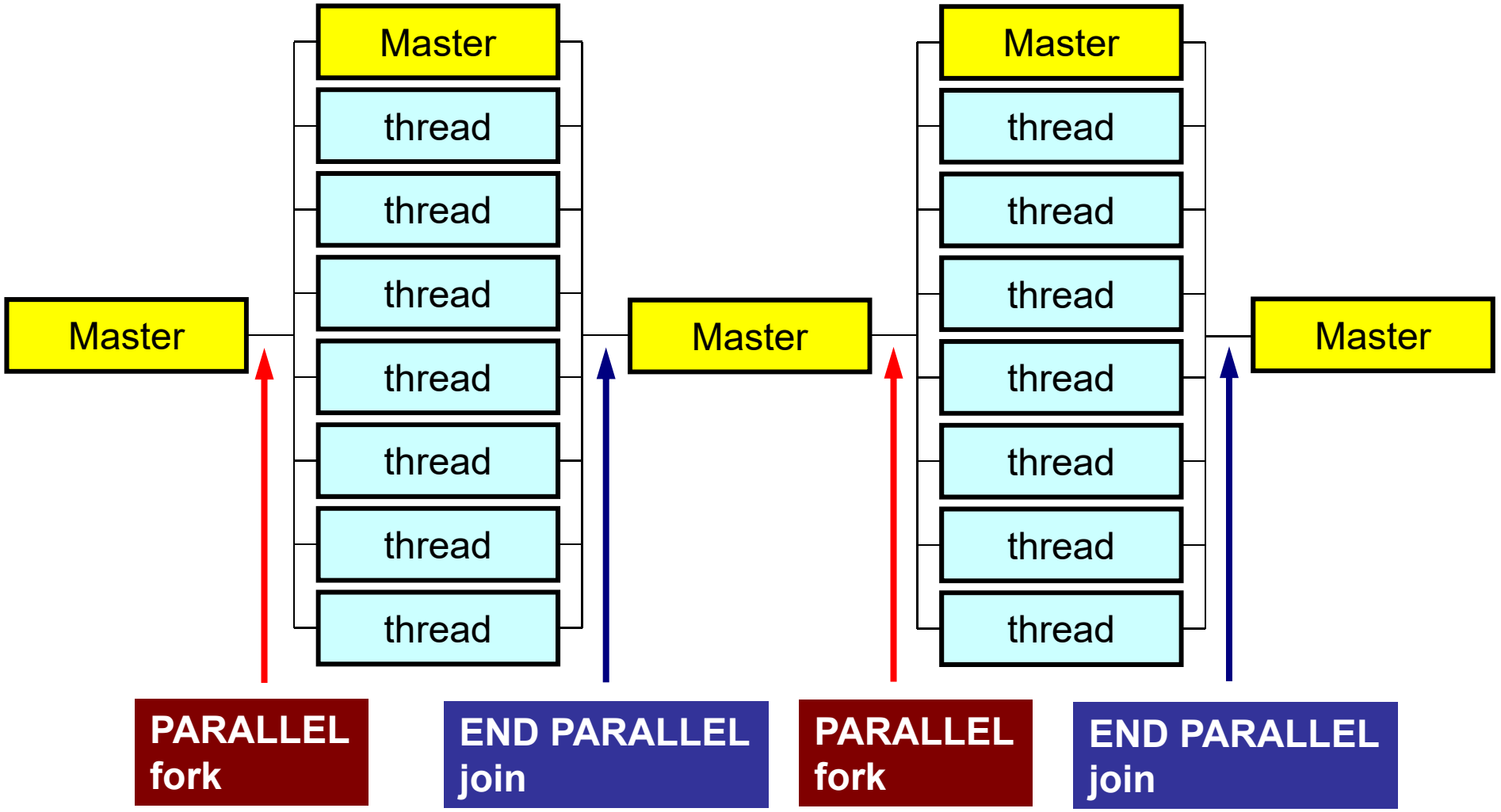
```
128  192  64
  4    6   1
pcube
```



HB 16x1

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

Fork-Join Parallel Execution Model



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

```
#pragma omp parallel for private (i)
 for (i=0; i<N; i++) {
      X[i] = 0.0;
      W[0][i] = 0.0;
      W[1][i] = 0.0;
      W[2][i] = 0.0;
 }
```

Dot Products

```
RHO = 0.0;
#pragma omp parallel for private (i)
 reduction (+:RHO)
 for(i=0; i<N; i++) {
     RHO += W[R][i] * W[Z][i];
 }
```

DAXPY

```
#pragma omp parallel for private (i)
 for (i=0; i<N; i++) {
    Y[i] = Y[i} + alpha*X[i];
 }
```

OpenMP/Direceives Matrix/Vector Products

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

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)

Features of OpenMP (cont.)

- “for” loops with “#pragma omp parallel for”
- Global (Shared) Variables, Private Variables
  - Default: Global (Shared)
  - Dot Products: reduction

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

```
RHO = 0.0;
#pragma omp parallel for private (i) reduction (+:RHO)
 for(i=0; i<N; i++) {
     RHO += W[R][i] * W[Z][i];
 }
```

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];
}
```

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

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

```
#pragma omp parllel for
 for(i=0; i<N; i++){
     B[i]= (A[i] + B[i]) * 0.50;
 }
```

- Default status of loop variables (“i” in this case) is private. Therefore, explicit declaration is not needed.

Example-1: REDUCTION

```
#pragma omp parallel default(private) reduction(+:A,B)
 for(i=0; i<N; i++){
     err= work(Alocal, Blocal);
     A= A + Alocal;
     B= B + Blocal;
 }
```

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= 0.0;
for(i=0; i<N; i++){
  VAL= VAL + W[R][i] * W[Z][i];
}
```

OpenMP for Dot Products

```
    VAL= 0.0;
    for(i=0; i<N; i++){
      VAL= VAL + W[R][i] * W[Z][i];
    }
```

```
    VAL= 0.0;
#pragma omp parallel for private (i) reduction(+:VAL)
    for(i=0; i<N; i++){
      VAL= VAL + W[R][i] * W[Z][i];
    }
```

Directives are just inserted.

OpenMP for Dot Products

```
      VAL= 0.0;
      for(i=0; i<N; i++){
        VAL= VAL + W[R][i] * W[Z][i];
      }
```

```
      VAL= 0.0;
#pragma omp parallel for private (i) reduction(+:VAL)
      for(i=0; i<N; i++){
        VAL= VAL + W[R][i] * W[Z][i];
      }
```

Directives are just inserted.

```
       VAL= 0.0;
#pragma omp parallel for private (i,ip)
 reduction(+:VAL)
      for(ip=0; ip<PEsmpTOT; ip++){
          for (i=INDEX[ip]; i<INDEX[ip+1]; i++){
             VAL= VAL + W[R][i] * W[Z][i];
          }
      }
```

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= 0.0;
#pragma omp parallel for private (i,ip)
 reduction(+:VAL)
    for(ip=0; ip<PEsmpTOT; ip++){
        for (i=INDEX[ip]; i<INDEX[ip+1]; i++){
           VAL= VAL + W[R][i] * W[Z][i];
        }
    }
```

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

```
for(i=0; i<N; i++) {
    VAL = D[i] * W[P][i];
    for(j=indexLU[i]; j<indexLU[i+1]; j++) {
        VAL += AMAT[j] * W[P][itemLU[j]-1];
    }

    W[Q][i] = VAL;
}
```

Matrix-Vector Multiply

```
#pragma omp parallel for private(ip,i,VAL,j)
 for (ip=0; ip<PEsmpTOT; ip++){
      for(i=SMPindexG[ip]; i<SMPindexG[ip+1]; i++){
          VAL = D[i] * W[P][i];
          for(j=indexLU[i]; j<indexLU[i+1]; j++) {
              VAL += AMAT[j] * W[P][itemLU[j]-1];
          }

          W[Q][i] = VAL;
      }
 }
```

Matrix-Vector Multiply: Other Approach

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

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

          W[Q][i] = VAL;
 }
```

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 {
```

- OpenMP
- **Parallel Version of the Code by OpenMP**
- STREAM

Target for Parallelization

- FVM code
- Preconditioned CG solver: PCG
  - Diagonal Scaling, Point Jacobi
- NO sample code.
- Please develop the parallel code by yourself

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)= p(i-1) + βi-1 z(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.

Files on Oakleaf-FX (1/2)

```
>$ cd

>$ cp /home/z30088/omp/omp2-c.tar .
>$ cp /home/z30088/omp/omp2-f.tar .

>$ tar xvf omp2-c.tar
>$ tar xvf omp2-f.tar

>$ cd multicore
```

Confirm Directories:

```
omp2  stream
```

```
<$O-omp2>, <$O-stream>
```

Files on Oakleaf-FX (2/2)

```
>$ cd <$O-omp2>
>$ cd src

>$ make

>$ cd ../run
>$ pjsub go.sh
```

<$O-omp2>/src/Makefile

NOT for parallel computing

```
CC         = fccpx          : Compiler
OPTFLAGS   = -Kfast         : Optimization
TARGET     = ../run/sol     : Exec File

.SUFFIXES:
.SUFFIXES: .o .c

.c.o:
        $(CC) -c $(CFLAGS) $(OPTFLAGS) $< -o $@

OBJS = input.o pointer_init.o ¥
       boundary_cell.o cell_metrics.o ¥
       rcm.o ...

HEADERS = ¥
        struct.h struct_ext.h ¥
        pcg.h ...

all: $(TARGET)
$(TARGET): $(OBJS)
        $(CC) $(CFLAGS) $(OPTFLAGS) -o $@ $(OBJS) $(LDFLAGS)

$(OBJS): $(HEADERS)

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

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 (16 cores) is occupied by each job.
  - Your node is not shared by other jobs.

Job Script

- **<$O-omp>/run/go.sh**
- Scheduling + Shell Script

```
#!/bin/sh
#PJM -L “node=1“                Number of Nodes
#PJM -L “elapse=00:10:00“       Computation Time
#PJM -L “rscgrp=lecture7“       Name of “QUEUE”
#PJM -g “gt17“                  Group Name (Wallet)
#PJM -j
#PJM -o “test.lst“              Standard Output

./sol                           Execs
```

Available QUEUE's

- Following 2 queues are available.
- 1 Tofu (12 nodes) can be used
  - **`lecture`**
    - 12 nodes (192 cores), 15 min., **valid until March 30 08:30**
    - Shared by all "educational" users
  - **`lecture7`**
    - 12 nodes (192 cores), 15 min., active during class time (09:00-17:00)
    - **More jobs (compared to `lecture`) can be processed up on availability.**
    - **Just during until Feb.23 17:00**
- **Please use "`lecture`" after Feb.24 !!**

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 --rsc -b`
• Limitation of submission	`pjstat --limit`

```
[z30088@oakleaf-fx-6 S2-ref]$ pjstat

Oakleaf-FX scheduled stop time: 2012/09/28(Fri) 09:00:00 (Remain: 31days 20:01:46)

JOB_ID     JOB_NAME   STATUS  PROJECT  RSCGROUP  START_DATE        ELAPSE          TOKEN NODE:COORD
334730     go.sh      RUNNING gt61     lecture   08/27 12:58:08    00:00:05          0.0 1
```

solve_PCG (1/3)

```
for(i=0; i<N; i++) {
    W[DD][i]= 1.e0/D[i];
}

...


for(L=0; L<(*ITR); L++) {

/*******************
 * {z} = [Minv]{r} *
 *******************/
    for(i=0; i<N; i++) {
        W[Z][i] = W[R][i]*W[DD][i];
    }


/*****************
 * RHO = {r}{z} *
 *****************/
    RHO = 0.0;
    for(i=0; i<N; i++) {
        RHO += W[R][i] * W[Z][i];
    }
```

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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
  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 (2/3)

```
/**********************************
 * {p}  = {z} if      ITER=0    *
 * BETA = RHO / RHO1  otherwise *
 **********************************/

if(L == 0) {
   for(i=0; i<N; i++) {
       W[P][i] = W[Z][i];
   }
   } else {
   BETA = RHO / RHO1;
   for(i=0; i<N; i++) {
       W[P][i] = W[Z][i] + BETA * W[P][i];
   }
}

/*****************
 * {q} = [A]{p} *
 *****************/

for(i=0; i<N; i++) {
    VAL = D[i] * W[P][i];
    for(j=indexLU[i]; j<indexLU[i+1]; j++) {
        VAL += AMAT[j] * W[P][itemLU[j]-1];
    }
    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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
  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 (3/3)

```
/*************************
 * ALPHA = RHO / {p}{q} *
 *************************/
C1 = 0.0;
for(i=0; i<N; i++) {
    C1 += W[P][i] * W[Q][i];
}
ALPHA = RHO / C1;

/*****************************
 * {x} = {x} + ALPHA * {p} *
 * {r} = {r} - ALPHA * {q} *
 *****************************/
for(i=0; i<N; i++) {
    X[i]    += ALPHA * W[P][i];
    W[R][i] -= ALPHA * W[Q][i];
}

DNRM2 = 0.0;
for(i=0; i<N; i++) {
    DNRM2 += W[R][i]*W[R][i];
}

ERR = sqrt(DNRM2/BNRM2);
if((L+1)%100 ==1) {
   fprintf(stderr, "%5d%16.6e¥n", L+1, ERR);
}
if(ERR < EPS) {
   *IER = 0; goto N900;
  } else {
   RHO1 = RHO;
  }
}
*IER = 1;
```

r= b-[A]x
DNRM2=|r|²
BNRM2=|b|²

ERR= |r|/|b|

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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
  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

Parallelization by OpenMP

- Focusing on “solver_PCG.c” (solve_PCG)
- Just insert OpenMP directives

```
>$ cd <$O-omp2>
>$ cd ex
(modify files)

>$ make
>$ cd ../run
>$ pjsub g.sh
```

```
#!/bin/sh
#PJM -L "node=1"
#PJM -L "elapse=00:10:00"
#PJM -L "rscgrp=lecture7"
#PJM -g "gt17"
#PJM -j
#PJM -o "100_08_002.lst"

export OMP_NUM_THREADS=8      1-16
./sol0
```

<$O-omp2>/ex/Makefile

parallel computing by OpenMP

```
CC         = fccpx           : Compiler
OPTFLAGS   = -Kfast,openmp   : Optimization + OpenMP
TARGET     = ../run/sol0     : Exec File

.SUFFIXES:
.SUFFIXES: .o .c

.c.o:
        $(CC) -c $(CFLAGS) $(OPTFLAGS) $< -o $@

OBJS = input.o pointer_init.o ¥
       boundary_cell.o cell_metrics.o ¥
       rcm.o ...

HEADERS = ¥
        struct.h struct_ext.h ¥
        pcg.h ...

all: $(TARGET)
$(TARGET): $(OBJS)
        $(CC) $(CFLAGS) $(OPTFLAGS) -o $@ $(OBJS) $(LDFLAGS)

$(OBJS): $(HEADERS)

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

solve_PCG (1/5)

parallel computing by OpenMP

```
#include <stdio.h>
#include <stdlib.h>
#include <string.h>
#include <errno.h>
#include <math.h>
#include <omp.h>

#include "solver_PCG.h"

extern int
solve_PCG (int N, int NPLU, int *indexLU, int *itemLU,
                  double *D, double *B, double *X, double *AMAT,
                  double EPS, int *ITR, int *IER, int *N2)
{
        double **W;
        double VAL, BNRM2, WVAL, SW, RHO, BETA, RHO1, C1, DNRM2, ALPHA, ERR;
        double Stime, Etime;
        int i, j, ic, ip, L, ip1, N3;
        int R = 0;
        int Z = 1;
        int Q = 1;
        int P = 2;
        int DD = 3;
```

solve_PCG (2/5)

```
#pragma omp parallel for private (i)
        for(i=0; i<N; i++) {
                X[i] = 0.0;
                W[1][i] = 0.0;
                W[2][i] = 0.0;
                W[3][i] = 0.0;
        }

#pragma omp parallel for private (i,VAL,j)
        for(i=0; i<N; i++) {
            VAL = D[i] * X[i];
            for(j=indexLU[i]; j<indexLU[i+1]; j++) {
               VAL += AMAT[j] * X[itemLU[j]-1];
            }
            W[R][i] = B[i] - VAL;
        }

BNRM2 = 0.0;
#pragma omp parallel for private (i) reduction
(+:BNRM2)
        for(i=0; i<N; i++) {
          BNRM2 += B[i]*B[i];
        }

#pragma omp parallel for private (i)
        for(i=0; i<N; i++) {
          W[DD][i]= 1.e0/D[i];
        }
```

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
  - $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
  - $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
- 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();

for(L=0; L<(*ITR); L++) {

#pragma omp parallel for private (i)
   for(i=0; i<N; i++) {
       W[Z][i] = W[R][i]*W[DD][i];
   }

RHO = 0.0;
#pragma omp parallel for private (i)
reduction(+:RHO)
    for(i=0; i<N; i++) {
        RHO += W[R][i] * W[Z][i];
    }

if(L == 0) {
#pragma omp parallel for private (i)
    for(i=0; i<N; i++) {
        W[P][i] = W[Z][i];
    }
    } else {
        BETA = RHO / RHO1;}
#pragma omp parallel for private (i)
    for(i=0; i<N; i++) {
        W[P][i] = W[Z][i] + BETA * W[P][i];
    }
}
```

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
    $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
    $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
  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)

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

C1 = 0.0;
#pragma omp parallel for private (i) reduction(+:C1)
    for(i=0; i<N; i++) {
        C1 += W[P][i] * W[Q][i];
    }
    ALPHA = RHO / C1;

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

DNRM2 = 0.0;
#pragma omp parallel for private (i) reduction(+:DNRM2)
    for(i=0; i<N; i++) {
        DNRM2 += W[R][i]*W[R][i];
    }
    ERR = sqrt(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
  - $\beta_{i-1}= \rho_{i-1}/\rho_{i-2}$
  - $p^{(i)}= z^{(i-1)} + \beta_{i-1}\ p^{(i)}$
- 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();

for(L=0; L<(*ITR); L++) {
...
        if(ERR < EPS) {
          *IER = 0;
          goto N900;
        } else {
          RHO1 = RHO;
        }
}
        *IER = 1;
N900:
        Etime = omp_get_wtime();

        fprintf(stderr, "%5d%16.6e¥n", L+1, ERR);
        fprintf(stderr, "%16.6e sec. (solver)¥n", Etime - Stime);

        *ITR = L;
        free(W);
        return 0;
}
```

Elapsed Time= Etime - Stime

Etime-Stime

NX=NY=NZ=100, 10^6 DOF

```
#!/bin/sh
#PJM -L "node=1"
#PJM -L "elapse=00:10:00"
#PJM -L "rscgrp=lecture7"
#PJM -g "gt17"
#PJM -j
#PJM -o "100_08_002.lst"

export OMP_NUM_THREADS=M      M=1,4 8,16
./sol
```

M	sec.	Speed-Up
1	33.7	1.00
4	8.73	3.86
8	4.95	6.80
16	3.30	10.20

Exercises

- Develop your own program by inserting OpenMP directives !

- Effect of problem size (NX, NY, NZ)
- Effect of Thread # (OMP_NUM_THREADS: 1-16)

- OpenMP
- Login to FX10
- Parallel Version of the Code by OpenMP
- **STREAM**

Why less than 16x ?

- Memory Contention
- Performance of memory per each thread decreases if number of threads on each node increases
- Sparse Matrix Solver: Memory-Bound
  - Effect of this decreasing is more significant
- Problem size is not so larger

Sparse/Dense Matrices

```
for(i=0;i<N;i++){
    Y[i] = Diag[i] * X[i];
    for(k=Index[i];k<Index[i+1];k++){
        Y[i] += AMat[k]*X[Item[k]];
    }
}
```

```
for(j=0;j<N;i++){
  Y[j]= 0.0;
  for (i=0;i<N;i++){
    Y[j]+= A[j][i]*X[i];
  }
}
```

- “X” in RHS
  - Dense: continuous on memory, easy to utilize cache
  - Sparse: continuity is not assured, difficult to utilize cache
    - more “memory-bound”

GeoFEM Benchmark

ICCG in FEM for Solid Mechanics

	SR11K/J2	SR16K/M1	T2K	FX10	京
Core #/Node	16	32	16	16	8
Peak Performance (GFLOPS)	147.2	980.5	147.2	236.5	128.0
STREAM Triad (GB/s)	101.0	264.2	20.0	64.7	43.3
B/F	0.686	0.269	0.136	0.274	0.338
GeoFEM (GFLOPS)	19.0	72.7	4.69	16.0	11.0
% to Peak	12.9	7.41	3.18	6.77	8.59
LLC/core (MB)	18.0	4.00	2.00	0.75	0.75

Sparse Linear Solver: Memory-Bound

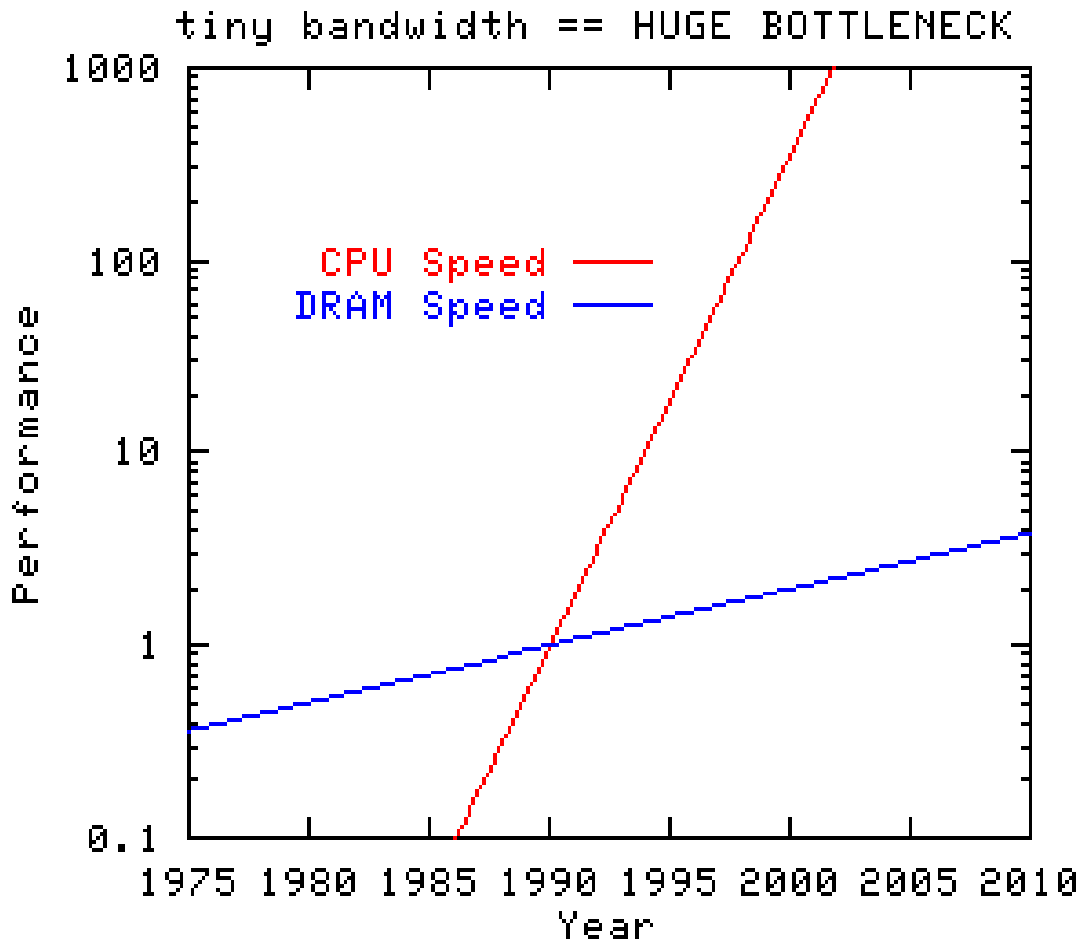
STREAM benchmark

http://www.cs.virginia.edu/stream/

- Benchmarks for Memory Bandwidth
  - Copy: c(i)= a(i)
  - Scale: c(i)= s*b(i)
  - Add: c(i)= a(i) + b(i)
  - Triad: c(i)= a(i) + s*b(i)

```
-------------------------------------------------
 Double precision appears to have 16 digits of accuracy
 Assuming 8 bytes per DOUBLE PRECISION word
-------------------------------------------------
 Number of processors =           16
 Array size =    2000000
 Offset     =          0
 The total memory requirement is     732.4 MB
(     45.8MB/task)
 You are running each test  10 times
 --
 The *best* time for each test is used
 *EXCLUDING* the first and last iterations
 -----------------------------------------------------
 -----------------------------------------------------
Function     Rate (MB/s)  Avg time   Min time  Max time
Copy:      18334.1898      0.0280      0.0279      0.0280
Scale:     18035.1690      0.0284      0.0284      0.0285
Add:       18649.4455      0.0412      0.0412      0.0413
Triad:     19603.8455      0.0394      0.0392      0.0398
```

Gap between performance of CPU and Memory



http://www.cs.virginia.edu/stream/

OpenMP version of STREAM

```
>$ cd <$O-stream>
>$ pjsub go.sh
```

- http://www.cs.virginia.edu/stream/
- C, Fortran, MPI, OpenMP etc.

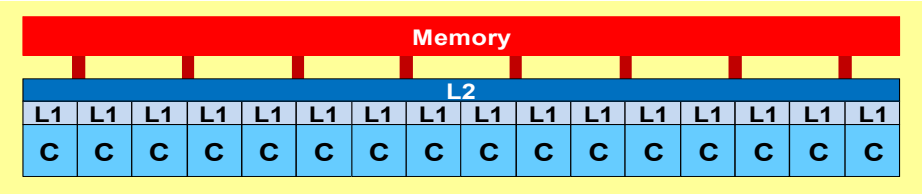
go.sh

```
#!/bin/sh
#PJM -L "rscgrp=lecture7"
#PJM -L "node=1"
#PJM -L "elapse=10:00"
#PJM -j

export PATH=…
export LD_LIBRARY_PATH=…
export PARALLEL=16
export OMP_NUM_THREADS=16        Number of threads (1-16)

./stream.out > 16-01.lst 2>&1    Name of output file
```

Results of Triad

<$O-stream>/stream/*.lst

Peak is 85.3 GB/sec., 75%



Thread #	MB/sec.	Speed-up
1	8606.14	1.00
2	16918.81	1.97
4	34170.72	3.97
8	59505.92	6.91
16	64714.32	7.52

Exercises

- Running the code
- Try various number of threads (1-16)
- MPI-version and Single PE version are available
  - Fortran, C
  - Web-site of STREAM