Report S1
C

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Technical & Scientific Computing II (4820-1028)
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Hybrid Distributed Parallel Computing (3747-111)

Report S1

- Problem S1-1
  - Read local files <$O-S1>/a1.0~a1.3, <$O-S1>/a2.0~a2.3.
  - Develop codes which calculate norm ||x|| of global vector for each case.
    - <$O-S1>file.c, <$O-S1>file2.c
- Problem S1-3
  - Develop parallel program which calculates the following numerical integration using “trapezoidal rule” by MPI_Reduce, MPI_Bcast etc.
  - Measure computation time, and parallel performance

$$\int_0^1 \frac{4}{1+x^2}\,dx$$

Copying files on Reedbush-U

Copy

```
>$ cd <$O-TOP>
>$ cp /lustre/gt29/z30088/class_eps/C/s1r-c.tar .
>$ tar xvf s1r-c.tar
```

Confirm directory

```
>$ ls
    mpi
>$ cd mpi/S1-ref
```

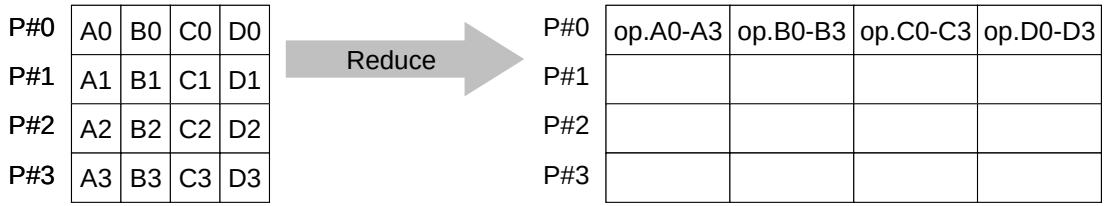
This directory is called as **<$O-S1r>**.

<$O-S1r> = <$O-TOP>/mpi/S1-ref

S1-1：Reading Local Vector, Calc. Norm

- Problem S1-1
  - Read local files <$O-S1>/a1.0~a1.3, <$O-S1>/a2.0~a2.3.
  - Develop codes which calculate norm ||x|| of global vector for each case.
- Use MPI_Allreduce (or MPI_Reduce)
- Advice
  - Checking each component of variables and arrays !

MPI_Reduce



- Reduces values on all processes to a single value
  - Summation, Product, Max, Min etc.

- **MPI_Reduce (sendbuf,recvbuf,count,datatype,op,root,comm)**
  - **sendbuf** choice I starting address of send buffer
  - **recvbuf** choice O starting address receive buffer
    type is defined by "**datatype**"
  - **count** int I number of elements in send/receive buffer
  - **datatype** MPI_Datatype I data type of elements of send/recive buffer
    FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.
    C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc
  - **op** MPI_Op I reduce operation
    MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD, MPI_LAND, MPI_BAND etc
    Users can define operations by **MPI_OP_CREATE**
  - **root** int I rank of root process
  - **comm** MPI_Comm I communicator

Send/Receive Buffer (Sending/Receiving)

- Arrays of “send (sending) buffer” and “receive (receiving) buffer” often appear in MPI.

- Addresses of “send (sending) buffer” and “receive (receiving) buffer” must be different.

“op” of MPI_Reduce/Allreduce

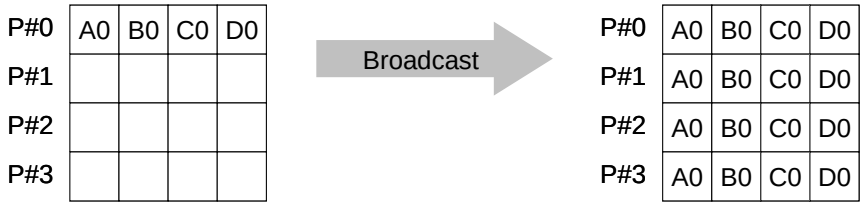
MPI_Reduce
(sendbuf,recvbuf,count,datatype,op,root,comm)

- **MPI_MAX**, **MPI_MIN** Max, Min
- **MPI_SUM**, **MPI_PROD** Summation, Product
- **MPI_LAND** Logical AND

```
double X0, XSUM;

MPI_Reduce
(&X0, &XSUM, 1, MPI_DOUBLE, MPI_SUM, 0, <comm>)
```

```
double X0[4];

MPI_Reduce
(&X0[0], &X0[2], 2, MPI_DOUBLE_PRECISION, MPI_SUM, 0, <comm>)
```

MPI_Bcast



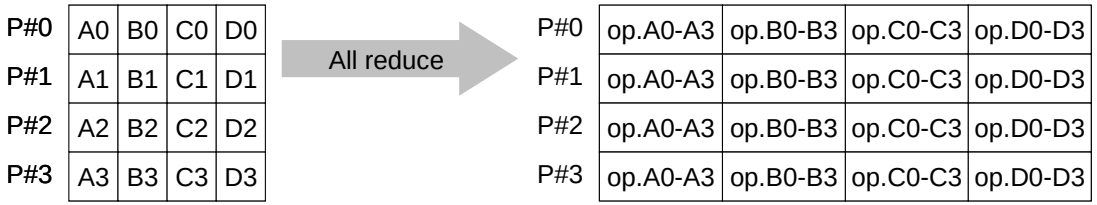
- Broadcasts a message from the process with rank "root" to all other processes of the communicator

- **MPI_Bcast (buffer,count,datatype,root,comm)**
  - **buffer** choice I/O starting address of buffer
    type is defined by "**datatype**"
  - **count** int I number of elements in send/receive buffer
  - **datatype** MPI_Datatype I data type of elements of send/recive buffer

    FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.

    C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc.
  - **root** int I rank of root process
  - **comm** MPI_Comm I communicator

MPI_Allreduce



- MPI_Reduce + MPI_Bcast
- Summation (of dot products) and MAX/MIN values are likely to utilized in each process

- **`call MPI_Allreduce`**
  `(sendbuf,recvbuf,count,datatype,op, comm)`
  - **`sendbuf`** choice I starting address of send buffer
  - **`recvbuf`** choice O starting address receive buffer
    type is defined by **"`datatype`"**
  - **`count`** int I number of elements in send/receive buffer
  - **`datatype`** MPI_Datatype I data type of elements of send/recive buffer
  - **`op`** MPI_Op I reduce operation
  - **`comm`** MPI_Comm I communicator

S1-1：Local Vector, Norm Calculation

Uniform Vectors (a1.*): s1-1-for_a1.c

```
#include <mpi.h>
#include <stdio.h>
#include <math.h>
#include <assert.h>

int main(int argc, char **argv){
        int i, N;
        int PeTot, MyRank;
        MPI_Comm SolverComm;
        double vec[8];
        double sum0, sum;
        char filename[80];
        FILE *fp;

        MPI_Init(&argc, &argv);
        MPI_Comm_size(MPI_COMM_WORLD, &PeTot);
        MPI_Comm_rank(MPI_COMM_WORLD, &MyRank);

        sprintf(filename, "a1.%d", MyRank);
        fp = fopen(filename, "r");
        assert(fp != NULL);

        N=8;
        for(i=0;i<N;i++){
                fscanf(fp, "%lf", &vec[i]);}
        sum0 = 0.0;
        for(i=0;i<N;i++){
                sum0 += vec[i] * vec[i];}

        MPI_Allreduce(&sum0, &sum, 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
        sum = sqrt(sum);

        if(!MyRank) printf("%27.20E¥n", sum);
        MPI_Finalize();
        return 0;
}
```

S1-1：Local Vector, Norm Calculation

Non-uniform Vectors (a2.*): s1-1-for_a2.c

```
#include <mpi.h>
#include <stdio.h>
#include <stdlib.h>
#include <math.h>
#include <assert.h>

int main(int argc, char **argv){
        int i, PeTot, MyRank, n;
        MPI_Comm SolverComm;
        double *vec, *vec2;
        int * Count, CountIndex;
        double sum0, sum;
        char filename[80];
        FILE *fp;

        MPI_Init(&argc, &argv);
        MPI_Comm_size(MPI_COMM_WORLD, &PeTot);
        MPI_Comm_rank(MPI_COMM_WORLD, &MyRank);

        sprintf(filename, "a2.%d", MyRank);
        fp = fopen(filename, "r");
        assert(fp != NULL);

        fscanf(fp, "%d", &n);
        vec = malloc(n * sizeof(double));
        for(i=0;i<n;i++){
                fscanf(fp, "%lf", &vec[i]);}
        sum0 = 0.0;
        for(i=0;i<n;i++){
                sum0 += vec[i] * vec[i];}

        MPI_Allreduce(&sum0, &sum, 1, MPI_DOUBLE, MPI_SUM, MPI_COMM_WORLD);
        sum = sqrt(sum);

        if(!MyRank) printf("%27.20E¥n", sum);
        MPI_Finalize();
        return 0;}
```

S1-1: Running the Codes

FORTRAN

```
$ cd <$O-S1r>
$ mpiifort -O3 s1-1-for_a1.f
$ mpiifort -O3 s1-1-for_a2.f

(modify "go4.sh")
$ qsub go4.sh
```

C

```
$ cd <$O-S1r>
$ mpicc -O3 s1-1-for_a1.c
$ mpicc -O3 s1-1-for_a2.c

(modify "go4.sh")
$ qsub go4.sh
```

S1-1：Local Vector, Calc. Norm

Results

Results using one core

```
a1.* 1.6208824756903259000E+03
a2.* 1.2221849287239636000E+03

$> ifort -O3 dot-a1.f
$> qsub go1.sh

$> ifort -O3 dot-a2.f
$> qsub go1.sh
```

Results

```
a1.* 1.6208824756903259000E+03
a2.* 1.2221849287239636000E+03
```

go1.sh

```
#!/bin/sh
#PBS -q u-lecture
#PBS -N test
#PBS -l select=1:mpiprocs=1
#PBS -Wgroup_list=gt29
#PBS -l walltime=00:05:00
#PBS -e err
#PBS -o test.lst

cd $PBS_O_WORKDIR
. /etc/profile.d/modules.sh

mpirun ./impimap.sh ./a.out
```

S1-1: Local Vector, Calc. Norm

If SENDBUF=RECVBUF, what happens ?

True

```
MPI_Allreduce(&sum0, &sum, 1, MPI_DOUBLE, MPI_SUM,
              MPI_COMM_WORLD)
```

False

```
MPI_Allreduce(&sum0, &sum0, 1, MPI_DOUBLE, MPI_SUM,
              MPI_COMM_WORLD)
```

S1-1: Local Vector, Calc. Norm

If SENDBUF=RECVBUF, what happens ?

True

```
MPI_Allreduce(&sum0, &sum, 1, MPI_DOUBLE, MPI_SUM,
              MPI_COMM_WORLD)
```

False

```
MPI_Allreduce(&sum0, &sum0, 1, MPI_DOUBLE, MPI_SUM,
              MPI_COMM_WORLD)
```

True

```
MPI_Allreduce(&sumK[1], &sumK[2], 1, MPI_DOUBLE, MPI_SUM,
              MPI_COMM_WORLD)
```

SENDBUF .ne. RECVBUF

S1-3: Integration by Trapezoidal Rule

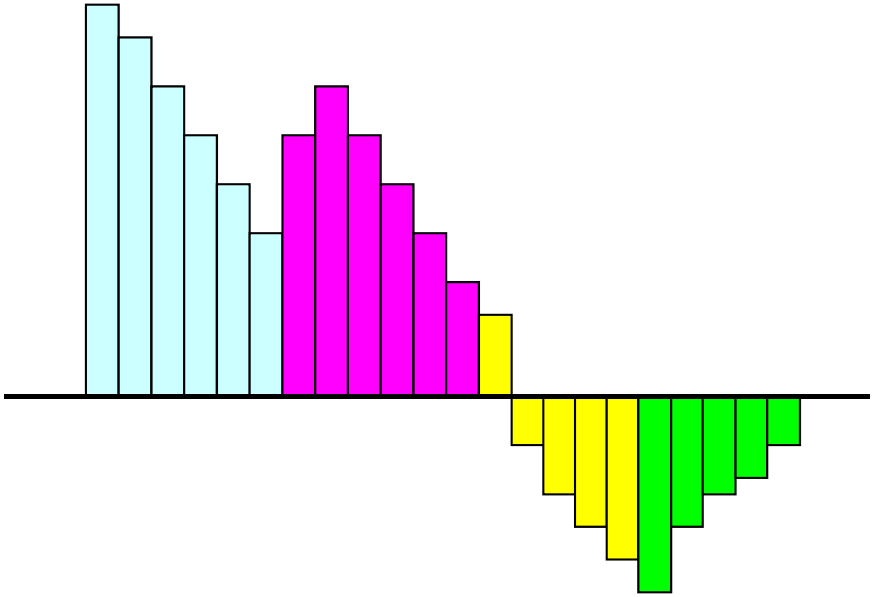
- Problem S1-3
  - Develop parallel program which calculates the following numerical integration using “trapezoidal rule” by MPI_Reduce, MPI_Bcast etc.
  - Measure computation time, and parallel performance

$$\int_0^1 \frac{4}{1+x^2}\,dx$$

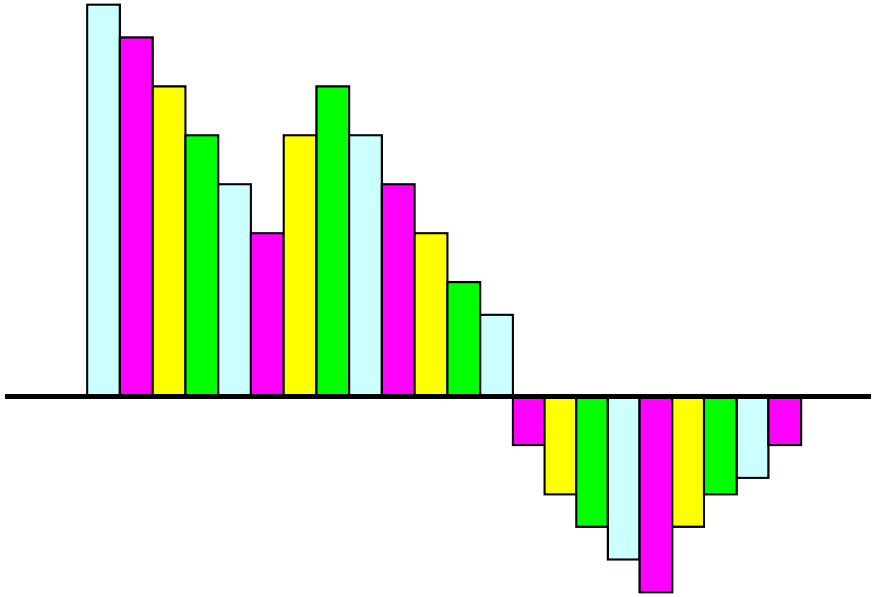
S1-3: Integration by Trapezoidal Rule

Two Types of Load Distribution

Type-A



Type-B



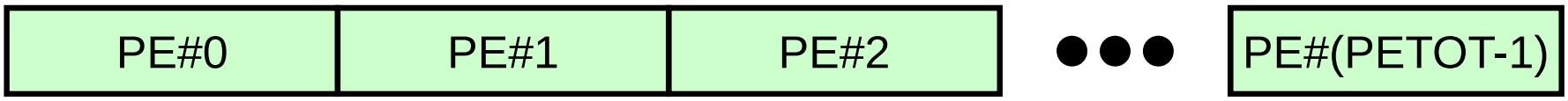
$$\frac{1}{2}\Delta x\left(f_1 + f_{N+1} + \sum_{i=2}^{N} 2 f_i \right)$$ corresponds to “Type-A”.

S1-3: Integration by Trapezoidal Rule

TYPE-A (1/2): `s1-3a.c`

```
#include <stdio.h>
#include <stdlib.h>
#include <assert.h>
#include <math.h>
#include "mpi.h"

int main(int argc, char **argv){
        int i;
        double TimeStart, TimeEnd, sum0, sum, dx;
        int PeTot, MyRank, n, int *index;
        FILE *fp;

        MPI_Init(&argc, &argv);
        MPI_Comm_size(MPI_COMM_WORLD, &PeTot);
        MPI_Comm_rank(MPI_COMM_WORLD, &MyRank);

        index = calloc(PeTot+1, sizeof(int));
        fp = fopen("input.dat", "r");
        fscanf(fp, "%d", &n);
        fclose(fp);
        if(MyRank==0) printf("%s%8d¥n", "N=", n);
        dx = 1.0/n;

        for(i=0;i<=PeTot;i++){
                index[i] = ((long long)i * n)/PeTot;}
```

“N (number of segments) “ is specified in “input.dat”

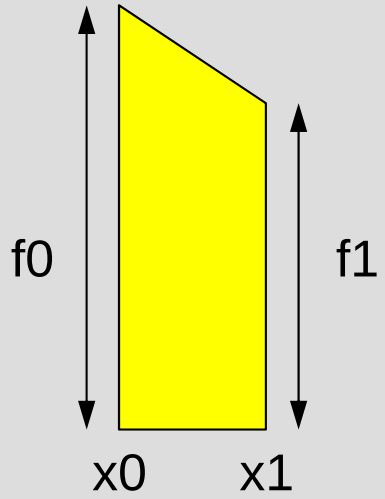


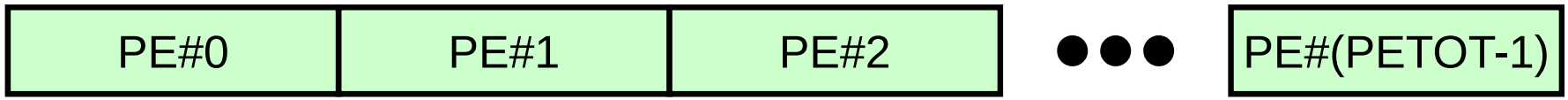
index[0] index[1] index[2] index[3] index[PETOT-1] index[PeTot] =N

S1-3: Integration by Trapezoidal Rule

TYPE-A (2/2): `s1-3a.c`

```
        TimeS = MPI_Wtime();
        sum0 = 0.0;
        for(i=index[MyRank]; i<index[MyRank+1]; i++)

        {
                double x0, x1, f0, f1;
                x0 = (double)i * dx;
                x1 = (double)(i+1) * dx;
                f0  = 4.0/(1.0+x0*x0);
                f1  = 4.0/(1.0+x1*x1);
                sum0 += 0.5 * (f0 + f1) * dx;
        }

        MPI_Reduce(&sum0, &sum, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
        TimeE = MPI_Wtime();

        if(!MyRank) printf("%24.16f%24.16f%24.16f¥n", sum, 4.0*atan(1.0), TimeE - TimeS);

        MPI_Finalize();
        return 0;
}
```



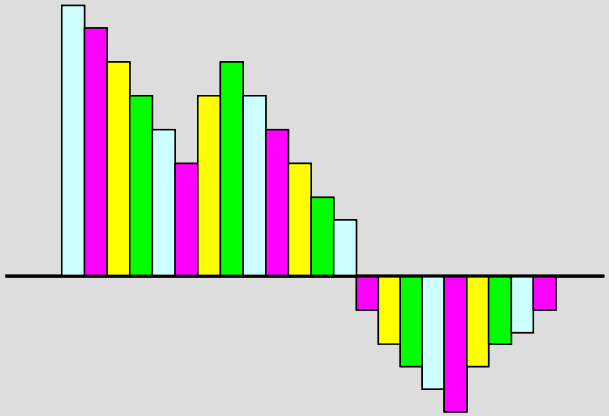


index[0] index[1] index[2] index[3] index[PETOT-1] index[PeTot] =N

S1-3: Integration by Trapezoidal Rule

TYPE-B: **s1-3b.c**

```
      TimeS = MPI_Wtime();
      sum0 = 0.0;
      for(i=MyRank; i<n; i+=PeTot)

      {
            double x0, x1, f0, f1;
            x0 = (double)i * dx;
            x1 = (double)(i+1) * dx;
            f0  = 4.0/(1.0+x0*x0);
            f1  = 4.0/(1.0+x1*x1);
            sum0 += 0.5 * (f0 + f1) * dx;
      }

      MPI_Reduce(&sum0, &sum, 1, MPI_DOUBLE, MPI_SUM, 0, MPI_COMM_WORLD);
      TimeE = MPI_Wtime();

      if(!MyRank) printf("%24.16f%24.16f%24.16f¥n", sum, 4.0*atan(1.0), TimeE-TimeS);

      MPI_Finalize();
      return 0;
}
```

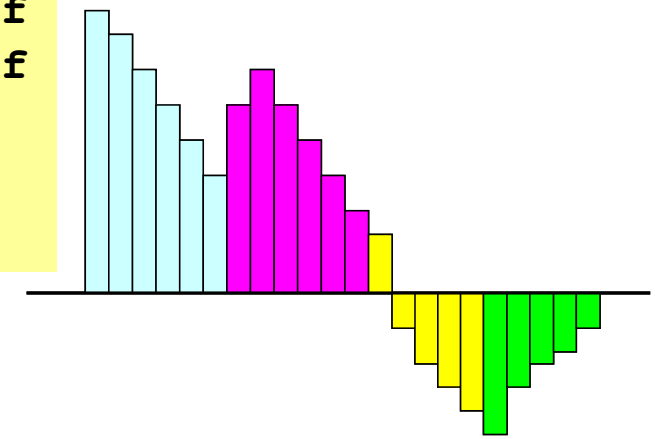


S1-3: Running the Codes

FORTRAN

```
$ mpiifort -O3 -xCORE-AVX2 -align array32byte s1-3a.f
$ mpiifort -O3 -xCORE-AVX2 -align array32byte s1-3b.f

(modify "go.sh")
$ qsub go.sh
```

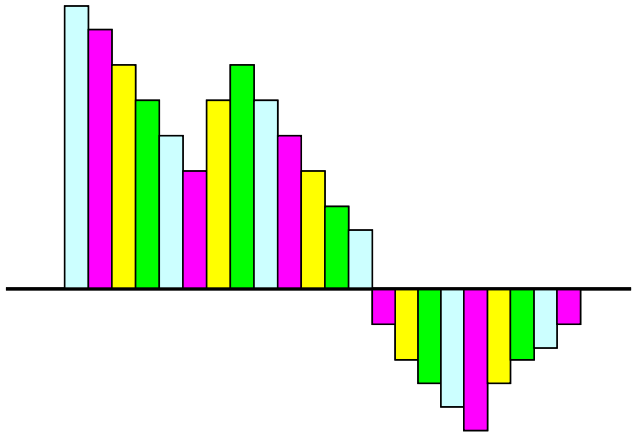
Type-A



C

```
$ mpicc -O3 -xCORE-AVX2 -align s1-3a.c
$ mpicc -O3 -xCORE-AVX2 -align s1-3b.c

(modify "go.sh")
$ qsub go.sh
```

Type-B

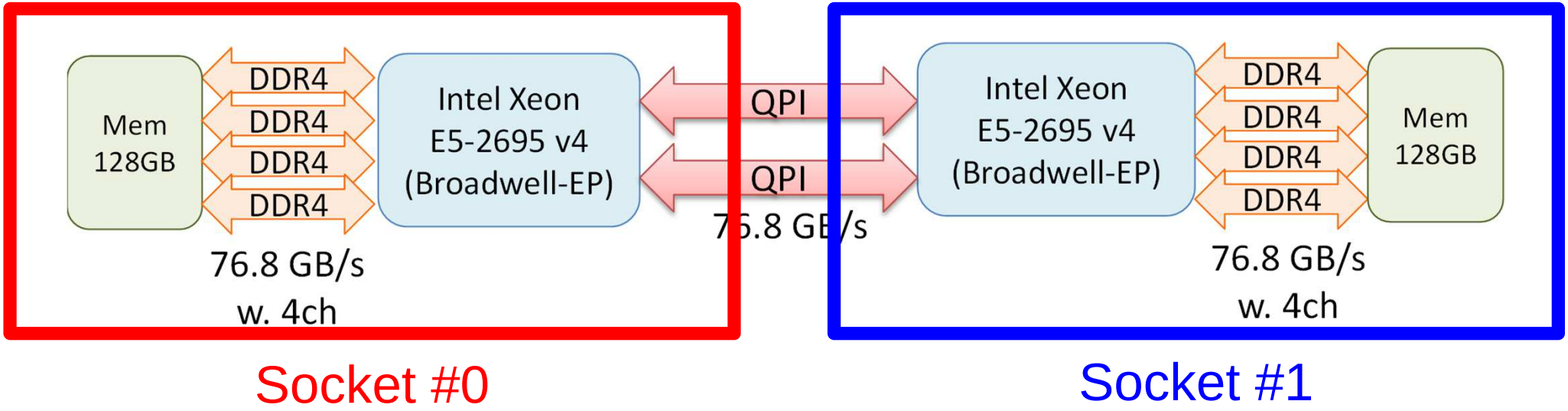


go.sh

```
#!/bin/sh
#PBS -q u-lecture                          Name of "QUEUE"
#PBS -N test                               Job Name
#PBS -l select=8:mpiprocs=32               node#, proc#/node
#PBS -Wgroup_list=gt29                     Group Name (Wallet)
#PBS -l walltime=00:05:00                  Computation Time
#PBS -e err                                Standard Error
#PBS -o test.lst                           Standard Outpt

cd $PBS_O_WORKDIR                          go to current dir
. /etc/profile.d/modules.sh                (ESSENTIAL)

export I_MPI_PIN_DOMAIN=socket             Execution on each socket
export I_MPI_PERHOST=32                    =mpiprocs
mpirun ./impimap.sh ./a.out                Exec's
```

```
#PBS -l select=1:mpiprocs=4     1-node, 4-proc's
#PBS -l select=1:mpiprocs=16    1-node, 16-proc's
#PBS -l select=1:mpiprocs=36    1-node, 36-proc's
#PBS -l select=2:mpiprocs=32    2-nodes, 32x2=64-proc's
#PBS -l select=8:mpiprocs=36    8-nodes, 36x8=288-proc's
```

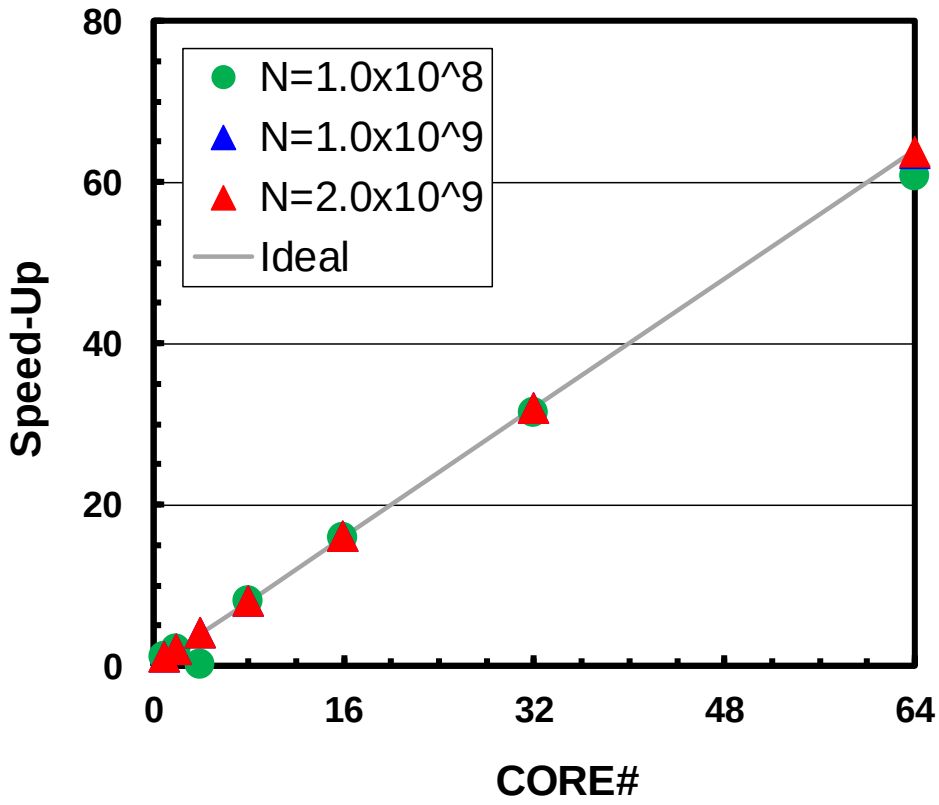
export I_MPI_PIN_DOMAIN=socket



- Each Node of Reedbush-U
  - 2 Sockets (CPU's) of Intel Broadwell-EP
  - Each socket has 18 cores
- Each core of a socket can access to the memory on the other socket : NUMA (Non-Uniform Memory Access)
  - I_MPI_PIN_DOMAIN=socket, impimap.sh: local memory to be used

S1-3: Performance on RB-U (1/3)

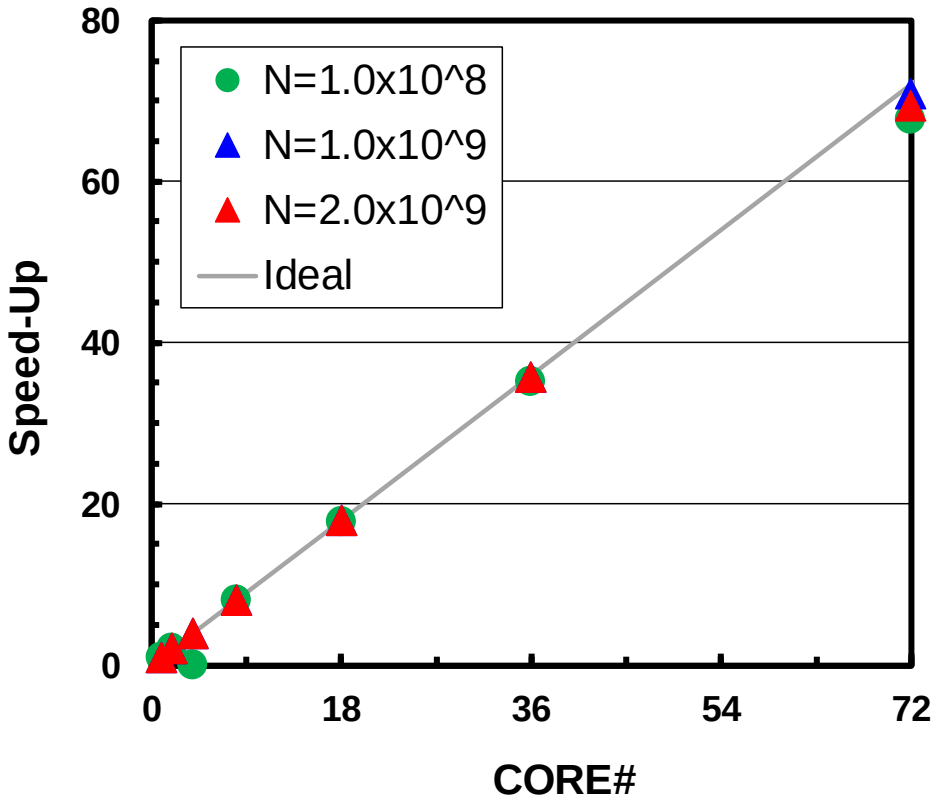
- ◆ : $N=10^8$, ● : 10^9, ▲ : $2x10^9$, — : Ideal
- Based on results (sec.) using a single core
- Strong Scaling
  - Entire problem size fixed
  - 1/N comp. time using N-x cores
- Weak Scaling
  - Problem size/core is fixed
  - Comp. time is kept constant for N-x scale problems using N-x cores



32 cores/node, 16 cores/socket up to 2 nodes (64 cores)

S1-3: Performance on RB-U (2/3)

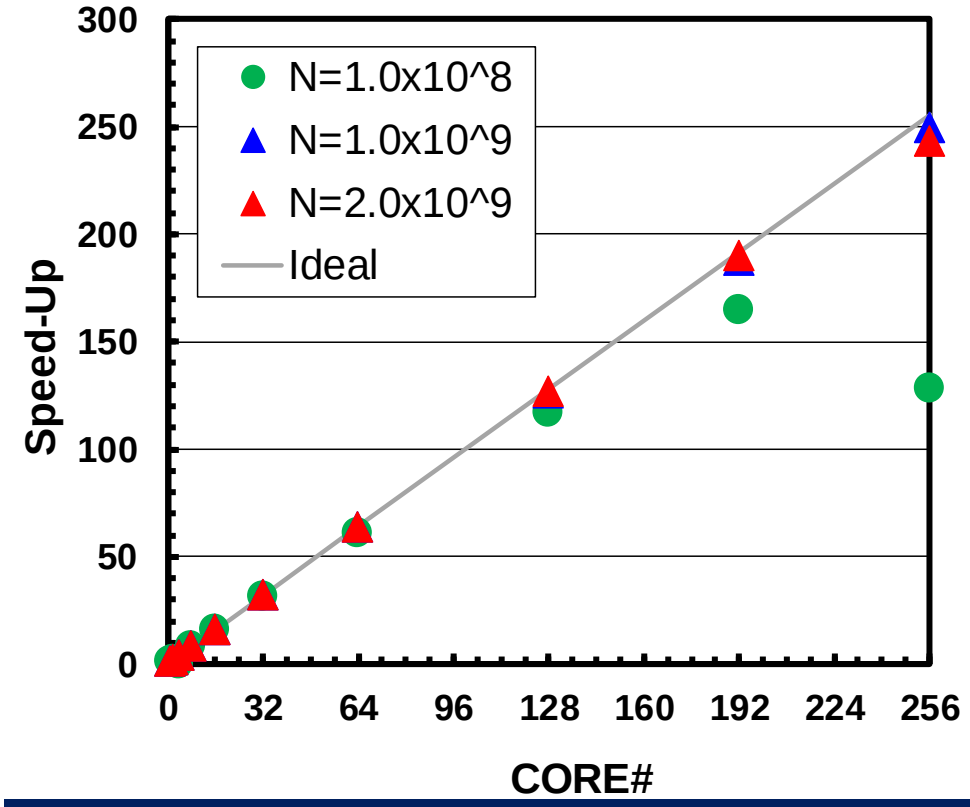
- ◆ : $N=10^8$, ● : 10^9, ▲ : $2x10^9$, — : Ideal
- Based on results (sec.) using a single core
- Strong Scaling
  - Entire problem size fixed
  - 1/N comp. time using N-x cores
- Weak Scaling
  - Problem size/core is fixed
  - Comp. time is kept constant for N-x scale problems using N-x cores



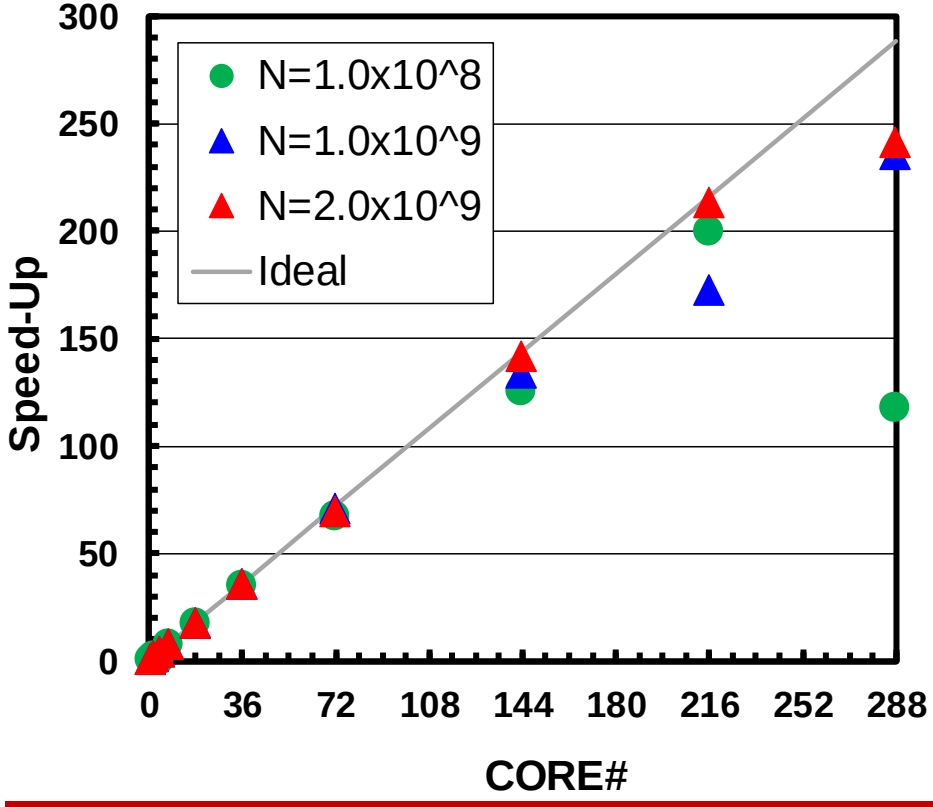
36 cores/node, 18 cores/socket up to 2 nodes (72 cores)

S1-3: Performance on RB-U (3/3)

- ◆ : N=10^8, ● : 10^9, ▲ : 2x10^9, — : Ideal
- 32cores/node (16cores/socket) cases are better
  - smaller number of MPI processes



32 cores/node, 16 cores/socket up to 8 nodes (256 cores)



36 cores/node, 18 cores/socket up to 8 nodes (288 cores)

Performance is lower than ideal one

- Time for MPI communication
  - Time for sending data
  - Communication bandwidth between nodes
  - Time is proportional to size of sending/receiving buffers
- Time for starting MPI
  - latency
  - does not depend on size of buffers
    - depends on number of calling, increases according to process #
  - $O(10^0)$-$O(10^1)$ μsec.
- Synchronization of MPI
  - Increases according to number of processes

Performance is lower than ideal one (cont.)

- If computation time is relatively small (N is small in S1-3), these effects are not negligible.
  - If the size of messages is small, effect of “latency” is significant.