Introduction to Programming by MPI for Parallel FEM Report S1 & S2 in Fortran (1/2)

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Motivation for Parallel Computing (and this class)

- Large-scale parallel computer enables fast computing in large-scale scientific simulations with detailed models. Computational science develops new frontiers of science and engineering.
- Why parallel computing ?
  - faster & larger
  - “larger” is more important from the view point of “new frontiers of science & engineering”, but “faster” is also important.
  - + more complicated
  - Ideal: Scalable
    - Weak Scaling, Strong Scaling

Scalable, Scaling, Scalability

- Solving N^x scale problem using N^x computational resources during same computation time
  - for large-scale problems: **Weak Scaling, Weak Scalability**
  - e.g. CG solver: more iterations needed for larger problems
- Solving a problem using N^x computational resources during 1/N computation time
  - for faster computation: **Strong Scaling, Strong Scalability**

Overview

- What is MPI ?
- Your First MPI Program: Hello World
- Collective Communication
- Point-to-Point Communication

What is MPI ? (1/2)

- Message Passing Interface
- “Specification” of message passing API for distributed memory environment
  - Not a program, Not a library
    - http://www.mcs.anl.gov/mpi/www/
    - https://www.mpi-forum.org/docs/
- History
  - 1992 MPI Forum
    - https://www.mpi-forum.org/
  - 1994 MPI-1
  - 1997 MPI-2: MPI I/O
  - 2012 MPI-3: Fault Resilience, Asynchronous Collective
- Implementation
  - mpich ANL (Argonne National Laboratory), OpenMPI, MVAPICH
  - H/W vendors
  - C/C++, FOTRAN, Java ; Unix, Linux, Windows, Mac OS

What is MPI ? (2/2)

- “mpich” (free) is widely used
  - supports MPI-2 spec. (partially)
  - MPICH2 after Nov. 2005.
  - http://www.mcs.anl.gov/mpi/
- Why MPI is widely used as *de facto standard* ?
  - Uniform interface through MPI forum
    - Portable, can work on any types of computers
    - Can be called from Fortran, C, etc.
  - mpich
    - free, supports every architecture
- PVM (Parallel Virtual Machine) was also proposed in early 90’s but not so widely used as MPI

References

- W.Gropp et al., Using MPI second edition, MIT Press, 1999.
- M.J.Quinn, Parallel Programming in C with MPI and OpenMP, McGrawhill, 2003.
- W.Gropp et al., MPI：The Complete Reference Vol.I, II, MIT Press, 1998.
- http://www.mcs.anl.gov/mpi/www/
  - API (Application Interface) of MPI

How to learn MPI (1/2)

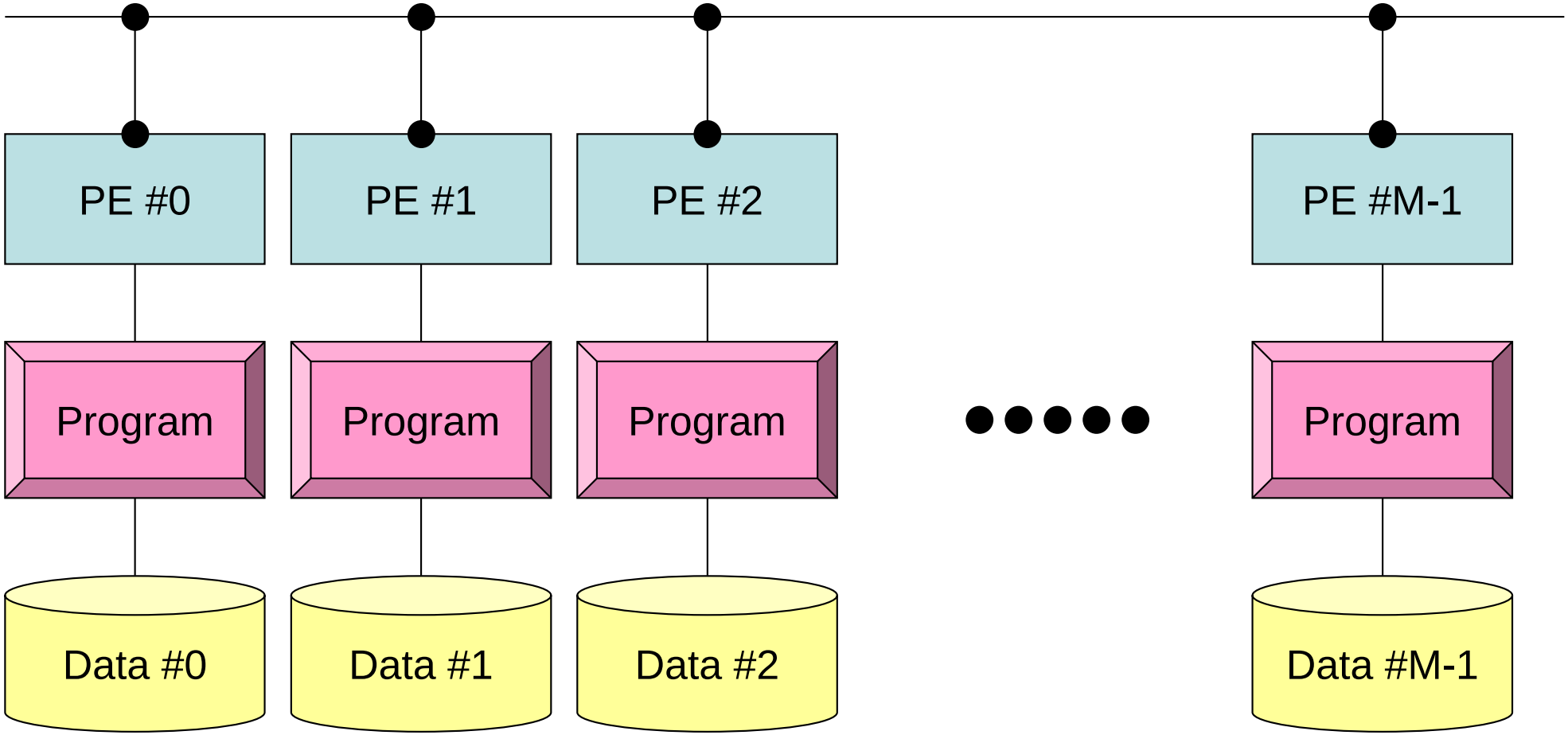
- Grammar
  - 10-20 functions of MPI-1 will be taught in the class
    - although there are many convenient capabilities in MPI-2
  - If you need further information, you can find information from web, books, and MPI experts.
- Practice is important
  - Programming
  - “Running the codes” is the most important
- Be familiar with or “grab” the idea of SPMD/SIMD op’s
  - Single Program/Instruction Multiple Data
  - Each process does same operation for different data
    - Large-scale data is decomposed, and each part is computed by each process
  - Global/Local Data, Global/Local Numbering

PE: Processing Element
Processor, Domain, Process

SPMD

You understand 90% MPI, if you understand this figure.

```
mpirun -np M <Program>
```



Each process does same operation for different data

Large-scale data is decomposed, and each part is computed by each process

It is ideal that parallel program is not different from serial one except communication.

Some Technical Terms

- Processor, Core
  - Processing Unit (H/W), Processor=Core for single-core proc's
- Process
  - Unit for MPI computation, nearly equal to "core"
  - Each core (or processor) can host multiple processes (but not efficient)
- PE (Processing Element)
  - PE originally mean "processor", but it is sometimes used as "process" in this class. Moreover it means "domain" (next)
    - In multicore proc's: PE generally means "core"
- Domain
  - domain=process (=PE), each of "MD" in "SPMD", each data set
- Process ID of MPI (ID of PE, ID of domain) starts from "0"
  - if you have 8 processes (PE's, domains), ID is 0~7

PE: Processing Element
Processor, Domain, Process

SPMD

You understand 90% MPI, if you understand this figure.

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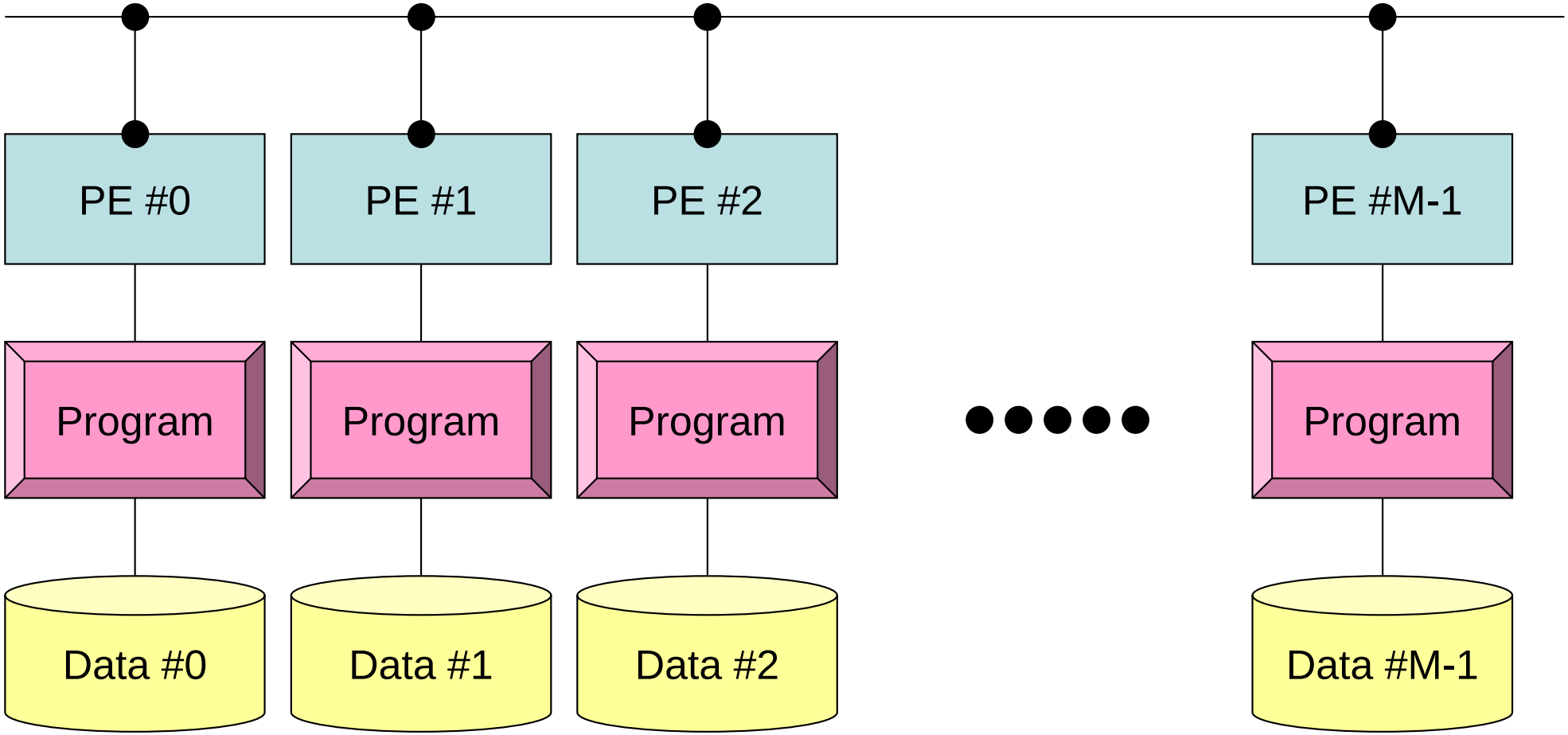
```



Each process does same operation for different data

Large-scale data is decomposed, and each part is computed by each process

It is ideal that parallel program is not different from serial one except communication.

How to learn MPI (2/2)

- NOT so difficult.
- Therefore, 5-6-hour lectures are enough for just learning grammar of MPI.

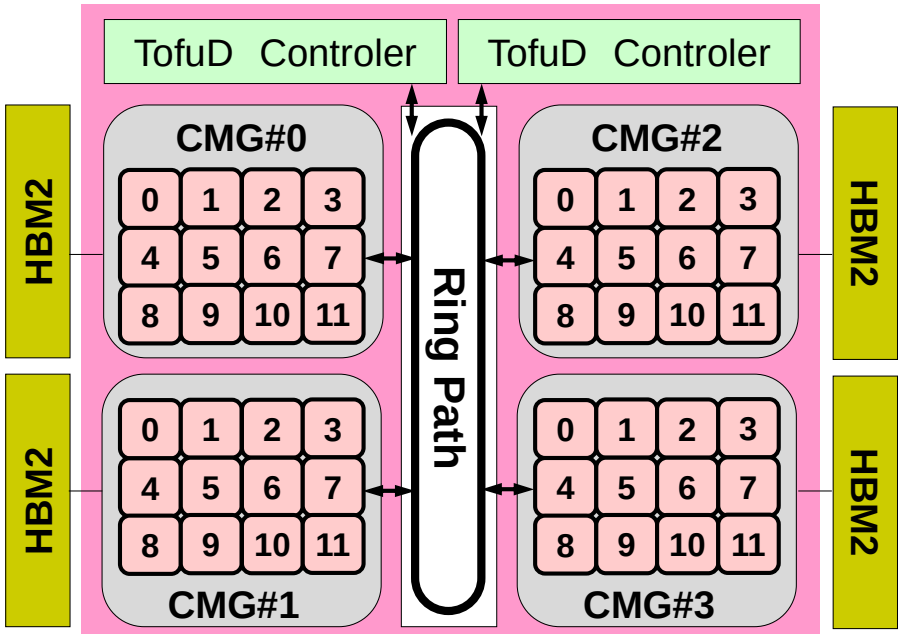
- Grab the idea of SPMD !

Schedule

- MPI
  - Basic Functions
  - Collective Communication
  - Point-to-Point (or Peer-to-Peer) Communication

- 90 min. x 4-5 lectures
  - Collective Communication
    - Report S1
  - Point-to-Point Communication
    - Report S2: Parallelization of 1D code
  - At this point, you are almost an expert of MPI programming

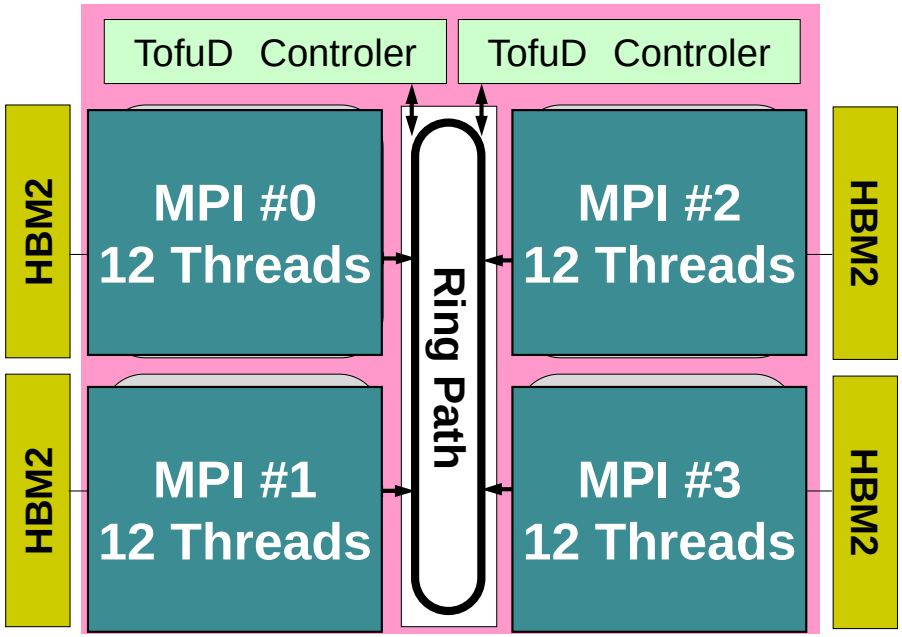
A64FX Processor on Odyssey



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
- Multiple Nodes: Recommended Programming Model
  - 1-MPI Process for each CMG with 12 OpenMP threads
  - 4-MPI processes for each node

A64FX Processor on Oddysey



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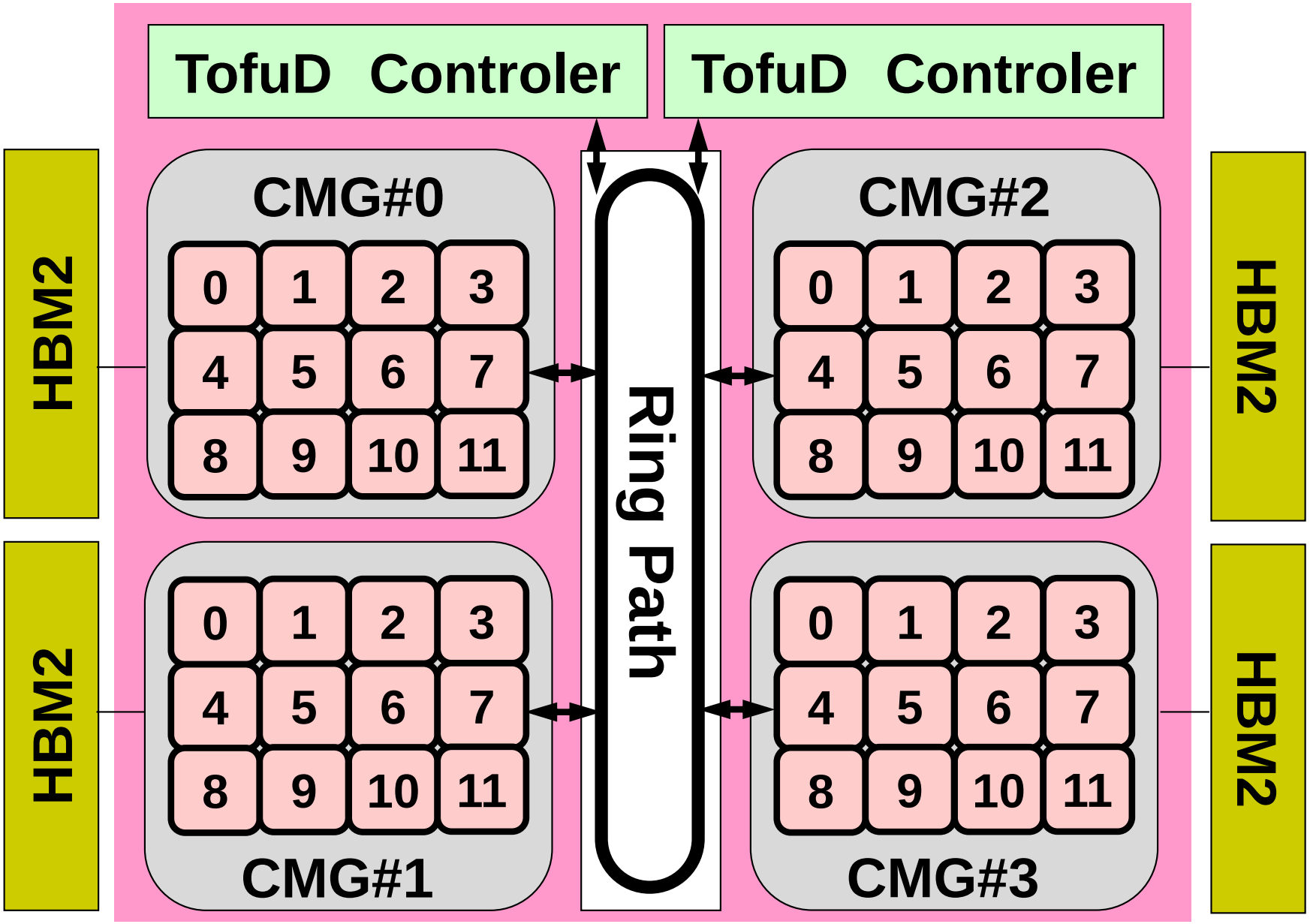
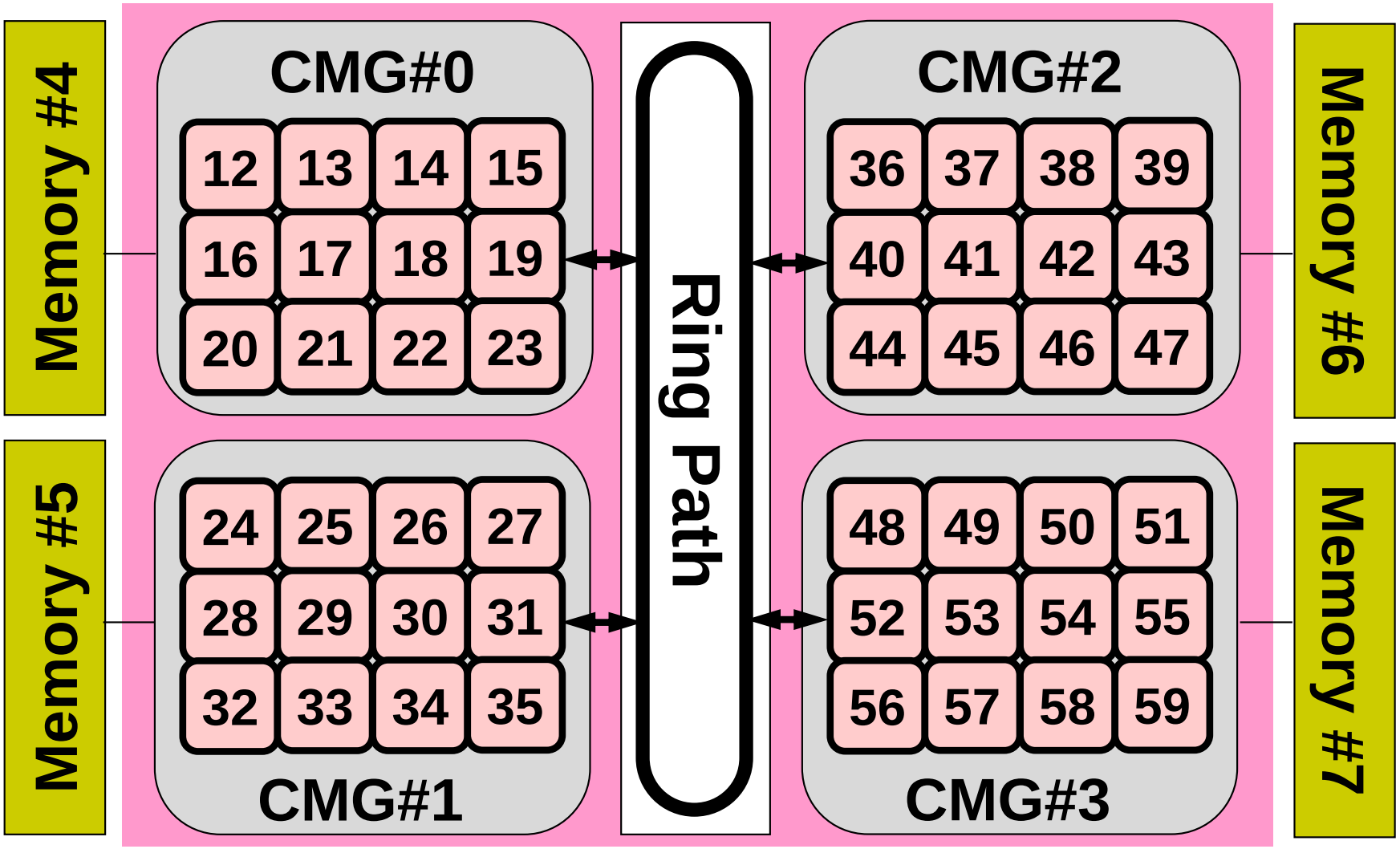
A64FX：CMG（Core Memory Group）



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

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



- What is MPI ?
- **Your First MPI Program: Hello World**
- Collective Communication
- Point-to-Point Communication

Login to Odyssey

ssh t36*@wisteria.cc.u-tokyo.ac.jp**

Create directory

```
>$ cd /work/gt36/t36***
>$ mkdir pFEM
>$ cd pFEM

>$ module load fj
```

Please type this every time you log-in !!

In this class this top-directory is called <$O-TOP>.
Files are copied to this directory.

Under this directory, S1, S2, S1-ref are created:

```
<$O-S1> = <$O-TOP>/mpi/S1
<$O-S2> = <$O-TOP>/mpi/S2
```

Odyssey **PC**

Copying files on Odyssey

FORTRAN

```
>$ cd /work/gt36/t36XXX/pFEM
>$ module load fj
>$ cp /work/gt00/z30088/pFEM/F/s1-f.tar .
>$ tar xvf s1-f.tar
```

C

```
>$ cd /work/gt36/t36XXX/pFEM
>$ module load fj
>$ cp /work/gt00/z30088/pFEM/C/s1-c.tar .
>$ tar xvf s1-c.tar
```

Confirmation

```
>$ ls
   mpi

>$ cd mpi/S1
```

This directory is called as <$O-S1>.

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

First Example

hello.f

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h‘
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

hello.c

```
#include "mpi.h"
#include <stdio.h>
int main(int argc, char **argv)
{
    int n, myid, numprocs, i;

    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD,&myid);
    printf ("Hello World %d¥n", myid);
    MPI_Finalize();
}
```

Compiling hello.f/c

```
>$ cd /work/gt36/t36XXX/pFEM/mpi/S1
>$ module load fj
>$ mpifrtpx -Kfast hello.f
>$ mpifccpx –Nclang -Kfast hello.c
```

FORTRAN

$> “mpifrtpx”:
required compiler & libraries are included for Fujitsu’s FORTRAN90+MPI

C

$> “mpifccpx”:
required compiler & libraries are included for Fujitsu’s C+MPI

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.

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Job Script

- **<$O-S1>/hello.sh**
- Scheduling + Shell Script

```
#!/bin/sh
#PJM -N "hello“                    Job Name
#PJM -L rscgrp=lecture6-o          Name of “Resource Group”
#PJM –L node=1                     Node#
#PJM –mpi proc=4                   Total MPI Process#
#PJM –L elapse=00:15:00            Computation Time
#PJM –g gt36                       Group Name (Wallet)
#PJM -j
#PJM -e err                        Standard Error
#PJM -o hello.lst                  Standard Output

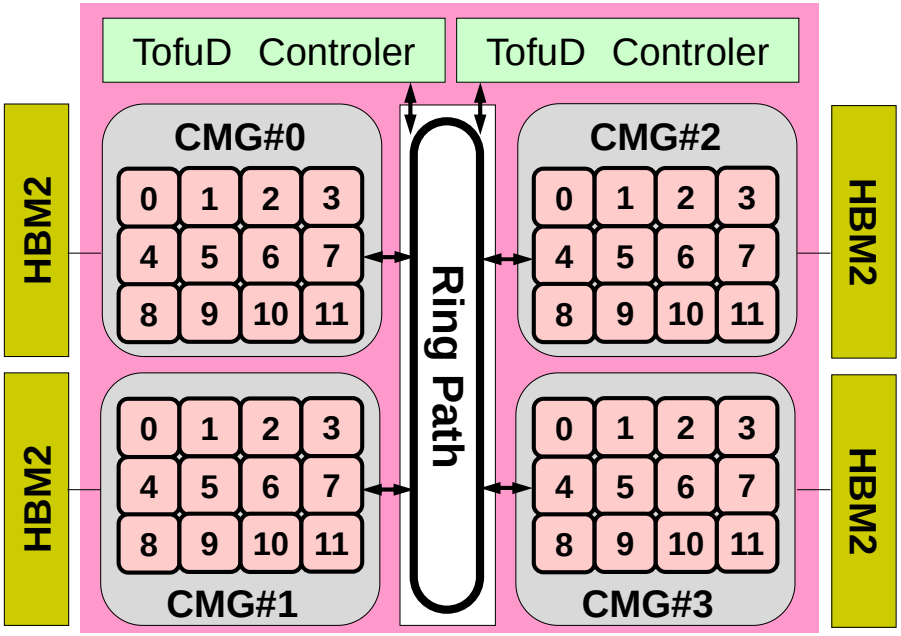
module load fj                     必須
module load fjmpi

mpiexec ./a.out
```

Number of Processes

```
#PJM -L node=1;#PJM --mpi proc= 1    1-node, 1-proc, 1-proc/n
#PJM -L node=1;#PJM --mpi proc= 4    1-node, 4-proc, 4-proc/n
#PJM -L node=1;#PJM --mpi proc=12    1-node,12-proc,12-proc/n
#PJM -L node=1;#PJM --mpi proc=24    1-node,24-proc,24-proc/n
#PJM -L node=1;#PJM --mpi proc=48    1-node,48-proc,48-proc/n

#PJM -L node= 4;#PJM --mpi proc=192   4-node,192-proc,48-proc/n
#PJM -L node= 8;#PJM --mpi proc=384   8-node,384-proc,48-proc/n
#PJM -L node=12;#PJM --mpi proc=576  12-node,576-proc,48-proc/n
```



Job Submission

```
>$ cd /work/gt36/t36XXX/pFEM/mpi/S1
>$ module load fj
>$ pjsub hello.sh

>$ cat hello.lst

  Hello World 0
  Hello World 3
  Hello World 2
  Hello World 1
```

Available Resource Groups (Queue's)

- Following 2 resource groups are available
- Up to 12 nodes are available
  - **`lecture-o`**
    - 12 nodes (576 cores), 15 min., valid until the end of August 2023
    - Shared by all "educational" users
  - **`lecture6-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
lecture6-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
lecture6-o              [DISABLE,STOP]           1       12   00:15:00      --:--:--       28 gt00

[t00XYZ@wisteria01 ~]$ pjstat --limit
SYSTEM: Odyssey
PROJECT        ACCEPT         RUN  BULK_ACCEPT    BULK_RUN          NODE
gt36          0/  128     0/   16       0/    8     0/   16       0/ 2304

SYSTEM: Aquarius
PROJECT        ACCEPT         RUN  BULK_ACCEPT    BULK_RUN           GPU
gt36          0/    4     0/    2       0/    0     0/    0       0/   64
```

Basic/Essential Functions

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

```
#include "mpi.h"
#include <stdio.h>
int main(int argc, char **argv)
{
    int n, myid, numprocs, i;

    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD,&myid);

    printf ("Hello World %d¥n", myid);
    MPI_Finalize();
}
```

‘mpif.h’, “mpi.h”

Essential Include file

“use mpi” is possible in F90

MPI_Init

Initialization

MPI_Comm_size

Number of MPI Processes

mpirun -np XX <prog>

MPI_Comm_rank

Process ID starting from 0

MPI_Finalize

Termination of MPI processes

Difference between FORTRAN/C

- (Basically) same interface
  - In C, UPPER/lower cases are considered as different
    - e.g.: **MPI_C**omm_size
      - MPI: UPPER case
      - First character of the function except “MPI_” is in UPPER case.
      - Other characters are in lower case.
- In Fortran, return value `ierr` has to be added at the end of the argument list.
- C needs special types for variables:
  - MPI_Comm, MPI_Datatype, MPI_Op etc.
- **`MPI_INIT`** is different:
  - `call MPI_INIT (ierr)`
  - `MPI_Init (int *argc, char ***argv)`

What's are going on ?

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

```
#!/bin/sh
#PJM -N "hello"                    Job Name
#PJM -L rscgrp=lecture7-o          Name of "Resource Group"
#PJM -L node=1                     Node#
#PJM -mpi proc=4                   Total MPI Process#
#PJM -L elapse=00:15:00            Computation Time
#PJM -g gt87                       Group Name (Wallet)
#PJM -j
#PJM -e err                        Standard Error
#PJM -o hello.lst                  Standard Output

module load fj                     必須
module load fjmpi

mpiexec ./a.out
```

- **`mpiexec`** starts up 4 MPI processes ("proc=4")
  - A single program runs on four processes.
  - each process writes a value of `myid`
- Four processes do same operations, but values of **`myid`** are different.
- Output of each process is different.
- That is SPMD !

mpi.h, mpif.h

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

```
#include "mpi.h"
#include <stdio.h>
int main(int argc, char **argv)
{
    int n, myid, numprocs, i;

    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD,&myid);

    printf ("Hello World %d¥n", myid);
    MPI_Finalize();
}
```

- Various types of parameters and variables for MPI & their initial values.
- Name of each var. starts from “MPI_”
- Values of these parameters and variables cannot be changed by users.
- Users do not specify variables starting from “MPI_” in users’ programs.

Fortran

MPI_INIT

- Initialize the MPI execution environment (required)
- It is recommended to put this BEFORE all statements in the program.

- **call MPI_INIT (ierr)**
  - **ierr** I O Completion Code

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

Fortran

MPI_FINALIZE

- Terminates MPI execution environment (required)
- It is recommended to put this AFTER all statements in the program.
- Please do not forget this.

- **call MPI_FINALIZE (ierr)**
  - **ierr** I O completion code

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

Fortran

MPI_COMM_SIZE

- Determines the size of the group associated with a communicator
- not required, but very convenient function

- **call MPI_COMM_SIZE (comm, size, ierr)**
  - **comm** I I communicator
  - **size** I O number of processes in the group of communicator
  - **ierr** I O completion code

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

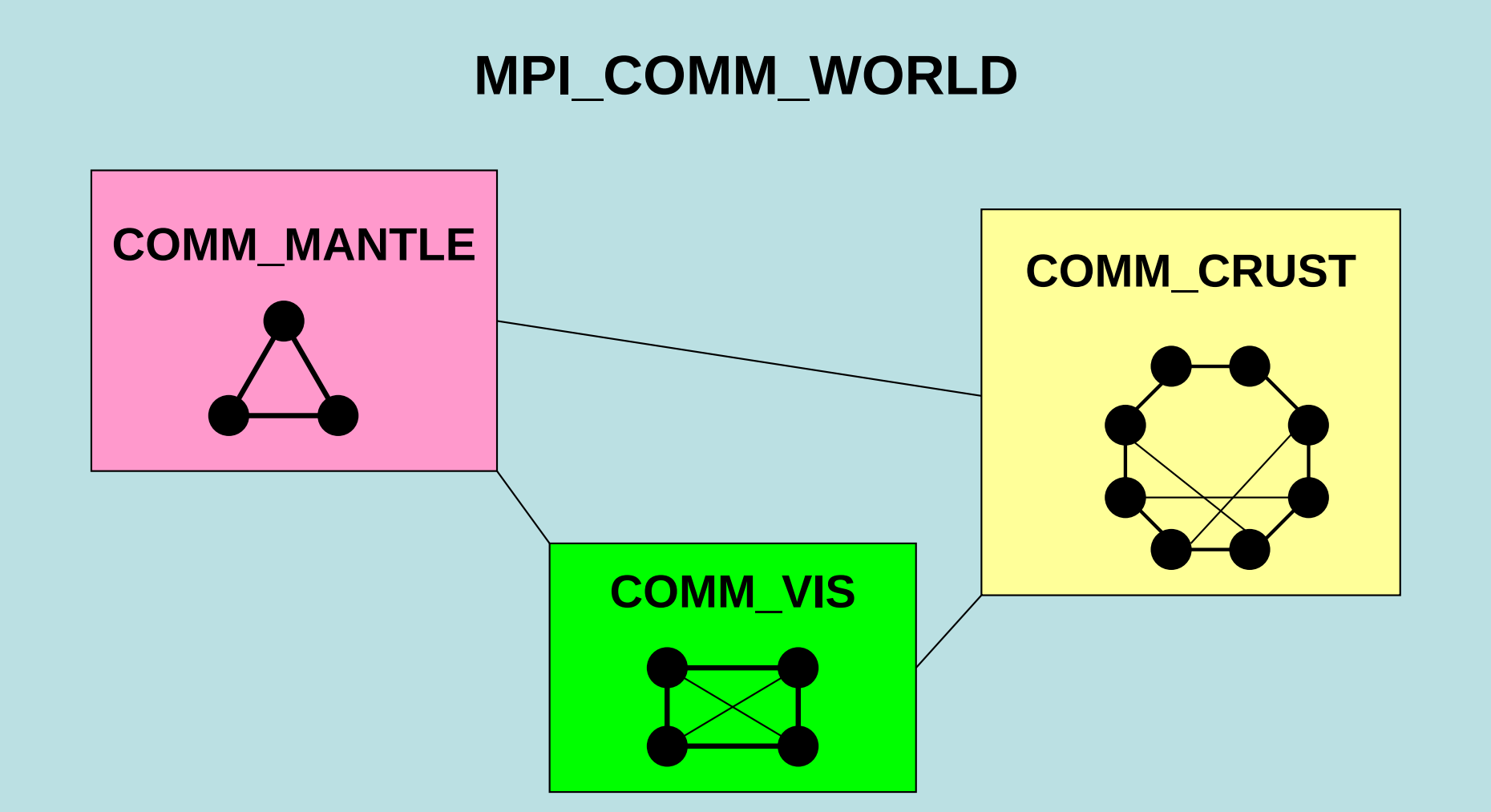
What is Communicator ?

```
MPI_Comm_Size (MPI_COMM_WORLD, PETOT)
```

- Group of processes for communication
- Communicator must be specified in MPI program as a unit of communication
- All processes belong to a group, named "**MPI_COMM_WORLD**" (default)
- Multiple communicators can be created, and complicated operations are possible.
  - Computation, Visualization
- Only "MPI_COMM_WORLD" is needed in this class.

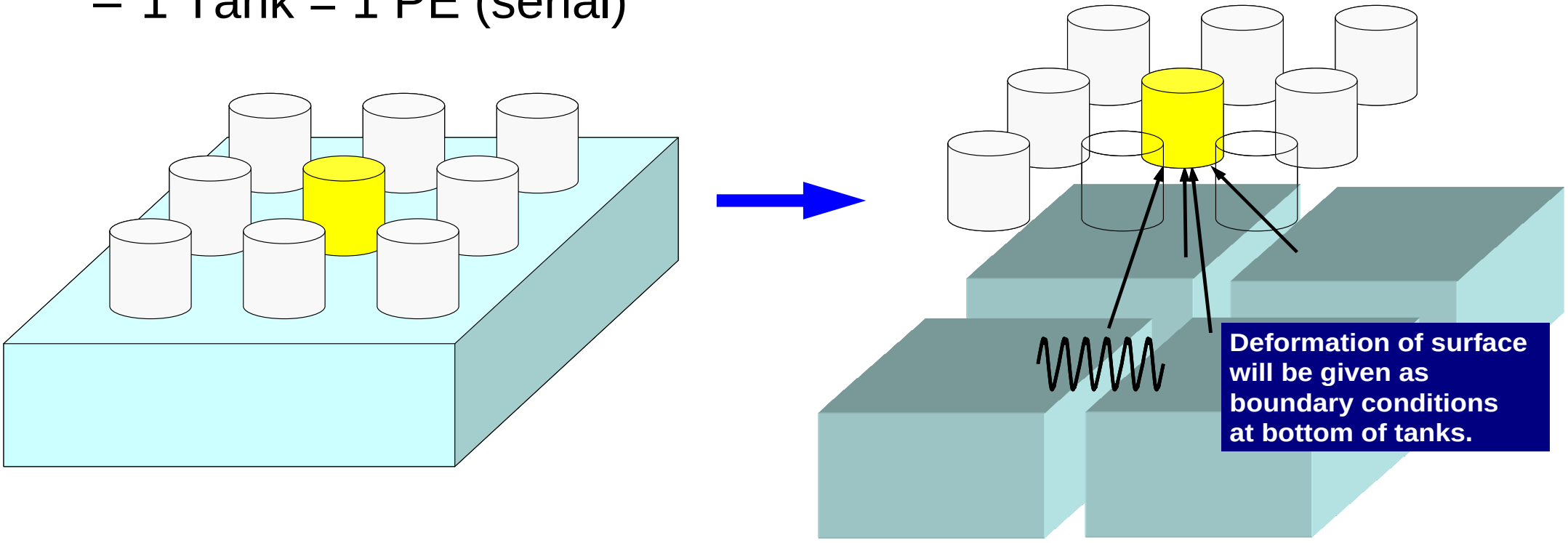
Communicator in MPI

One process can belong to multiple communicators



Target Application

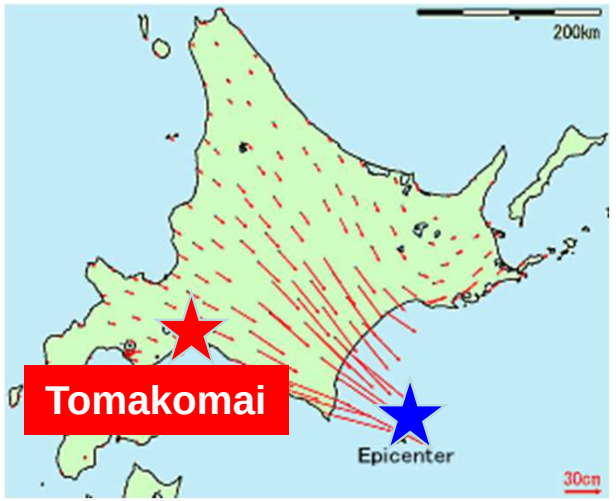
- Coupling between “Ground Motion” and “Sloshing of Tanks for Oil-Storage”
  - “One-way” coupling from “Ground Motion” to “Tanks”.
  - Displacement of ground surface is given as forced displacement of bottom surface of tanks.
  - 1 Tank = 1 PE (serial)



2003 Tokachi Earthquake (M8.0)

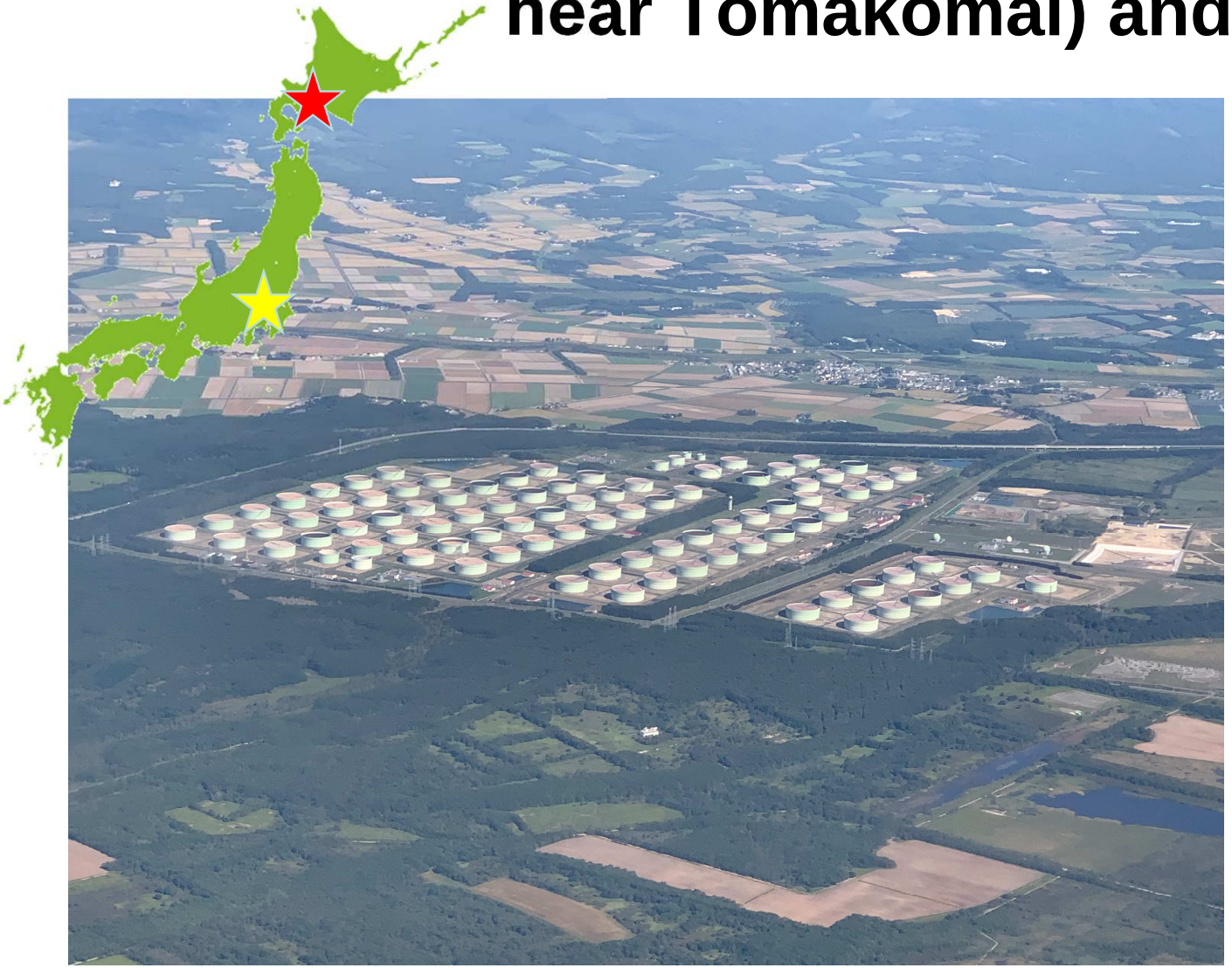
Fire accident by sloshing due to long-period ground motion

- Oil tanks in Tomakomai shook violently by the earthquake
- Sparks with rubbed metal fittings ignited the oil that swung on the liquid level
- The fire was so large that it was impossible to extinguish it
- We needed to wait a few days for all the oil to burn out.



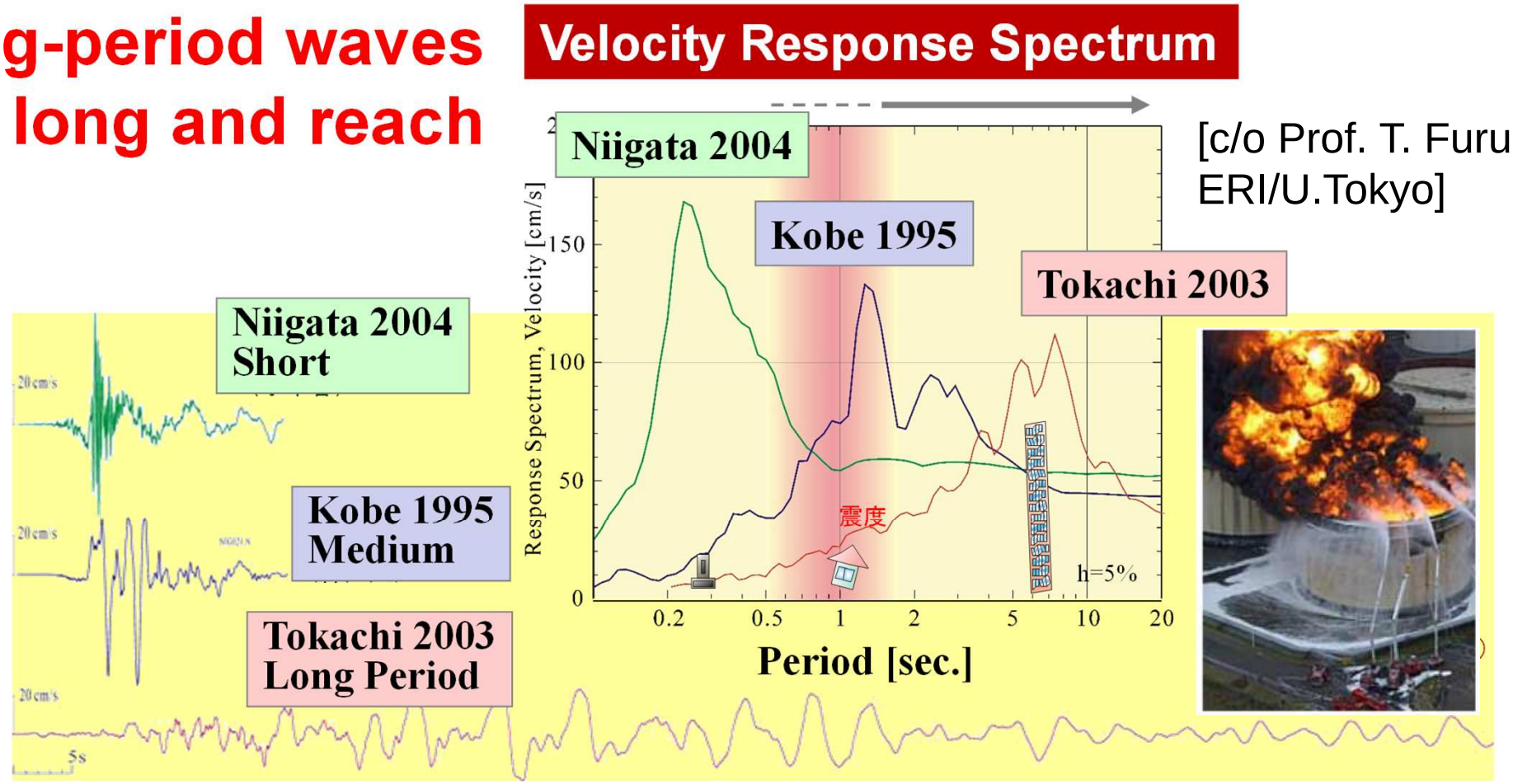
The Tanks on September 10, 2022

View from flight between Sapporo (Capital of Hokkaido, near Tomakomai) and Tokyo



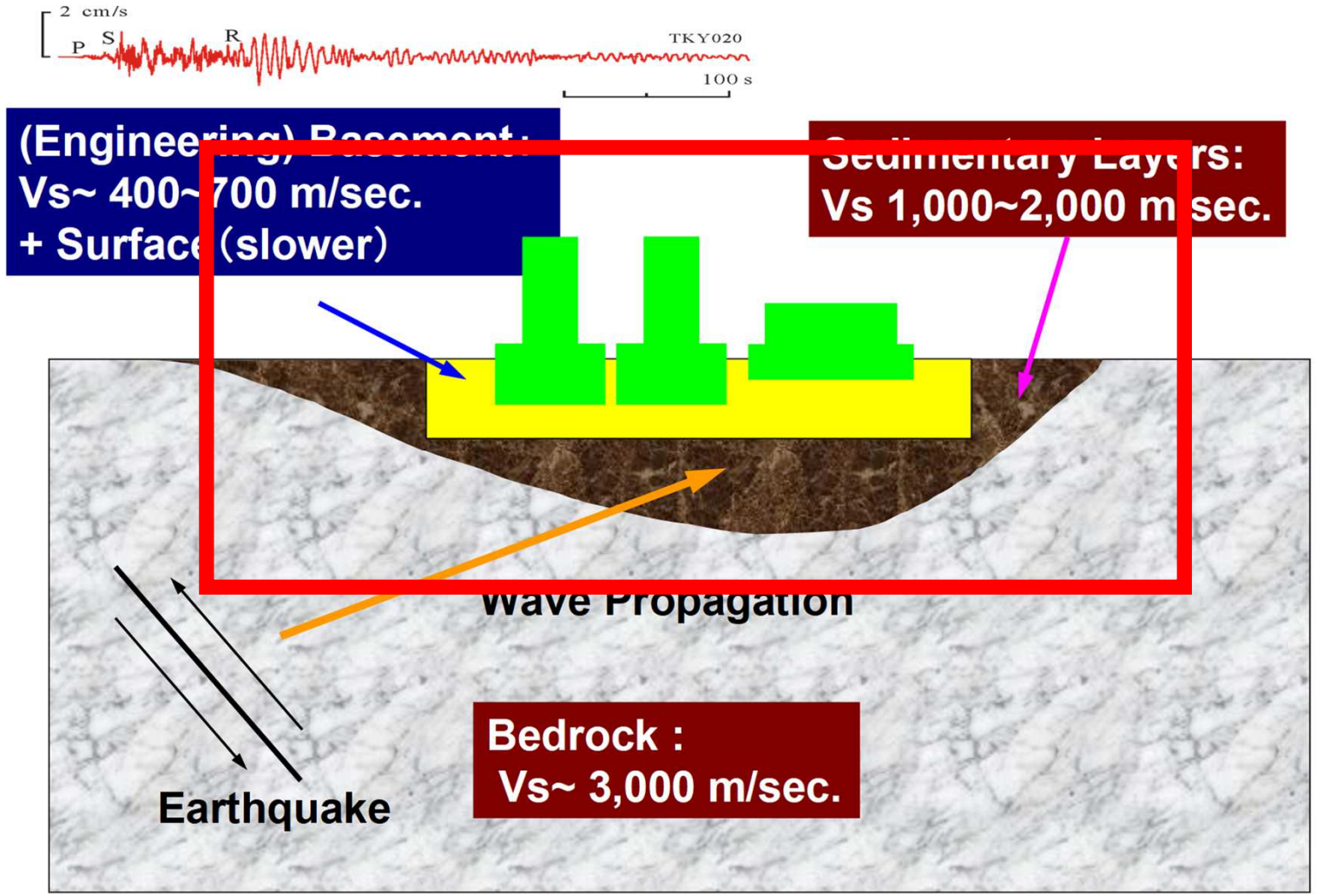
Seismic Wave

- Various Components of Wavelength
- Buildings with the same natural period as the predominant component of seismic waves shake most violently (0.1-10 sec.): a kind of "resonance"
- **Long-period waves last long and reach far**



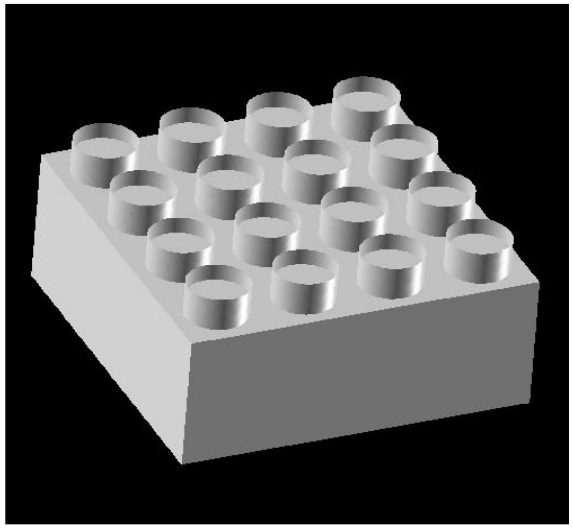
[c/o Prof. T. Furumura, ERI/U.Tokyo]

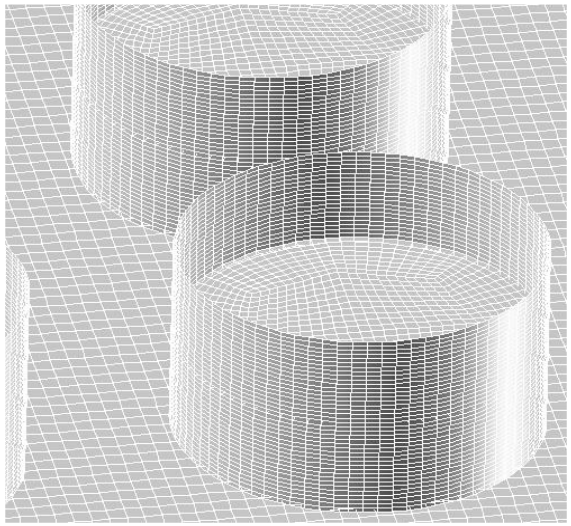
Seismic Wave Propagation, Underground Structure



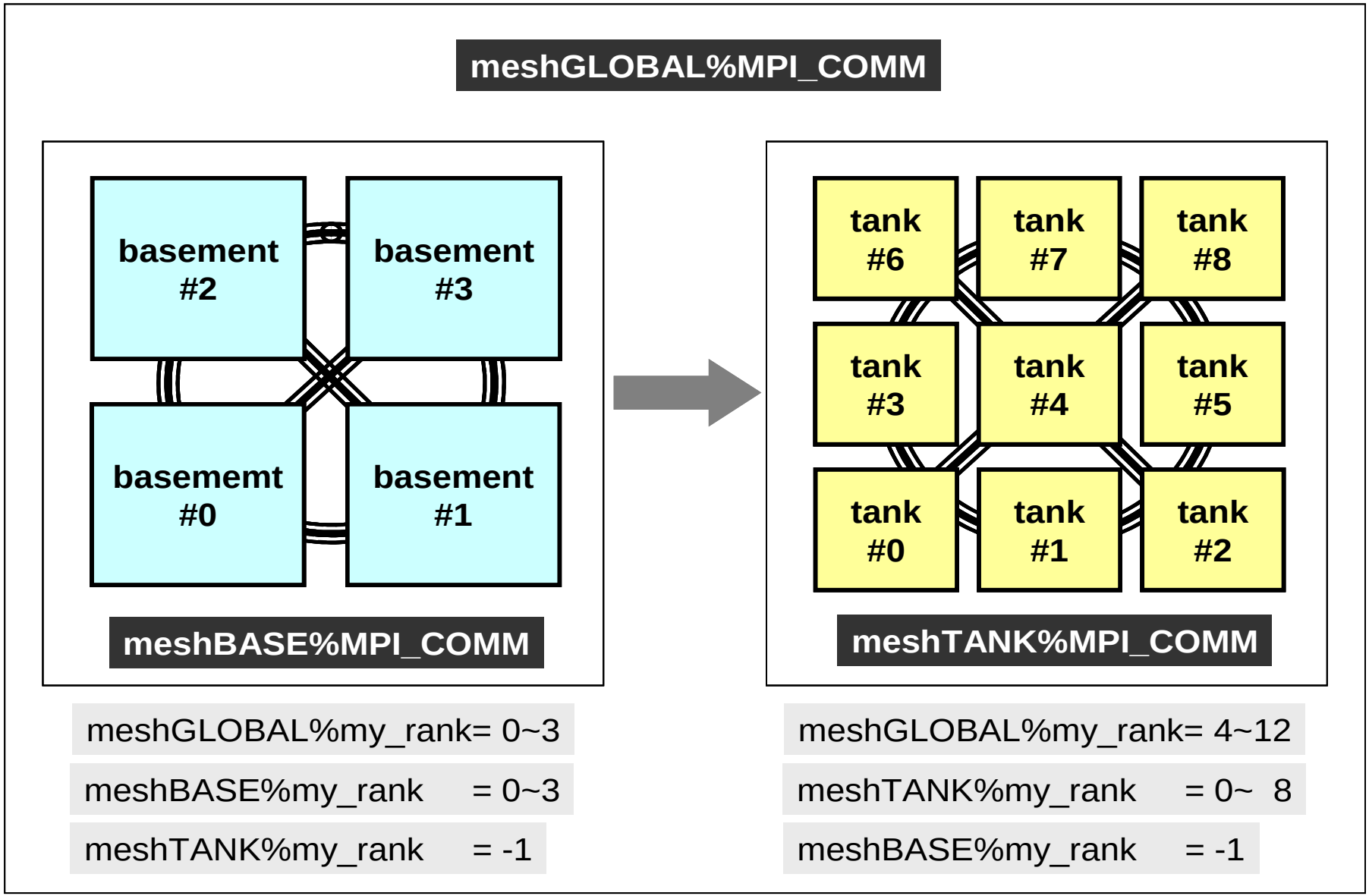
Simulation Codes

- Ground Motion (Ichimura): Fortran
  - Parallel FEM, 3D Elastic/Dynamic
    - Explicit forward Euler scheme
  - Each element: 2m × 2m × 2m cube
  - 240m × 240m × 100m region
- Sloshing of Tanks (Nagashima): C
  - Serial FEM (Embarrassingly Parallel)
    - Implicit backward Euler, Skyline method
    - Shell elements + Inviscid potential flow
  - D: 42.7m, H: 24.9m, T: 20mm,
  - Frequency: 7.6sec.
  - 80 elements in circ., 0.6m mesh in height
  - Tank-to-Tank: 60m, 4 × 4
- Total number of unknowns: 2,918,169

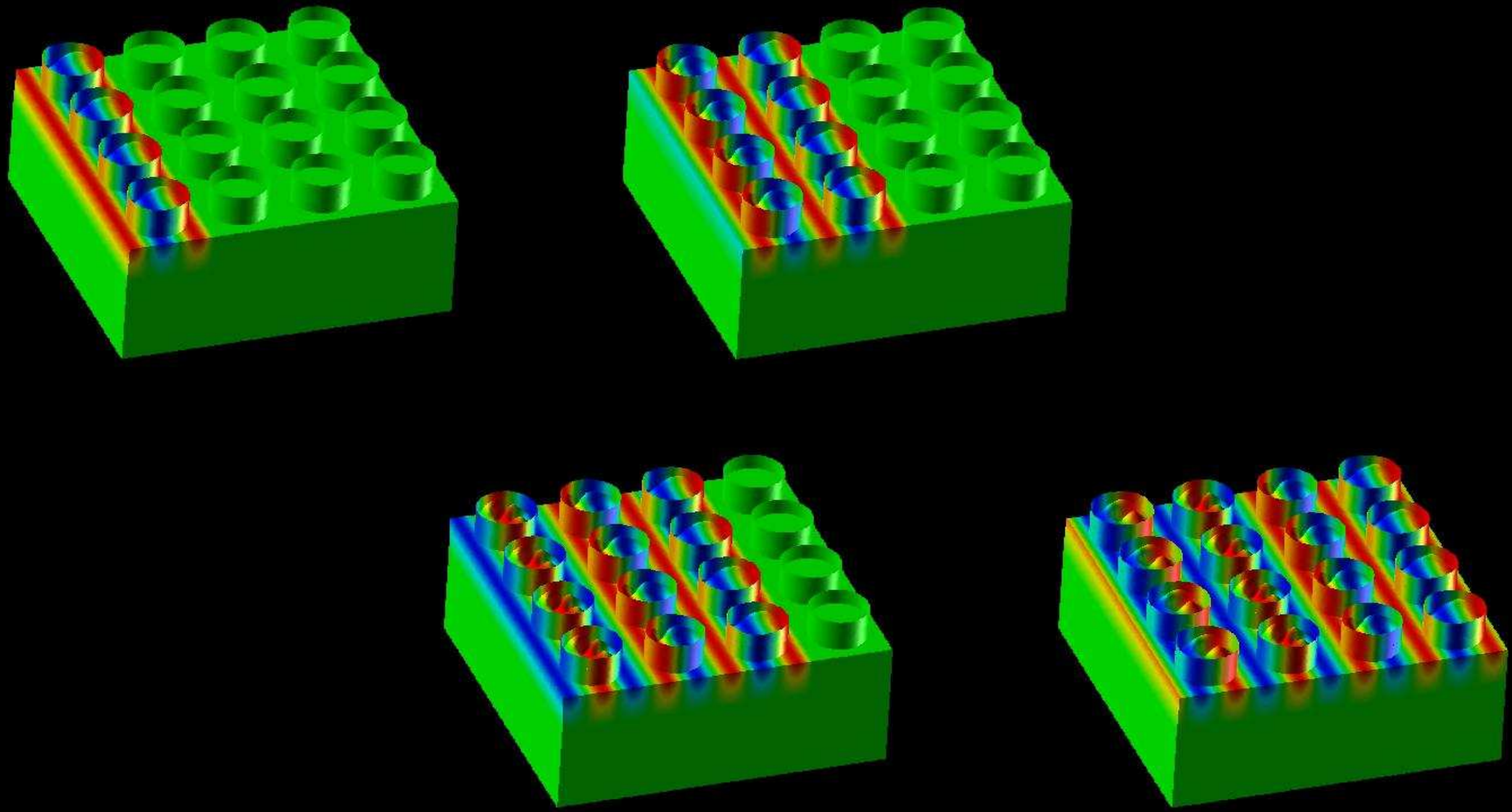


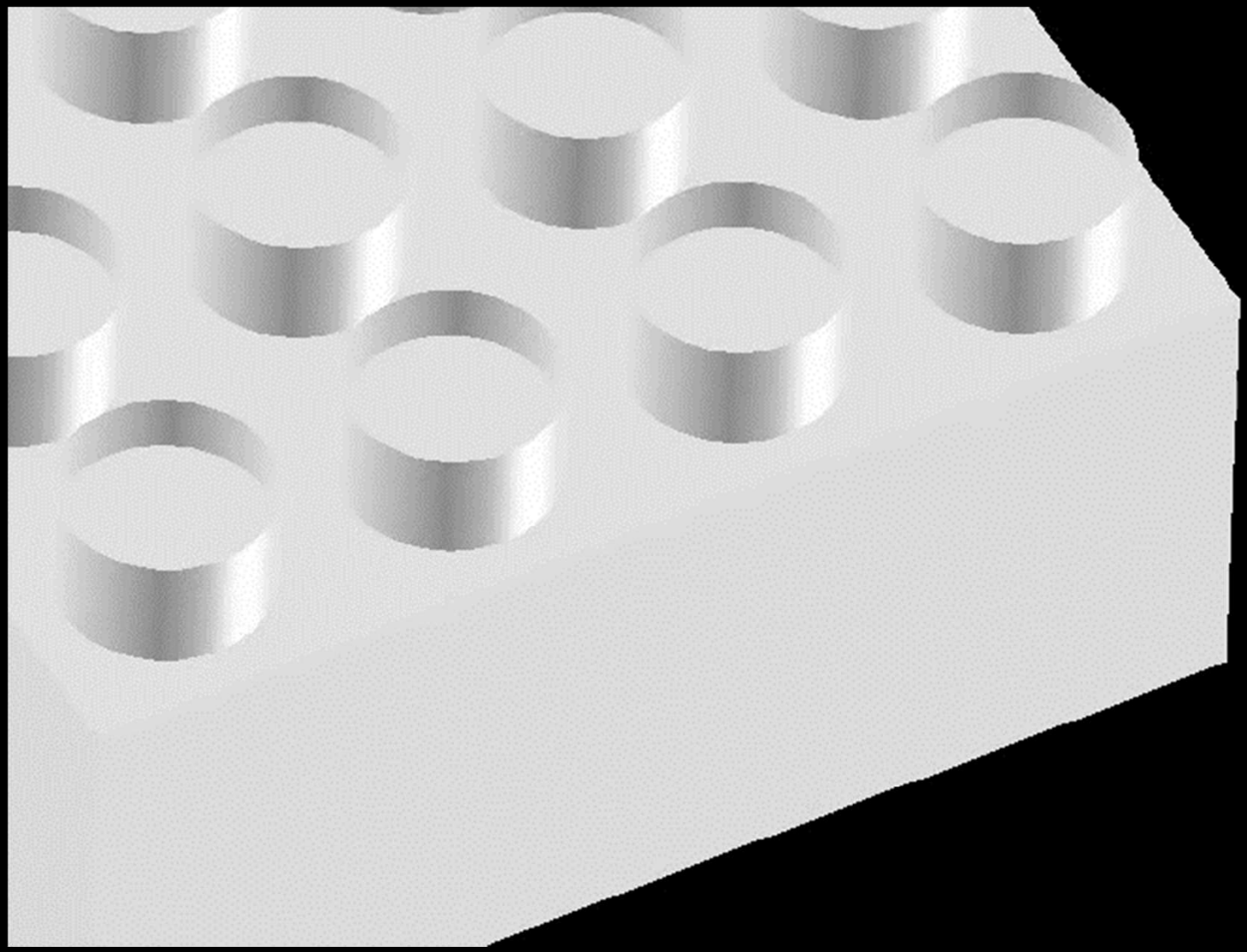


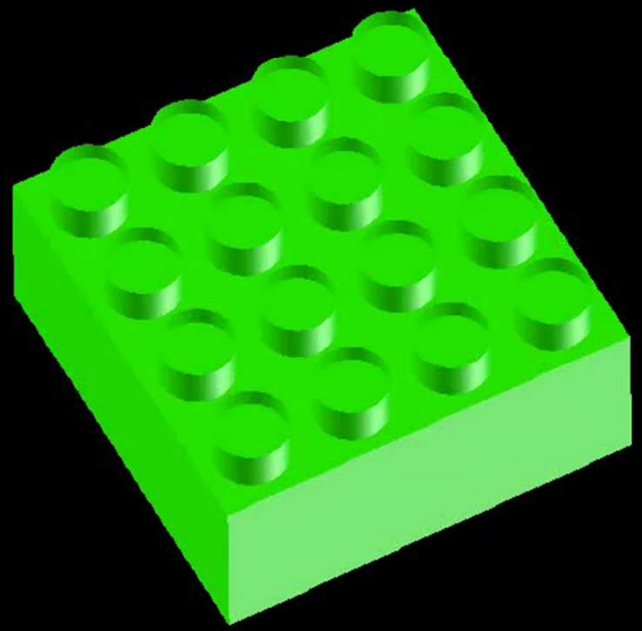
Three Communicators



Coupling between “Ground Motion” and “Sloshing of Tanks for Oil-Storage”







Fortran

MPI_COMM_RANK

- Determines the rank of the calling process in the communicator
  - "ID of MPI process" is sometimes called "rank"

- **MPI_COMM_RANK (comm, rank, ierr)**
  - **comm** I I communicator
  - **rank** I O rank of the calling process in the group of comm
    Starting from "0"
  - **ierr** I O completion code

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

write (*,'(a,2i8)') 'Hello World FORTRAN', my_rank, PETOT

call MPI_FINALIZE (ierr)

stop
end
```

Fortran

MPI_ABORT

- Aborts MPI execution environment

- **`call MPI_ABORT (comm, errcode, ierr)`**
  - **`comm`** I I communication
  - **`errcode`** I O error code
  - **`ierr`** I O completion code

Fortran

MPI_WTIME

- Returns an elapsed time on the calling processor
- **time= MPI_WTIME ()**
  - **time** R8 O Time in seconds since an arbitrary time in the past.

```
…
real(kind=8):: Stime, Etime

Stime= MPI_WTIME ()
do i= 1, 100000000
  a= 1.d0
enddo
Etime= MPI_WTIME ()

write (*,'(i5,1pe16.6)') my_rank, Etime-Stime
```

Example of MPI_Wtime

```
$> cd /work/gt36/t36XXX/pFEM/mpi/S1
$> module load fj

$> mpifccpx –Nclang –O1 time.c
$> mpifrtpx –O1 time.f

(modify go4.sh, 4 processes)
$> pjsub go4.sh

     0    1.113281E+00
     3    1.113281E+00
     2    1.117188E+00
     1    1.117188E+00

 Process      Time
   ID
```

go4.sh

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture6-o
#PJM -L node=1
#PJM --mpi proc=4
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o test.lst

module load fj
module load fjmpi

mpiexec ./a.out
```

MPI_Wtick

- Returns the resolution of MPI_Wtime
- depends on hardware, and compiler

- **`time= MPI_Wtick ()`**
  - **`time`** `double O` Time in seconds of resolution of MPI_Wtime

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'

…
TM= MPI_WTICK ()
write (*,*) TM
…
```

```
double Time;

…
Time = MPI_Wtick();
printf("%5d%16.6E¥n", MyRank, Time);
…
```

Example of MPI_Wtick

```
$> cd /work/gt36/t36XXX/pFEM/mpi/S1
$> module load fj

$> mpifccpx –Nclang –O1 wtick.c
$> mpifrtpx –O1 wtick.f

(modify go1.sh, 1 process)
$> pjsub go1.sh
```

go1.sh

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture6-o
#PJM -L node=1
#PJM --mpi proc=1
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o test.lst

module load fj
module load fjmpi

mpiexec ./a.out
```

Fortran

MPI_BARRIER

- Blocks until all processes in the communicator have reached this routine.
- Mainly for debugging, huge overhead, not recommended for real code.

- **`call MPI_BARRIER (comm, ierr)`**
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

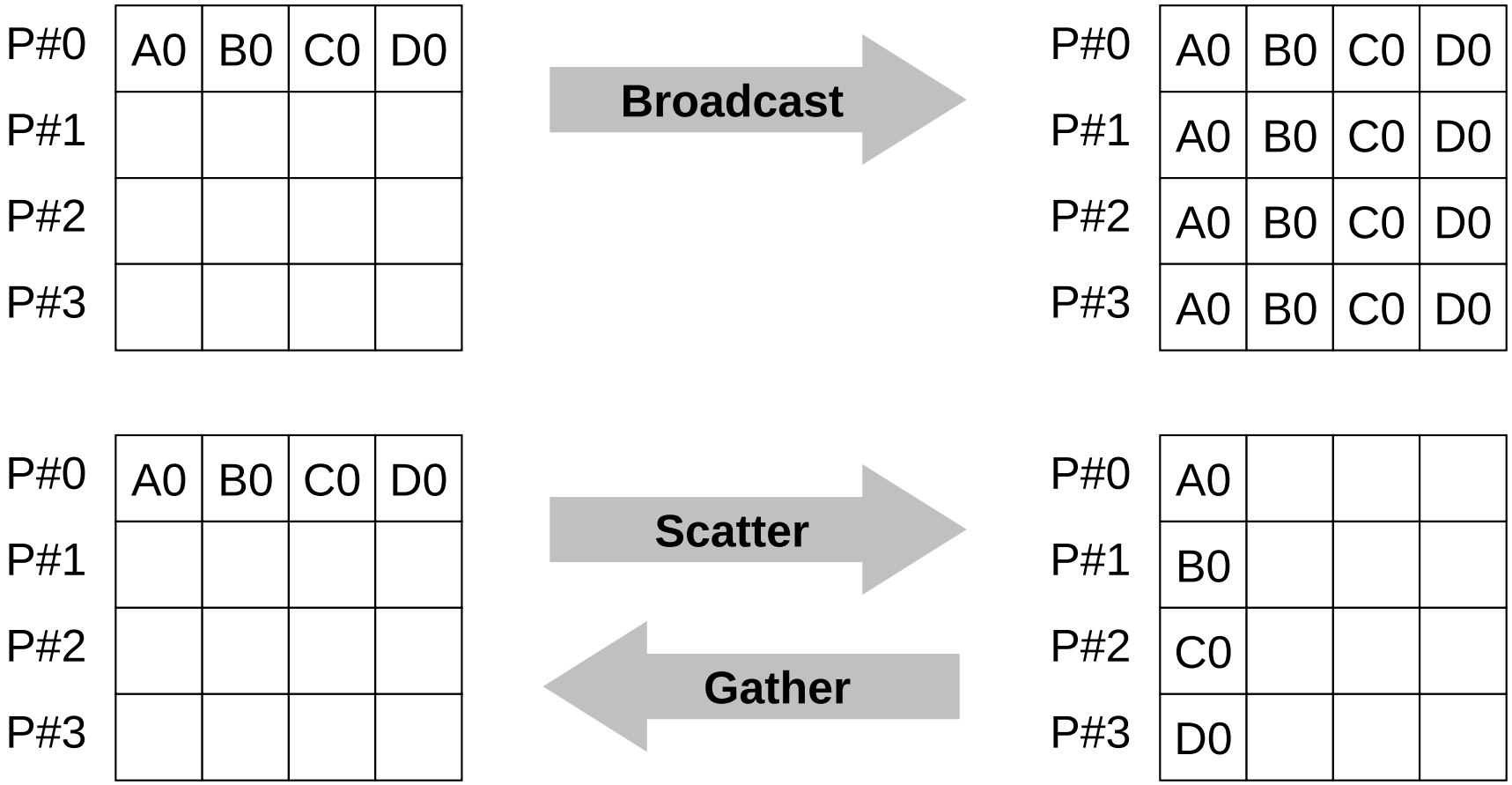
- What is MPI ?
- Your First MPI Program: Hello World
- **Collective Communication**
- Point-to-Point Communication

What is Collective Communication ?
集団通信, グループ通信

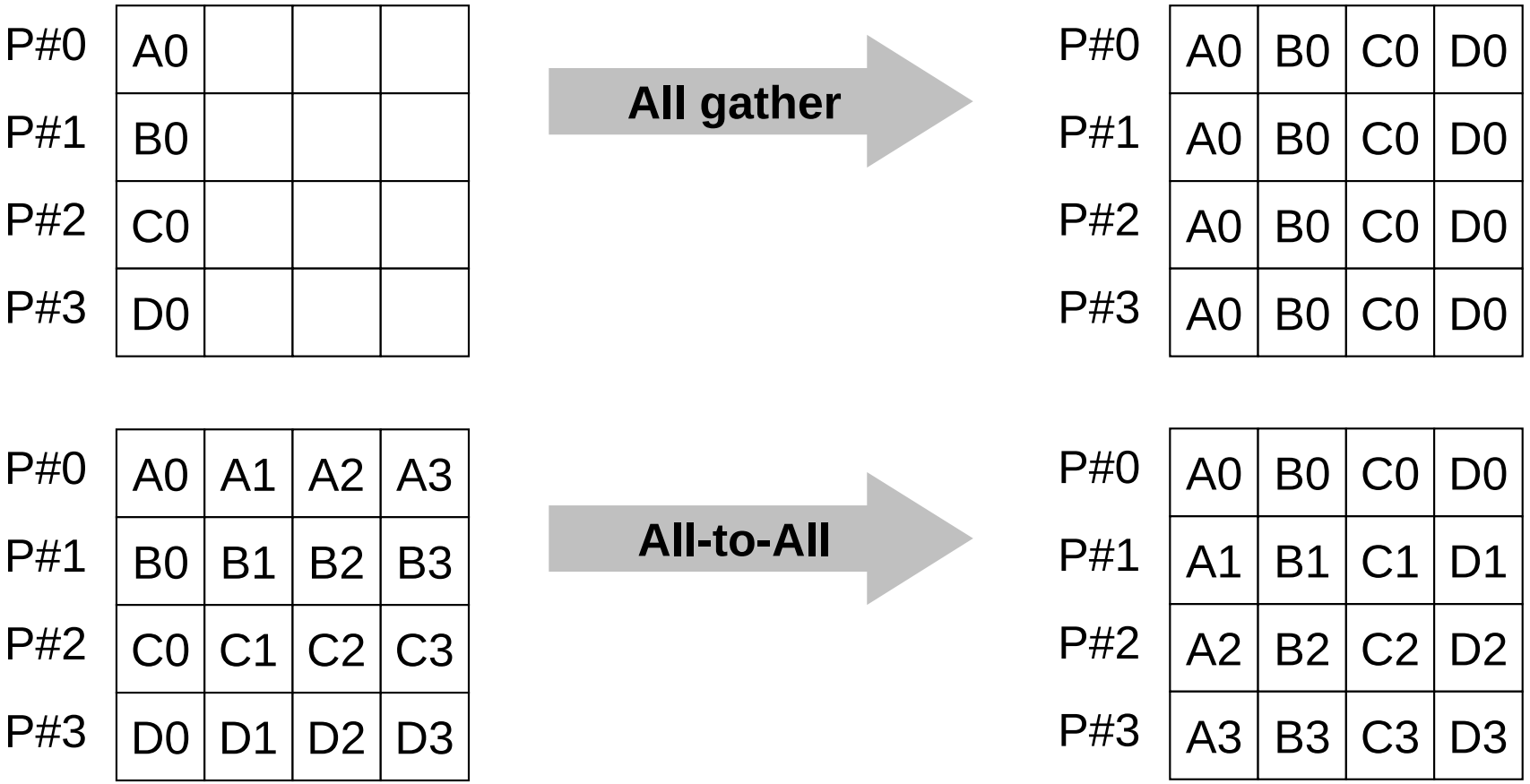
- Collective communication is the process of exchanging information between multiple MPI processes in the communicator: one-to-all or all-to-all communications.

- Examples
  - Broadcasting control data
  - Max, Min
  - Summation
  - Dot products of vectors
  - Transformation of dense matrices

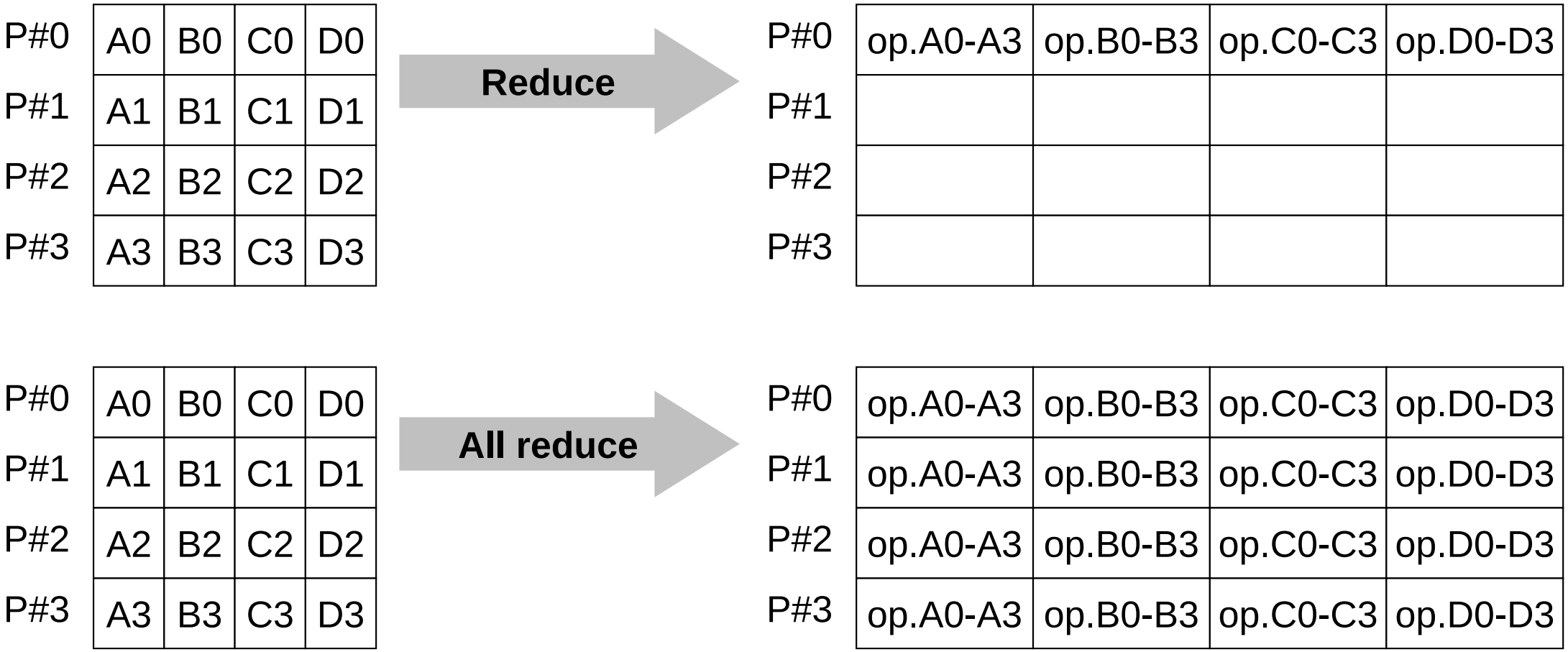
Example of Collective Communications (1/4)



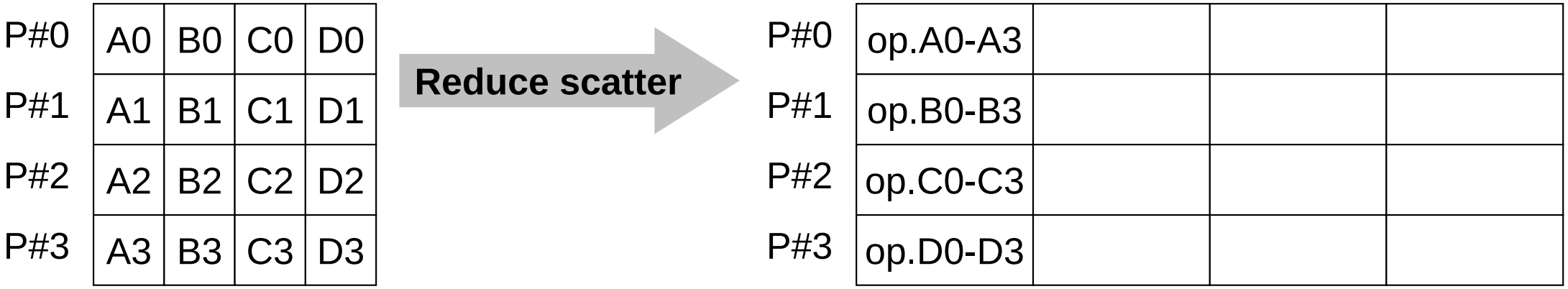
Example of Collective Communications (2/4)



Example of Collective Communications (3/4)



Example of Collective Communications (4/4)



Examples by Collective Comm.

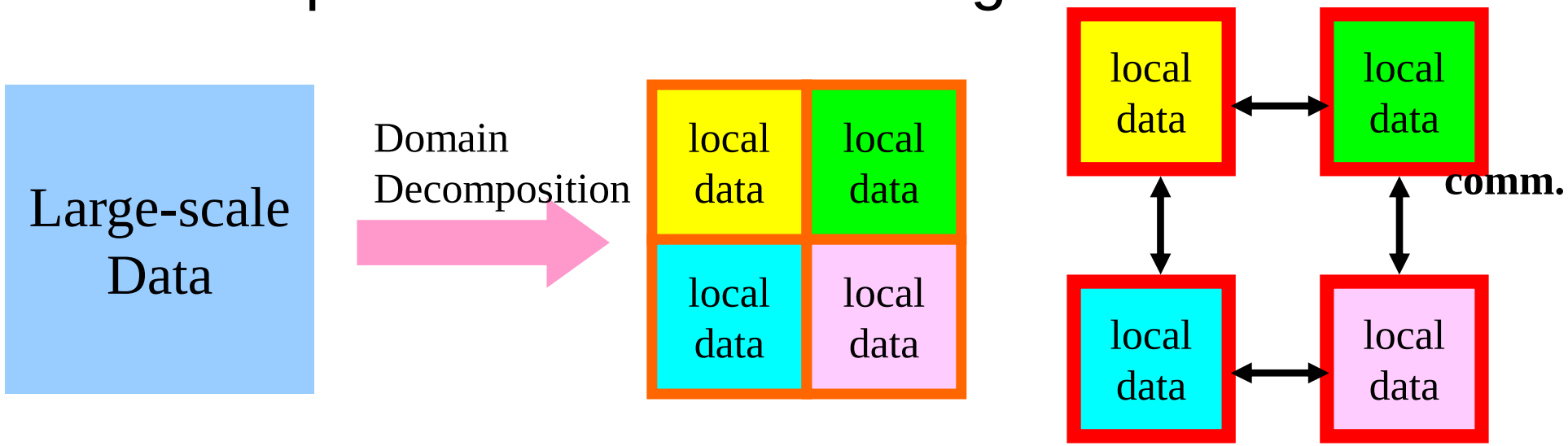
- **Dot Products of Vectors**
- Scatter/Gather
- Reading Distributed Files
- MPI_Allgatherv

Global/Local Data

- Data structure of parallel computing based on SPMD, where large scale “global data” is decomposed to small pieces of “local data”.

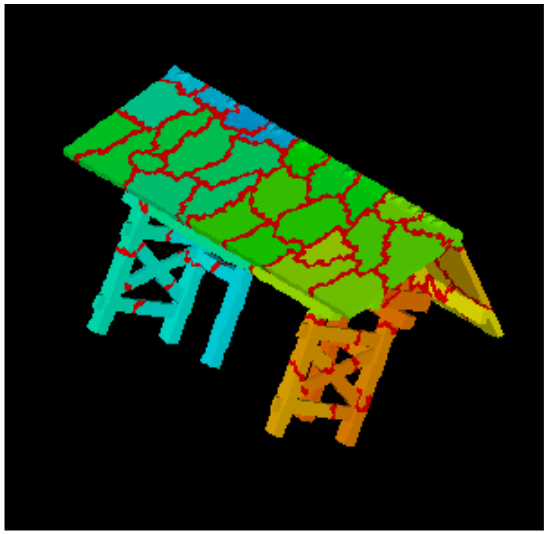
Domain Decomposition/Partitioning

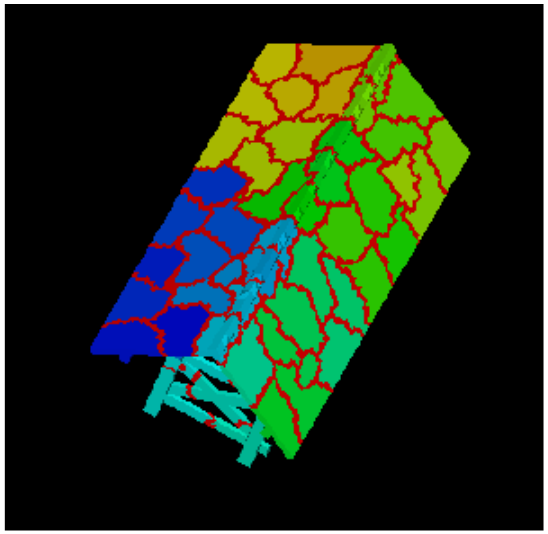
- PC with 1GB RAM: can execute FEM application with up to 10^6 meshes
  - 10^3km × 10^3 km × 10^2 km (SW Japan): 10^8 meshes by 1km cubes
- Large-scale Data: Domain decomposition, parallel & local operations
- Global Computation: Comm. among domains needed



Local Data Structure

- It is important to define proper local data structure for target computation (and its algorithm)
  - Algorithms= Data Structures
- Main objective of this class !





Global/Local Data

- Data structure of parallel computing based on SPMD, where large scale “global data” is decomposed to small pieces of “local data”.

- Consider the dot product of following VECp and VECs with length=20 by parallel computation using 4 processors

```
VECp( 1)=  2
    ( 2)=  2
    ( 3)=  2
…
    (18)=  2
    (19)=  2
    (20)=  2
```

```
VECs( 1)=  3
    ( 2)=  3
    ( 3)=  3
…
    (18)=  3
    (19)=  3
    (20)=  3
```

```
VECp[ 0]=  2
    [ 1]=  2
    [ 2]=  2
…
    [17]=  2
    [18]=  2
    [19]=  2
```

```
VECs[ 0]=  3
    [ 1]=  3
    [ 2]=  3
…
    [17]=  3
    [18]=  3
    [19]=  3
```

<$O-S1>/dot.f, dot.c

```
implicit REAL*8 (A-H,O-Z)
real(kind=8),dimension(20):: &
    VECp,  VECs

do i= 1, 20
  VECp(i)= 2.0d0
  VECs(i)= 3.0d0
enddo

sum= 0.d0
do ii= 1, 20
  sum= sum + VECp(ii)*VECs(ii)
enddo

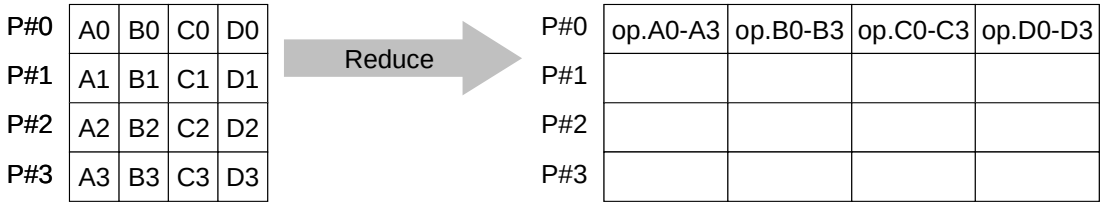
stop
end
```

```
#include <stdio.h>
int main(){
   int i;
   double VECp[20], VECs[20]
   double sum;

   for(i=0;i<20;i++){
     VECp[i]= 2.0;
     VECs[i]= 3.0;
   }

   sum = 0.0;
   for(i=0;i<20;i++){
     sum += VECp[i] * VECs[i];
   }
   return 0;
}
```

MPI_REDUCE



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

- **`call MPI_REDUCE (sendbuf,recvbuf,count,datatype,op,root,comm,ierr)`**
  - **`sendbuf`** choice I starting address of send buffer
  - **`recvbuf`** choice O starting address receive buffer
    type is defined by "**`datatype`**"
  - **`count`** I I number of elements in send/receive buffer
  - **`datatype`** I 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`** I 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`** I I rank of root process
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

Fortran

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.

Send/Receive Buffer (1/3)
A: Scalar

```
call MPI_REDUCE
(A,recvbuf, 1,datatype,op,root,comm,ierr)

MPI_Reduce
(A,recvbuf,1,datatype,op,root,comm)
```

Send/Receive Buffer (2/3)
A: Array

```
call MPI_REDUCE
(A,recvbuf, 3,datatype,op,root,comm,ierr)

MPI_Reduce
(A,recvbuf,3,datatype,op,root,comm)
```

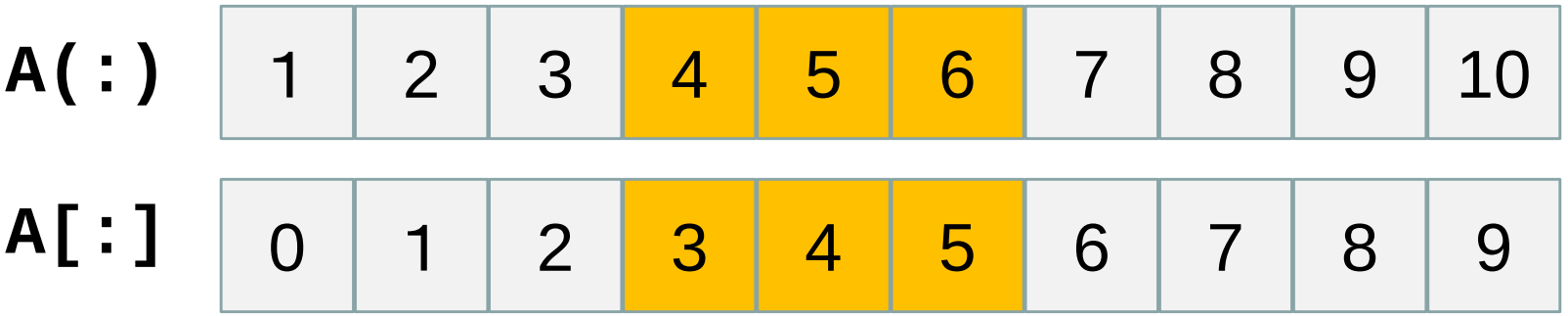
- Starting Address of Send Buffer
  - A(1): Fortran, A[0]: C
  - 3 (continuous) components of A (A(1)-A(3), A[0]-A[2]) are sent

Send/Receive Buffer (3/3)
A: Array

```
call MPI_REDUCE
(A(4),recvbuf, 3,datatype,op,root,comm,ierr)

MPI_Reduce
(A[3],recvbuf,3,datatype,op,root,comm)
```

- Starting Address of Send Buffer
  - A(4): Fortran, A[3]: C
  - 3 (continuous) components of A (A(4)-A(6), A[3]-A[5]) are sent



Fortran

Example of MPI_Reduce (1/2)

```
call MPI_REDUCE
(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

```
real(kind=8):: X0, X1

call MPI_REDUCE
(X0, X1, 1, MPI_DOUBLE_PRECISION, MPI_MAX, 0, <comm>, ierr)
```

```
real(kind=8):: X0(4), XMAX(4)

call MPI_REDUCE
(X0, XMAX, 4, MPI_DOUBLE_PRECISION, MPI_MAX, 0, <comm>, ierr)
```

Global Max. values of X0(i) go to XMAX(i) on #0 process (i=1-4)

Fortran

Example of MPI_Reduce (2/2)

```
call MPI_REDUCE
(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

```
real(kind=8):: X0, XSUM

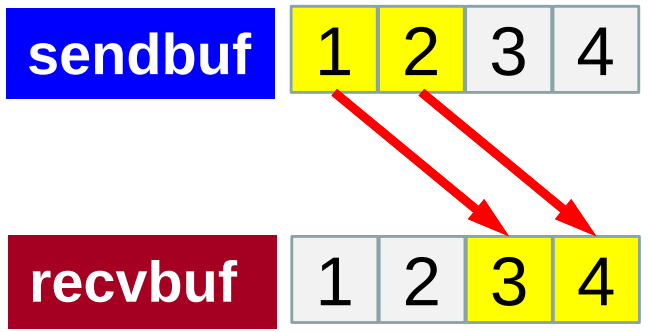
call MPI_REDUCE
(X0, XSUM, 1, MPI_DOUBLE_PRECISION, MPI_SUM, 0, <comm>, ierr)
```

Global summation of X0 goes to XSUM on #0 process.

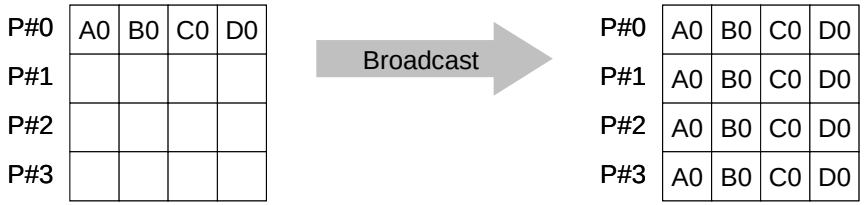
```
real(kind=8):: X0(4)

call MPI_REDUCE
(X0(1), X0(3), 2, MPI_DOUBLE_PRECISION, MPI_SUM, 0, <comm>, ierr)
```

- Global summation of X0(1) goes to X0(3) on #0 process.
- Global summation of X0(2) goes to X0(4) on #0 process.



MPI_BCAST

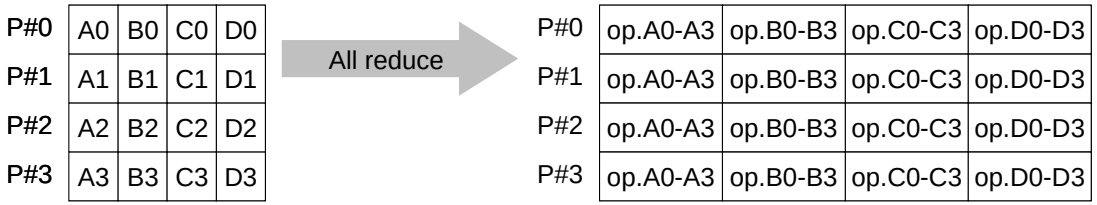


- Broadcasts a message from the process with rank "root" to all other processes of the communicator

- **`call MPI_BCAST (buffer,count,datatype,root,comm,ierr)`**
  - **`buffer`** `choice I/O` starting address of buffer
    type is defined by "**`datatype`**"
  - **`count`** `I I` number of elements in send/recv buffer
  - **`datatype`** `I I` data type of elements of send/recv buffer
    `FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.`
    `C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc.`
  - **`root`** `I I` rank of root process
  - **`comm`** `I I` communicator
  - **`ierr`** `I O` completion code

Fortran

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,ierr)`**
  - **`sendbuf`** choice I — starting address of send buffer
  - **`recvbuf`** choice O — starting address receive buffer
    type is defined by **"`datatype`"**
  - **`count`** I I — number of elements in send/recv buffer
  - **`datatype`** I I — data type of elements in send/recv buffer
  - **`op`** I I — reduce operation
  - **`comm`** I I — commuinicator
  - **`ierr`** I O — completion code

Fortran

“op” of MPI_Reduce/Allreduce

Fortran

```
call MPI_REDUCE
(sendbuf,recvbuf,count,datatype,op,root,comm,ierr)
```

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

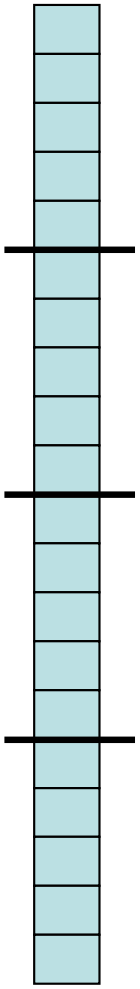
Local Data (1/2)

Fortran

- Decompose vector with length=20 into 4 domains (processes)
- Each process handles a vector with length= 5

```
VECp( 1)=  2
    ( 2)=  2
    ( 3)=  2
…
    (18)=  2
    (19)=  2
    (20)=  2
```

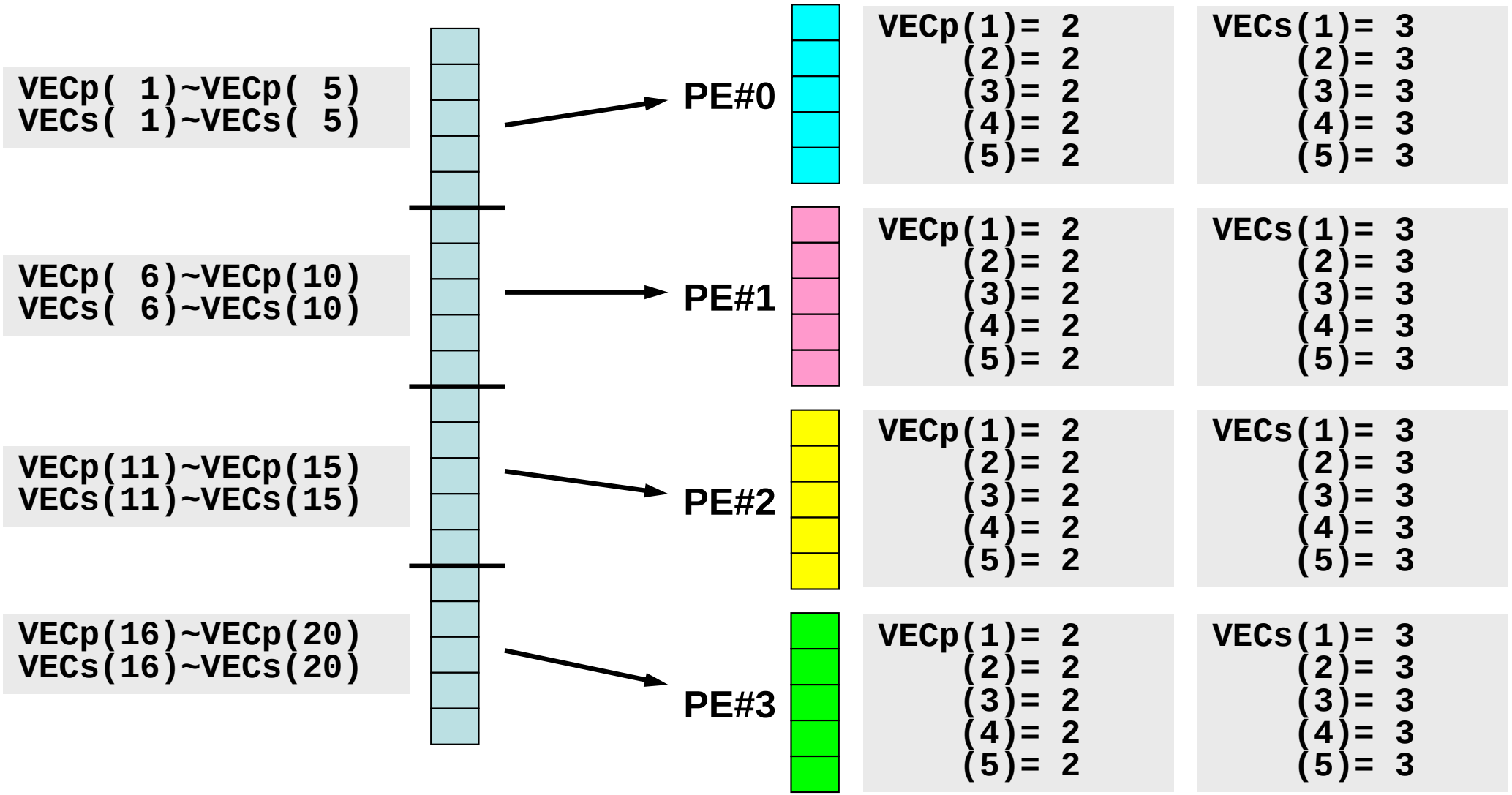
```
VECs( 1)=   3
    ( 2)=   3
    ( 3)=   3
…
    (18)=   3
    (19)=   3
    (20)=   3
```



Local Data (2/2)

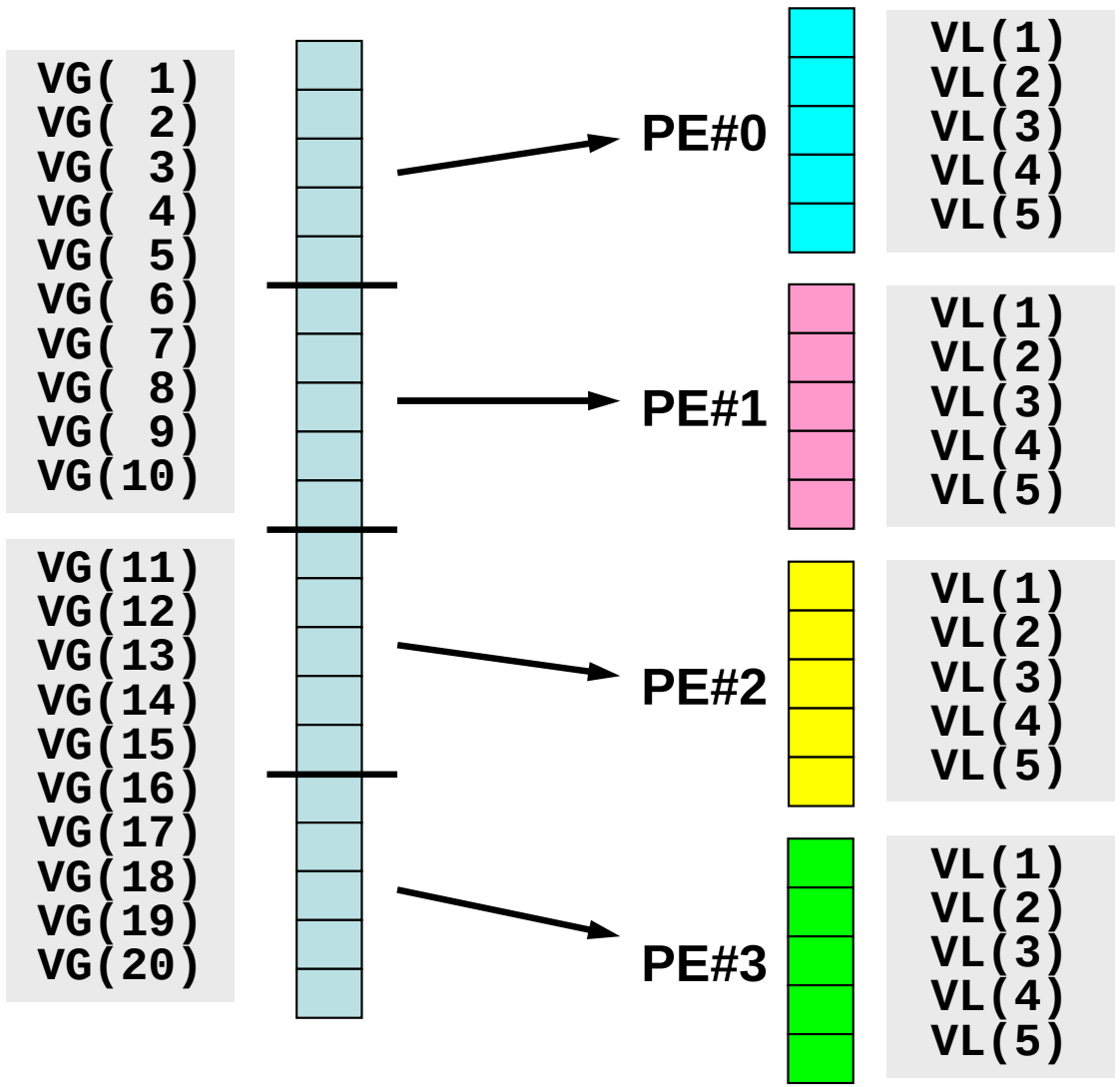
Fortran

- 1th-5th components of original global vector go to 1th-5th components of PE#0, 6th-10th -> PE#1, 11th-15th -> PE#2, 16th-20th -> PE#3.



But ...

- It is too easy !! Just decomposing and renumbering from 1 (or 0).
- Of course, this is not enough. Further examples will be shown in the latter part.



Example: Dot Product (1/3)

<$O-S1>/allreduce.f

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr
real(kind=8), dimension(5) :: VECp,  VECs

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

sumA= 0.d0
sumR= 0.d0
do i= 1, 5
  VECp(i)= 2.d0
  VECs(i)= 3.d0
enddo

sum0= 0.d0
do i= 1, 5
  sum0= sum0 + VECp(i) * VECs(i)
enddo

if (my_rank.eq.0) then
  write (*,'(a)') '(my_rank, sumALLREDUCE, sumREDUCE)‘
endif
```

Local vector is generated at each local process.

Example: Dot Product (2/3)

<$O-S1>/allreduce.f

```
!C
!C-- REDUCE
  call MPI_REDUCE (sum0, sumR, 1, MPI_DOUBLE_PRECISION, MPI_SUM, 0, &
                   MPI_COMM_WORLD, ierr)

!C
!C-- ALL-REDUCE
  call MPI_Allreduce (sum0, sumA, 1, MPI_DOUBLE_PRECISION, MPI_SUM, &
                      MPI_COMM_WORLD, ierr)

  write (*,'(a,i5, 2(1pe16.6))') 'before BCAST', my_rank, sumA, sumR
```

Dot Product

Summation of results of each process (sum0)

“sumR” has value only on PE#0.

“sumA” has value on all processes by MPI_Allreduce

Example: Dot Product (3/3)

<$O-S1>/allreduce.f

```
!C
!C-- BCAST
  call MPI_BCAST (sumR, 1, MPI_DOUBLE_PRECISION, 0, MPI_COMM_WORLD, &
                  ierr)
  write (*,'(a,i5, 2(1pe16.6))') 'after  BCAST', my_rank, sumA, sumR

  call MPI_FINALIZE (ierr)

  stop
  end
```

“sumR” has value on PE#1-#3 by MPI_Bcast

Execute <$O-S1>/allreduce.f/c

```
$> cd /work/gt36/t36XXX/pFEM/mpi/S1
$> module load fj
$> mpifrtpx -Kfast allreduce.f
$> mpifccpx –Nclang -Kfast allreduce.c
(modify go4.sh, 4-processes)
$> pjsub go4.sh

(my_rank, sumALLREDUCE,sumREDUCE)
before BCAST    0    1.200000E+02    1.200000E+02
after  BCAST    0    1.200000E+02    1.200000E+02

before BCAST    1    1.200000E+02    0.000000E+00
after  BCAST    1    1.200000E+02    1.200000E+02

before BCAST    3    1.200000E+02    0.000000E+00
after  BCAST    3    1.200000E+02    1.200000E+02

before BCAST    2    1.200000E+02    0.000000E+00
after  BCAST    2    1.200000E+02    1.200000E+02
```

Examples by Collective Comm.

- Dot Products of Vectors
- **Scatter/Gather**
- Reading Distributed Files
- MPI_Allgatherv

Global/Local Data (1/3)

- Parallelization of an easy process where a real number α is added to each component of real vector **VECg**:

```
      do i= 1, NG
        VECg(i)= VECg(i) + ALPHA
      enddo
```

```
for (i=0; i<NG; i++{
    VECg[i]= VECg[i] + ALPHA
}
```

Global/Local Data (2/3)

- Configurationa
  - **NG= 32 (length of the vector)**
  - **ALPHA=1000.**
  - Process # of MPI= 4

- Vector VECg has following 32 components (<$O-S1>/a1x.all):

```
(101.0,  103.0,  105.0,  106.0,  109.0,  111.0,  121.0,  151.0,
 201.0,  203.0,  205.0,  206.0,  209.0,  211.0,  221.0,  251.0,
 301.0,  303.0,  305.0,  306.0,  309.0,  311.0,  321.0,  351.0,
 401.0,  403.0,  405.0,  406.0,  409.0,  411.0,  421.0,  451.0)
```

Global/Local Data (3/3)

- Procedure
  - ① Reading vector **VECg** with length=32 from one process (*e.g.* 0th process)
    - Global Data
  - ② Distributing vector components to 4 MPI processes equally (*i.e.* length= 8 for each processes)
    - Local Data, Local ID/Numbering
  - ③ Adding **ALPHA** to each component of the local vector (with length= 8) on each process.
  - ④ Merging the results to global vector with length= 32.

- Actually, we do not need parallel computers for such a kind of small computation.

Operations of Scatter/Gather (1/8)

Reading **VECg** (length=32) from a process (*e.g.* #0)

- Reading global data from #0 process

```
include   'mpif.h'
integer,  parameter :: NG= 32
real(kind=8), dimension(NG):: VECg

call MPI_INIT (ierr)
call MPI_COMM_SIZE (<comm>, PETOT  , ierr)
call MPI_COMM_RANK (<comm>, my_rank, ierr)

if (my_rank.eq.0) then
  open (21, file= 'a1x.all', status= 'unknown')
  do i= 1, NG
    read (21,*) VECg(i)
  enddo
  close (21)
endif
```

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

int main(int argc, char **argv){
  int i, NG=32;
  int PeTot, MyRank, MPI_Comm;
  double VECg[32];
  char filename[80];
  FILE *fp;

  MPI_Init(&argc, &argv);
  MPI_Comm_size(<comm>, &PeTot);
  MPI_Comm_rank(<comm>, &MyRank);

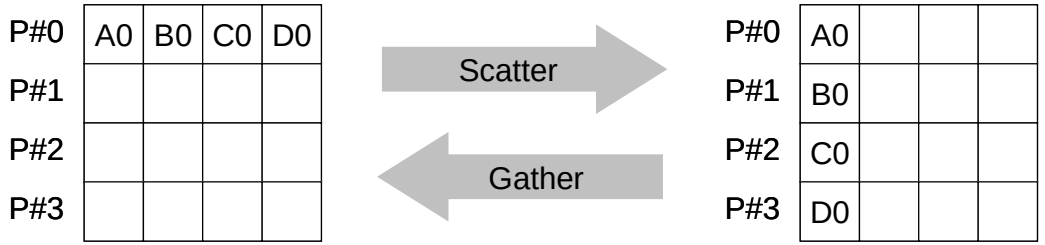
        fp = fopen("a1x.all", "r");
        if(!MyRank) for(i=0;i<NG;i++){
                fscanf(fp, "%lf", &VECg[i]);
        }
```

Operations of Scatter/Gather (2/8)

Distributing global data to 4 process equally (*i.e.* length=8 for each process)

- MPI_Scatter

MPI_SCATTER



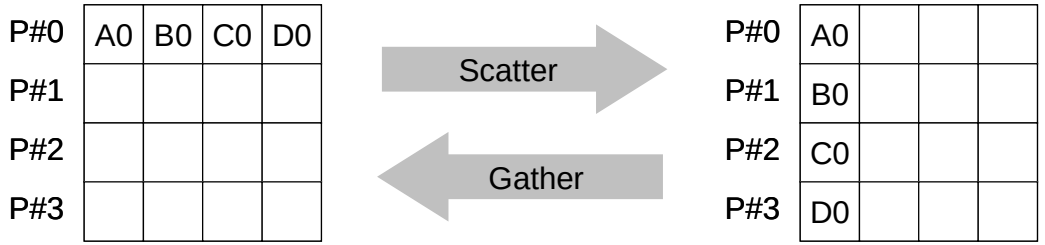
- Sends data from one process to all other processes in a communicator
  - scount-size messages are sent to each process

- **call MPI_SCATTER (sendbuf, scount, sendtype, recvbuf, rcount, recvtype, root, comm, ierr)**
  - **sendbuf** choice I starting address of sending buffer
    type is defined by "**datatype**"
  - **scount** I I number of elements sent to each process
  - **sendtype** I I data type of elements of sending buffer

    FORTRAN MPI_INTEGER, MPI_REAL, MPI_DOUBLE_PRECISION, MPI_CHARACTER etc.
    C MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR etc.
  - **recvbuf** choice O starting address of receiving buffer
  - **rcount** I I number of elements received from the root process
  - **recvtype** I I data type of elements of receiving buffer
  - **root** I I rank of root process
  - **comm** I I communicator
  - **ierr** I O completion code

Fortran

MPI_SCATTER (cont.)



- **call MPI_SCATTER (sendbuf, scount, sendtype, recvbuf, rcount, recvtype, root, comm, ierr)**
  - **sendbuf** choice I — starting address of sending buffer; type is defined by "**datatype**"
  - **scount** I I — number of elements sent to each process
  - **sendtype** I I — data type of elements of sending buffer
  - **recvbuf** choice O — starting address of receiving buffer
  - **rcount** I I — number of elements received from the root process
  - **recvtype** I I — data type of elements of receiving buffer
  - **root** I I — rank of root process
  - **comm** I I — communicator
  - **ierr** I O — completion code
- Usually
  - **scount = rcount**
  - **sendtype= recvtype**
- This function sends **scount** components starting from **sendbuf** (sending buffer) at process **#root** to each process in **comm**. Each process receives **rcount** components starting from **recvbuf** (receiving buffer).

Fortran

Operations of Scatter/Gather (3/8)

Distributing global data to 4 processes equally

- Allocating receiving buffer **VEC** (length=8) at each process.
- 8 components sent from sending buffer **VECg** of process #0 are received at each process #0-#3 as 1st-8th components of receiving buffer **VEC**.

```
integer, parameter :: N =  8
real(kind=8), dimension(N ) :: VEC
...
call MPI_Scatter                              &
     (VECg, N, MPI_DOUBLE_PRECISION, &
      VEC , N, MPI_DOUBLE_PRECISION, &
      0, <comm>, ierr)
```

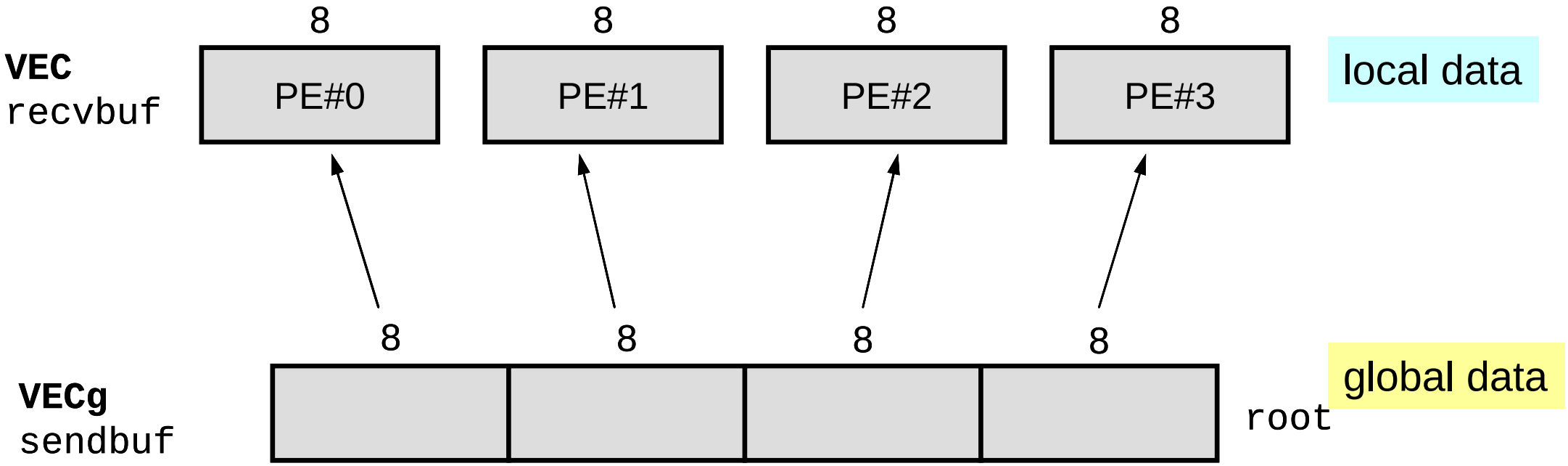
```
int  N=8;
double VEC [8];
...
MPI_Scatter  (VECg,  N,  MPI_DOUBLE,  VEC,  N,
MPI_DOUBLE, 0, <comm>);
```

```
call MPI_SCATTER
(sendbuf, scount, sendtype, recvbuf, rcount,
 recvtype, root, comm, ierr)
```

Operations of Scatter/Gather (4/8)

Distributing global data to 4 processes equally

- 8 components are *scattered* to each process from root (#0)
- 1st-8th components of **VECg** are stored as 1st-8th ones of **VEC** at **#0**, 9th-16th components of **VECg** are stored as 1st-8th ones of **VEC** at **#1**, etc.
  - **VECg**: Global Data, **VEC**: Local Data



Operations of Scatter/Gather (5/8)

Distributing global data to 4 processes equally

- Global Data: 1st-32nd components of **VECg** at **#0**
- Local Data: 1st-8th components of **VEC** at each process
- Each component of **VEC** can be written from each process in the following way:

```
do i= 1, N
  write (*,'(a, 2i8,f10.0)') 'before',  my_rank, i, VEC(i)
enddo
```

```
for(i=0;i<N;i++){
printf("before %5d %5d %10.0F¥n", MyRank, i+1, VEC[i]);}
```

Operations of Scatter/Gather (5/8)

Distributing global data to 4 processes equally

- Global Data: 1st-32nd components of **VECg** at **#0**
- Local Data: 1st-8th components of **VEC** at each process
- Each component of **VEC** can be written from each process in the following way:

```
PE#0
before 0 1   101.
before 0 2   103.
before 0 3   105.
before 0 4   106.
before 0 5   109.
before 0 6   111.
before 0 7   121.
before 0 8   151.
```

```
PE#1
before 1 1   201.
before 1 2   203.
before 1 3   205.
before 1 4   206.
before 1 5   209.
before 1 6   211.
before 1 7   221.
before 1 8   251.
```

```
PE#2
before 2 1   301.
before 2 2   303.
before 2 3   305.
before 2 4   306.
before 2 5   309.
before 2 6   311.
before 2 7   321.
before 2 8   351.
```

```
PE#3
before 3 1   401.
before 3 2   403.
before 3 3   405.
before 3 4   406.
before 3 5   409.
before 3 6   411.
before 3 7   421.
before 3 8   451.
```

Operations of Scatter/Gather (6/8)

On each process, **ALPHA** is added to each of 8 components of **VEC**

- On each process, computation is in the following way

```
real(kind=8), parameter :: ALPHA= 1000.
do i= 1, N
  VEC(i)= VEC(i) + ALPHA
enddo
```

```
double ALPHA=1000.;
...
for(i=0;i<N;i++){
  VEC[i]= VEC[i] + ALPHA;}
```

- Results:

PE#0
```
after 0 1  1101.
after 0 2  1103.
after 0 3  1105.
after 0 4  1106.
after 0 5  1109.
after 0 6  1111.
after 0 7  1121.
after 0 8  1151.
```

PE#1
```
after 1 1  1201.
after 1 2  1203.
after 1 3  1205.
after 1 4  1206.
after 1 5  1209.
after 1 6  1211.
after 1 7  1221.
after 1 8  1251.
```

PE#2
```
after 2 1  1301.
after 2 2  1303.
after 2 3  1305.
after 2 4  1306.
after 2 5  1309.
after 2 6  1311.
after 2 7  1321.
after 2 8  1351.
```

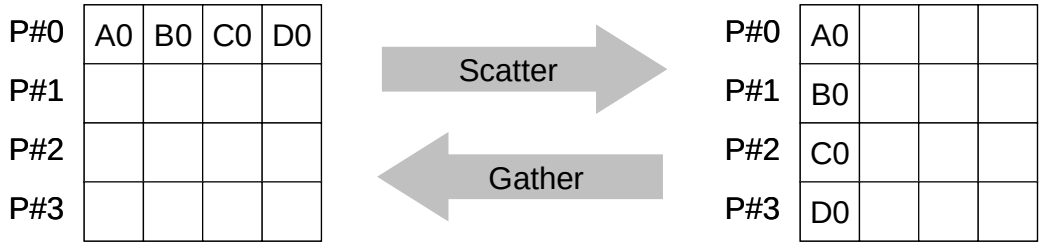
PE#3
```
after 3 1  1401.
after 3 2  1403.
after 3 3  1405.
after 3 4  1406.
after 3 5  1409.
after 3 6  1411.
after 3 7  1421.
after 3 8  1451.
```

Operations of Scatter/Gather (7/8)

Merging the results to global vector with length= 32

- Using MPI_Gather (inverse operation to MPI_Scatter)

MPI_GATHER



- Gathers together values from a group of processes, inverse operation to MPI_Scatter

- **`call MPI_GATHER (sendbuf, scount, sendtype, recvbuf, rcount, recvtype, root, comm, ierr)`**
  - **`sendbuf`** choice I starting address of sending buffer
  - **`scount`** I I number of elements sent to each process
  - **`sendtype`** I I data type of elements of sending buffer
  - **`recvbuf`** choice O starting address of receiving buffer
  - **`rcount`** I I number of elements received from the root process
  - **`recvtype`** I I data type of elements of receiving buffer
  - **`root`** I I rank of root process
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

- **`recvbuf`** is on **`root`** process.

Fortran

Operations of Scatter/Gather (8/8)

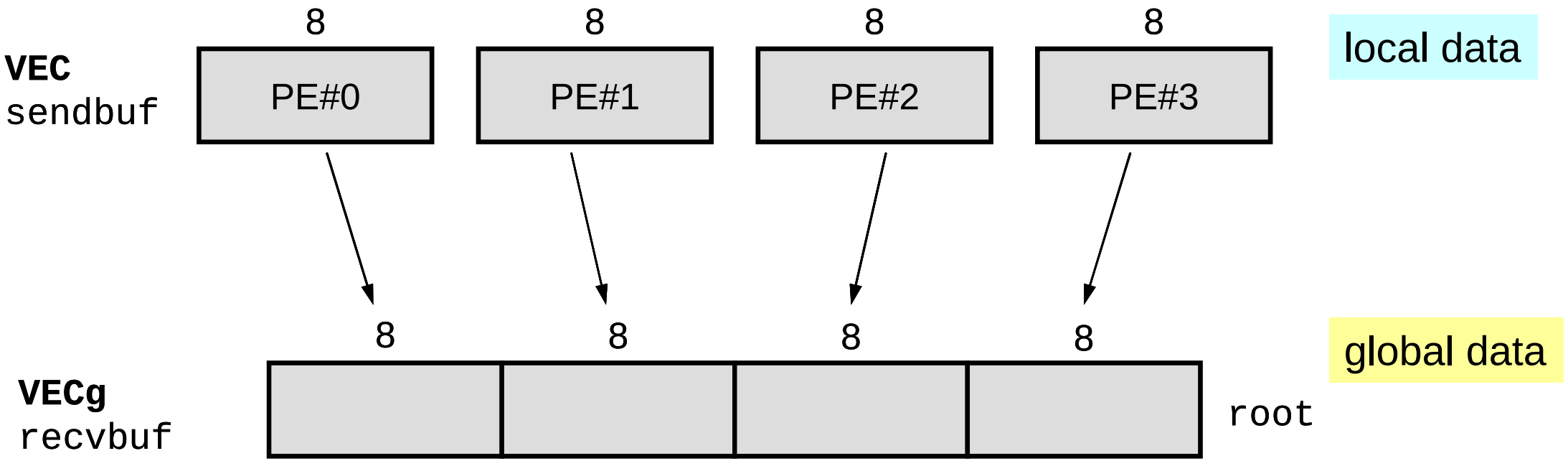
Merging the results to global vector with length= 32

- Each process components of **VEC** to **VECg** on root (#0 in this case).

```
call MPI_Gather                                    &
     (VEC , N, MPI_DOUBLE_PRECISION, &
      VECg, N, MPI_DOUBLE_PRECISION, &
      0, <comm>, ierr)
```

```
MPI_Gather (VEC, N, MPI_DOUBLE, VECg, N,
MPI_DOUBLE, 0, <comm>);
```

- 8 components are gathered from each process to the root process.



<$O-S1>/scatter-gather.f/c

```
$> cd /work/gt36/t36XXX/pFEM/mpi/S1
$> module load fj
$> mpifccpx –Nclang –Kfast scatter-gather.c
$> mpifrtpx –Kfast scatter-gather.f

(modify go4.sh, 4-processes)
$> pjsub go4.sh
```

```
PE#0
before 0 1   101.
before 0 2   103.
before 0 3   105.
before 0 4   106.
before 0 5   109.
before 0 6   111.
before 0 7   121.
before 0 8   151.
```

```
PE#1
before 1 1   201.
before 1 2   203.
before 1 3   205.
before 1 4   206.
before 1 5   209.
before 1 6   211.
before 1 7   221.
before 1 8   251.
```

```
PE#2
before 2 1   301.
before 2 2   303.
before 2 3   305.
before 2 4   306.
before 2 5   309.
before 2 6   311.
before 2 7   321.
before 2 8   351.
```

```
PE#3
before 3 1   401.
before 3 2   403.
before 3 3   405.
before 3 4   406.
before 3 5   409.
before 3 6   411.
before 3 7   421.
before 3 8   451.
```

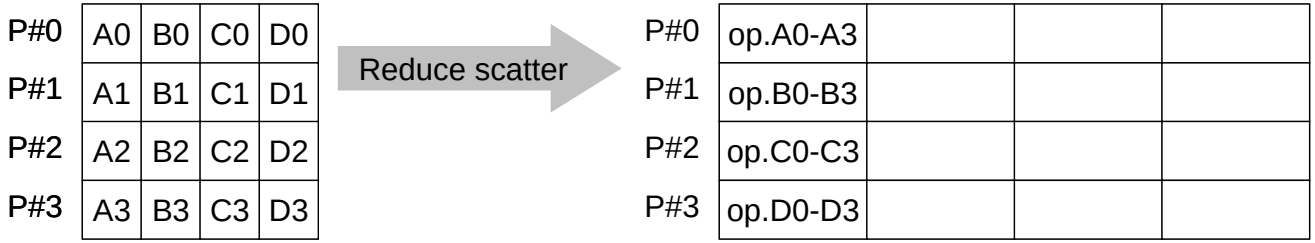
```
PE#0
after 0 1   1101.
after 0 2   1103.
after 0 3   1105.
after 0 4   1106.
after 0 5   1109.
after 0 6   1111.
after 0 7   1121.
after 0 8   1151.
```

```
PE#1
after 1 1   1201.
after 1 2   1203.
after 1 3   1205.
after 1 4   1206.
after 1 5   1209.
after 1 6   1211.
after 1 7   1221.
after 1 8   1251.
```

```
PE#2
after 2 1   1301.
after 2 2   1303.
after 2 3   1305.
after 2 4   1306.
after 2 5   1309.
after 2 6   1311.
after 2 7   1321.
after 2 8   1351.
```

```
PE#3
after 3 1   1401.
after 3 2   1403.
after 3 3   1405.
after 3 4   1406.
after 3 5   1409.
after 3 6   1411.
after 3 7   1421.
after 3 8   1451.
```

MPI_REDUCE_SCATTER

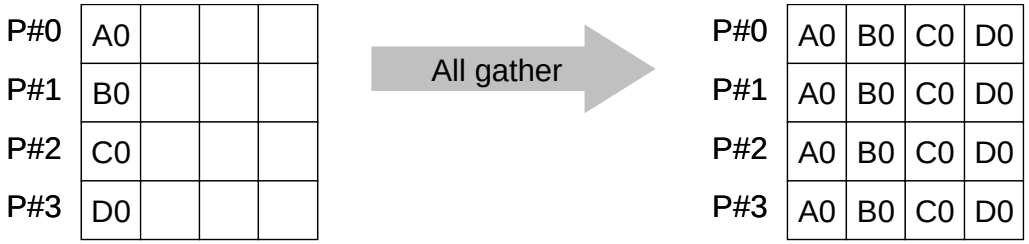


- MPI_REDUCE + MPI_SCATTER

- **`call MPI_REDUCE_SCATTER (sendbuf, recvbuf, rcount, datatype, op, comm, ierr)`**
  - **`sendbuf`** choice I starting address of sending buffer
  - **`recvbuf`** choice O starting address of receiving buffer
  - **`rcount`** I I integer array specifying the number of elements in result distributed to each process. Array must be identical on all calling processes.
  - **`datatype`** I I data type of elements of sending/receiving buffer
  - **`op`** I I reduce operation
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

Fortran

MPI_ALLGATHER

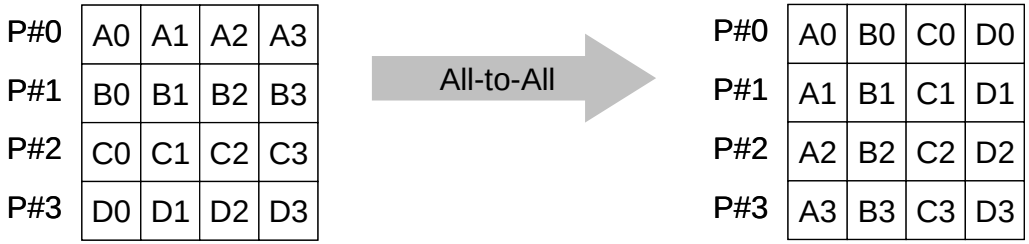


- MPI_GATHER＋MPI_BCAST
  - Gathers data from all tasks and distribute the combined data to all tasks

- **`call MPI_ALLGATHER (sendbuf, scount, sendtype, recvbuf, rcount, recvtype, comm, ierr)`**
  - **`sendbuf`** choice I starting address of sending buffer
  - **`scount`** I I number of elements sent to each process
  - **`sendtype`** I I data type of elements of sending buffer
  - **`recvbuf`** choice O starting address of receiving buffer
  - **`rcount`** I I number of elements received from each process
  - **`recvtype`** I I data type of elements of receiving buffer
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

Fortran

MPI_ALLTOALL



- Sends data from all to all processes: transformation of dense matrix

- **`call MPI_ALLTOALL (sendbuf, scount, sendtype, recvbuf, rcount, recvrype, comm, ierr)`**
  - **`sendbuf`** choice I starting address of sending buffer
  - **`scount`** I I number of elements sent to each process
  - **`sendtype`** I I data type of elements of sending buffer
  - **`recvbuf`** choice O starting address of receiving buffer
  - **`rcount`** I I number of elements received from each process
  - **`recvtype`** I I data type of elements of receiving buffer
  - **`comm`** I I communicator
  - **`ierr`** I O completion code

Fortran

Examples by Collective Comm.

- Dot Products of Vectors
- Scatter/Gather
- **Reading Distributed Files**
- MPI_Allgatherv

Operations of Distributed Local Files

- In Scatter/Gather example, PE#0 reads global data, that is *scattered* to each processer, then parallel operations are done.

- If the problem size is very large, a single processor may not read entire global data.
  - If the entire global data is decomposed to distributed local data sets, each process can read the local data.
  - If global operations are needed to a certain sets of vectors, MPI functions, such as MPI_Gather etc. are available.

Reading Distributed Local Files: Uniform Vec. Length (1/2)

```
>$ cd /work/gt36/t36XXX/pFEM/mpi/S1
>$ module load fj
>$ ls a1.*
   a1.0 a1.1 a1.2 a1.3
>$ mpifccpx –Nclang -Kfast file.c
>$ mpifrtpx –Kfast file.f
(modify go4.sh for 4 processes)
>$ pjsub go4.sh
```

a1x.all is decomposed to 4 files.

a1.0
101.0
103.0
105.0
106.0
109.0
111.0
121.0
151.0

a1.1
201.0
203.0
205.0
206.0
209.0
211.0
221.0
251.0

a1.2
301.0
303.0
305.0
306.0
309.0
311.0
321.0
351.0

a1.3
401.0
403.0
405.0
406.0
409.0
411.0
421.0
451.0

go4.sh

```
#!/bin/sh
#PJM -N “test“                          Job Name
#PJM -L rscgrp=lecture6-o               Name of “QUEUE”
#PJM -L node=1                          Node#
#PJM --mpi proc=4                       Total MPI Process#
#PJM -L elapse=00:15:00                 Computation Time
#PJM -g gt36                            Group Name (Wallet)
#PJM -j
#PJM -e err                             Standard Error
#PJM -o test.lst                        Standard Output

module load fj
module load fjmpi

mpiexec ./a.out
```

Reading Distributed Local Files: Uniform Vec. Length (2/2)

<$O-S1>/file.f

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr
real(kind=8), dimension(8) :: VEC
character(len=80)          :: filename

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

if (my_rank.eq.0) filename= 'a1.0'
if (my_rank.eq.1) filename= 'a1.1'
if (my_rank.eq.2) filename= 'a1.2'
if (my_rank.eq.3) filename= 'a1.3'

open (21, file= filename, status= 'unknown')
  do i= 1, 8
    read (21,*) VEC(i)
  enddo
close (21)

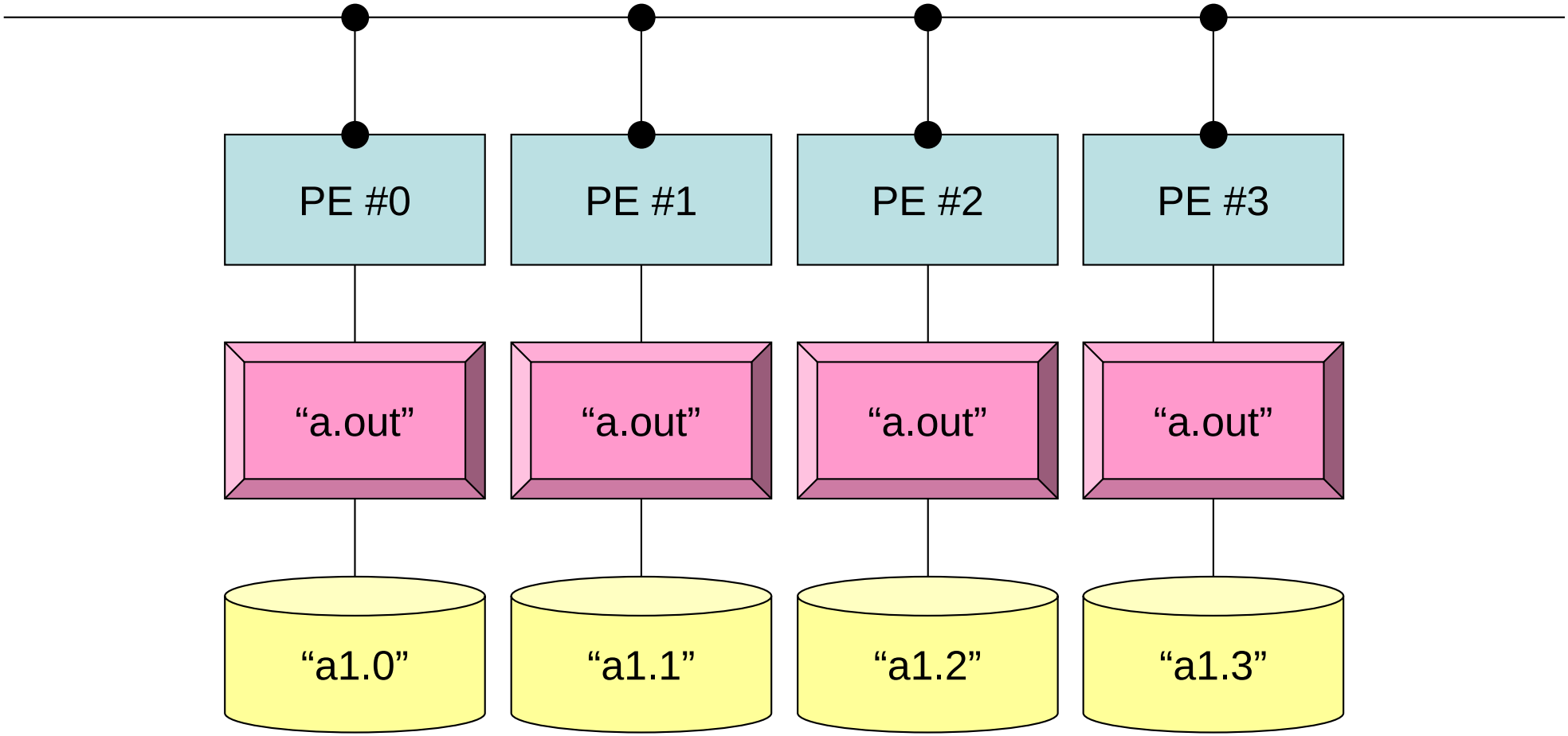
call MPI_FINALIZE (ierr)

stop
end
```

Similar to “Hello”

Local ID is 1-8

Typical SPMD Operation




```
mpirun -np 4 a.out
```

Non-Uniform Vector Length (1/2)

```
>$ cd /work/gt36/t36XXX/pFEM/mpi/S1
>$ module load fj
>$ ls a2.*
   a2.0 a2.1 a2.2 a2.3
>$ cat a2.1
  5          Number of Components at each Process
  201.0      Components
  203.0
  205.0
  206.0
  209.0

>$ mpifccpx –Nclang -Kfast file2.c
>$ mpifrtpx -Kfast file2.f

(modify go4.sh for 4 processes)
>$ pjsub go4.sh
```

a2.0~a2.3

PE#0

```
   8
101.0
103.0
105.0
106.0
109.0
111.0
121.0
151.0
```

PE#1

```
   5
201.0
203.0
205.0
206.0
209.0
```

PE#2

```
   7
301.0
303.0
305.0
306.0
311.0
321.0
351.0
```

PE#3

```
   3
401.0
403.0
405.0
```

Non-Uniform Vector Length (2/2)

<$O-S1>/file2.f

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'
integer :: PETOT, my_rank, ierr
real(kind=8), dimension(:), allocatable :: VEC
character(len=80)                       :: filename

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

 if (my_rank.eq.0) filename= 'a2.0'
 if (my_rank.eq.1) filename= 'a2.1'
 if (my_rank.eq.2) filename= 'a2.2'
 if (my_rank.eq.3) filename= 'a2.3'

 open (21, file= filename, status= 'unknown')
   read (21,*) N
   allocate (VEC(N))
   do i= 1, N
     read (21,*) VEC(i)
   enddo
 close(21)

call MPI_FINALIZE (ierr)
stop
end
```

“N” is different at each process

How to generate local data

- Reading global data (N=NG)
  - Scattering to each process
  - Parallel processing on each process
  - (If needed) reconstruction of global data by gathering local data
- Generating local data (N=NL), or reading distributed local data
  - Generating or reading local data on each process
  - Parallel processing on each process
  - (If needed) reconstruction of global data by gathering local data
- In future, latter case is more important, but former case is also introduced in this class for understanding of operations of global/local data.

Examples by Collective Comm.

- Dot Products of Vectors
- Scatter/Gather
- Reading Distributed Files
- **MPI_Allgatherv**

MPI_GATHERV, MPI_SCATTERV

- MPI_Gather, MPI_Scatter
  - Length of message from/to each process is uniform

- MPI_XXXv extends functionality of MPI_XXX by allowing a varying count of data from each process:
  - MPI_Gatherv
  - MPI_Scatterv
  - MPI_Allgatherv
  - MPI_Alltoallv

Fortran

MPI_ALLGATHERV

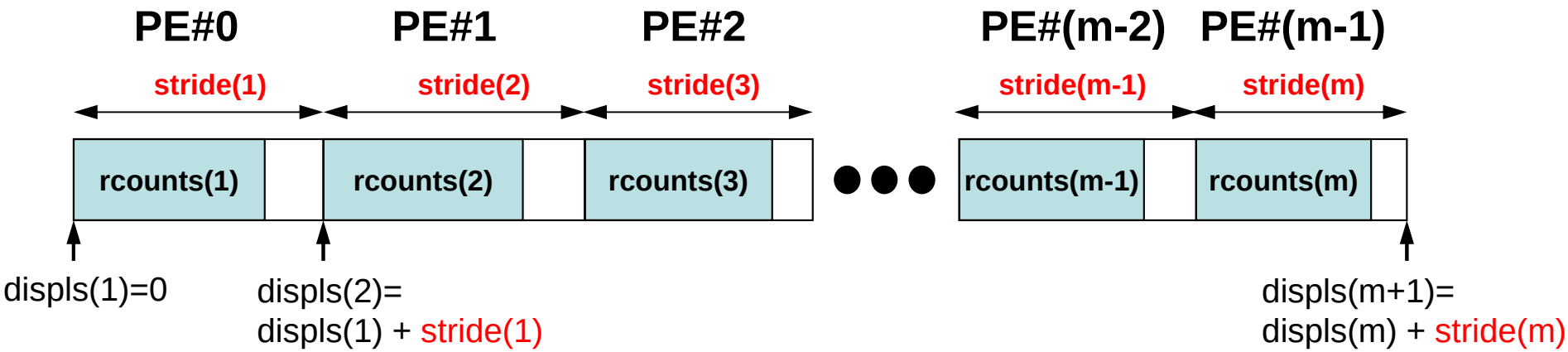
- Variable count version of MPI_Allgather
  - creates “global data” from “local data”

- **call MPI_ALLGATHERV (sendbuf, scount, sendtype, recvbuf, rcounts, displs, recvtype, comm, ierr)**
  - **sendbuf** choice I starting address of sending buffer
  - **scount** I I number of elements sent to each process
  - **sendtype** I I data type of elements of sending buffer
  - **recvbuf** choice O starting address of receiving buffer
  - **rcounts** I I integer array (of length *groupsize*) containing the number of elements that are to be received from each process (array: size= PETOT)
  - **displs** I I integer array (of length *groupsize*). Entry *i* specifies the displacement (relative to recvbuf) at which to place the incoming data from process *i* (array: size= PETOT+1)
  - **recvtype** I I data type of elements of receiving buffer
  - **comm** I I communicator
  - **ierr** I O completion code

MPI_ALLGATHERV (cont.)

Fortran

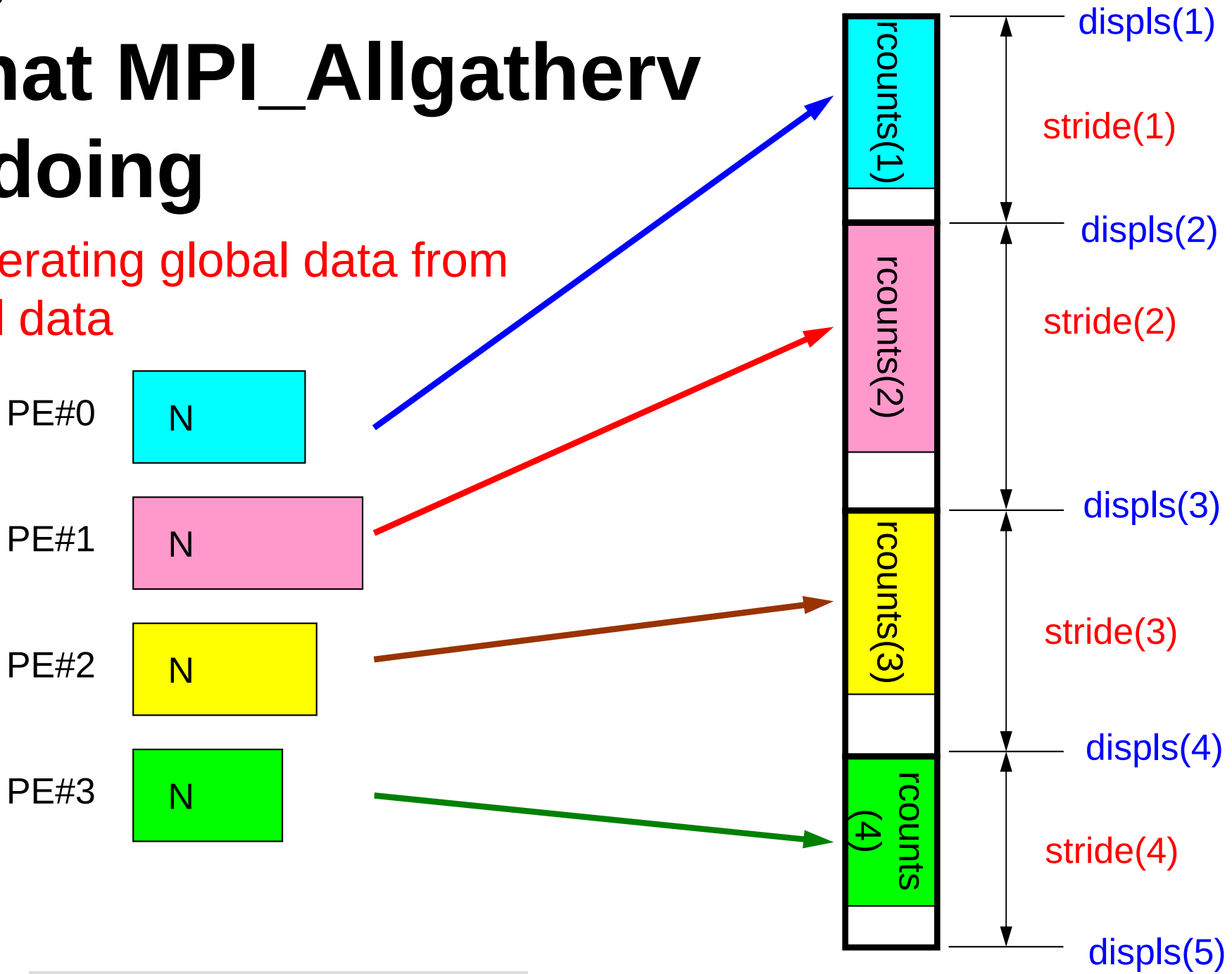
- **`call MPI_ALLGATHERV (sendbuf, scount, sendtype, recvbuf, rcounts, displs, recvtype, comm, ierr)`**
  - **`rcounts`** I I integer array (of length *groupsize*) containing the number of elements that are to be received from each process (array: size= PETOT)
  - **`displs`** I I integer array (of length *groupsize*). Entry *i* specifies the displacement (relative to recvbuf) at which to place the incoming data from process *i* (array: size= PETOT+1)
  - These two arrays are related to size of final "global data", therefore each process requires information of these arrays (`rcounts, displs`)
    - Each process must have same values for all components of both vectors
  - Usually, **`stride(i)=rcounts(i)`**



size(recvbuf)= displs(PETOT+1)= sum(stride)

What MPI_Allgatherv is doing

Generating global data from local data

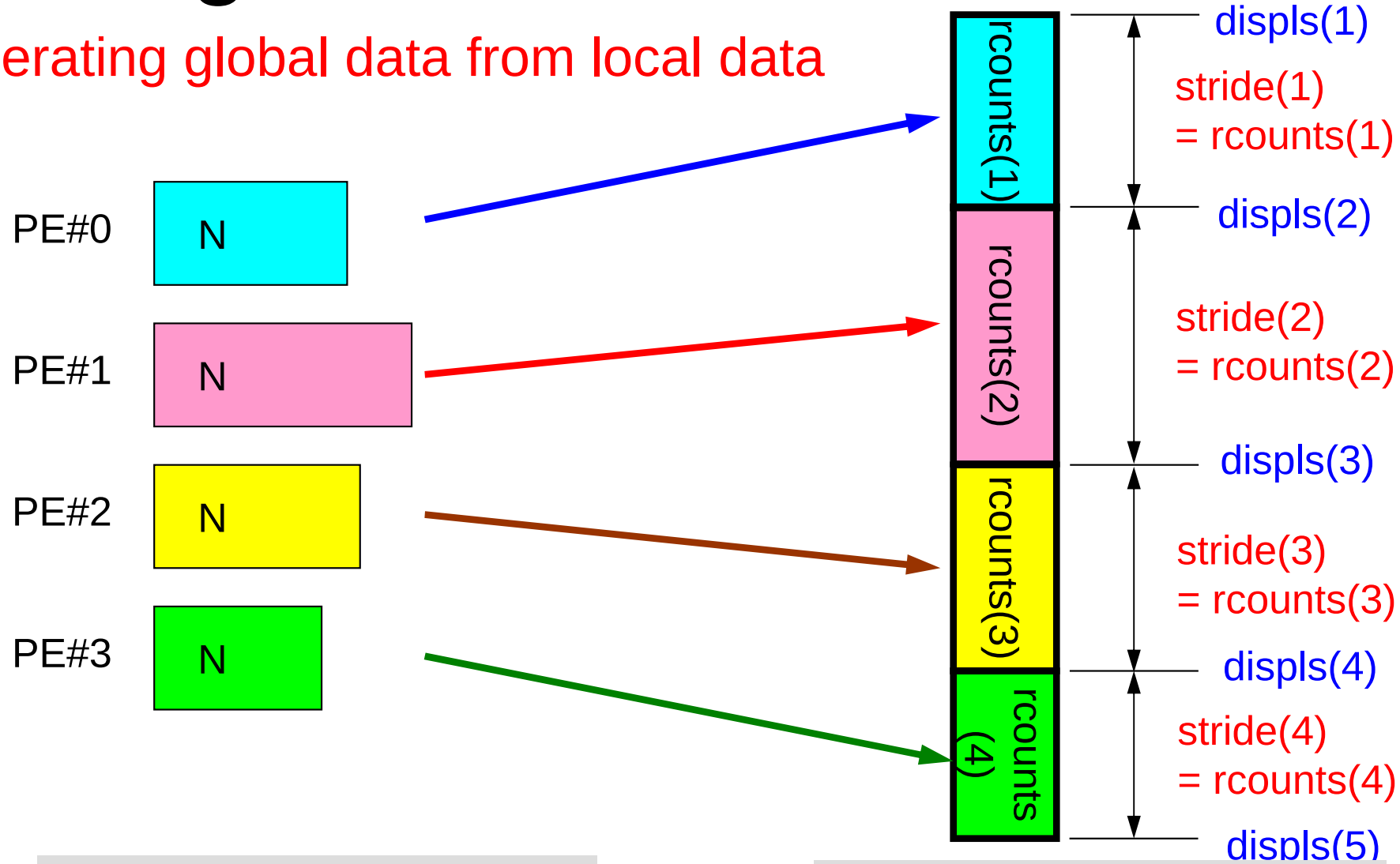


Local Data: sendbuf

Global Data: recvbuf

What MPI_Allgatherv is doing

Generating global data from local data



Local Data: sendbuf

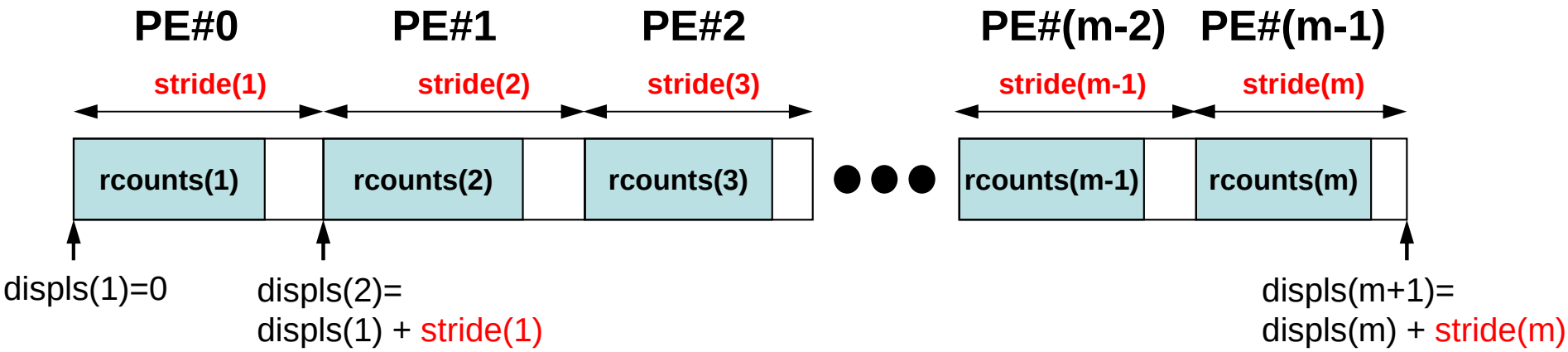
Global Data: recvbuf

MPI_Allgatherv in detail (1/2)

Fortran

- **`call MPI_ALLGATHERV (sendbuf, scount, sendtype, recvbuf, rcounts, displs, recvtype, comm, ierr)`**

- **`rcounts`**
  - Size of message from each PE: Size of Local Data (Length of Local Vector)
- **`displs`**
  - Address/index of each local data in the vector of global data
  - **`displs(PETOT+1)`**= Size of Entire Global Data (Global Vector)

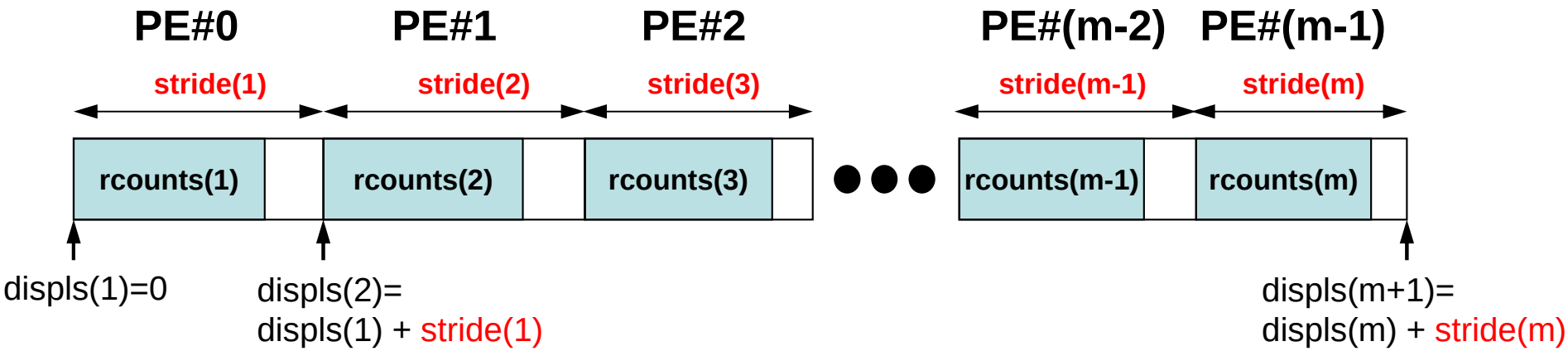


size(recvbuf)= displs(PETOT+1)= sum(stride)

MPI_Allgatherv in detail (2/2)

Fortran

- Each process needs information of **rcounts** & **displs**
  - **"rcounts"** can be created by gathering local vector length **"N"** from each process.
  - On each process, **"displs"** can be generated from **"rcounts"** on each process.
    - **stride[i]= rcounts[i]**
  - Size of **"recvbuf"** is calculated by summation of **"rcounts".**



size(recvbuf)= displs(PETOT+1)= sum(stride)

Preparation for MPI_Allgatherv <$O-S1>/agv.f

- Generating global vector from “a2.0”~”a2.3”.
- Length of the each vector is 8, 5, 7, and 3, respectively. Therefore, size of final global vector is 23 (= 8+5+7+3).

a2.0~a2.3

PE#0

```
   8
101.0
103.0
105.0
106.0
109.0
111.0
121.0
151.0
```

PE#1

```
   5
201.0
203.0
205.0
206.0
209.0
```

PE#2

```
   7
301.0
303.0
305.0
306.0
311.0
321.0
351.0
```

PE#3

```
   3
401.0
403.0
405.0
```

Preparation: MPI_Allgatherv (1/4)

Fortran

<$O-S1>/agv.f

```
implicit REAL*8 (A-H,O-Z)
include 'mpif.h'

integer :: PETOT, my_rank, SOLVER_COMM, ierr
real(kind=8), dimension(:), allocatable :: VEC
real(kind=8), dimension(:), allocatable :: VEC2
real(kind=8), dimension(:), allocatable :: VECg
integer(kind=4), dimension(:), allocatable :: rcounts
integer(kind=4), dimension(:), allocatable :: displs
character(len=80)                          :: filename

call MPI_INIT      (ierr)
call MPI_COMM_SIZE (MPI_COMM_WORLD, PETOT, ierr )
call MPI_COMM_RANK (MPI_COMM_WORLD, my_rank, ierr )

if (my_rank.eq.0) filename= 'a2.0'
if (my_rank.eq.1) filename= 'a2.1'
if (my_rank.eq.2) filename= 'a2.2'
if (my_rank.eq.3) filename= 'a2.3'

open (21, file= filename, status= 'unknown')
  read (21,*) N
  allocate (VEC(N))
  do i= 1, N
    read (21,*) VEC(i)
  enddo
```

N(NL) is different at each process

Preparation: MPI_Allgatherv (2/4)

Fortran

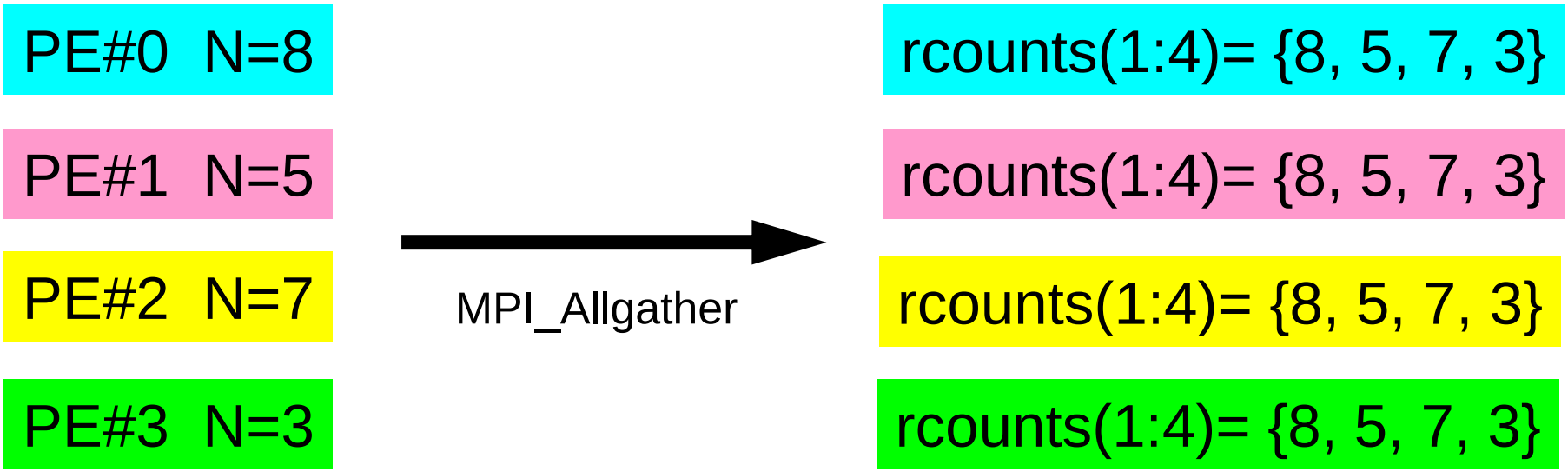
<$O-S1>/agv.f

```
 allocate (rcounts(PETOT), displs(PETOT+1))
 rcounts= 0
 write (*,'(a,10i8)') "before", my_rank, N, rcounts

 call MPI_allGATHER ( N     , 1, MPI_INTEGER,              &
&                     rcounts, 1, MPI_INTEGER,              &
&                     MPI_COMM_WORLD, ierr)

 write (*,'(a,10i8)') "after ", my_rank, N, rcounts
 displs(1)= 0
```

Rcounts on each PE



Preparation: MPI_Allgatherv (2/4)

Fortran

<$O-S1>/agv.f

```
 allocate (rcounts(PETOT), displs(PETOT+1))
 rcounts= 0
 write (*,'(a,10i8)') "before", my_rank, N, rcounts

 call MPI_allGATHER ( N     , 1, MPI_INTEGER,              &
&                     rcounts, 1, MPI_INTEGER,              &
&                     MPI_COMM_WORLD, ierr)

 write (*,'(a,10i8)') "after ", my_rank, N, rcounts
 displs(1)= 0

 do ip= 1, PETOT
   displs(ip+1)= displs(ip) + rcounts(ip)
 enddo

 write (*,'(a,10i8)') "displs", my_rank, displs

 call MPI_FINALIZE (ierr)

 stop
 end
```

Rcounts on each PE

Displs on each PE

Preparation: MPI_Allgatherv (3/4)

```
> cd /work/gt36/t36XXX/pFEM/mpi/S1
> module load fj
> mpifrtpx –Kfast agv.f

(modify go4.sh for 4 processes)

> pjsub go4.sh


before       0       8       0       0       0       0
after        0       8       8       5       7       3
Displs       0       0       8      13      20      23

before       1       5       0       0       0       0
after        1       5       8       5       7       3
Displs       1       0       8      13      20      23

before       3       3       0       0       0       0
after        3       3       8       5       7       3
Displs       3       0       8      13      20      23

before       2       7       0       0       0       0
after        2       7       8       5       7       3
Displs       2       0       8      13      20      23
write (*,‘(a,10i8)’) “before”, my_rank, N, rcounts
write (*,'(a,10i8)') "after ", my_rank, N, rcounts
write (*,'(a,10i8)') "displs", my_rank, displs
```

Preparation: MPI_Allgatherv (4/4)

- Only ”recvbuf” is not defined yet.
- Size of ”recvbuf” = ”displs(PETOT+1)”

```
call MPI_allGATHERv
     ( VEC , N, MPI_DOUBLE_PRECISION,
       recvbuf, rcounts, displs, MPI_DOUBLE_PRECISION,
       MPI_COMM_WORLD, ierr)
```

Report S1 (1/2)

- ~~Deadline: January 24th (Wed), 2024, 17:00@ITC-LMS~~

- Problem S1-1
  - Read local files <$O-S1>/a1.0~a1.3, <$O-S1>/a2.0~a2.3.
  - Develop codes which calculate norm $||x||_2$ of global vector for each case.
    - <$O-S1>file.c, <$O-S1>file2.c
- Problem S1-2
  - Read local files <$O-S1>/a2.0~a2.3.
  - Develop a code which constructs “global vector” using MPI_Allgatherv.

Report S1 (2/2)

- 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

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

- Report
  - Cover Page: Name, ID, and Problem ID (S1) must be written.
  - Less than two pages including figures and tables (A4) for each of three sub-problems
    - Strategy, Structure of the Program, Remarks
  - Source list of the program (if you have bugs)
  - Output list (as small as possible)

a012.sh

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture6-o
#PJM -L node=1
#PJM --mpi proc=12
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o test.lst

module load fj
module load fjmpi
mpiexec ./a.out
mpiexec numactl –l ./a.out
```

a048.sh

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture6-o
#PJM -L node=1
#PJM --mpi proc=48
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o test.lst

module load fj
module load fjmpi
mpiexec ./a.out
mpiexec numactl –l ./a.out
```

a384.sh

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture6-o
#PJM -L node=8
#PJM --mpi proc=384
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o test.lst

module load fj
module load fjmpi
mpiexec ./a.out
mpiexec numactl –l ./a.out
```

a576.sh

```
#!/bin/sh
#PJM -N "test"
#PJM -L rscgrp=lecture6-o
#PJM -L node=12
#PJM --mpi proc=576
#PJM -L elapse=00:15:00
#PJM -g gt36
#PJM -j
#PJM -e err
#PJM -o test.lst

module load fj
module load fjmpi
mpiexec ./a.out
mpiexec numactl –l ./a.out
```

`numactl –l/--localalloc` for utilizing local memory (no effects)

Number of Processes

```
#PJM -L node=1;#PJM --mpi proc= 1    1-node, 1-proc, 1-proc/n
#PJM -L node=1;#PJM --mpi proc= 4    1-node, 4-proc, 4-proc/n
#PJM -L node=1;#PJM --mpi proc=12    1-node,12-proc,12-proc/n
#PJM -L node=1;#PJM --mpi proc=24    1-node,24-proc,24-proc/n
#PJM -L node=1;#PJM --mpi proc=48    1-node,48-proc,48-proc/n

#PJM -L node= 4;#PJM --mpi proc=192   4-node,192-proc,48-proc/n
#PJM -L node= 8;#PJM --mpi proc=384   8-node,384-proc,48-proc/n
#PJM -L node=12;#PJM --mpi proc=576  12-node,576-proc,48-proc/n
```