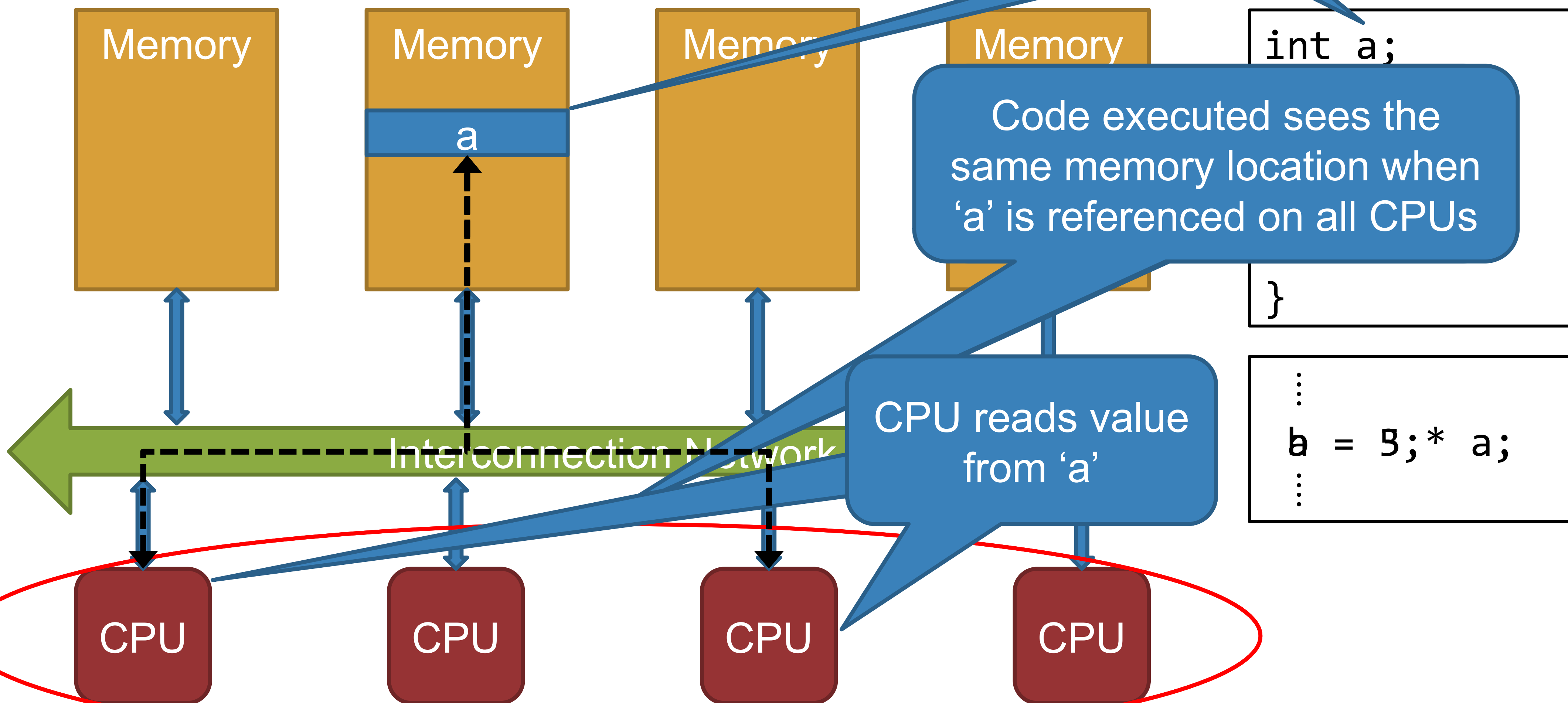
An introduction to MPI

Asst. Prof. Ioannis E. Venetis

University of Piraeus, Greece

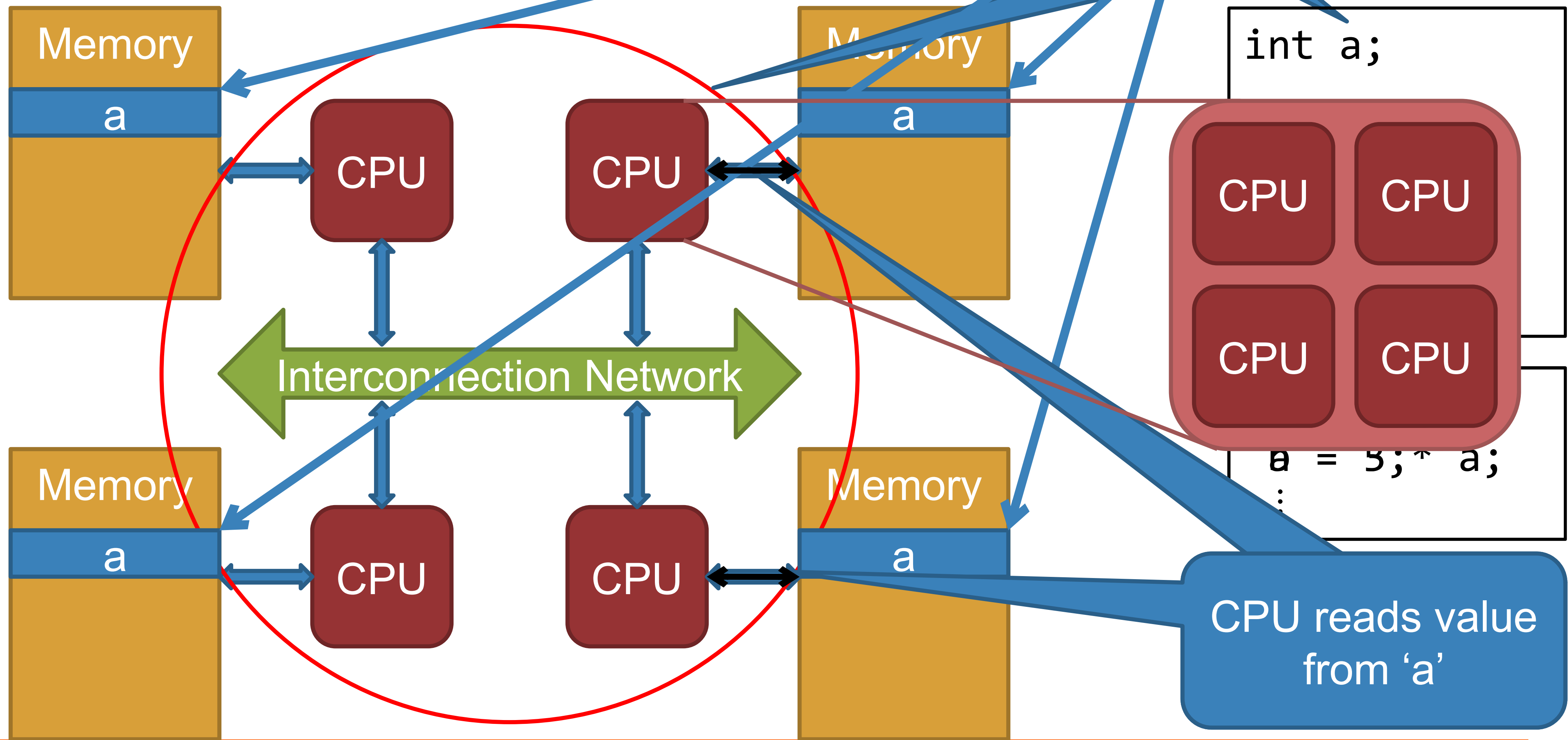
Classification of parallel architectures

- There are many classification schemes for parallel architectures
- One of the most useful ones is according to the memory architecture of the system
  - Shared memory
  - Distributed memory
  - Distributed shared memory
- Largely determines the programming models that can be used to program the specific architecture

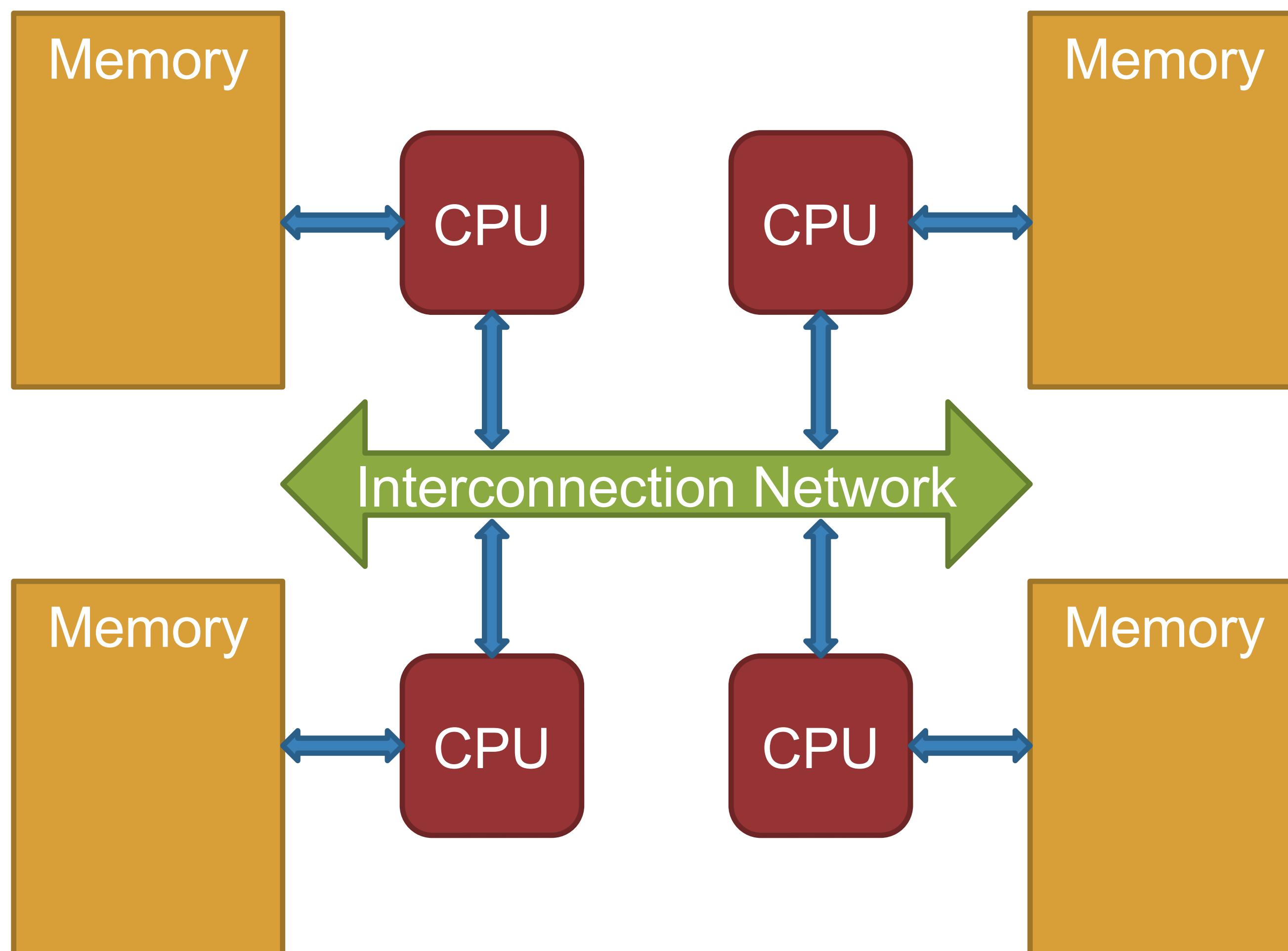


Definit
vari
Memory location to store the variable
Shared memory parallel architectures
Memory
Memory
Memory
Memory
a
int a;
Code executed sees the same memory location when ‘a’ is referenced on all CPUs
}
Interconnection Network
CPU reads value from ‘a’
⋮
b = 3;* a;
⋮
CPU
CPU
CPU
CPU

Distributed memory parallel architectures



Distributed shared memory parallel architectures



Same organization as distributed memory systems

But memory behaves as in shared memory systems

- Hardware ensures this kind of behavior

Programming models for shared memory parallel architectures

- Threads
  - POSIX Threads as well as other threading libraries
- OpenMP
- Cilk
- Cilk Plus
- Threading Building Blocks
- …

Programming models for distributed memory parallel architectures

- MPI
- PVM
- …

Ultimate winner!

What is the goal when using a parallel programming model?

- Problem to be solved is large
  - Requires too much time to run on single CPU

- Divide input data into smaller chunks
  - Smaller size of input ⇒ Faster calculation
- Assign every chunk to a CPU
  - Using appropriate software abstraction (thread or process)
- Every CPU processes its chunk and creates part of the solution
- Combine partial solutions into global solution

MPI (Message Passing Interface)

- It is a standard
  - Not a specific implementation
- It defines a set of functions, data structures, data types, etc. to exchange messages of data among processes
  - Implemented as a library
- Layered design
- At a high level
  - Provides an API for the programmer
- At a low level
  - Interacts with the interconnection network to send and receive data
- Supports C, C++, Fortran 77 and Fortran 90

MPI implementations

Open MPI: http://www.open-mpi.org

MPICH: http://www-unix.mcs.anl.gov/mpi/mpich

MPICH2: http://www-unix.mcs.anl.gov/mpi/mpich2

MPICH-GM: http://www.myri.com/scs

LAM/MPI: http://www.lam-mpi.org

LA-MPI: http://public.lanl.gov/lampi

SCI-MPICH: http://www.lfbs.rwth-aachen.de/users/joachim/SCI-MPICH

MPI/Pro: http://www.mpi-softtech.com

A basic subset of MPI functions

The following six MPI functions allow implementation of any MPI program:

- MPI_Init
- MPI_Finalize
- MPI_Comm_size
- MPI_Comm_rank
- MPI_Send
- MPI_Recv

Why are then other functions provided?

- Patterns occur in parallel programming
  - *Simplification of programming*
- Performance optimization
  - *e.g., smarter algorithms, non-blocking data exchange, …*

Initialization/Finalization of MPI processes

- int MPI_Init(int *argc, char ***argv);
  - Initializes an MPI program
  - Must be called by every MPI process
    - *Must be called exactly once*
    - *Must be called before calling any other MPI function*
  - Initializes the implementation of MPI in use
- int MPI_Finalize(void);
  - Finalizes an MPI program
  - Must be called by every MPI process
    - *Must be called exactly once*
  - Cleans up the implementation of MPI in use

Identification of MPI processes

int MPI_Comm_size(MPI_Comm comm, int *size);

Stores in variable size the number of MPI processes that constitute the communicator defined by the parameter comm

int MPI_Comm_rank(MPI_Comm comm, int *rank);

Stores in variable rank the rank of the calling MPI process within the communicator defined by the parameter comm

Communicators

Parameter comm in the functions presented earlier

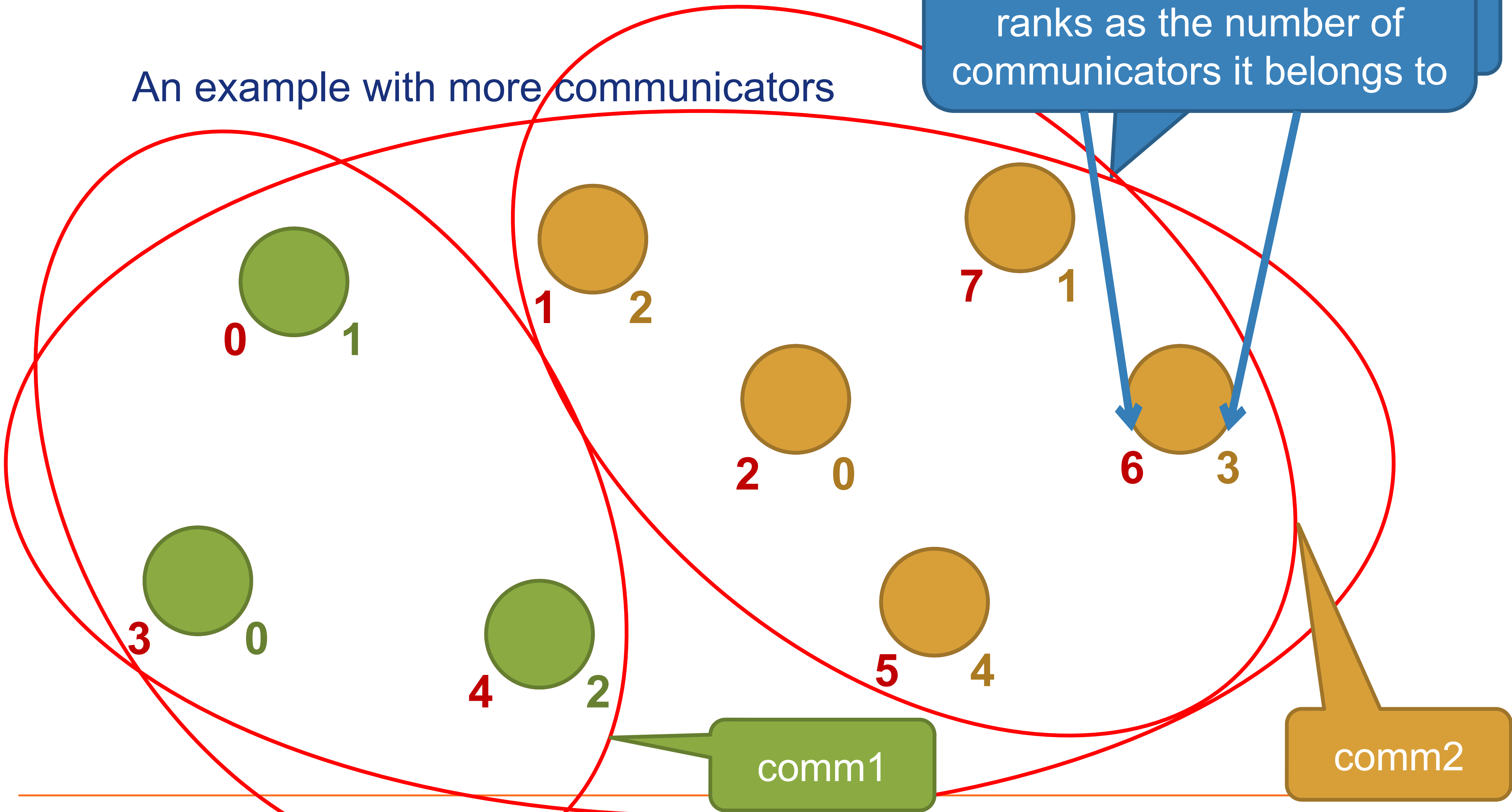
Defines a communication domain

- A subset of the processes that constitute the MPI application
- Processes in a subset can easily communicate
  - *Collective communication will be analyzed later*

We will use MPI_COMM_WORLD

- A constant defined by any implementation
- Defines a communicator that is comprised of all processes of the MPI application

An example with more communicators



A first, simple example

```
#include "mpi.h"
#include <stdio.h>

int main(int  argc, char *argv[]) {
    int rank, size;

    MPI_Init(&argc, &argv);

    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);

    printf("Hello world! I'm %d of %d\n", rank, size);

    MPI_Finalize();

    return(0);
}
```

Compilation/Execution of MPI programs

Compilation

```
mpicc -O3 -Wall -o my_prog my_prog.c
```

Execution:

Typically using “mpirun” command

```
mpirun -np 4 ./my_prog
```

Creates and executes (at least) one process on a number of nodes of the system

Depending on the implementation of MPI there are other commands that can be used to start execution of an MPI program

When using the SLURM batch system then “srun” should be used in the SLURM scripts

Works with all MPI implementations

Differentiation of execution according to the rank

```
#include "mpi.h"
#include <stdio.h>

int main(int  argc, char *argv[]) {
    int rank, size;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &size);
    if (rank == 2) {
    printf("I am process 2 and I am different!\n");
    } else {
    printf("Hello world! I'm %d of %d\n", rank, size);
    }
    MPI_Finalize();

    return(0);
}
```

Communication in MPI

- From one process to another: point-to-point
- Among sets of processes (communicators): collecti
- Can be standard, buffered, synchronous or ready
  - When can transmission of data start, with respect to the corr e operation?
- Can be blocking or non-blocking
  - When does the call to the MPI function return?
    - *Before or after the actual data transfer has taken place?*

Typically this is used

Typically this is used

Point-to-point communication

Point-to-point communication

- Exchange of data between specific processes of an MPI program
  - Identified using the ranks of these processes

Sending a message in MPI

```
int MPI_Send(void *buf, int count, MPI_Datatype datatype, int dest,
             int tag, MPI_Comm comm);
```

buf: Starting address of data to be sent

count: Number of elements to be sent

datatype: Data type of each element to be sent

dest: Rank of the process to receive the message

tag: Tag of the message

comm: Communicator

Used to determine the size (in bytes) of the message

The rank is determined according to the provided communicator

Receiving a message in MPI

```
int MPI_Recv(void *buf, int count, MPI_Datatype datatype, int source,
             int tag, MPI_Comm comm, MPI_Status *status);
```

buf: Starting address in memory where received data will be stored

count: Number of elements to be received

datatype: Data type of each element to be received

source: Rank of the process that sent the message to be received

tag: Tag of the message

comm: Communicator

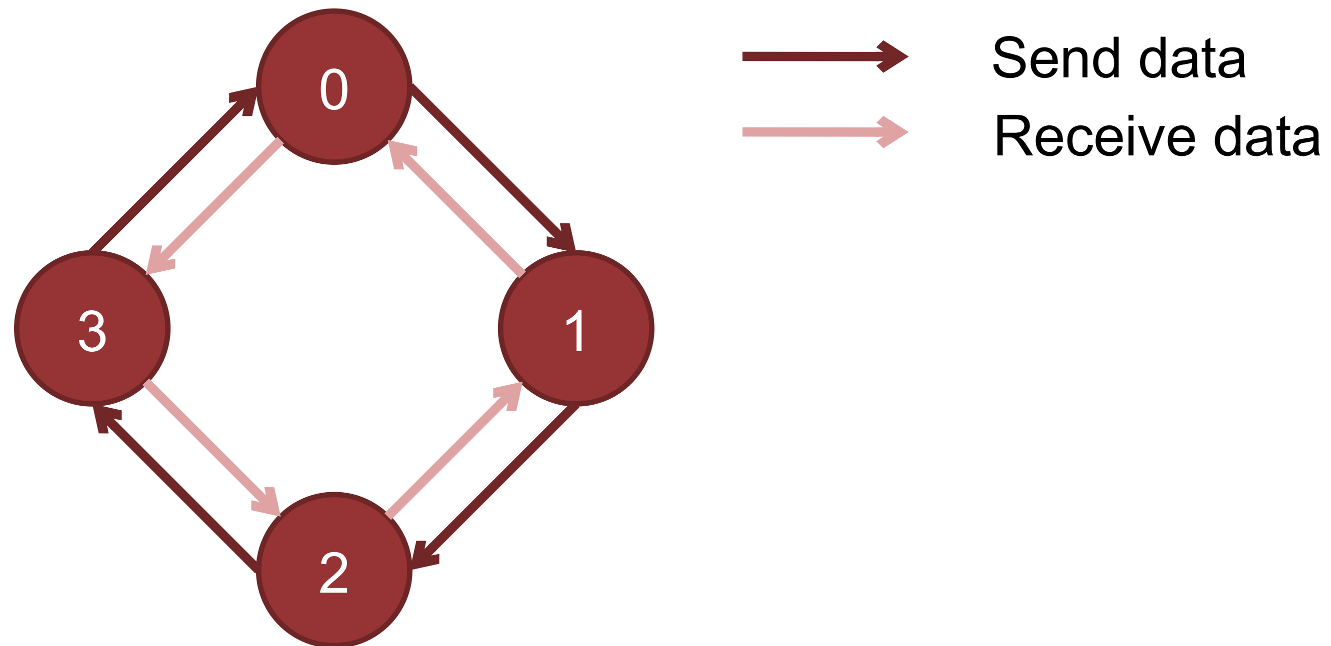
status: The MPI implementation can return details about the message received

Data types in MPI

- MPI defines its own data types
  - Allows portability of MPI programs among different architectures
  - Allows definition of new data types
    - *Derived data types*
- Most predefined data types in MPI correspond to predefined data types of the language, e.g. in C:
  - MPI_SHORT . short int
  - MPI_INT . int
  - MPI_LONG . long int
  - MPI_FLOAT . float
  - MPI_DOUBLE . double
  - MPI_CHAR . char
  - …

Creating a virtual ring (1/3)

- Each MPI process will send its rank to the “next” process
  - What happens with the last process (with the largest rank)?



Creating a virtual ring (2/3)

```
#include <stdio.h>
#include "mpi.h"

int main(int argc, char *argv[]) {
    int my_rank, p, next_rank, prev_rank, other_rank, tag1 = 5;
    MPI_Status status;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
    MPI_Comm_size(MPI_COMM_WORLD, &p);

    if (my_rank == p - 1)  {
    next_rank = 0;
    } else {
    next_rank = my_rank + 1;
    }
```

Creating a virtual ring (3/3)

What would happen if we changed the order of the send and receive calls?

```
    if (my_rank == 0)  {
         prev_rank = p – 1;
    } else {
         prev_rank = my_rank - 1;
    }

    MPI_Send(&my_rank, 1, MPI_INT, next_rank, tag1, MPI_COMM_WORLD);
    MPI_Recv(&other_rank, 1, MPI_INT, prev_rank, tag1, MPI_COMM_WORLD, &status);

    printf("I am process %d and I received the value %d.\n", my_rank, other_rank);

    MPI_Finalize();

    return(0);
}
```

Important notice

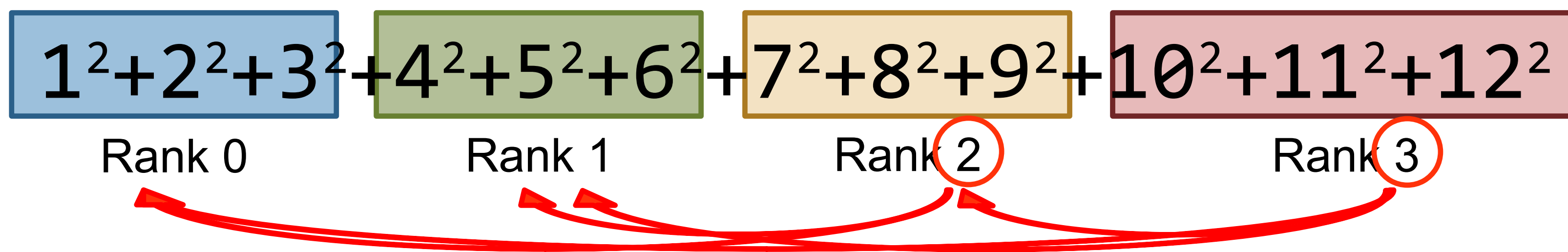
- Most of the examples we will look at are “embarrassingly parallel”
  - No exchange of data is required during execution
  - Except at the beginning and end of the calculation
- In this training we focus on making things clear with respect to using MPI
  - The simplicity of these examples helps towards this goal
- Real problems are typically not embarrassingly parallel

Calculation of $1^2+2^2+...+N^2$

Ask the user to provide a number N

Calculate in parallel $1^2+2^2+...+N^2$

Assume: N = 12
p = 4
num = 3



How many elements for each process?

num = N / p = 3

How will each process calculate the first number it has to process?

It has to bypass rank * num numbers

Calculation of $1^2+2^2+...+N^2$ (1/3)

```
#include <stdio.h>
#include "mpi.h"

int main(int argc, char *argv[]) {
    int my_rank, p, i, res, finres, start, end, num, N, source, target, tag1 = 5, tag2 = 6;
    MPI_Status status;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
    MPI_Comm_size(MPI_COMM_WORLD, &p);

    if (my_rank == 0)  {
    printf("Enter last number: ");
    scanf("%d", &N);
    for (target = 1; target < p; target++) {
    MPI_Send(&N, 1, MPI_INT, target, tag1, MPI_COMM_WORLD);
    }
    } else {
    MPI_Recv(&N, 1, MPI_INT, 0, tag1, MPI_COMM_WORLD, &status);
    }
```

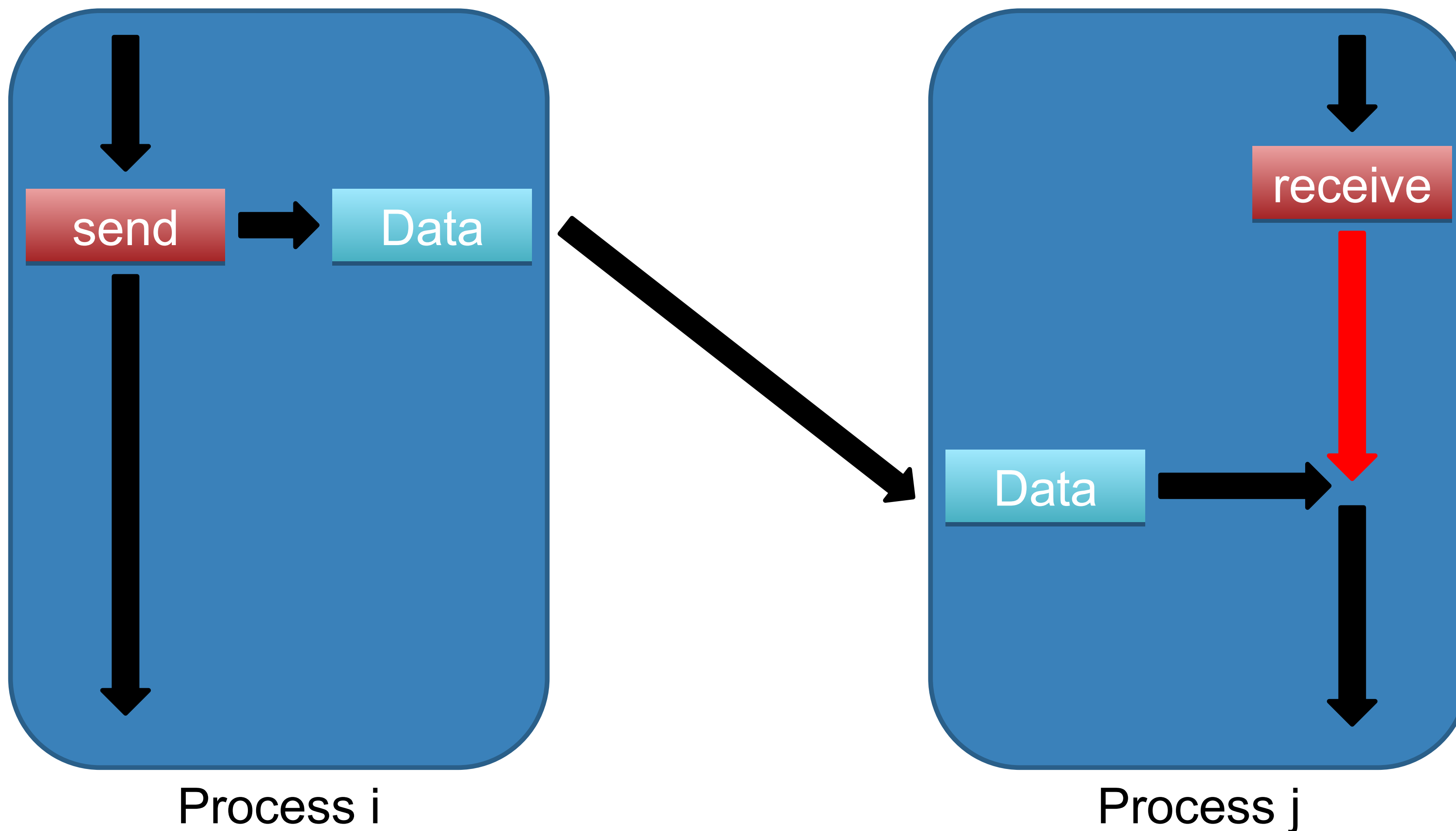
Calculation of $1^2+2^2+...+N^2$ (2/3)

```
res   = 0;
num   = N / p;
start = (my_rank * num) + 1;
end   = start + num;

for (i = start; i < end; i++) {
     res += (i * i);
}
```

Calculation of $1^2+2^2+...+N^2$ (3/3)

```
    if (my_rank != 0)  {
    MPI_Send(&res, 1, MPI_INT, 0, tag2, MPI_COMM_WORLD);
    } else {
    finres = res;

    printf("\nResult of process %d: %d\n", my_rank, res);

    for (source = 1; source < p; source++)  {
    MPI_Recv(&res, 1, MPI_INT, source, tag2, MPI_COMM_WORLD, &status);
    finres += res;
    printf("\nResult of process %d: %d\n", source, res);
    }
    printf("\n\n\nFinal result: %d\n", finres);
    }

    MPI_Finalize();

    return(0);
}
```

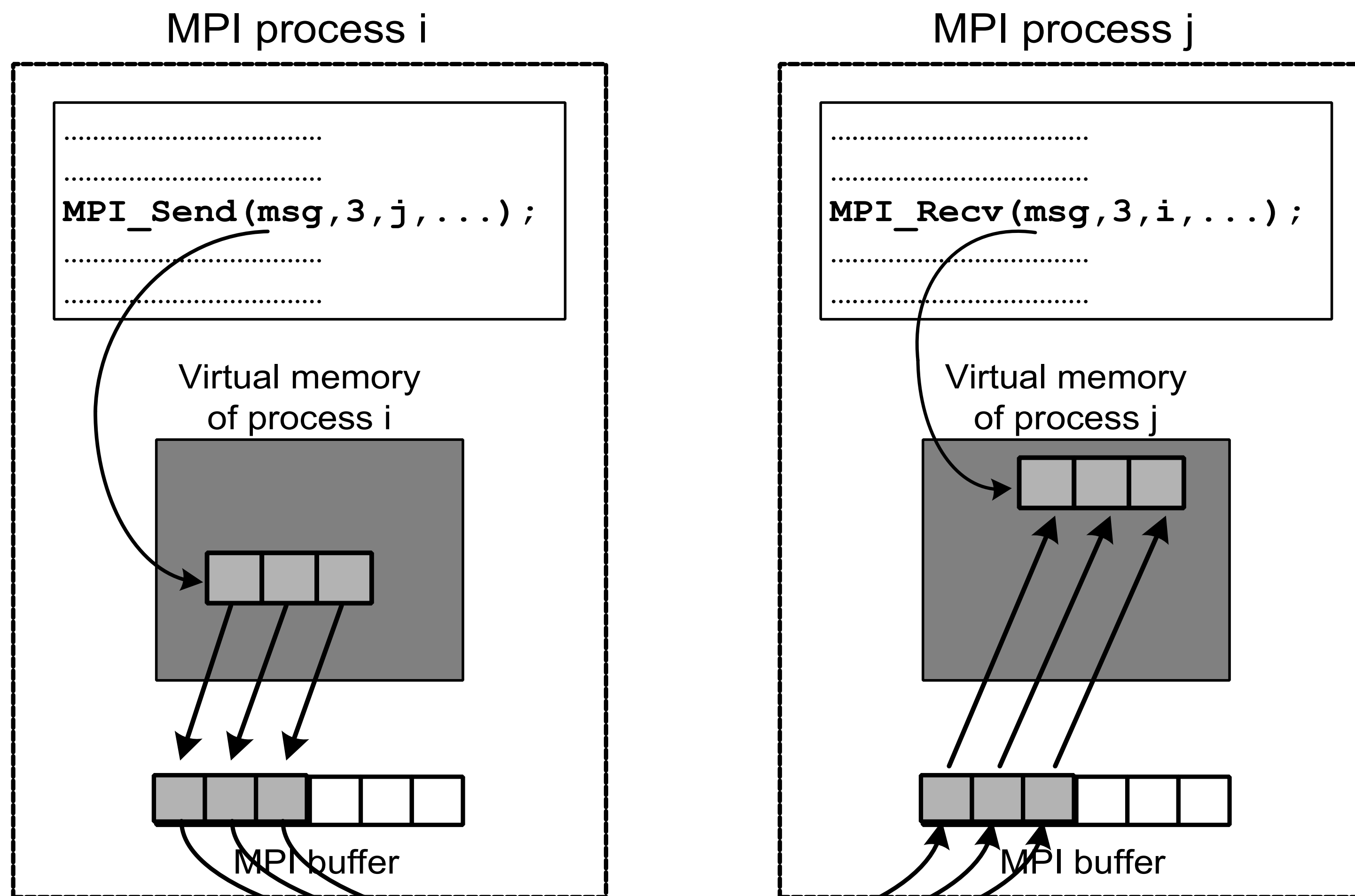
Relative execution speed:
Receive is executed before corresponding send



Relative execution speed:
Send is executed before corresponding receive

send
Data
?
Data
receive
Process i
Process j

Send and receive in MPI



Sum of squares of vector elements (1/3)

```
#include <stdio.h>
#include "mpi.h"

int main(int argc, char *argv[])
{
     int my_rank, p, i, res, finres, num, N;
     int source, target;
     int tag1=50, tag2=60, tag3=70;
     int data[100];
     MPI_Status status;

     MPI_Init(&argc, &argv);
     MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
     MPI_Comm_size(MPI_COMM_WORLD, &p);
```

Sum of squares of vector elements (2/3)

```
if (my_rank == 0)  {
     printf(“Enter size of vector: ");
     scanf("%d", &N);

     printf(“Enter %d vector elements: ”, N);
     for (i = 0; i < N; i++) {
          scanf(“%d”, &data[i]);
     }

     for (target = 1; target < p; target++) {
          MPI_Send(&N, 1, MPI_INT, target, tag1, MPI_COMM_WORLD);
     }

     num = N / p;
     i   = num;
     for (target = 1; target < p; target++)  {
          MPI_Send(&data[i], num, MPI_INT, target, tag2, MPI_COMM_WORLD);
          i += num;
     }
} else {
     MPI_Recv(&N, 1, MPI_INT, 0, tag1, MPI_COMM_WORLD, &status);
     num = N / p;
     MPI_Recv(&data[0], num, MPI_INT, 0, tag2, MPI_COMM_WORLD, &status);
}
```

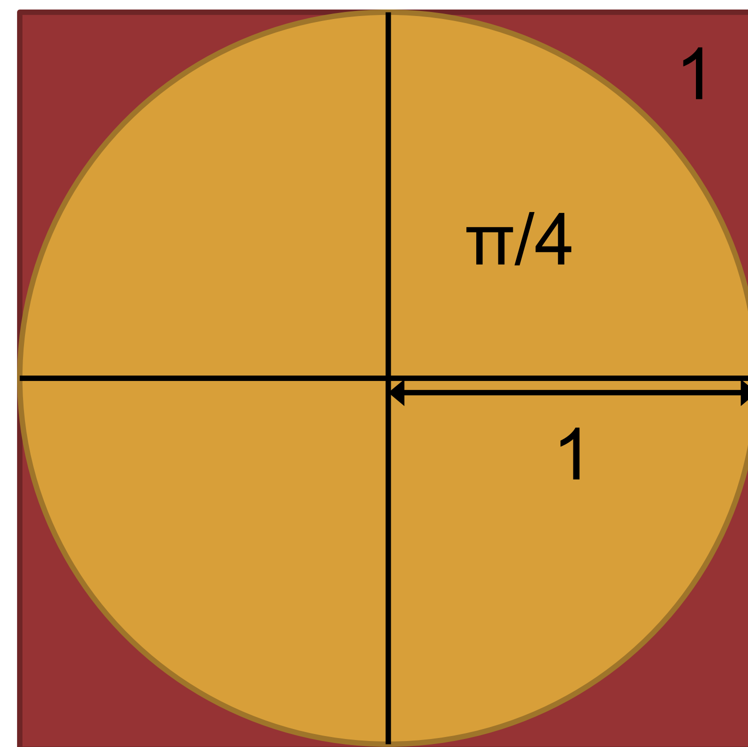
Sum of squares of vector elements (3/3)

```
    res = 0;
    for (i = 0; i < num; i++) {
         res += (data[i] * data[i]);
    }

    if (my_rank != 0) {
         MPI_Send(&res, 1, MPI_INT, 0, tag3, MPI_COMM_WORLD);
    } else {
         finres = res;

         printf("\nResult of process %d: %d\n", my_rank, res);

         for (source = 1; source < p; source++) {
              MPI_Recv(&res, 1, MPI_INT, source, tag3, MPI_COMM_WORLD, &status);
              finres += res;
              printf("\nResult of process %d: %d\n", source, res);
         }
         printf("\n\n\nFinal result: %d\n", finres);
    }

    MPI_Finalize();

    return(0);
}
```

Calculating π with a Monte Carlo method (1/3)

Idea

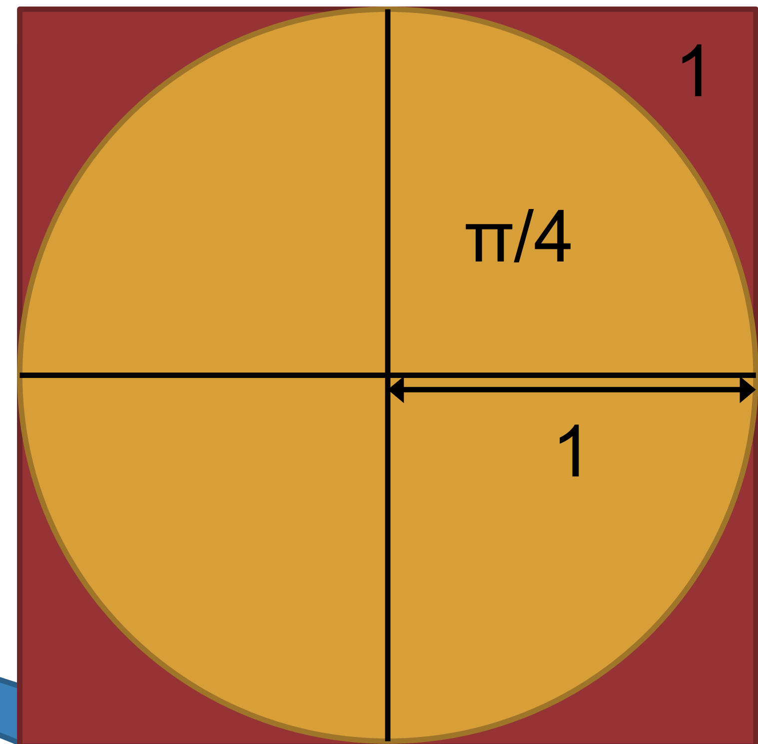
- Create a square with a side of 1 and a quartile with a radius of 1
  - *Area of square = 1*
  - *Area of quartile = π/4*
- Put N random points in to the square
  - *Assume that M fall into the quartile*



$$\frac{\text{Area of quartile}}{\text{Area of square}} = \frac{\pi/4}{1} \approx \frac{M}{N} \Rightarrow \pi \approx 4 \cdot \frac{M}{N}$$

Calculating π with a Monte Carlo method (2/3)

```
int main(int argc, char* argv[])
{
    int i, rank, np, c, local_c, local_N, N=1000000;
    int tag = 5, source;
    double x, y;
    MPI_status status;

    MPI_Init(&argc, &argv);
    MPI_Comm_rank(MPI_COMM_WORLD, &rank);
    MPI_Comm_size(MPI_COMM_WORLD, &np);

    srand48(rank);
    local_c = 0;
    local_N = N / np;

    for (i = 0; i < local_N; i++) {
    x = drand48();
    y = drand48();
    if (((x * x) + (y * y)) <= 1.0) {
    local_c++;
    }
    }
```



Avoids creation of the same pseudo-random series of numbers on all MPI processes

Calculating π with a Monte Carlo method (3/3)

```
    if (rank != 0)  {
    MPI_Send(&local_c, 1, MPI_INT, 0, tag, MPI_COMM_WORLD);
    } else {
    c = local_c;

    for (source = 1; source < np; source++)  {
    MPI_Recv(&local_c,1,MPI_INT,source,tag,MPI_COMM_WORLD,&status);
    c += local_c;
    }
    printf("Estimate of Pi = %24.16f\n", (4.0 * c) / N);
    }

    MPI_Finalize();

    return(0);
}
```

Collective communication

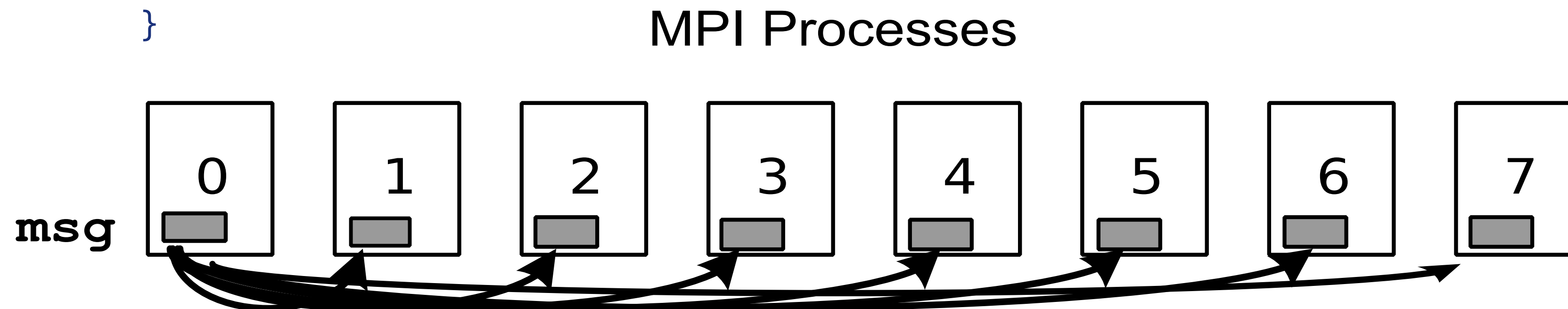
Collective communication

- Allows exchange of data among processes of an MPI program that belong to the same communicator
  - Broadcast
  - Reduction
  - Gather/Gatherv, Scatter/Scatterv, AllGather/AllGatherv
  - All-to-All
  - Barrier
- Support for topologies
  - More on this later during the presentation
- More efficient use of MPI buffers
  - Optimized use for multiple operations
- Support for MPI data types

Why support and use collective communication operations? (1/2)

Sending the same message from process 0 to processes 1-7

```
if (rank == 0) {
for (dest = 1; dest < size; dest++)
MPI_Send(msg, count, MPI_FLOAT, dest, tag, MPI_COMM_WORLD);
} else {
MPI_Recv(msg, count, MPI_FLOAT, 0, tag, MPI_COMM_WORLD, &status);
}
```

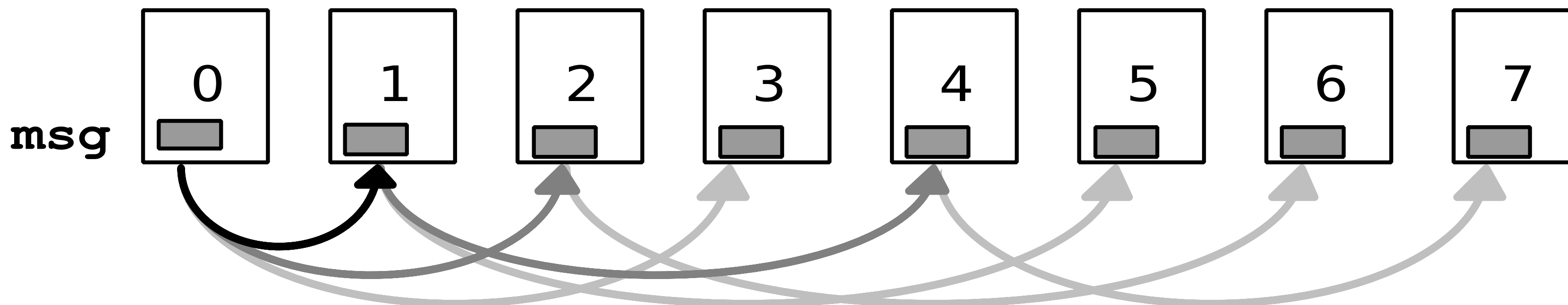


For p processes we need p-1 communication steps

Why support and use collective communication operations? (2/2)

Sending the same message from process 0 to processes 1-7

```
MPI_Bcast(msg, count, MPI_FLOAT, 0, MPI_COMM_WORLD);
```



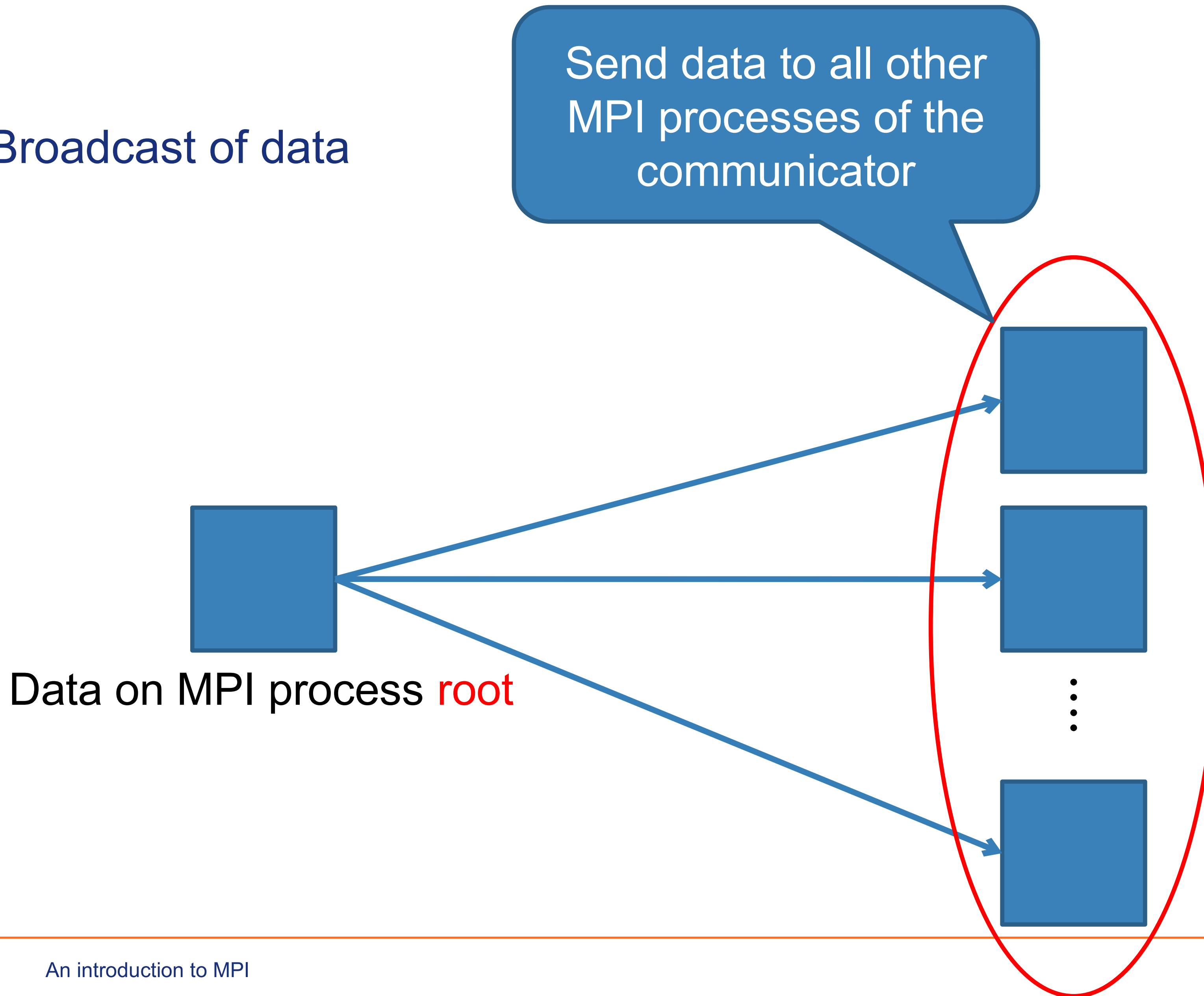
For p processes we need $\lceil \log_2 p \rceil$ communication steps

Broadcast

```
int MPI_Bcast(void *buffer, int count, MPI_Datatype datatype,
              int root, MPI_Comm comm);
```

- buffer: Has double semantics
  - *Process that sends data: Starting address of data to be sent*
  - *Processes that receive data: Starting address in memory where received data will be stored*
- count: Number of elements to be sent/received
- datatype: Data type of each element to be sent/received
- root: Rank of process that is sending data
  - *All other processes in the communicator will receive data*
- comm: Communicator

Broadcast of data

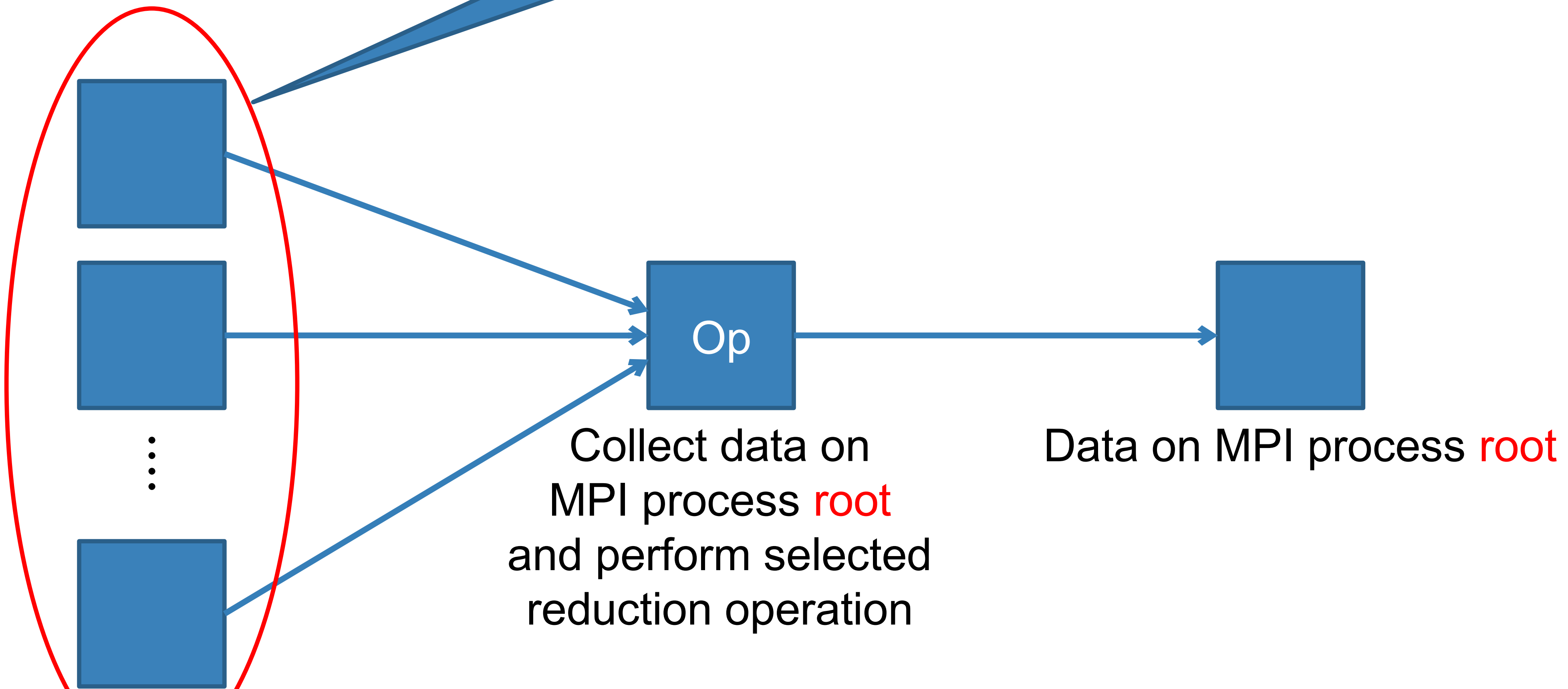


Reduction

```
int MPI_Reduce(void *sendbuf, void *recvbuf, int count,
               MPI_Datatype datatype, MPI_Op op, int root, MPI_Comm comm);
```

- sendbuf: Starting address of data to be sent
- recvbuf: Starting address in memory where received data will be stored
  - *Data stored only on the process with rank root*
- count: Number of elements to be sent/received
- datatype: Data type of each element to be sent/received
- op: Reduction operation to be performed
- root: The rank of the process that receives data and performs the reduction operation
  - *All processes in the communicator send data (including root)*
- comm: Communicator

Reduction of data



Reduction operations

- MPI_MAX . Maximum value
- MPI_MIN . Minimum value
- MPI_SUM . Sum
- MPI_PROD . Product
- MPI_LAND . Logical AND
- MPI_BAND . Bitwise AND
- MPI_LOR . Logical OR
- MPI_BOR . Bitwise OR
- MPI_LXOR . Logical Exclusive OR (XOR)
- MPI_BXOR . Bitwise Exclusive OR (XOR)
- MPI_MAXLOC . Maximum value and position within a vector
- MPI_MINLOC . Minimum value and position within a vector

Calculation of $1^2+2^2+...+N^2$ (1/2)

```
#include <stdio.h>
#include “mpi.h”

int main(int argc, char *argv[])
{
     int my_rank, p, i, res, finres, start, end, num, N;

     MPI_Init(&argc, &argv);
     MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
     MPI_Comm_size(MPI_COMM_WORLD, &p);

     if (my_rank == 0) {
          printf(“Enter last number: ”);
          scanf(“%d”, &N);
     }
```

Calculation of $1^2+2^2+...+N^2$ (2/2)

```
    MPI_Bcast(&N, 1, MPI_INT, 0, MPI_COMM_WORLD);

    res   = 0;
    num   = N / p;
    start = (my_rank * num) + 1;
    end   = start + num;
    for (i = start; i < end; i++) {
         res += (i * i);
    }

    printf("\nResult of process %d: %d\n", my_rank, res);

    MPI_Reduce(&res, &finres, 1, MPI_INT, MPI_SUM, 0, MPI_COMM_WORLD);

    if (my_rank == 0) {
         printf("\n Total result for N = %d is equal to : %d \n", N, finres);
    }
    MPI_Finalize();
    return(0);
}
```

Scatter

```
int MPI_Scatter(void *sendbuf, int sendcount, MPI_Datatype sendtype,
                void *recvbuf,  int recvcount,  MPI_Datatype recvtype,
                int root, MPI_Comm comm);
```

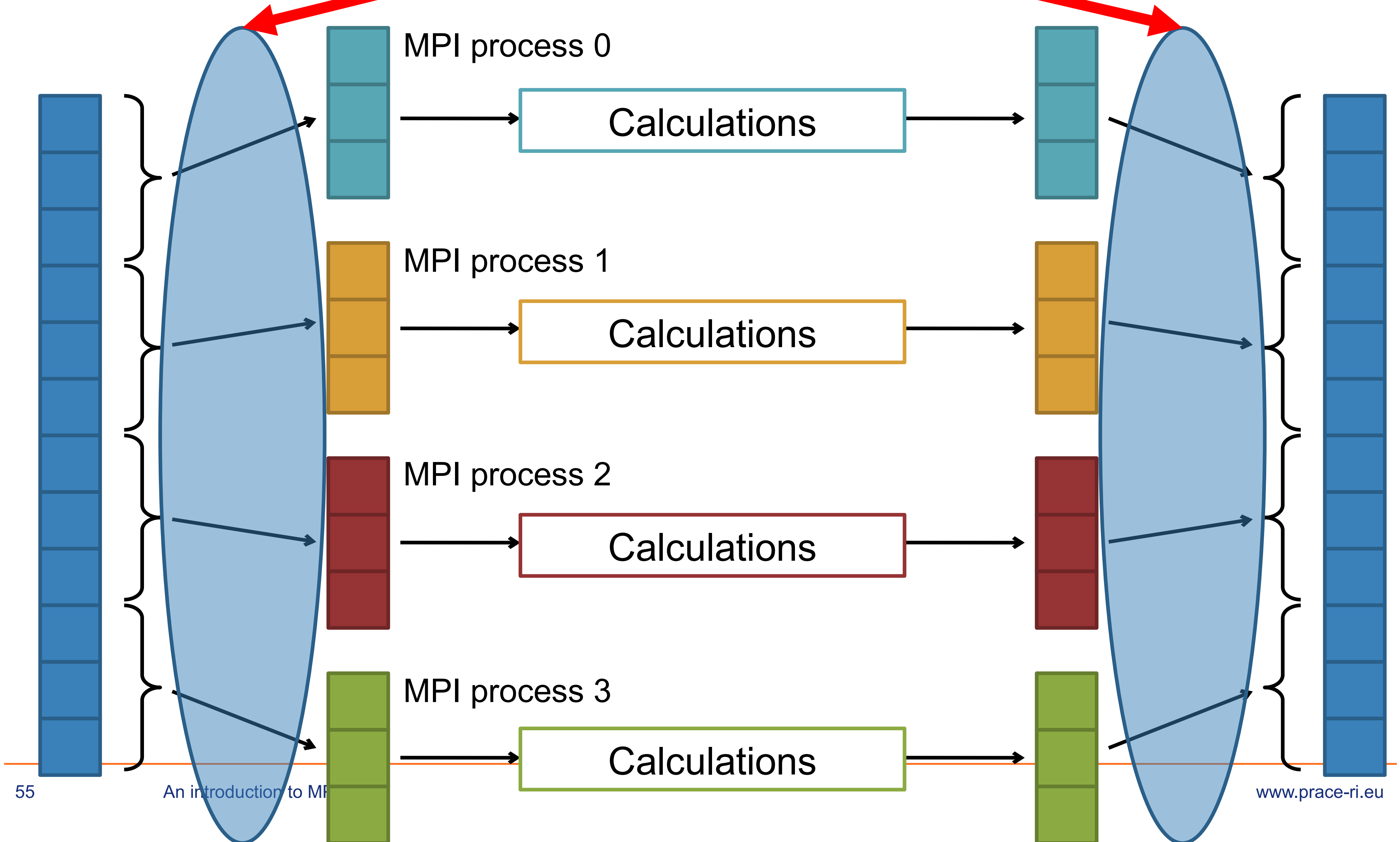
- sendbuf: Starting address of data to be sent
  - *Only on the process with rank root*
- sendcount: Number of elements to be sent to each process
- sendtype: Data type of each element to be sent
- recvbuf: Starting address in memory where received data will be stored
  - *On all processes, including root*
- recvcount: Number of elements to be received on each process
- recvtype: Data type of each element to be received
- root: The rank of the process that will distribute the data
  - *All other processes in the communicator will receive part of the data*
- comm: Communicator

Gather

```
int MPI_Gather(void *sendbuf, int sendcount, MPI_Datatype sendtype,
               void *recvbuf,  int recvcount,  MPI_Datatype recvtype,
               int root, MPI_Comm comm);
```

- sendbuf: Starting address of data to be collected
  - *From every process, including root*
- sendcount: Number of elements to be sent from each process
- sendtype: Data type of each element to be sent
- recvbuf: Starting address in memory where received data will be stored
  - *Only on the process with rank root*
- recvcount: Number of elements to be received from each process
- recvtype: Data type of each element to be received
- root: The rank of the process that will collect all the data
  - *All other processes in the communicator will send part of the data*
- comm: Communicator

Scatter/Gather



Scalar-Vector multiplication (1/3)

```
int main(int argc, char *argv[])
{
     int my_rank, p, i, num, b, size, A[100], local_A[100];

     MPI_Init(&argc, &argv);
     MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
     MPI_Comm_size(MPI_COMM_WORLD, &p);

     if (my_rank == 0) {
          printf("Calculating b * A\n\n");
          printf("Enter value for b: ");
          scanf("%d", &b);
          printf("Enter size of vector A:");
          scanf("%d", &size);
          printf("Enter values of vector elements: ");
          for (i = 0; i < size; i++) {
               scanf("%d", &A[i]);
          }
     }
```

Scalar-Vector multiplication (2/3)

```
MPI_Bcast(&size, 1, MPI_INT, 0, MPI_COMM_WORLD);
MPI_Bcast(&b, 1, MPI_INT, 0, MPI_COMM_WORLD);

num = size / p;

MPI_Scatter(A, num, MPI_INT, local_A, num, MPI_INT, 0, MPI_COMM_WORLD);

for (i = 0; i < num; i++) {
local_A[i] *= b;
}

printf("\nLocal results for process %d:\n", my_rank);
for (i = 0; i < num; i++) {
     printf("%d ", local_A[i]);
}
printf("\n\n");
```

Scalar-Vector multiplication (3/3)

```
    MPI_Gather(local_A, num, MPI_INT, A, num, MPI_INT, 0, MPI_COMM_WORLD);

    if (my_rank == 0) {
        printf("\nFinal result:\n");
        for (i = 0; i < size; i++) {
            printf("%d ", A[i]);
        }
        printf("\n\n");
    }

    MPI_Finalize();

    return(0);
}
```

Scatterv

```
int MPI_Scatterv(void *sendbuf, int *sendcounts, int *displs, MPI_Datatype sendtype,
                 void *recvbuf, int recvcount, MPI_Datatype recvtype,
                 int root, MPI_Comm comm);
```

“sendbuf”: Η διεύθυνση των δεδομένων προς διαμοίραση

Στον επεξεργαστή root

“sendcounts”: Διάνυσμα με το πλήθος στοιχείων που αποστέλλονται προς κάθε επεξεργαστή

“displs”: Διάνυσμα με τις μετατοπίσεις από την αρχή του διανύσματος “sendbuf” για κάθε επεξεργαστή

“sendtype”: Ο τύπος κάθε στοιχείου που αποστέλλεται

“recvbuf”: Η διεύθυνση αποθήκευσης των δεδομένων που θα παραληφθούν

Σε κάθε επεξεργαστή

“recvcount”: Πλήθος στοιχείων που παραλαμβάνονται από κάθε επεξεργαστή

“recvtype”: Ο τύπος κάθε στοιχείου που παραλαμβάνεται

“root”: Ο επεξεργαστής ο οποίος αποστέλλει δεδομένα

Όλοι οι άλλοι στον communicator θα παραλάβουν

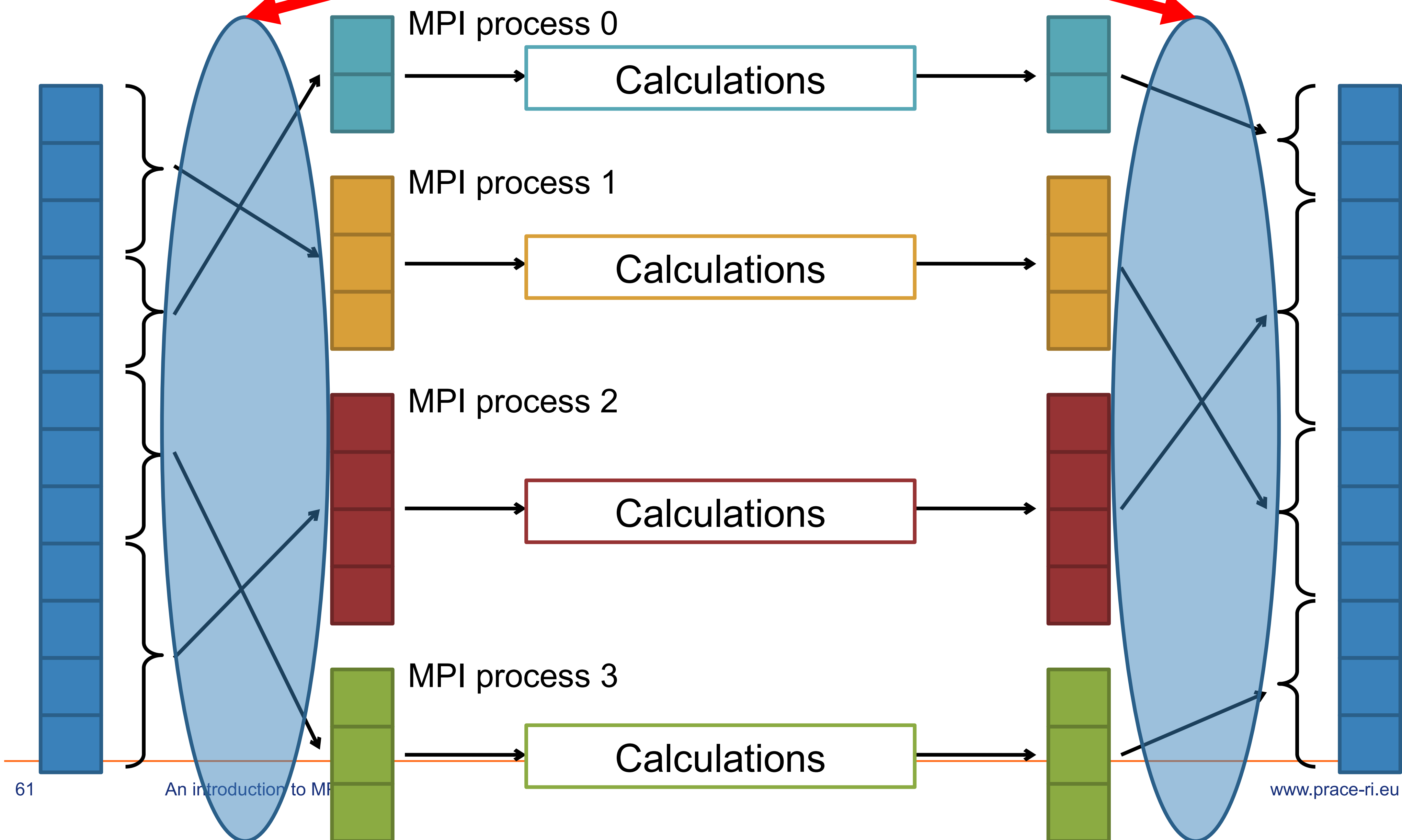
“comm”: Communicator

Gatherv

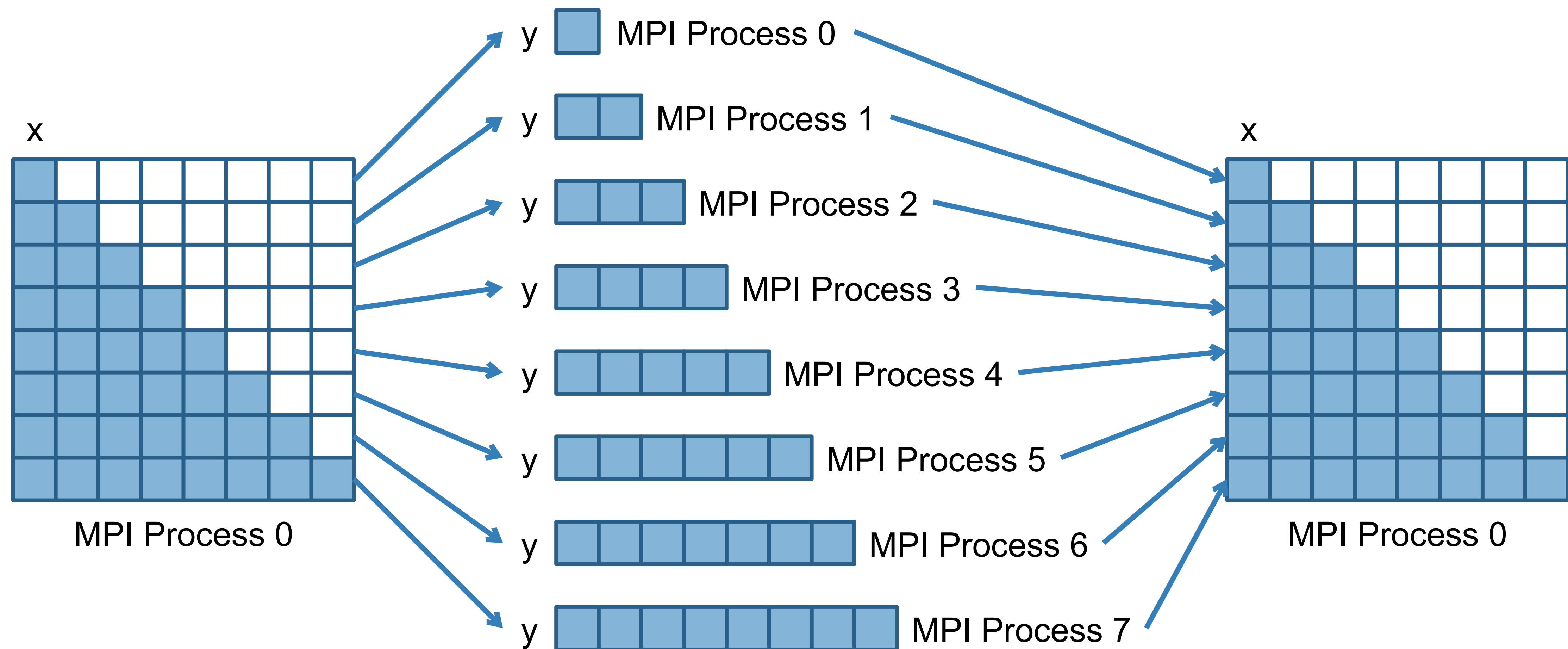
```
int MPI_Gatherv(void *sendbuf, int sendcount, MPI_Datatype sendtype, void *recvbuf,
                int *recvcounts, int *displs, MPI_Datatype recvtype,
                int root, MPI_Comm comm);
```

- “sendbuf”: Η διεύθυνση των δεδομένων προς συγκέντρωση
  - *Σε κάθε επεξεργαστή*
- “sendcount”: Πλήθος στοιχείων που αποστέλλονται προς τον επεξεργαστή root από κάθε επεξεργαστή
- “sendtype”: Ο τύπος κάθε στοιχείου που αποστέλλεται
- “recvbuf”: Η διεύθυνση αποθήκευσης των δεδομένων που θα παραληφθούν
  - *Στον επεξεργαστή root*
- “recvcounts”: Διάνυσμα με το πλήθος στοιχείων που παραλαμβάνονται από κάθε επεξεργαστή
- “displs”: Διάνυσμα με τις μετατοπίσεις από την αρχή του διανύσματος “recvbuf” για κάθε επεξεργαστή
- “recvtype”: Ο τύπος κάθε στοιχείου που παραλαμβάνεται
- “root”: Ο επεξεργαστής ο οποίος συγκεντρώνει δεδομένα
  - *Όλοι οι άλλοι στον communicator θα αποστείλουν*
- “comm”: Communicator

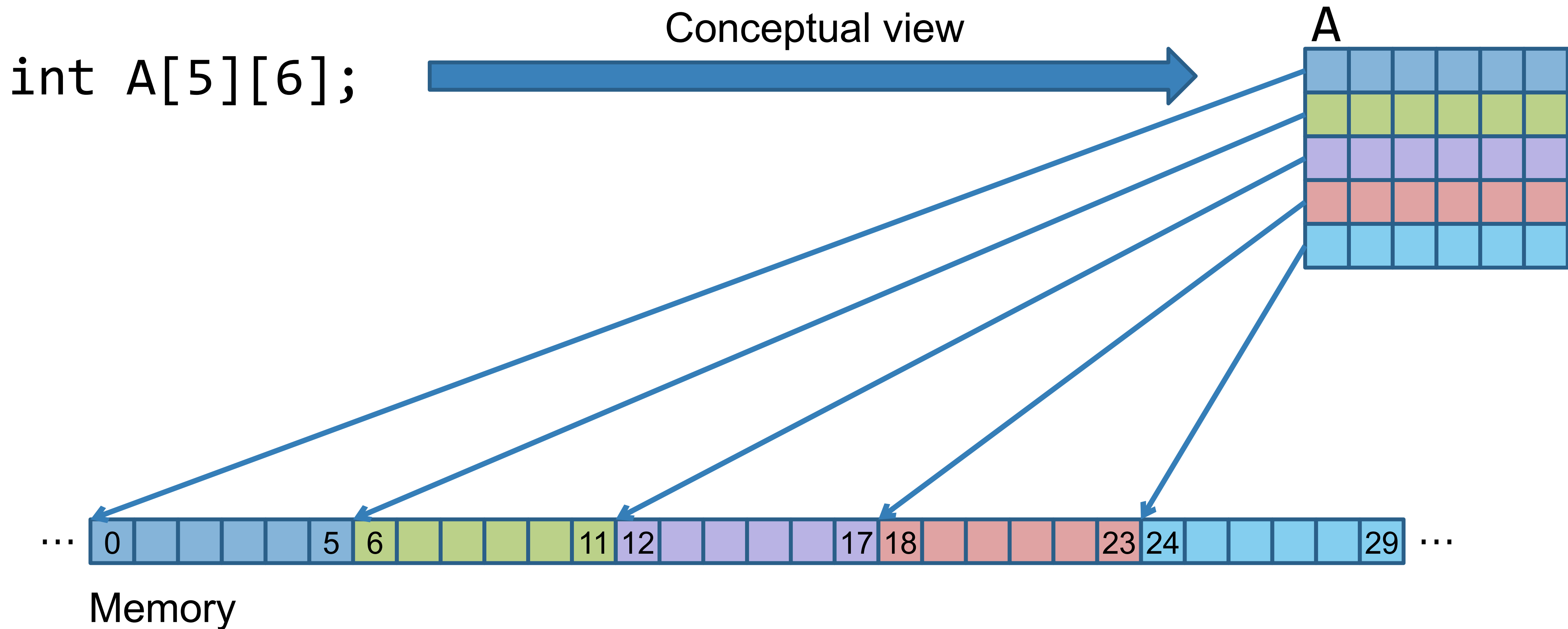
Scatterv/Gatherv



Example: Handling a lower triangular matrix



2-D matrix representation in memory (row-major)



Handling a lower triangular matrix (1/7)

```
#include <stdio.h>
#include “mpi.h”

#define MAXPROC 8        /* Max number of procsses */
#define LENGTH  8        /* Size of matrix is LENGTH * LENGTH */

int main(int argc, char *argv[]) {
     int i, j, np, my_rank;
     int x[LENGTH][LENGTH];    /* Send buffer */
     int y[LENGTH]; /* Receive buffer */
     int res[LENGTH][LENGTH]; /* Final receive buffer */
     int *sendcount, *recvcount;    /* Arrays for sendcounts and recvcounts */
     int *displs1, *displs2;   /* Arrays for displacements */
```

Handling a lower triangular matrix (2/7)

```
MPI_Init(&argc, &argv);              /* Initialize MPI     */
MPI_Comm_size(MPI_COMM_WORLD, &np);      /* Get # of processes */
MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);      /* Get own rank       */

/* Check that we have one process for each row in the matrix */
if (np != LENGTH) {
     if (my_rank == 0) {
         printf("You have to use %d processes\n", LENGTH);
     }
     MPI_Finalize();
     exit(0);
}
```

Handling a lower triangular matrix (3/7)

```
/* Allocate memory for the sendcount, recvcount and displacements arrays */
sendcount = (int *)malloc(LENGTH*sizeof(int));
recvcount = (int *)malloc(LENGTH*sizeof(int));
displs1   = (int *)malloc(LENGTH*sizeof(int));
displs2   = (int *)malloc(LENGTH*sizeof(int));

if (my_rank == 0) {
     for (i = 0; i < LENGTH; i++) {
         for (j = 0; j < LENGTH; j++) {
             x[i][j] = i * LENGTH + j;
         }
     }
}
```

Handling a lower triangular matrix (4/7)

```
/* Initialize sendcount and displacements arrays */
for (i = 0; i < LENGTH; i++) {
     sendcount[i] = i + 1;
     displs1[i] = i * LENGTH;
}

/* Scatter the lower triangular part of array x to all proceses, place it in y */
MPI_Scatterv(x, sendcount, displs1, MPI_INT, y, sendcount[my_rank], MPI_INT, 0,
                  MPI_COMM_WORLD);
```

Handling a lower triangular matrix (5/7)

```
if (my_rank == 0) {
     /* Initialize the result matrix res with 0 */
     for (i = 0; i < LENGTH; i++) {
         for (j = 0; j < LENGTH; j++) {
             res[i][j] = 0;
         }
     }

     /* Print out the result matrix res before gathering */
     printf("The result matrix before gathering is\n");
     for (i = 0; i < LENGTH; i++) {
         for (j = 0; j < LENGTH; j++) {
             printf("%4d ", res[i][j]);
         }
         printf("\n");
     }
}
```

Handling a lower triangular matrix (6/7)

```
for (i = 0; i < LENGTH; i++) {
     recvcount[i] = i + 1;
     displs2[i] = i * LENGTH;
}

/* Gather the local elements of each process to form a triangular matrix in the root */
MPI_Gatherv(y, recvcount[my_rank], MPI_INT, res, recvcount, displs2, MPI_INT, 0,
                 MPI_COMM_WORLD);
```

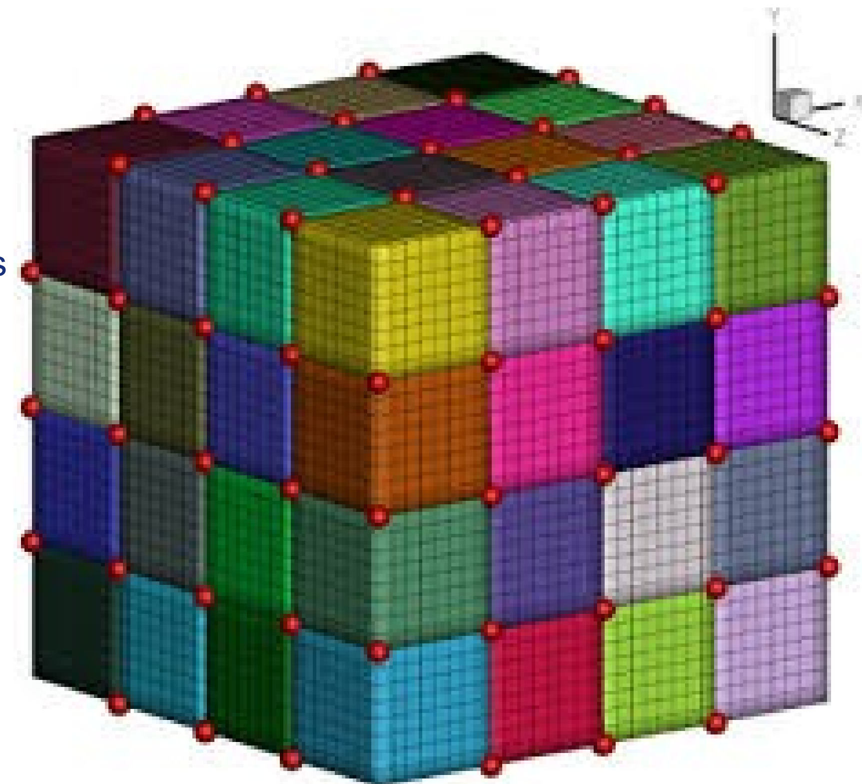
Handling a lower triangular matrix (7/7)

```
    if (my_rank == 0) {
        /* Print out the result matrix after gathering */
        printf("The result matrix after gathering is\n");
        for (i = 0; i < LENGTH; i++) {
            for (j = 0; j < LENGTH; j++) {
                printf("%4d ", res[i][j]);
            }
            printf("\n");
        }
    }

    MPI_Finalize();

    exit(0);
}
```

Virtual Topologies

Virtual Topologies

- Physical problems are in 1D, 2D or 3D
  - Domain is decomposed into smaller parts
  - Each part is assigned to an MPI process
- Algorithms that solve such problems typically require MPI processes to exchange data that resides close to the borders of each part
- Virtual topologies
  - Allows easy determination of neighboring MPI processes that must exchange data
  - Two types supported
    - *Cartesian (regular mesh)*
    - *Graph*



Creating a communication topology

```
int MPI_Cart_create(MPI_Comm comm_old, int ndims, int *dims, int *periods, int reorder, MPI_Comm *comm_cart)
```

- “comm_old”: The original communicator that includes the MPI processes to be used in creating the Cartesian topology
- “ndims”: Dimensionality of the Cartesian topology
- “dims”: integer array (of size “ndims”) that defines the number of processes in each dimension
- “periods”: array (of size “ndims”) that defines the periodicity of each dimension
  - *0 for a dimension ⇒ Not periodic*
  - *1 for a dimension ⇒ Periodic*
- “reorder”: MPI is allowed to renumber (reassign ranks) of the MPI processes
- “comm_cart”: New communicator that includes information about the Cartesian topology

Ranks and coordinates

Translate a rank to coordinates within a Cartesian topology

```
int MPI_Cart_coords(MPI_Comm comm, int rank, int maxdims, int *coords)
```

- “comm”: Cartesian communicator
- “rank”: Rank of MPI process who’s coordinates in the Cartesian topology are to be found
- “maxdim”: Dimension of “coords”
- “coords”: Coordinates in the Cartesian topology that correspond to “rank”

Translate coordinates of a Cartesian topology to a rank

```
int MPI_Cart_rank(MPI_Comm comm, int *coords, int *rank)
```

- “comm”: Cartesian communicator
- “coords”: Array of coordinates
- “rank”: The rank of the MPI processes corresponding to “coords”

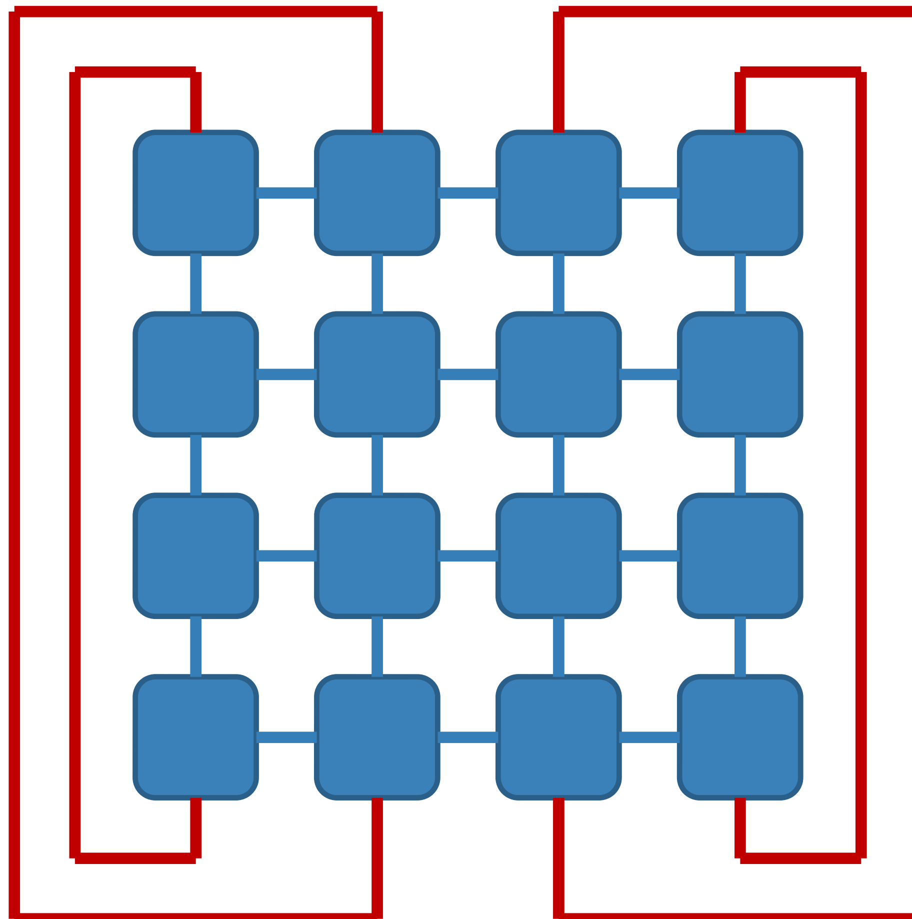
Finding neighbors

Find ranks of neighboring MPI processes on s single dimension

```
int MPI_Cart_shift(MPI_Comm comm, int direction, int disp,
                   int *rank_source, int *rank_dest)
```

- "comm": Cartesian communicator
- "direction": Shift direction, e.g., dimension for which neighbors will be returned
  - *0 on 1D topology*
  - *0 or 1 on 2D topology*
  - *0, 1 or 2 for 3D dimension, etc*
- "disp": Shift displacement
- "rank_source": Rank of source MPI process
- "rank_dest": Rank of destination process

2D grid with periodicity on one dimension



2D grid with periodicity on one dimension (1/3)

```
#include "mpi.h"
#include <stdio.h>
#define SIZE 16
#define UP    0
#define DOWN  1
#define LEFT  2
#define RIGHT 3

int main(int argc, char *argv[])
{
  int numtasks, rank, source, dest, outbuf, i, tag=1, dims[2]={4,4}, periods[2]={0,1}, nbrs[4],
      inbuf[4]={MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,MPI_PROC_NULL,},reorder=0,coords[2];

  MPI_Request reqs[8];
  MPI_Status stats[8];
  MPI_Comm cartcomm;

  MPI_Init(&argc,&argv);
  MPI_Comm_size(MPI_COMM_WORLD, &numtasks);
```

2D grid with periodicity on one dimension (2/3)

```
if (numtasks == SIZE) {
    MPI_Cart_create(MPI_COMM_WORLD, 2, dims, periods, reorder, &cartcomm);

    MPI_Comm_rank(cartcomm, &rank);

    MPI_Cart_coords(cartcomm, rank, 2, coords);

    MPI_Cart_shift(cartcomm, 0, 1, &nbrs[UP], &nbrs[DOWN]);
    MPI_Cart_shift(cartcomm, 1, 1, &nbrs[LEFT], &nbrs[RIGHT]);
```

2D grid with periodicity on one dimension (3/3)

```
    outbuf = rank;

    for (i = 0; i < 4; i++) {
      dest = nbrs[i];
      source = nbrs[i];
      MPI_Isend(&outbuf, 1, MPI_INT, dest, tag, MPI_COMM_WORLD, &reqs[i]);
      MPI_Irecv(&inbuf[i], 1, MPI_INT, source, tag, MPI_COMM_WORLD, &reqs[i+4]);
    }
    MPI_Waitall(8, reqs, stats);

    printf("rank= %d, coords= (%d, %d), neighbors(u,d,l,r) = (%d %d %d %d)\n",
            rank,coords[0],coords[1],nbrs[UP],nbrs[DOWN],nbrs[LEFT], nbrs[RIGHT]);

    printf("rank= %d,                       inbuf(u,d,l,r) = (%d %d %d %d)\n",
            rank,inbuf[UP],inbuf[DOWN],inbuf[LEFT],inbuf[RIGHT]);
  } else {
    printf("Must specify %d processors. Terminating.\n",SIZE);
  }
  MPI_Finalize();
}
```

Communication modes

Send modes

- To this point, we have studied non-blocking send routines using **standard mode**
  - In standard mode, the implementation determines whether buffering occurs
- MPI includes three other send modes that give the user explicit control over buffering.
  - Buffered
  - Synchronous
  - Ready
- Corresponding MPI functions
  - MPI_Bsend
  - MPI_Ssend
  - MPI_Rsend

MPI_Bsend

Buffered Send: allows user to explicitly create buffer space and attach buffer to send operations:

```
MPI_BSend(void *buf, int count, MPI_Datatype type, int dest, int tag,
          MPI_Comm comm)
```

Note: this is same as standard send arguments

```
MPI_Buffer_attach(void *buf, int size)
```

Create buffer space to be used with BSend

```
MPI_Buffer_detach(void *buf, int *size)
```

Note: call blocks until message has been safely sent

It is up to the user to properly manage the buffer and ensure space is available for any Bsend call

MPI_Ssend

Synchronous Send

Ensures that no buffering is used

Couples send and receive operation – send cannot complete until matching receive is posted and message is fully copied to remove processor

Very good for testing buffer safety of program

MPI_Rsend

Ready Send

Matching receive must be posted before send, otherwise program is incorrect

Can be implemented to avoid handshake overhead when program is known to meet this condition

Not very typical + dangerous

MPI’s Non-blocking Operations

Non-blocking operations return (immediately) “request handles” that can be tested and waited on.

```
MPI_Isend(start, count, datatype, dest, tag, comm, request)
MPI_Irecv(start, count, datatype, dest, tag, comm, request)
MPI_Wait(&request, &status)
```

One can also test without waiting:

```
MPI_Test(&request, &flag, status)
```

Multiple Completions

It is sometimes desirable to wait on multiple requests:

```
MPI_Waitall(count, array_of_requests, array_of_statuses)
MPI_Waitany(count, array_of_requests, &index, &status)
MPI_Waitsome(count, array_of_requests, array_of indices, array_of_statuses)
```

There are corresponding versions of test for each of these.

THANK YOU FOR YOUR ATTENTION

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