COMP 4901Q: High Performance Computing (HPC)

Lecture 10: Collective Communication Algorithms in MPI

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Outline

- Blocking vs. Nonblocking Communications
- MPI Derived Datatypes

- Collective Communications
  - Basic collective communications
  - Advanced collective algorithms

- A Case Study

Blocking Message Passing

- A blocking message passing operation means that it won't return until the desired operation has been finished.
  - It can guarantee the correctness of semantic.
  - Its performance may not be good, because while data is being transmitted, the sender/receiver can do nothing (i.e., being blocked!).

- MPI_Send and MPI_Recv are blocking operations.

- Case 1: blocking non-buffered Send/Receive
  - The send operation doesn't return until the matching receive has been encountered at the receiving process.

  - Once the receive operation is encountered, the message is sent and the send operation returns upon completion of the communication operation.

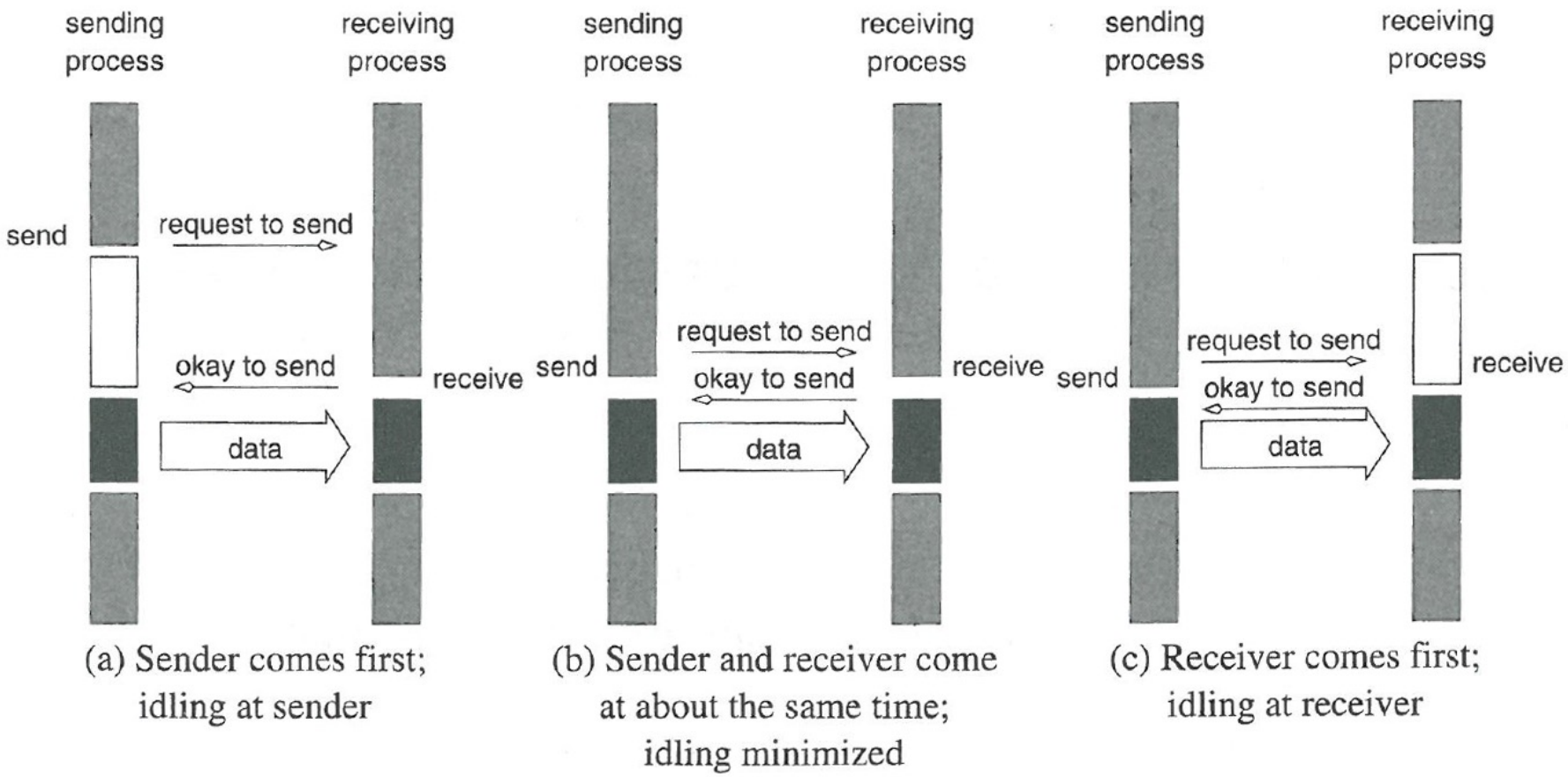
Blocking Non-Buffered Send/Receive

- Two issues of blocking non-buffered operations
  - Idling overhead
    - Since the send operation and receive operation may be executed at different time, either the sender or receiver will be idling for a period, waiting for the other side.
  - Deadlocks
    - The below example shows a deadlock scenario, in which two processes try to exchange two values, a and b.

Process 0	Process 1
Send(&a, 1, 1); Receive(&b, 1, 1);	Send(&a, 1, 0); Receive(&b, 1, 0);

Question: how to correct the above code?

Blocking Non-Buffered Send/Receive



(a) Sender comes first; idling at sender

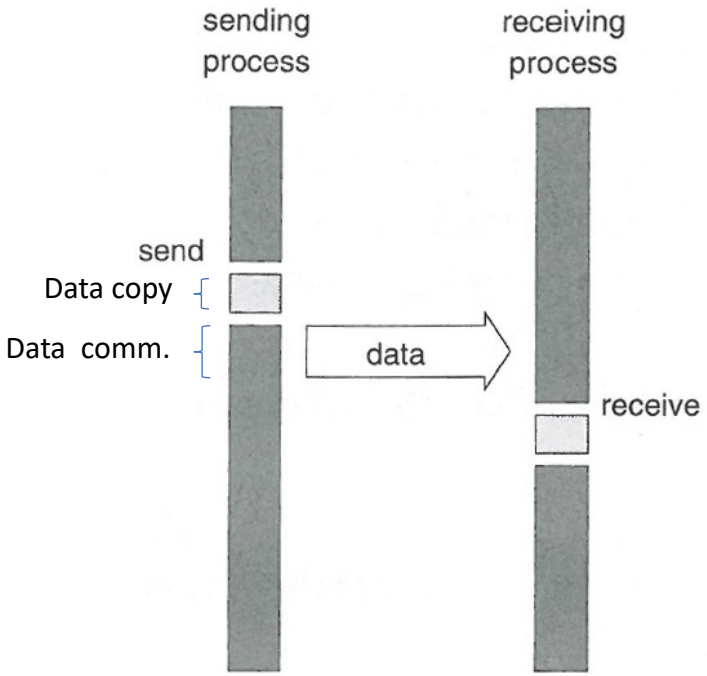
(b) Sender and receiver come at about the same time; idling minimized

(c) Receiver comes first; idling at receiver

Source: Fig. 6.1 of Ref. [1].

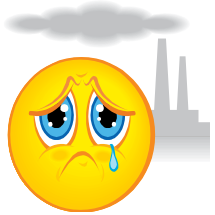
Blocking Message Passing

- Case 2: blocking buffered Send/Receive
  - The "idling overheads" and "deadlocks" issues of Case 1 can be alleviated by introducing "buffers".
- Example: The communication hardware has buffers at send and receive ends.
  - For the send operation, the sender copies the data into a buffer, and returns immediately after the copy operation.
  - The sender can continue with other jobs.
  - The actual communication can be accomplished in many ways, depending on the hardware resources.



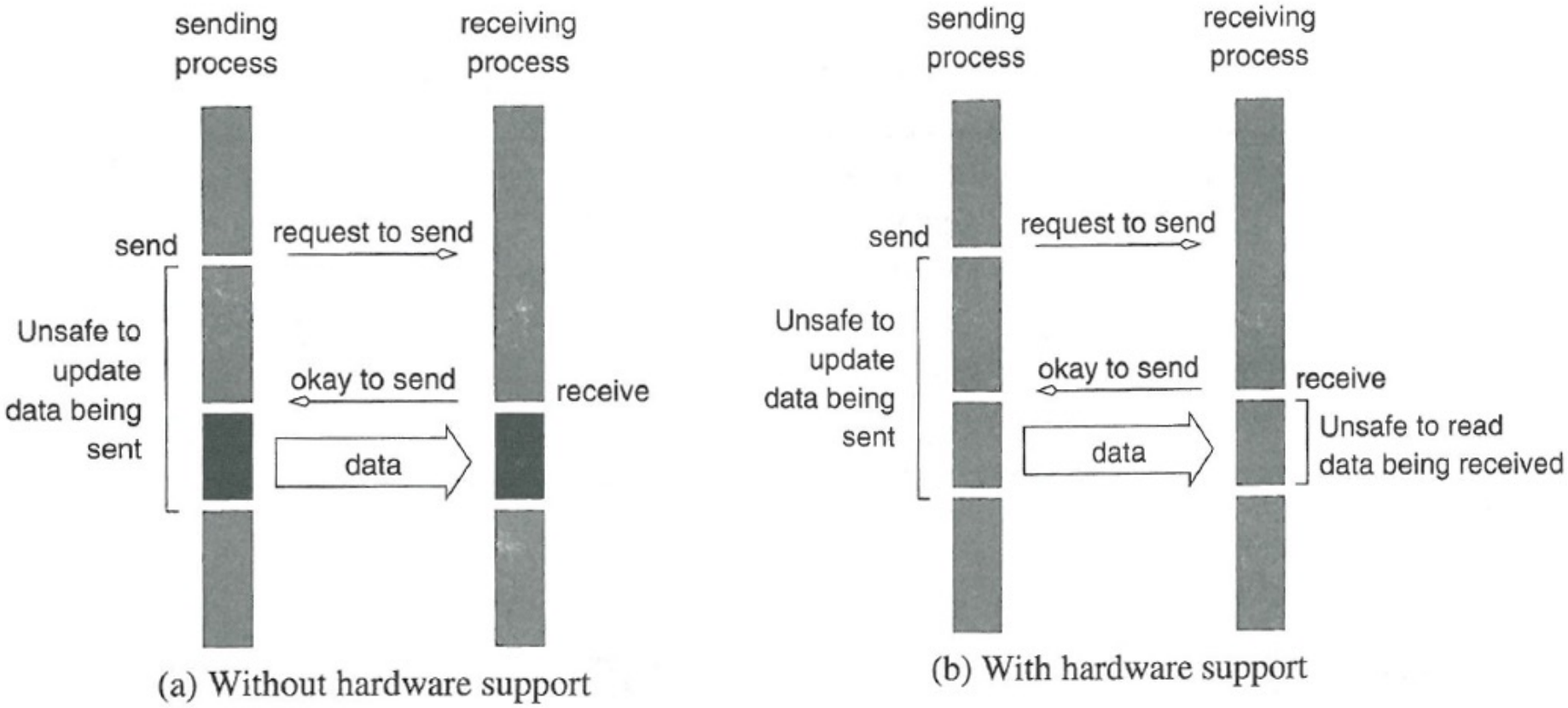
Source: Fig. 6.2 (a) of Ref. [1].

Non-blocking Message Passing

- Non-blocking send/receive operations return immediately, even if the communication is not finished.
  - It can avoid most deadlocks. 
  - It can achieve better performance by overlapping communication with computation. 
  - It requires a complicated program design. 

Non-blocking Message Passing

Non-blocking non-buffered send and receive operations



Source: Fig. 6.4 of Ref. [1].

Non-blocking Message Passing

- Problem: how does a process know that the data communication task is finished?

- Answer: the programmer needs to check the status of the previous non-blocking operation
  - If the data communication is finished, you can start to process the data;
  - If the data communication is not finished, you can either sleep or do some other safe computing tasks.

Non-blocking Message Passing in MPI

- MPI provides a pair of functions for non-blocking send and receive operations: MPI_Isend and MPI_Irecv

- int MPI_Isend(void* buf,
  int count,
  MPI_Datatype datatype,
  int dest,
  int tag,
  MPI_Comm comm,
  MPI_Request *request /* out */);
  - <buf, count, datatype> specify the message
  - dest specifies the rank of the process that should receive the message
  - tag (a nonnegative integer) is used to distinguish messages
  - comm specifies the process group
  - Request is a pointer to a request object, which is used by MPI_Test and MPI_Wait functions to identify the operation whose status we want to query or to wait for its completion.

Non-blocking Message Passing in MPI

- int MPI_Irecv(void* buf,
  int maxsize,
  MPI_Datatype datatype,
  int source,
  int tag,
  MPI_Comm comm,
  MPI_Request* request);
  - <buf, maxsize, datatype> specify where to store the message
  - source specifies the rank of the process from which the message should be received
  - tag should match the "tag" specified by the sender
  - comm specifies the process group
  - Request is a pointer to a request object, which is used by MPI_Test and MPI_Wait functions to identify the operation whose status we want to query or to wait for its completion.

- Remark: there is no status_p argument. The status information associated with the receive operation is returned by MPI_Test and MPI_Wait functions.

MPI_Test

- MPI_Test tests whether or not a non-blocking send or receive operation has finished.
  - The send or receive operation is identified by a request object with type MPI_Request

- int MPI_Test(MPI_Request *request,

  int *flag,

  MPI_Status *status);
  - **request** identifies the non-blocking operation. If the operation has finished, the request object will be deallocated.
  - **flag** is set to true (non-zero in C/C++) if the non-blocking operation has finished, or false (0 in C/C++) otherwise.
  - **status** is set to contain information about the operation if the non-blocking operation has finished.

MPI_Wait

- MPI_Wait blocks until the non-blocking operation (identified by an argument) completes.

- int MPI_Wait(MPI_Request *request,
  MPI_Status *status);
  - request identifies the non-blocking operation.
  - status is set to contain information about the operation.

A Simple Example

```
int main(int argc, char *argv[])
{
    int myid, numprocs, tag;
    int buffer;
    MPI_Status status;
    MPI_Request request;

    MPI_Init(&argc,&argv);
    MPI_Comm_size(MPI_COMM_WORLD,&numprocs);
    MPI_Comm_rank(MPI_COMM_WORLD,&myid);
    tag=1234;
    if(myid == 0){
        buffer = 5678;
        MPI_Isend(&buffer, 1, MPI_INT, 1, tag, MPI_COMM_WORLD, &request);
    }
    if(myid == 1){
        MPI_Irecv(&buffer, 1, MPI_INT, 0, tag, MPI_COMM_WORLD, &request);
    }
    MPI_Wait(&request, &status);
    if(myid == 0){
        printf("Process %d  sent %d\n", myid, buffer);
    }
    if(myid == 1){
        printf("Process %d  got %d\n", myid, buffer);
    }
    MPI_Finalize();
}
```

Process 0 sends an integer to process 1.

Both processes use non-blocking message passing.

Blocking and Non-Blocking

- A non-blocking communication operation can be matched with a corresponding blocking operation.

- For example, a process sends a message using a non-blocking send operation, and the message can be received by the other process using a blocking receive operation.

Derived Datatypes

- Previously, MPI programs only exchange data which are stored as a continuous array and all data elements in a message must have the same type.

- Motivations
  1. In today's distributed memory systems, communication is much more expensive than local computation.

  2. The cost of sending a fixed amount of data in multiple messages is much greater than the cost of sending a single message with the same amount of data

- In MPI, derived datatype is an approach to consolidating multiple data into a single message, even if they are not stored continuously in memory.
  - Once you created a derived datatype, you can use it just like other basic MPI datatypes.

Derived Datatypes

- A derived datatype is used to represent a collection of data items in memory by storing both the types of the items and their relative locations in memory.
  - Idea: if a function that sends data knows the information about a collection of data items, it can collect the items from memory before they are sent.
  - Similarly, a function that receives data can distribute the items into their correct destinations in memory when they're received.

Example of Derived Datatypes

- Assume a process wants to broadcast the following three variables
  - double a, b;
  - int n.
- A simple solution: call MPI_Bcast three times.
- Or, we can create a new datatype that can consolidate a, b, n into a single message, and then call a single MPI_Bcast.
  - Remember that data types in MPI have the type MPI_Datatype. So we are trying to create a variable with type MPI_Datatype.
- Formally, the derived datatype consists of a sequence of basic MPI data types together with a displacement for each of the data types.
  - Each data type is called a block, which can have multiple data elements.

Variable	Address
a	24
b	40
n	48

displacement

0

16

24

In the left example, the derived datatype consists of three blocks, each with a single data element.

$$\{(\texttt{MPI\_DOUBLE}, 0), (\texttt{MPI\_DOUBLE}, 16), (\texttt{MPI\_INT}, 24)\}$$

MPI_Type_create_struct

- MPI_Type_create_struct() builds a derived datatype that consists of individual elements that have different basic types.

- int MPI_Type_create_struct(

```
int          count, /* in */
int          array_of_blocklengths[], /* in */
MPI_Aint          array_of_displacements[], /* in */
MPI_Datatype   array_of_types[], /* in */
MPI_Datatype*  new_type_p /* out */)
```

  - count is the number of blocks in the new datatype
  - array_of_blocklengths[] stores the number of data elements in each block
  - array_of_displacement[] stores the displacements (in bytes) of each block
  - array_of_types[] stores the MPI datatypes of elements in each block
  - new_type_p is a pointer to the MPI derived datatype

MPI_Get_address

- How to find out the displacements?
  - Get the addresses of the memory location of each element by MPI_Get_address();
  - Calculate the displacements by subtractions

- A special MPI type MPI_Aint is used to store memory address

- int MPI_Get_address(

```
        void*        location_p,  /* in */
        MPI_Aint*    address_p /* out */)
```

  - location_p is the pointer to the target variable
  - address_p is the variable used to store the memory address of the target variable

MPI_Type_commit and MPI_Type_free

- A derived datatype must be committed by MPI_Type_commit() before it can be used.
  - MPI_Type_commit() allows the MPI implementation to optimize its internal representation of the datatype for use in communication functions.

- int MPI_Type_commit(MPI_Datatype* new_type_p);

- After using the new datatype, we can free its additional storage with MPI_Type_free()

- int MPI_Type_free(MPI_Datatype* old_type_p);

Derived Datatype: Example

```
1 #include "mpi.h"
2 #include <stdio.h>
3 struct mystruct {
4     char x;
5     double y[6];
6     int z[4];
7 };
8
9 int main(int argc, char *argv[]) {
10     struct mystruct mydata[1000];
11     int i, j, myid;
12     MPI_Status status;
13     MPI_Datatype mytype;
14     MPI_Datatype type[3] = {MPI_CHAR, MPI_DOUBLE, MPI_INT};
15     int blocklen[3] = {1, 6, 4};
16     MPI_Aint disp[3];
17     MPI_Init(&argc, &argv);
18     disp[0] = &mydata[0].x - &mydata[0];
19     disp[1] = &mydata[0].y - &mydata[0];
20     disp[2] = &mydata[0].z - &mydata[0];
21     MPI_Type_create_struct(3, blocklen, disp, type, &mytype);
22     MPI_Type_commit(&mytype);
23     MPI_Comm_rank(MPI_COMM_WORLD, &myid);
```

C/C++ structure for a single data element.
We will convert it into an MPI derived datatype.

Derived Datatype: Example

```
    if (myid == 0) {
        /* the code of initializing mydata[] should be put here */
        MPI_Send(mydata, 1000, mytype, 1, 0, MPI_COMM_WORLD);
    } else if (myid == 1){
        MPI_Recv(mydata, 1000, mytype, 0, 0, MPI_COMM_WORLD, &status);
    }
    MPI_Type_free (mytype);
    MPI_Finalize();
    return 0;
}
```

Collective Communication

- Point-to-point communication happens between two processes.

- Collective communication is a method of communication which involves participation of all processes in a communicator.
  - Example 1: process 0 needs to broadcast a vector to all other processes
  - Example 2: process 0 needs to receive data from all other processes and then perform a calculation

Motivation

- Consider the following example: how to sum up 8 numbers owned by 8 different processes?
  - Solution 1:

```
for( i = 1; i < 8; i++)
    Process i sends its number to process 0;
```

Process 0 adds the received 7 numbers with its own number.

  - Analysis:
    - Solution 1 involves 7 network transmissions, all with Process 0 as the destination. In a typical cluster, these 7 network transmissions take place sequentially (assuming the host of process 0 has a single network interface).

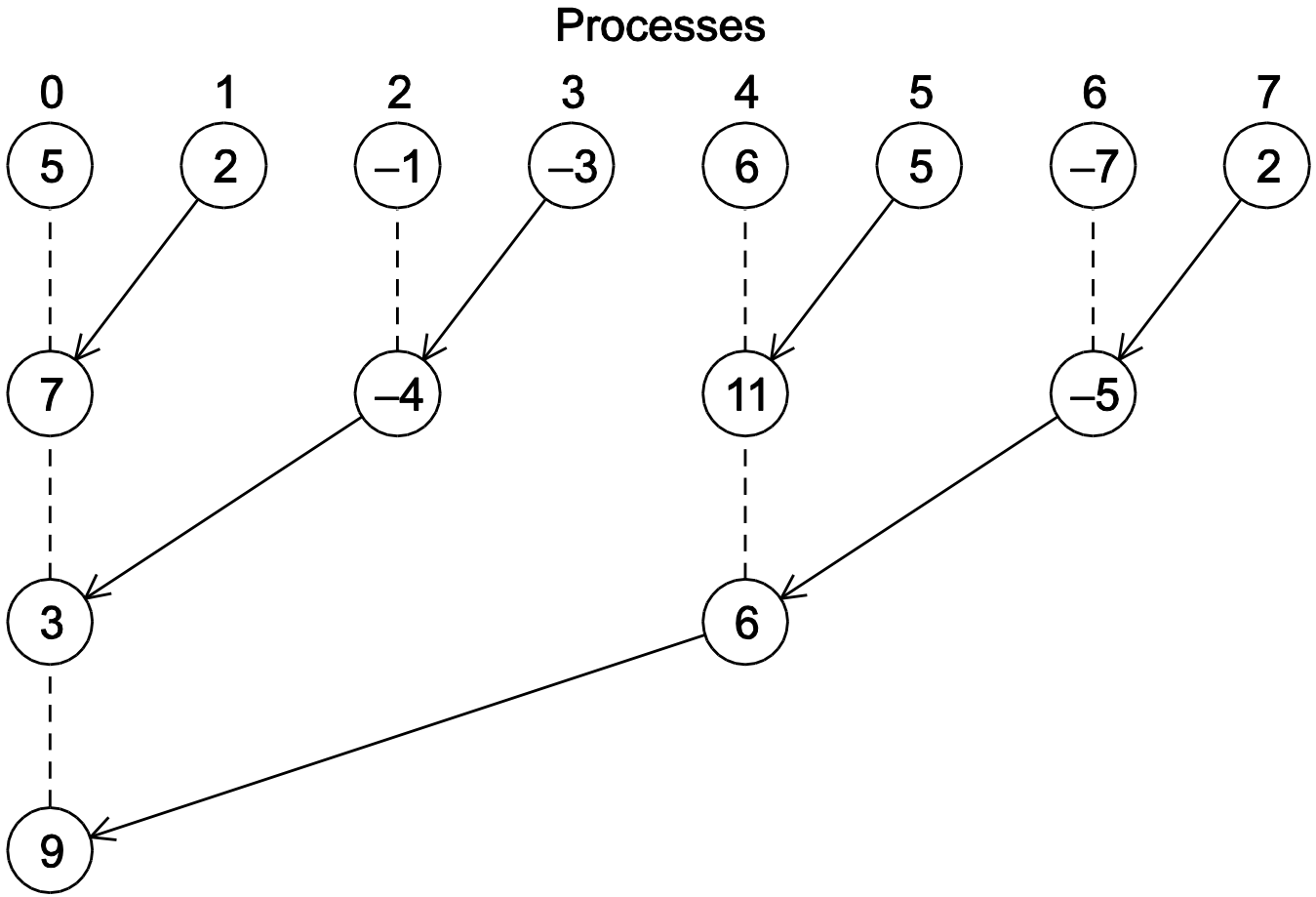
Motivation (Cont.)

- Solution 2 (a better one)
  - (1.a) Process 1 sends to 0, 3 sends to 2, 5 sends to 4, and 7 sends to 6.
  - (1.b) Processes 0, 2, 4, and 6 add in the received values.

  - (2.a) Processes 2 and 6 send their new values to processes 0 and 4, respectively.
  - (2.b) Processes 0 and 4 add the received values into their new values.

  - (3.a) Process 4 sends its newest value to process 0.
  - (3.b) Process 0 adds the received value to its newest value.

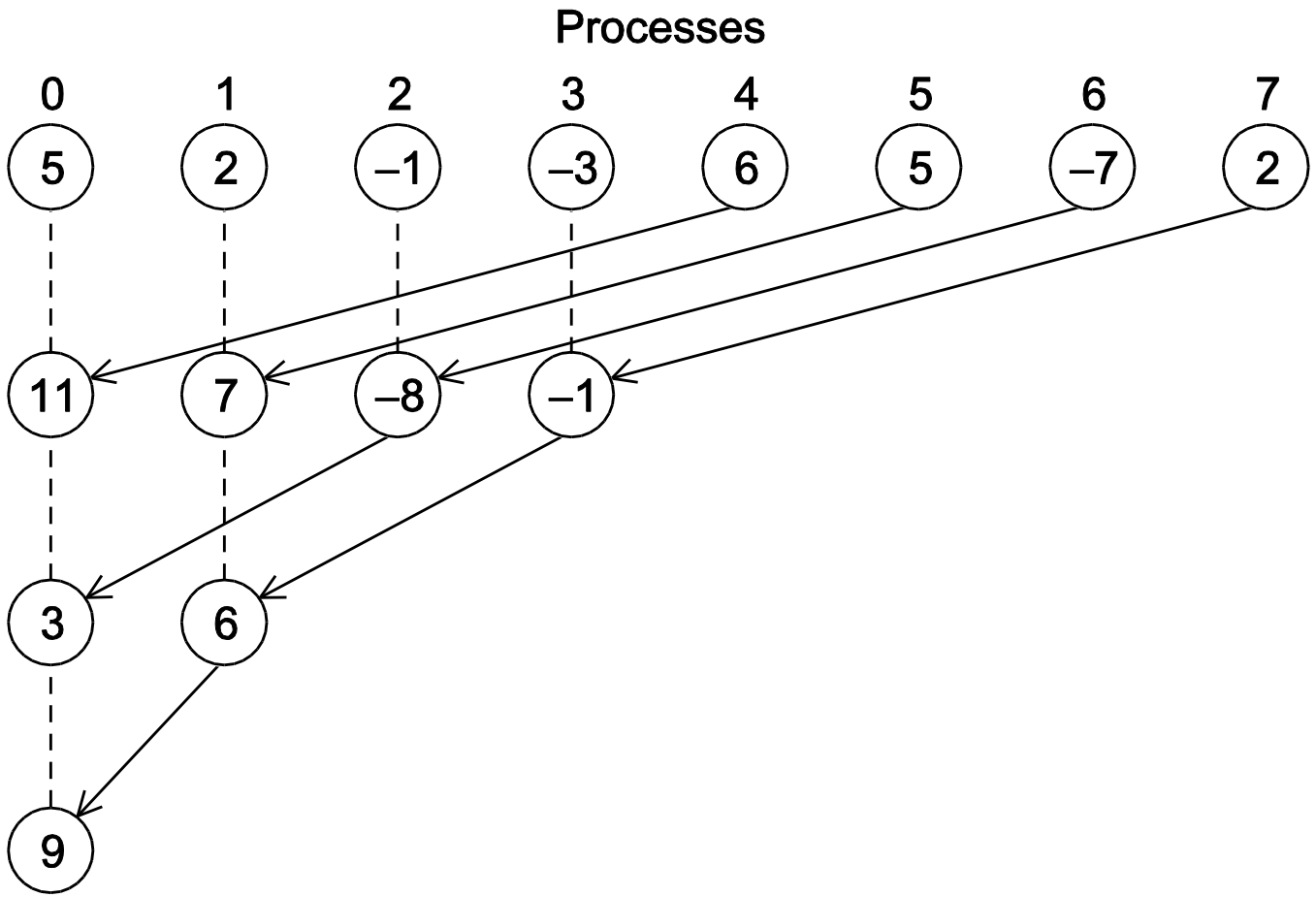
Solution 2: A Tree-Structured Global Sum



Analysis of Solution 2

- By using a network switch, multiple data communications can happen simultaneously if there is no common source/destination
- Solution 2 also needs a total of 7 data communications
- But, these 7 communications can happen in just 3 steps
  - Because some communications can take place in parallel
- It's easy to see that, summing up n numbers takes $\log_2 n$ steps only. Solution 1 takes n-1 steps.

An Alternative Tree-Structured Global Sum



Data Reduction in MPI

- The previous example is a typical pattern called "reduction", i.e., to reduce a set of messages into a single message within a process group.
  - Good solutions are much better than a simple solution.
  - There are different ways to implement a good solution.
  - A message can include multiple data elements. The reduction operation is applied element-wise on each data element.

MPI_Reduce

- MPI provides an optimized library function MPI_Reduce for reduction operation. The reduced results will be stored in a "destination process".

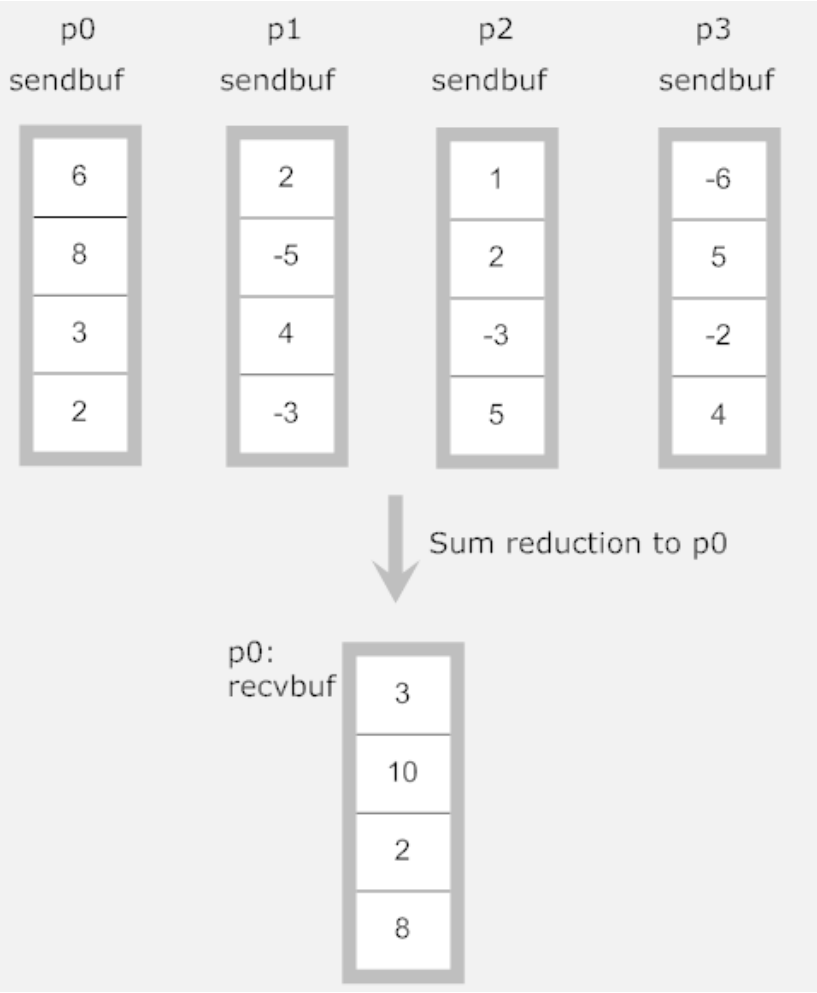
- int MPI_Reduce(void *sendbuf,
  void *recvbuf,
  int count,
  MPI_Datatype datatype,
  MPI_Op operator,
  int root,
  MPI_Comm comm)

  - <sendbuf, count, datatype> specify the "message"
  - <recvbuf, root> specify where to store the reduced result (i.e., recvbuf at process root)
  - operator specify the reduction operation (see next slide)
  - comm specifies the process group

MPI_Reduce

- The reduction operations are performed element-wise.

- Can recvbuf be the same as sendbuf at process 0?
  - Answer: NO!



MPI Reduction Operators

- The following operators are supported by MPI:

Operation Value	Meaning
MPI_MAX	Maximum
MPI_MIN	Minimum
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
MPI_BXOR	Bitwise exclusive or
MPI_MAXLOC	Maximum and location of maximum
MPI_MINLOC	Minimum and location of minimum

Collective vs. Point-to-Point Communications

- All processes in the communicator must call the same collective function.

- For example, a program that attempts to match a call to MPI_Reduce on one process with a call to MPI_Recv on another process is erroneous, and, in all likelihood, the program will hang or crash.

Collective vs. Point-to-Point Communications

- The arguments passed by each process to an MPI collective communication must be "compatible".

- For example, if one process passes in 0 as the root and another passes in 1, then the outcome of a call to MPI_Reduce is erroneous, and, once again, the program is likely to hang or crash.

Collective vs. Point-to-Point Communications

- The recvbuf argument is only used on dest_process.
- However, all of the processes still need to pass in an actual argument corresponding to recvbuf, even if it's just NULL.

Collective vs. Point-to-Point Communications

- Point-to-point communications are matched on the basis of tags and communicators.
- Collective communications don't use tags.
- They're matched solely on the basis of the communicator and the order in which they're called.

Test Yourself

- Suppose that each process calls MPI_Reduce with operator MPI_SUM, and destination process 0.
  - At the end, what will be the value of b and d at process 0, respectively?

Time	Process 0	Process 1	Process 2
0	`a = 1; c = 2`	`a = 1; c = 2`	`a = 1; c = 2`
1	`MPI_Reduce(&a, &b, ...)`	`MPI_Reduce(&c, &d, ...)`	`MPI_Reduce(&a, &b, ...)`
2	`MPI_Reduce(&c, &d, ...)`	`MPI_Reduce(&a, &b, ...)`	`MPI_Reduce(&c, &d, ...)`

Some Major Collective Communications

- MPI_Reduce
- MPI_Bcast
- MPI_Scatter
- MPI_Gather

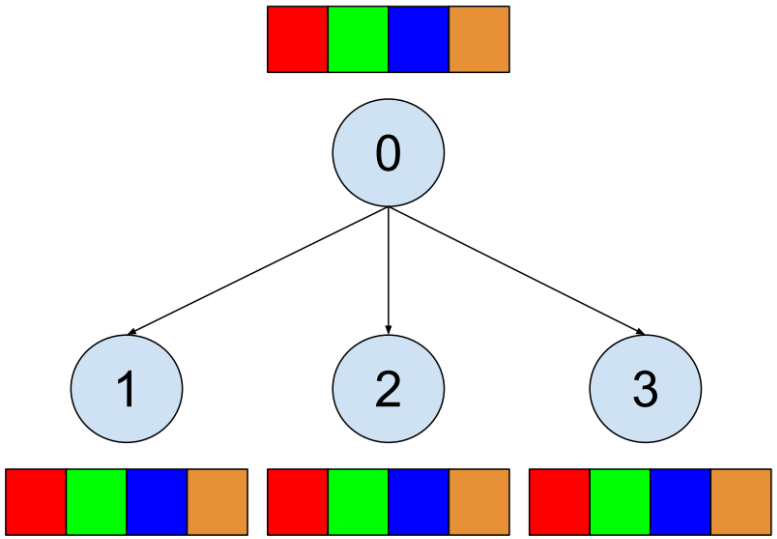
- MPI_Allgather
- MPI_Allreduce
- MPI_Alltoall
- MPI_Reduce_scatter

- MPI_Barrier

MPI_Bcast

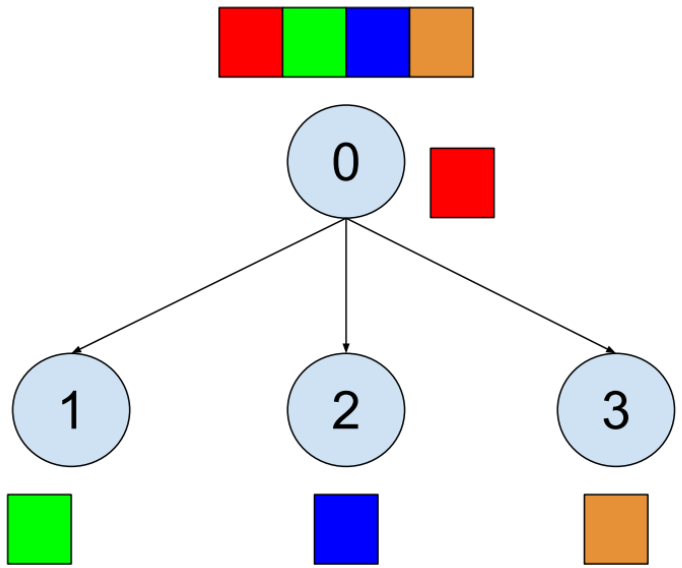
- Data belonging to a single process is sent to all of the processes in the process group.

- int MPI_Bcast(void *buf,
  int count,
  MPI_Datatype datatype,
  int root,
  MPI_Comm comm)
  - <buf, count, datatype> specify the "message"
  - root specifies the rank of the source process
  - comm specifies the process group



MPI_Scatter

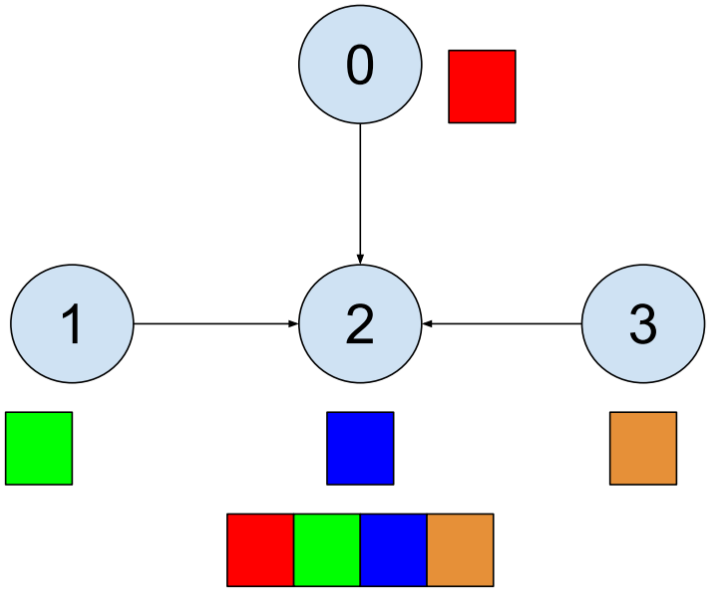
- MPI_Scatter evenly divides a vector of data owned by a root process into a number of pieces, and sends each piece to each of the other processes.
  - # of pieces equals # of processes in the process group
  - Assumption: the # of data items can be evenly divided by the # of processes



- int MPI_Scatter(void *sendbuf, int sendcount,
  MPI_Datatype senddatatype,
  void *recvbuf, int recvcount,
  MPI_Datatype recvdatatype,
  int root, MPI_Comm comm)
  - <sendbuf, sendcount, senddatatype> specify the "source message", where sendcount is the amount of data sent to each process, NOT the total amount of data in the sendbuf
  - <recvbuf, recvcount, recvdatatype> specify the "received message", where recvcount is the amount of data received by each process
  - root specifies the rank of the source process
  - comm specifies the process group

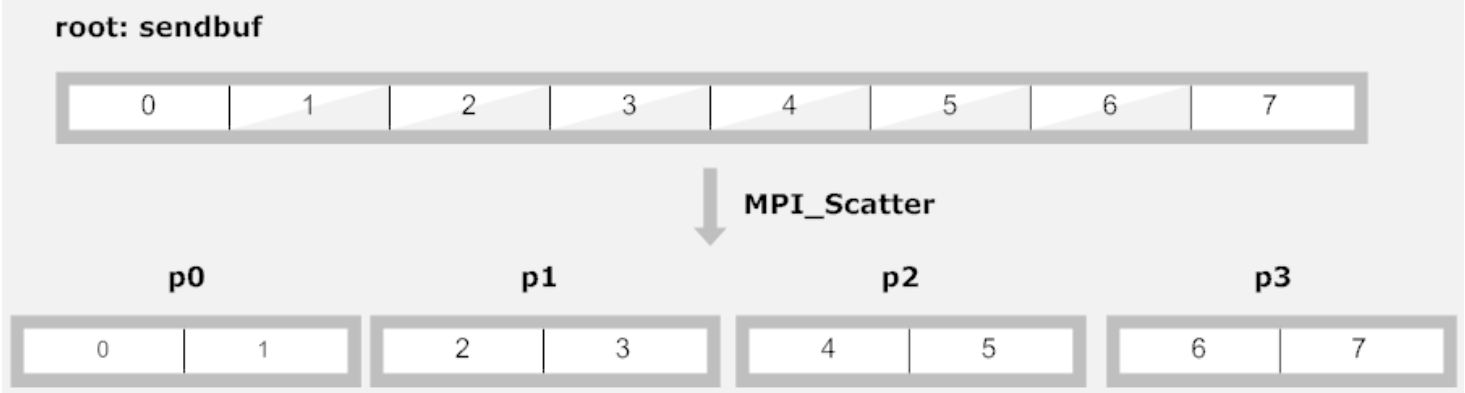
MPI_Gather

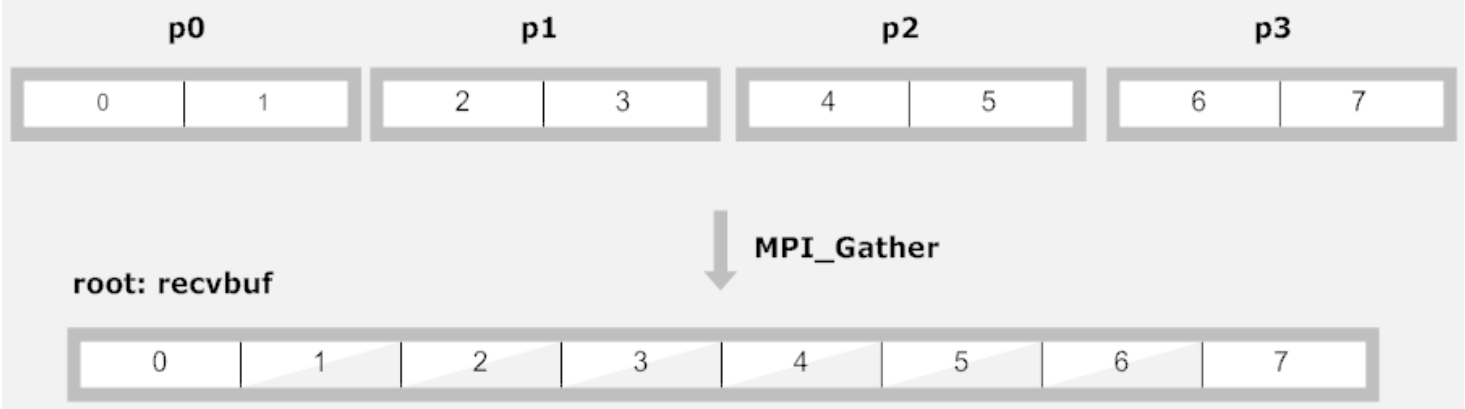
- MPI_Gather collects data from all processes in a process group onto a single process.
  - Remark: each process has to contribute the same amount of data items



- int MPI_Gather(void *sendbuf,
  int sendcount,
  MPI_Datatype senddatatype,
  void *recvbuf,
  int recvcount,
  MPI_Datatype recvdatatype,
  int root,
  MPI_Comm comm)
  - <sendbuf, sendcount, senddatatype> specify the "source message", where sendcount is the amount of data sent out by each process
  - <recvbuf, recvcount, recvdatatype> specify the "received message", where recvcount is the amount of data received from **each process**
  - root specifies the rank of the destination process
  - comm specifies the process group

MPI_Scatter and MPI_Gather





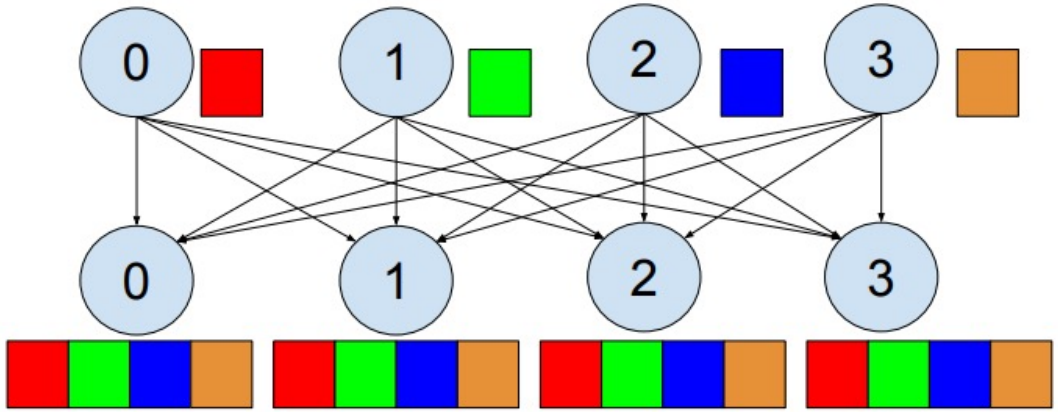
Example of MPI_Scatter: Distribute an Array

```
4     int n, local_n, my_rank, comm_sz;
5     MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
6     MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
7     if (my_rank == 0) {
8         scanf("%d", &n);
9         MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
10    } else {
11        MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
12    }
13    local_n = n / comm_sz;
14    local_a = malloc(local_n * sizeof(double));
15    if (my_rank == 0) {
16        a = malloc(n * sizeof(double));
17        for (i = 0; i < n; i++)
18            scanf("%lf", &a[i]);
19        MPI_Scatter(a, local_n, MPI_DOUBLE, local_a, local_n, MPI_DOUBLE, 0, MPI_COMM_WORLD);
20    } else {
21        MPI_Scatter(a, local_n, MPI_DOUBLE, local_a, local_n, MPI_DOUBLE, 0, MPI_COMM_WORLD);
22    }
```

MPI_Allgather

- MPI_Allgather concatenates the data of each process and stores the concatenated data in each process.

- int MPI_Allgather(void *sendbuf,
  int sendcount,
  MPI_Datatype senddatatype,
  void *recvbuf,
  int recvcount,
  MPI_Datatype recvdatatype,
  MPI_Comm comm)

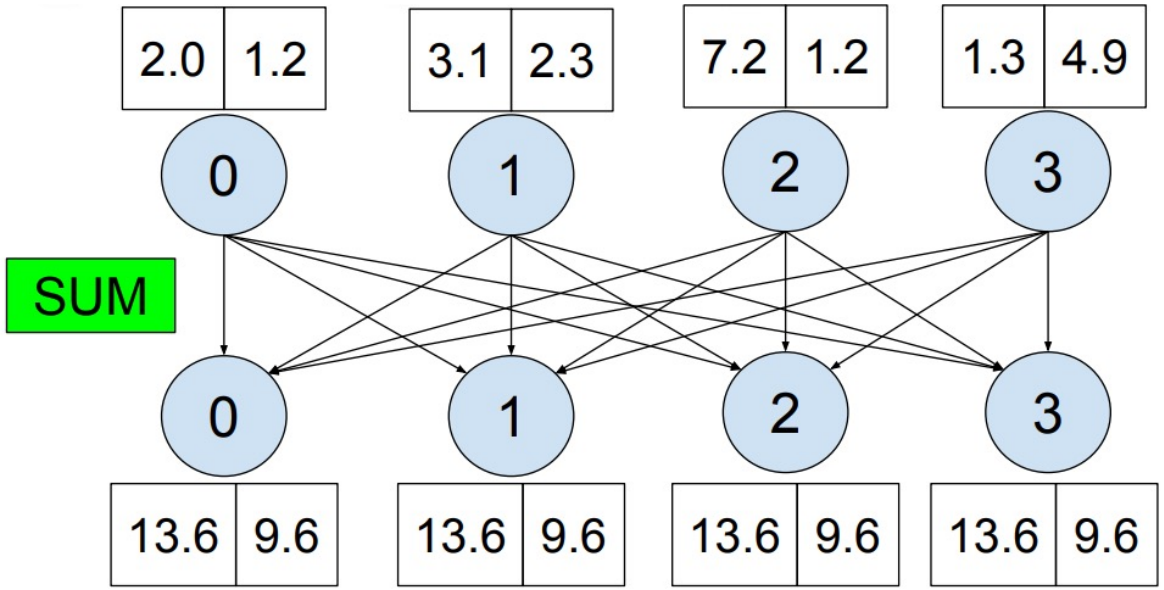


  - <sendbuf, sendcount, senddatatype> specify the "source message", where sendcount is the amount of data sent out by each process
  - <recvbuf, recvcount, recvdatatype> specify the "received message", where recvcount is the amount of data received from each process
  - comm specifies the process group

MPI_Allreduce

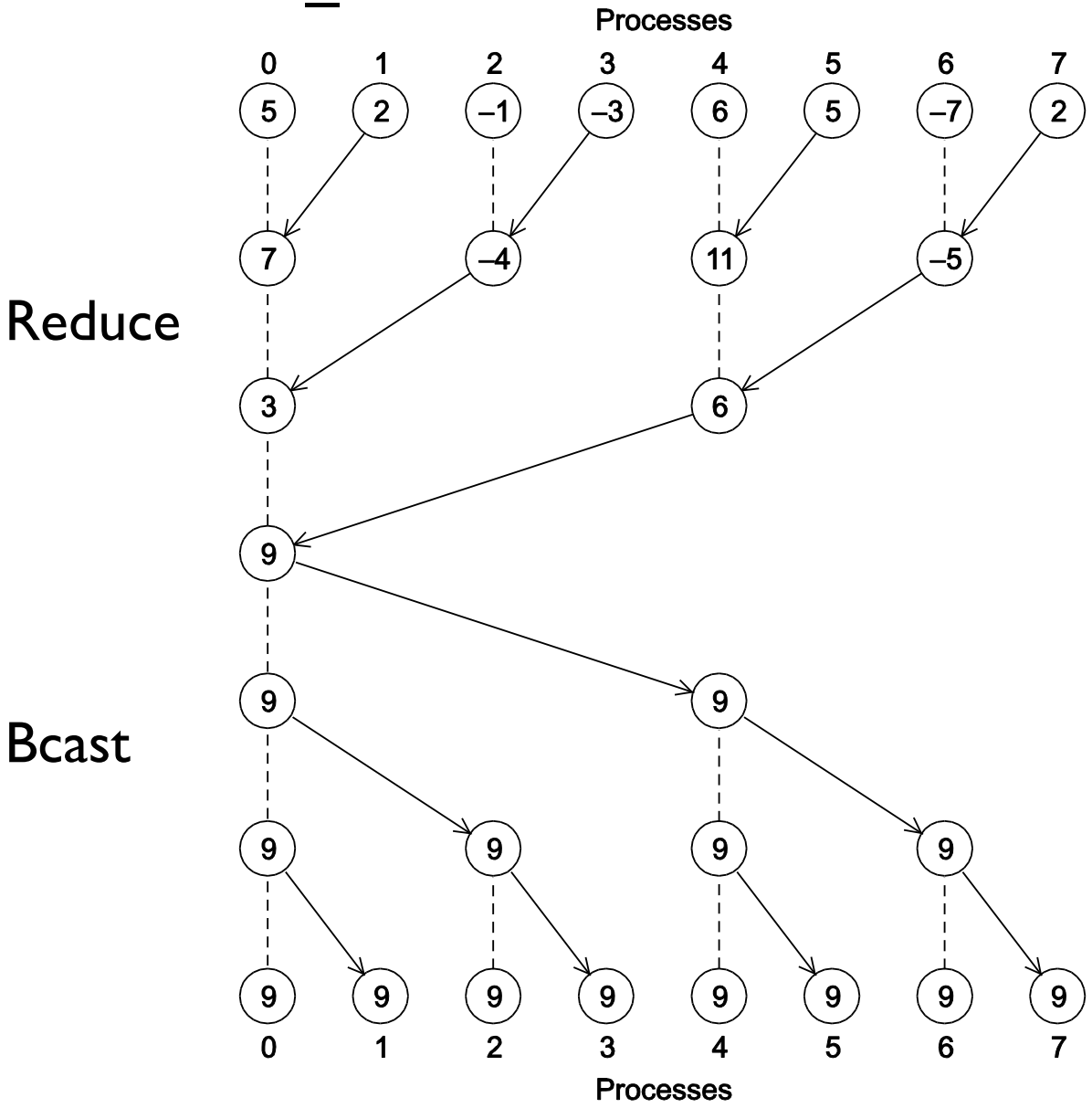
- int MPI_Allreduce(void *sendbuf,
  void *recvbuf,
  int count,
  MPI_Datatype datatype,
  MPI_Op operator,
  MPI_Comm comm)

- Similar to MPI_Reduce, but the reduced results are stored in ALL processes



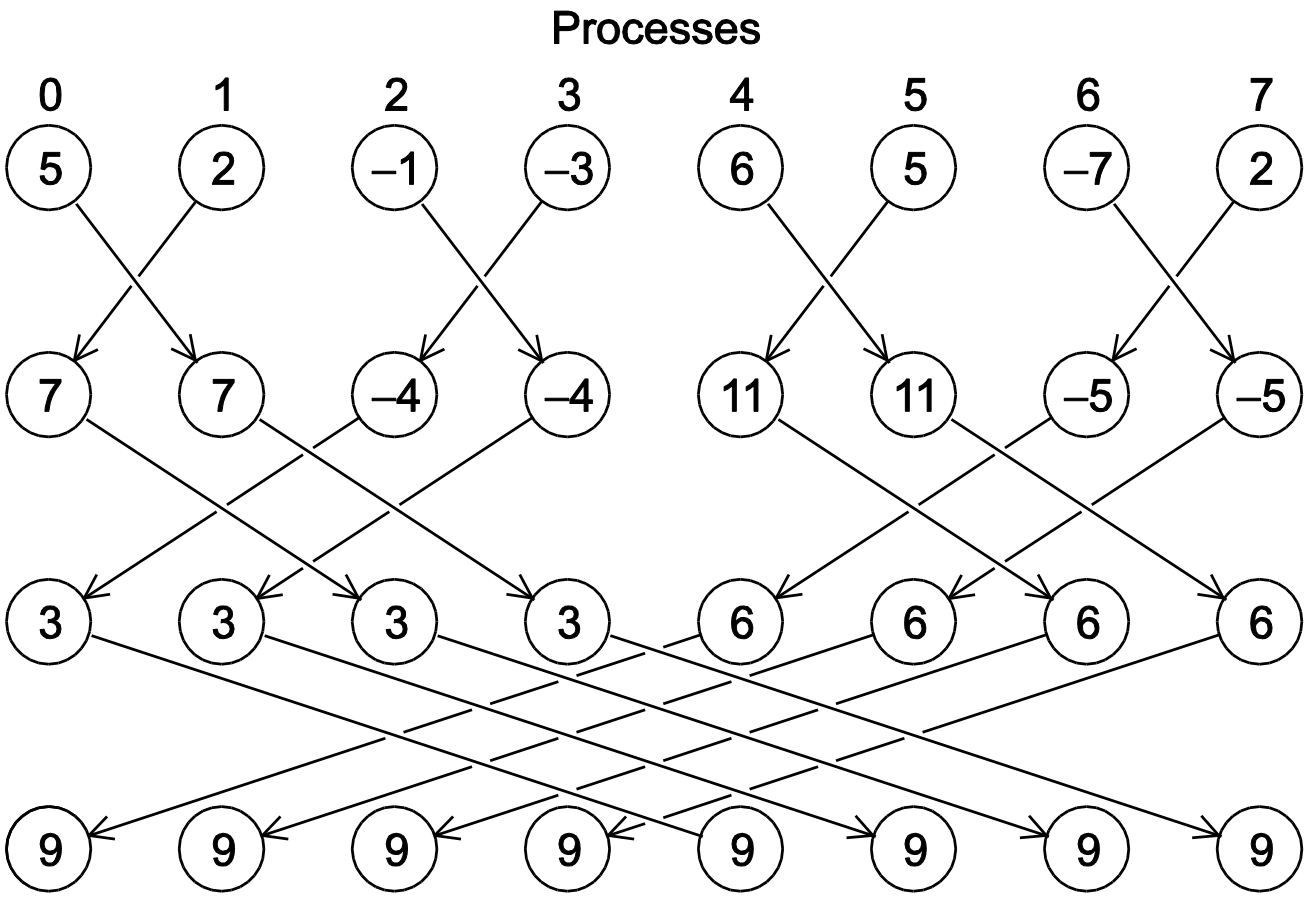
MPI_Allreduce: Algorithm 1

- A $2\log_2 n$ solution to MPI_Allreduce:



MPI_Allreduce: Algorithm 2

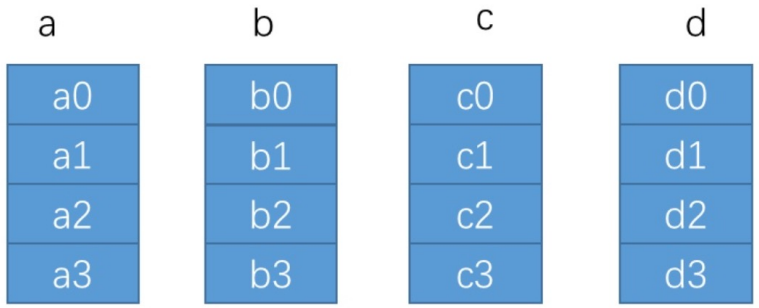
- A $\log_2 n$ solution to MPI_Allreduce: butterfly-structure
- It exploits the fact that today's network interface card and network switch support simultaneous send and receive operations.

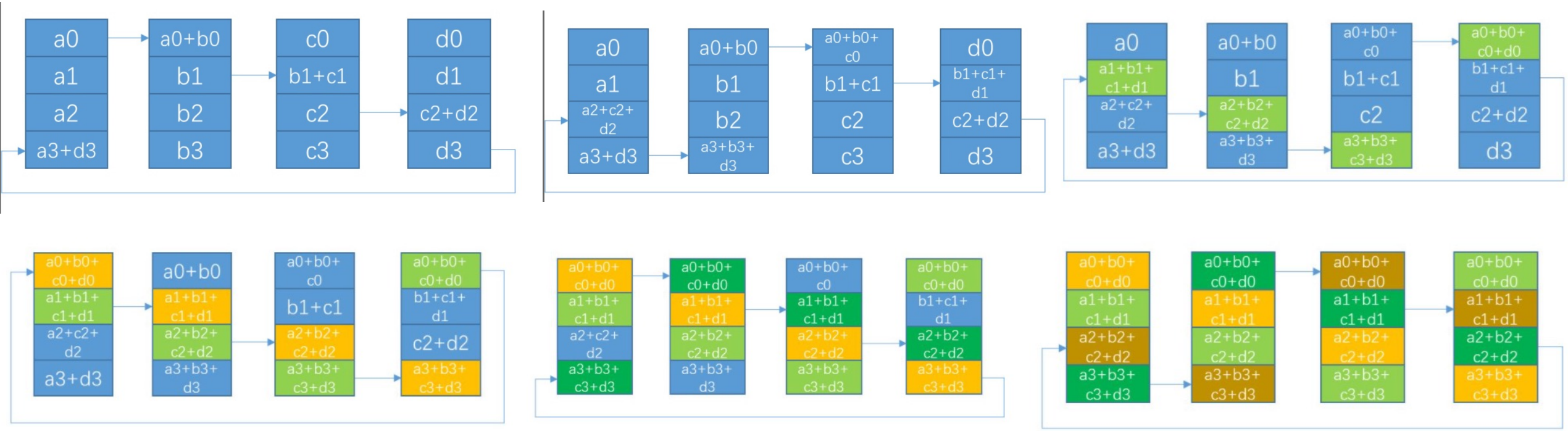


MPI_Allreduce: Algorithm 3

- A bandwidth friendly solution to MPI_Allreduce: ring-based

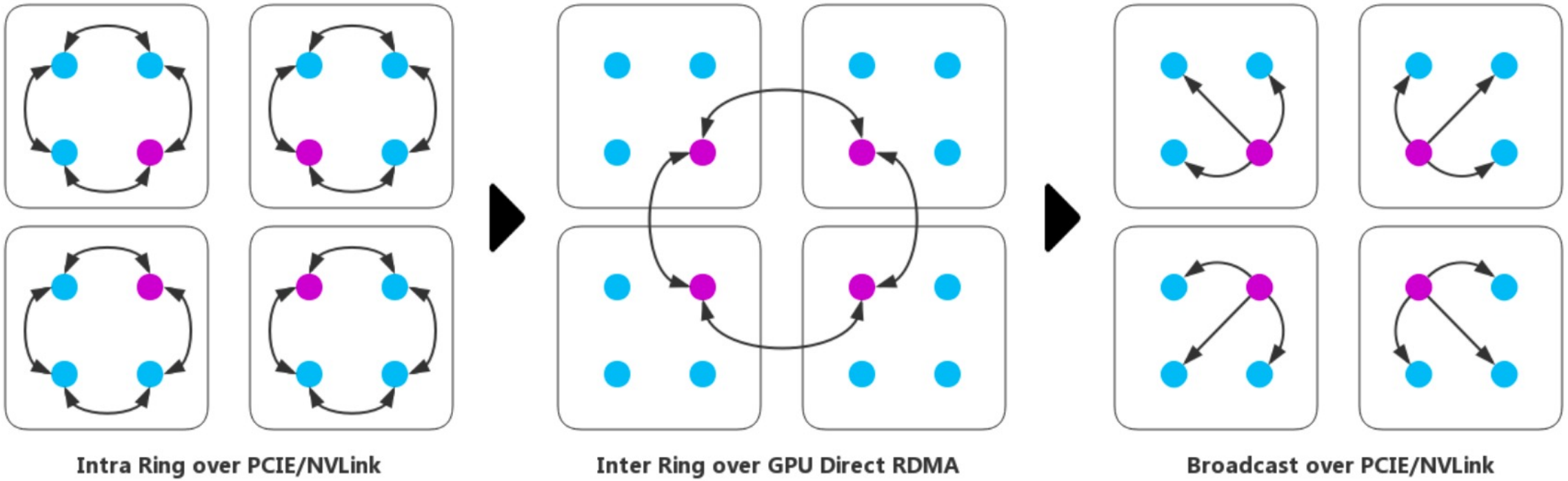
$$2(n-1)\alpha + 2(n-1)\beta m/n$$





Allreduce: Algorithm 4

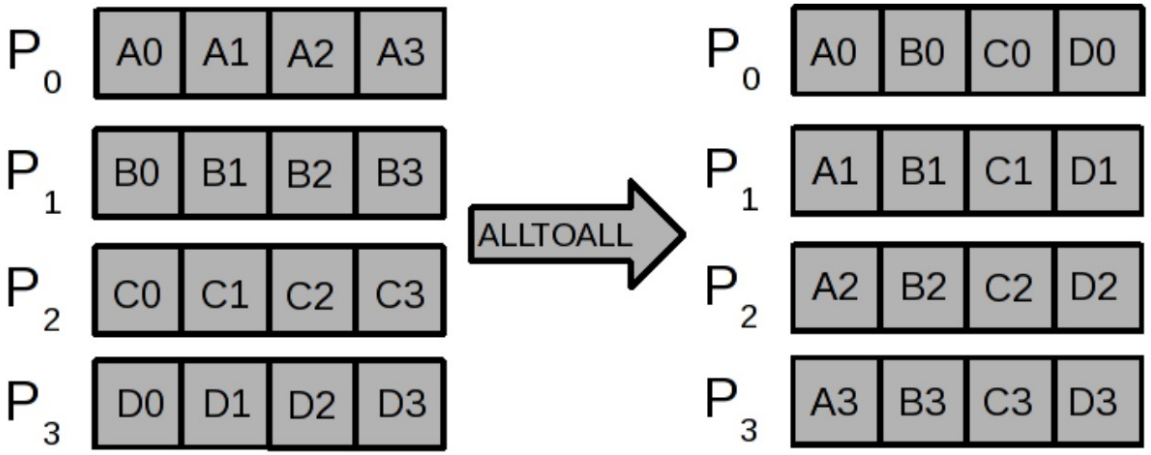
- A solution to balance the latency and bandwidth: hierarchical Allreduce [1]



[1] Jia et al., Highly Scalable Deep Learning Training System with Mixed-Precision: Training ImageNet in Four Minutes, *NIPS Workshop 2018*

MPI_Alltoall

- int MPI_Alltoall (void *sendbuf,
  int sendcount,
  MPI_Datatype sendtype,
  void *recvbuf,
  int recvcount,
  MPI_Datatype recvtype,
  MPI_Comm comm)



- Like a transpose
- Can be seen as a collection of simultaneous scatters or simultaneous gathers

MPI_Alltoall Example

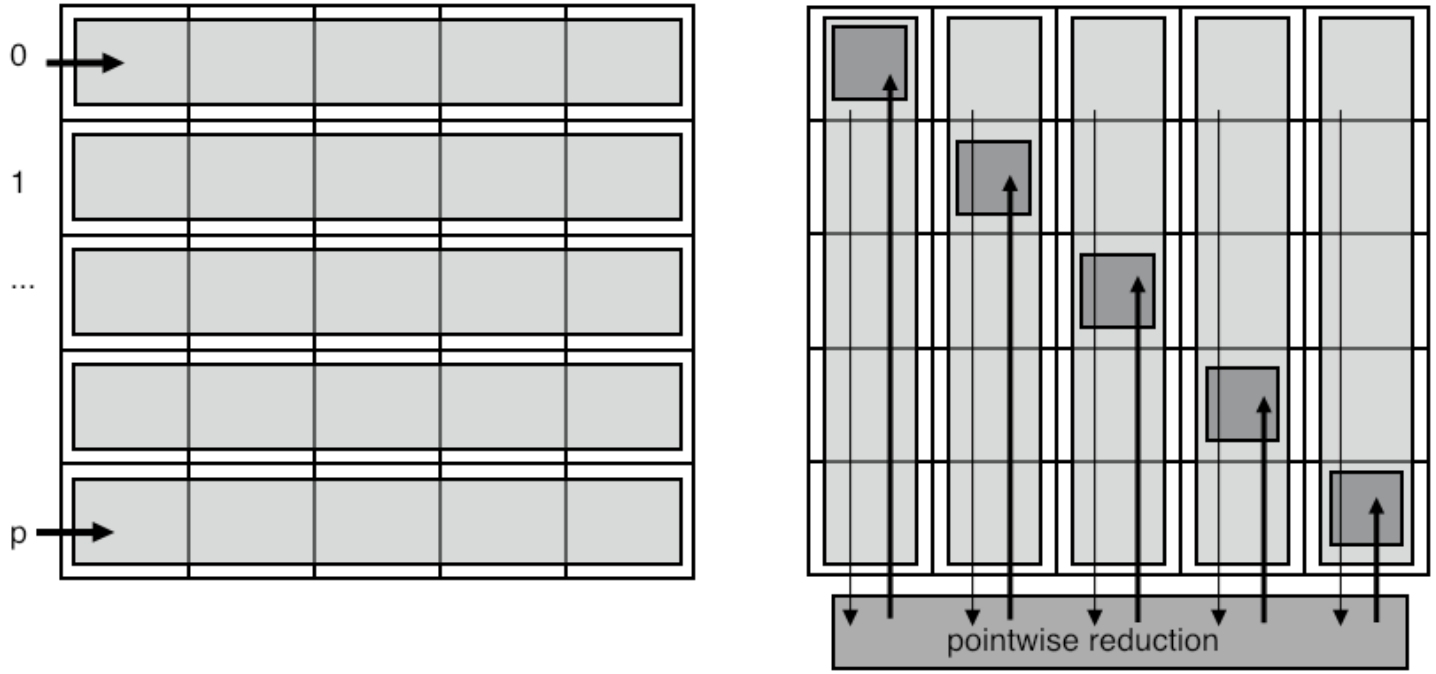
- Suppose there are four processes including the root, each with arrays u and v. After the all-to-all operation

MPI_Alltoall(u, 2, MPI_INT, v, 2, MPI_INT, MPI_COMM_WORLD);

array u								Rank	array v							
10	11	12	13	14	15	16	17	0	10	11	20	21	30	31	40	41
20	21	22	23	24	25	26	27	1	12	13	22	23	32	33	42	43
30	31	32	33	34	35	36	37	2	14	15	24	25	34	35	44	45
40	41	42	43	44	45	46	47	3	16	17	26	27	36	37	46	47

MPI_Reduce_scatter

- int MPI_Reduce_scatter(void *sendbuf, void *recvbuf,
  const int recvcounts[], MPI_Datatype datatype,
  MPI_Op op, MPI_Comm comm)
  - *sendbuf*: Starting address of send buffer.
  - *recvbuf*: Starting address of receive buffer (choice)
  - *recvcounts*: Integer array specifying the number of elements in result distributed to each process. Array must be identical on all calling processes.



MPI_Barrier

- Barrier is a commonly used synchronization method for a group of processes or threads.
  - Each member needs to wait at the barrier, until all members in the group have arrived at the barrier.

- MPI_Barrier implements the barrier synchronization operation.
  - The call to MPI_Barrier returns only after all the processes in the group have called this function.

- int MPI_Barrier(MPI_Comm comm)

Matrix-Vector Multiplication: Scatter and Gather

```c
int main(int argc, char** argv)
{
    int m = 0, n = 0, myid, numprocs, i;
    int srow = 0;
    double *A, *x, *y, *local_A, *local_y;
    double start, end;

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

    if(myid == 0) {
        while ( m <= 0 || n <= 0 || m%numprocs != 0) {
            printf("Please input positive integers m and n: ");
            scanf("%d %d", &m, &n);
        }
        A = (double*) malloc( m * n * sizeof(double) );
        x = (double*) malloc(n * sizeof(double) );
        y = (double*) malloc(m * sizeof(double) );
        init_array(A, m * n);
        init_array(x, n);
    }
```

Prepare the data at Process 0

Matrix-Vector Multiplication: Scatter and Gather

```
27      MPI_Bcast(&m, 1, MPI_INT, 0, MPI_COMM_WORLD);
28      MPI_Bcast(&n, 1, MPI_INT, 0, MPI_COMM_WORLD);
29
30      srow = m / numprocs;
31
32      local_A = (double*) malloc( srow * n * sizeof(double) );
33      local_y = (double*) malloc( srow * sizeof(double) );
34      if(myid != 0)     x = (double*) malloc(n * sizeof(double) );
35
36      MPI_Bcast(x, n, MPI_DOUBLE, 0, MPI_COMM_WORLD);
37
38      MPI_Scatter(A, srow * n, MPI_DOUBLE, local_A, srow * n, MPI_DOUBLE, 0, MPI_COMM_WORLD);
39
40      Mat_vect_mul(local_A, x, local_y, srow, n);
41
42      MPI_Gather(local_y, srow, MPI_DOUBLE, y, srow, MPI_DOUBLE, 0, MPI_COMM_WORLD);
43      if (myid == 0) { free(A); free(y); }
44      free(local_A); free(x); free(local_y);
45      MPI_Finalize();
46      return 0;
47  }
```

Broadcast m and n

Memory allocation

Scatter matrix A

Gather vector y

A Case Study

- Solving A System of Linear Equations by Gaussian Elimination

$$\mathbf{A\,x = b}$$

- It was used to evaluate the TOP500 supercomputers.
  - http://www.top500.org/project/linpack/

Linear Equations

- Consider the problem of solving the following linear equations:

$$
\begin{array}{ccccccccc}
a_{0,0}x_0 & + & a_{0,1}x_1 & + & \cdots & + & a_{0,n-1}x_{n-1} & = & b_0, \\
a_{1,0}x_0 & + & a_{1,1}x_1 & + & \cdots & + & a_{1,n-1}x_{n-1} & = & b_1, \\
\vdots & & \vdots & & & & \vdots & & \vdots \\
a_{n-1,0}x_0 & + & a_{n-1,1}x_1 & + & \cdots & + & a_{n-1,n-1}x_{n-1} & = & b_{n-1}.
\end{array}
$$

- This is written as $\boldsymbol{Ax} = \boldsymbol{b}$, where $\boldsymbol{A}$ is an $n \times n$ matrix with $\boldsymbol{A}[i, j] = a_{i,j}$, $\boldsymbol{b}$ is an $n \times 1$ vector $[\, b_0, b_1, \ldots, b_{n-1} \,]^T$, and $\boldsymbol{x}$ is the solution.

Solution: Gaussian Elimination

- Two steps: (1) reduction **A** to upper triangular form, and (2) back-substitution.

- The upper triangular form is as:

$$
\begin{array}{rcrcrcrcrcl}
x_0 & + & u_{0,1}x_1 & + & u_{0,2}x_2 & + & \cdots & + & u_{0,n-1}x_{n-1} & = & y_0, \\
 & & x_1 & + & u_{1,2}x_2 & + & \cdots & + & u_{1,n-1}x_{n-1} & = & y_1, \\
 & & & & & & & & \vdots & & \vdots \\
 & & & & & & & & x_{n-1} & = & y_{n-1}.
\end{array}
$$

- We write this as: $\boldsymbol{Ux} = \boldsymbol{y}$. Notice that we choose a **unit upper-triangular matrix** for $\boldsymbol{U}$, whose diagonal entries are all equal to one.

- A commonly used method for transforming a given matrix into an upper-triangular matrix is Gaussian Elimination.

Gaussian Elimination Example

$$
\begin{array}{rrrrcr}
4x_0 & +6x_1 & +2x_2 & -2x_3 & = & 8 \\
2x_0 & & +5x_2 & -2x_3 & = & 4 \\
-4x_0 & -3x_1 & -5x_2 & +4x_3 & = & 1 \\
8x_0 & +18x_1 & -2x_2 & +3x_3 & = & 40
\end{array}
$$

Gaussian Elimination Example

$$\boxed{x_0 \quad +1.5x_1 \quad +0.5x_2 \quad -0.5x_3 \quad = \quad 2}$$

$$2x_0 \quad +5x_2 \quad -2x_3 \quad = \quad 4$$

$$-4x_0 \quad -3x_1 \quad -5x_2 \quad +4x_3 \quad = \quad 1$$

$$8x_0 \quad +18x_1 \quad -2x_2 \quad +3x_3 \quad = \quad 40$$

Gaussian Elimination Example

$$
\begin{array}{lllll}
x_0 & +1.5x_1 & +0.5x_2 & -0.5x_3 & = & 2 \\
 & -3x_1 & +4x_2 & -1x_3 & = & 0 \\
 & +3x_1 & -3x_2 & +2x_3 & = & 9 \\
 & +6x_1 & -6x_2 & +7x_3 & = & 24
\end{array}
$$

Gaussian Elimination Example

$$
\begin{array}{lllll}
x_0 & +1.5x_1 & +0.5x_2 & -0.5x_3 & = & 2 \\
 & \boxed{x_1 \quad -4/3x_2 \quad +1/3x_3 \quad = \quad 0} \\
 & +3x_1 & -3x_2 & +2x_3 & = & 9 \\
 & +6x_1 & -6x_2 & +7x_3 & = & 24
\end{array}
$$

Gaussian Elimination Example

$$
\begin{array}{ccccccc}
x_0 & +1.5x_1 & +0.5x_2 & -0.5x_3 & = & 2 \\
 & x_1 & -4/3x_2 & +1/3x_3 & = & 0 \\
 & & 1x_2 & +1x_3 & = & 9 \\
 & & 2x_2 & +5x_3 & = & 24
\end{array}
$$

Gaussian Elimination Example

$$
\begin{array}{lllll}
x_0 & +1.5x_1 & +0.5x_2 & -0.5x_3 & = & 2 \\
 & x_1 & -4/3x_2 & +1/3x_3 & = & 0 \\
 & & \boxed{x_2 \quad +x_3 \quad = \quad 9} & & & \\
 & & & 3x_3 & = & 6
\end{array}
$$

Gaussian Elimination Example

$$
\begin{array}{ccccccc}
x_0 & +1.5x_1 & +0.5x_2 & -0.5x_3 & = & 2 \\
 & x_1 & -4/3x_2 & +1/3x_3 & = & 0 \\
 & & x_2 & +x_3 & = & 9 \\
 & & & x_3 & = & 2
\end{array}
$$

Back Substitution

$$x_3 = 2$$

$$x_2 = 9 - x_3 = 7$$

$$x_1 = 4/3x_2 - 1/3x_3 = 26/3$$

$$x_0 = 2 - 1.5x_1 - 0.5x_2 + 0.5x_3 = -27/2$$

Serial Gaussian Elimination

- A serial Gaussian Elimination algorithm that converts **Ax=b** to **Ux=y**

Input: ***A***, ***b***

Output: ***U***, ***y***

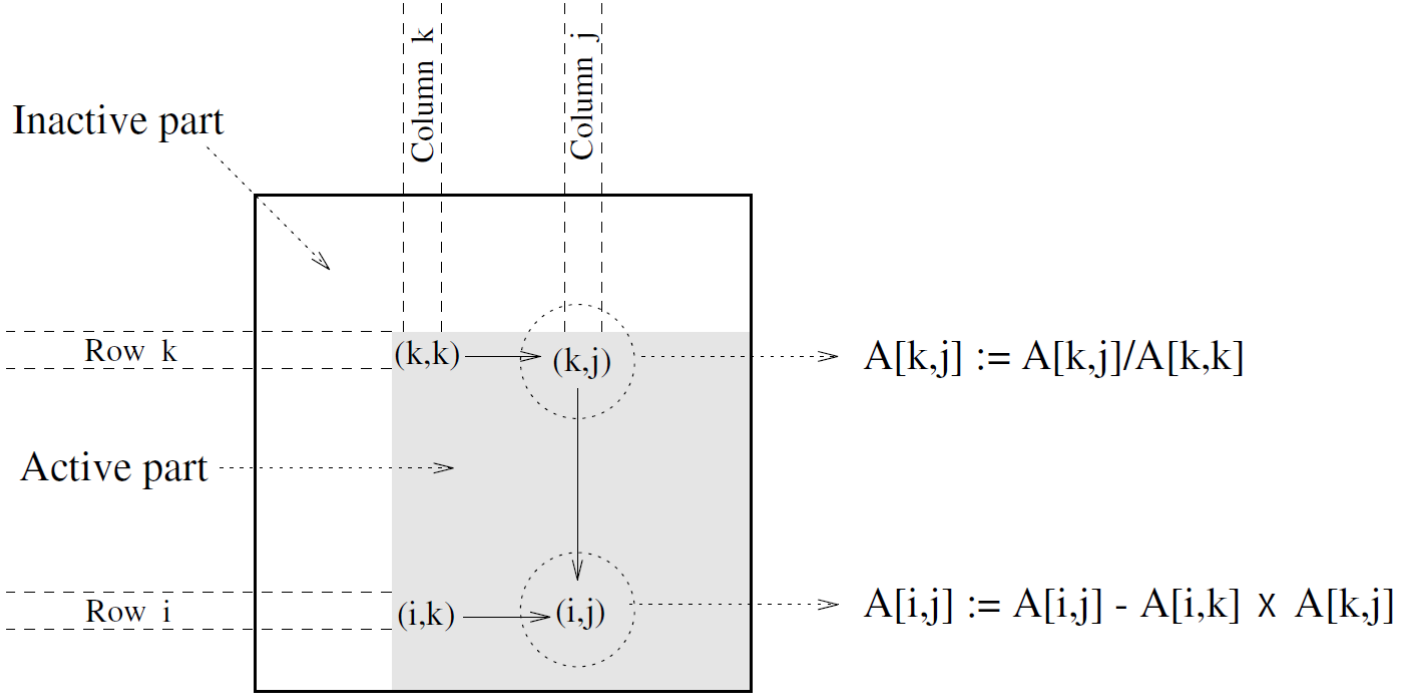
U is stored in the upper-triangular locations of ***A***.

```
1.  procedure GAUSSIAN_ELIMINATION (A, b, y)
2.  begin
3.      for k := 0 to n − 1 do                /* Outer loop */
4.      begin
5.          for j := k + 1 to n − 1 do
6.              A[k, j] := A[k, j]/A[k, k];   /* Division step */
7.          y[k] := b[k]/A[k, k];
8.          A[k, k] := 1;
9.          for i := k + 1 to n − 1 do
10.         begin
11.             for j := k + 1 to n − 1 do
12.                 A[i, j] := A[i, j] − A[i, k] × A[k, j]; /* Elimination step */
13.             b[i] := b[i] − A[i, k] × y[k];
14.             A[i, k] := 0;
15.         endfor;            /* Line 9 */
16.     endfor;                /* Line 3 */
17. end GAUSSIAN_ELIMINATION
```

Source: Algorithm 8.4 of Ref. [1]

A Typical Computation in Gaussian Elimination

- The computation has three nested loops.
  - In the *k*th iteration of the outer loop, the algorithm performs $(n-k)^2$ computations.
  - Summing from $k = 1 \ldots n$, we have roughly $n^3/3$ multiplications-subtractions, or $2n^3/3$ operations.



Source: Figure 8.5 of Ref. [1]

Back-Substitution

- Sequential back-substitution algorithm for solving an upper-triangular system of equations Ux=y
  - ***U*** is a unit upper-triangular matrix (i.e., ***U***[*k*,*k*] = 1)
  - It takes $n^2/2$ multiplications and subtractions

```
procedure BACK_SUBSTITUTION (U, x, y)
begin
    for k := n − 1 downto 0 do   /* Main loop */
        begin
            x[k] := y[k];
            for i := k − 1 downto 0 do
                y[i] := y[i] − x[k] × U[i, k];
        endfor;
end BACK_SUBSTITUTION
```

Source: Algorithm 8.5 of Ref. [1]

A Small Test

- Tianhe-2 is one of the fastest supercomputers in the world (rank 6th as of 2020)
  - http://www.top500.org/system/177999

- Its Linkpack performance (i.e., R_{max}) is 33,862.7 TFlop/s, measured by solving a linear system with 9,960,000 (i.e., N_{max}) linear equations.

- Can you estimate how long does Tianhe-2 take to solve the linear system with N_{max} equations?

Partial Pivoting

- In the previous algorithm, we implicitly assume that A[k,k] is not zero or close to zero.
  - Why?

- Partial pivoting (by column exchange)
  - At the beginning of the outer loop in the *k*th iteration, select a column *i* such that $\boldsymbol{A}[k, i]$ is the largest in magnitude among all $\boldsymbol{A}[k, j]$, $k \leq j < n$. We call column *i* the **pivot column**.
  - Exchange the *k*th and the *i*th columns before starting the iteration.

- Partial pivoting (by row exchange)

Parallel Gaussian Elimination: 1-D Partitioning

- We can apply rowwise 1-D partitioning on the coefficient matrix A.

- Assume each row is assigned to a process
  - An n x n matrix requires n processes.
  - Process i (P_i) initially stores data $\boldsymbol{A}[i, j]$, $0 \leq j < n$

- How to parallelize Algorithm 8.4 shown in Page 68?

Parallel Gaussian Elimination: 1-D Partitioning

- In the outer loop (line 3), each iteration has a dependency on the previous iterations (in the general sense)
  - We cannot easily parallelize at this level

- In the inner level (lines 9-15), the elimination step for each row is independent from each other
  - These computations can be done in parallel by different processes

An Example: n = 8, k = 3

P_0	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
P_1	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
P_2	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
P_3	0	0	0	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)
P_4	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
P_5	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P_6	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
P_7	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

Source: Figure 8.6 (a) of Ref. [1]

Lines 5-8:

```
for j := k+1 to n-1 do
    A[k,j] := A[k,j] / A[k,k];
y[k] := b[k] / A[k,k];
A[k,k] := 1;
```

The above codes are executed by Process P_3 only.

No communication is required.

An Example: n = 8, k = 3

P_0	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
P_1	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
P_2	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
P_3	0	0	0	1	(3,4)	(3,5)	(3,6)	(3,7)
P_4	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
P_5	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P_6	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
P_7	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

Source: Figure 8.6 (b) of Ref. [1]

After the calculations of lines 5-8, data ***A***[*k*, *j*], *k*<*j*<*n*, need to be broadcast to processes P_4 – P_7.

We call these data "**active data**".

An Example: n = 8, k = 3

P_0	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
P_1	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
P_2	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
P_3	0	0	0	1	(3,4)	(3,5)	(3,6)	(3,7)
P_4	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
P_5	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P_6	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
P_7	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

Source: Figure 8.6 (c) of Ref. [1]

Lines 9-15:

```
for i := k+1 to n-1 do
begin
   for j := k+1 to n-1 do
      A[i,j] -= A[i,k] * A[k,j];
   b[i] -= A[i,k] * y[k];
   A[i,k] := 0;
end
```

The above codes are executed by Processes P_4-P_7 in parallel.

No communication is required.

Analysis for the Case of n Processors

- The first step of the algorithm normalizes the row. This is a serial operation and takes time (*n*-*k*-1) in the *k*-th iteration.

- In the second step, the active data in the normalized row are broadcast to (n-k-1) processors. This takes time

$$(t_s + t_w(n-k-1))\log n$$

- Each processor can independently eliminate this row from its own. This requires (*n*-*k*-1) multiplications and subtractions.

- To summarize, the *k*-th iteration takes 3(*n*-*k*-1) calculations and

$$(t_s + t_w(n-k-1))\log n$$

communications.

Analysis for the Case of n Processors

- The total parallel run time can be computed by summing from $k = 0 \ldots n\text{-}1$ as

$$T_P = \frac{3}{2}n(n-1) + t_s n \log n + \frac{1}{2}t_w n(n-1)\log n.$$

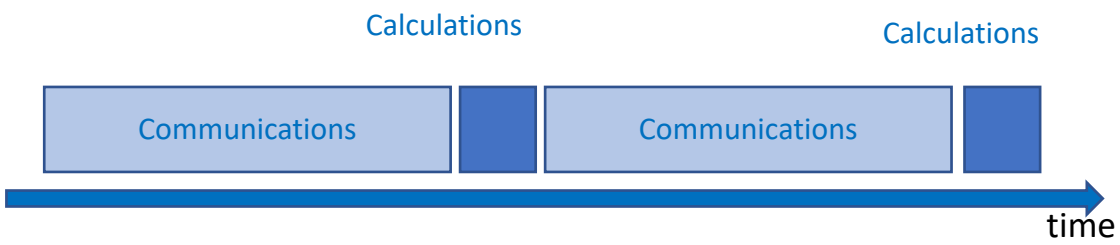
- The cost of the parallel solution is nT_p, which is

$$\Theta(n^3 \log n)$$

- So this solution is not cost-optimal!

Two Inefficiencies

- Communications overhead
  - For each iteration k, each process performs $\Theta(n\text{-}k)$ calculations in parallel. But the communication time for each iteration is $\Theta(n\text{-}k)\log_2 n$!



- Load imbalance
  - Process P_i will become totally idle after the $(i+1)$-th iteration
  - Process P_o has the lightest workload of $\Theta(n)$, while $P_{n\text{-}1}$ has the heaviest workload of $\Theta(n^2)$.

How to Improve?

- In the previous method, the (k+1)-th iteration starts only after all the computation and communication for the k-th iteration is complete.
  - Is it a must?
- Inside each iteration of k, the calculations happen after the data communications.
  - Is it a must?
- To answer the above questions, we need to have an in-depth analysis of serial Algorithm 8.4.

In-depth Analysis of Algorithm 8.4

- In iteration k, Process P_k broadcasts its active data to Processes $P_{k+1}, \ldots, P_{n-1}$.
  - This can be done by a sequential forwarding: $P_k \rightarrow P_{k+1}, P_{k+1} \rightarrow P_{k+2}, \ldots, P_{n-2} \rightarrow P_{n-1}$.

- For process P_{k+1}, after forwarding the active data to P_{k+2}, it need not wait for all processes to receive the active data. Instead, it can start to perform the elimination step (Line 12)!
  - We can overlap communications with computations!

- After P_{k+1} performs its elimination step in the k-th iteration, it can start to perform the division step (Line 6) for the (k+1)-th iteration. Then it can start to send its active data to process P_{k+2}.
  - We can overlap iteration K+1 with iteration k! It can further overlap communications with computations, and also simultaneous communications!

- Next, we will show a "pipelined" parallel solution by a 5x5 example.

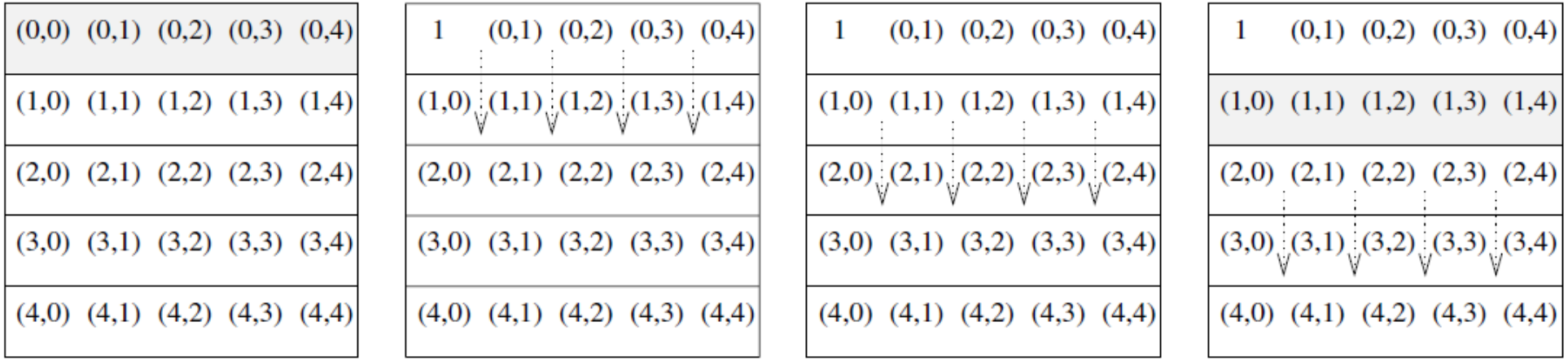
An Example of 5x5 Matrix

(a) P_0 performs the division on row 0.

(b) P_0 forwards its active data to P_1 .

(c) P_1 forwards its active data to P_2 .

(d) P_1 performs elimination. Meanwhile, P_2 forwards its active data to P_3.



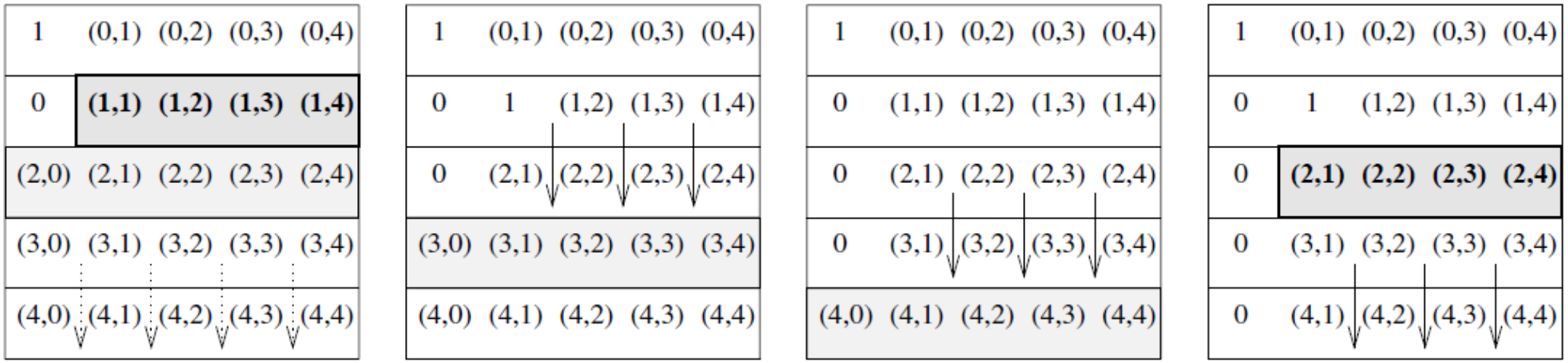
(a) Iteration k = 0 starts (b) (c) (d)

Source: Figure 8.7 (a-d) of Ref. [1]

An Example of 5x5 Matrix

(e) P_2 performs the elimination. Meanwhile, P_3 forwards its active data to P_4. Furthermore, P_1 performs the division on row 1 – iteration k=1 starts while iteration k=0 has not finished yet!

(f-p) Go through them by yourselves.



(e) Iteration k = 1 starts (f) (g) Iteration k = 0 ends (h)

Source: Figure 8.7 (e-h) of Ref. [1]

An Example of 5x5 Matrix

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	**(2,2)**	**(2,3)**	**(2,4)**
0	**(3,1)**	**(3,2)**	**(3,3)**	**(3,4)**
0	(4,1)	(4,2)	(4,3)	(4,4)

(i) Iteration k = 2 starts

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	(3,2)	(3,3)	(3,4)
0	**(4,1)**	**(4,2)**	**(4,3)**	**(4,4)**

(j) Iteration k = 1 ends

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	(3,2)	(3,3)	(3,4)
0	0	(4,2)	(4,3)	(4,4)

(k)

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	**(3,2)**	**(3,3)**	**(3,4)**
0	0	(4,2)	(4,3)	(4,4)

(l)

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	0	(3,3)	(3,4)
0	0	**(4,2)**	**(4,3)**	**(4,4)**

(m) Iteration k = 3 starts

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	0	1	(3,4)
0	0	0	(4,3)	(4,4)

(n)

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	0	1	(3,4)
0	0	0	(4,3)	(4,4)

(o) Iteration k = 3 ends

1	(0,1)	(0,2)	(0,3)	(0,4)
0	1	(1,2)	(1,3)	(1,4)
0	0	1	(2,3)	(2,4)
0	0	0	1	(3,4)
0	0	0	0	**(4,4)**

(p) Iteration k = 4

Source: Figure 8.7 (i-p) of Ref. [1]

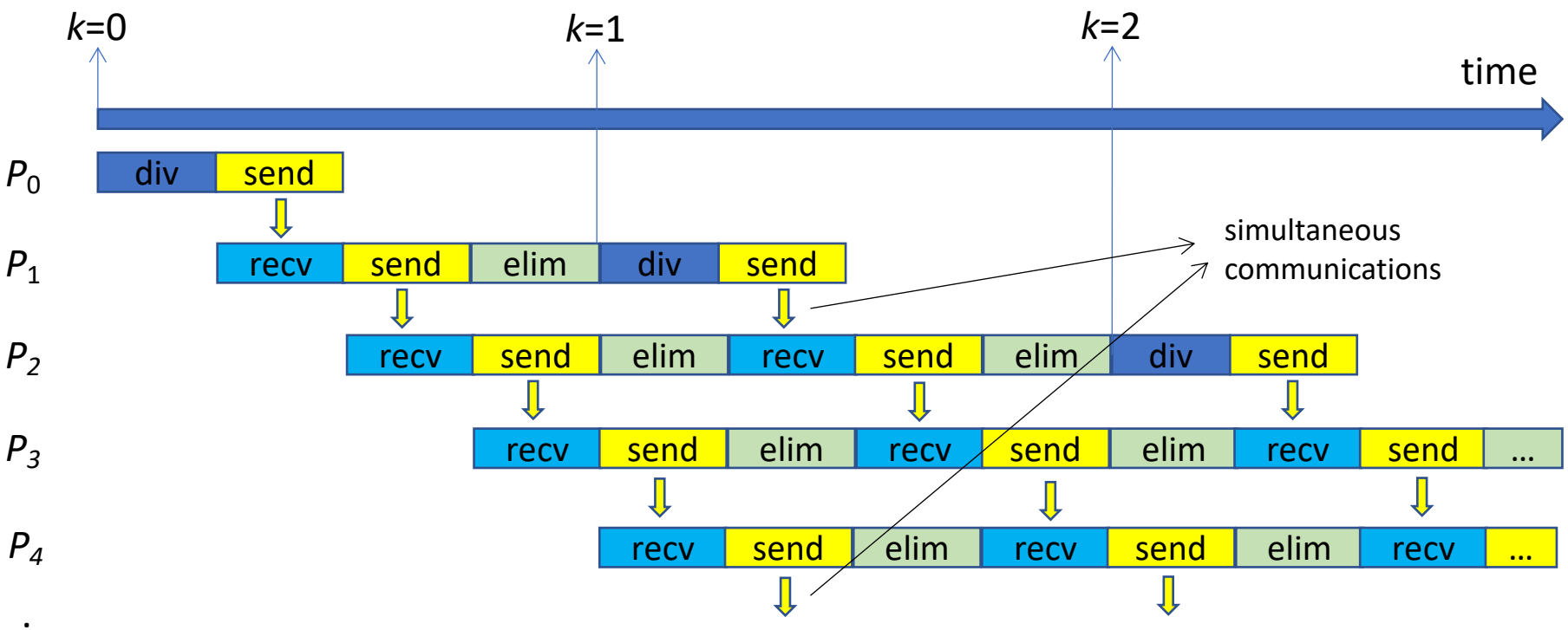
Pipelined Parallel Solution

- In the pipelined version, each process P_i performs the followings:

```
step = 0;
while (step < i) {
   Receive the "active data" from P_{i-1};
   Send the "active data" to P_{i+1} ;
   Perform the elimination ;
   step++;
}
perform the division;
send the active data to P_{i+1};
```

Analysis of Pipelined Solution

Remark: We simply assume div, recv, send, elim take the same time.



div: division step
send: send data to next process
recv: receive data from the previous process
elim: elimination step

Analysis of Pipelined Solution

- From the previous pipeline diagram, it is obvious that the time interval between two iterations is $\Theta(n)$.
- There is a total of n iterations. So the last iteration starts from $\Theta(n^2)$.
- The last iteration takes $\Theta(1)$ only.
- So the parallel run time is $\Theta(n^2)$, which is cost optimal.

Back to Reality: p < n

- Previously, we assume the number of processes (or processors) $p = n$
- In most scenarios, the number of processors p is much smaller than n
- Block 1-D rowwise partition: each process is assigned n/p contiguous rows of the matrix

Example of Block 1-D Partitioning

P_0	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
P_1	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
	0	0	0	1	(3,4)	(3,5)	(3,6)	(3,7)
P_2	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P_3	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

Source: Figure 8.8 of Ref. [1]

In the k=3 iteration, the active data on P_1 need to be sent to P_2 and P_3.

As compared with the case of $p = n$, the communication cost is reduced by a factor of n/p.

When $n >> p$, computations dominate communications.

Load Balancing Issue

P_0	1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)
	0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)
P_1	0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)
	0	0	0	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)
P_2	0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)
	0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)
P_3	0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)
	0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)

(a) Block 1-D mapping

Source: Figure 8.9 (a) of Ref. [1]

The cost of the block 1-D partitioning is n^3, while the cost of the serial algorithm is $2n^3/3$.

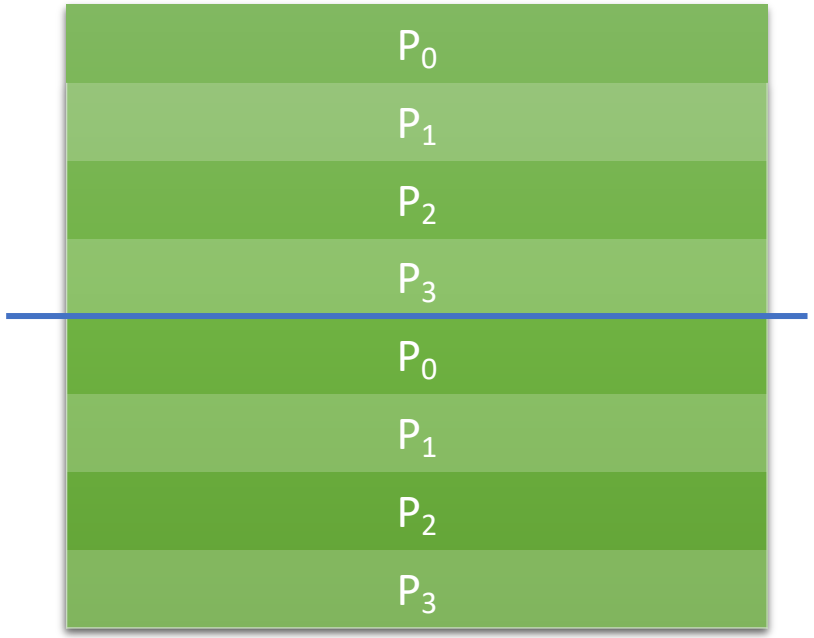
This is caused by the uneven load distribution among p processes.

In the left example, P_0 is completely idle, P_1 is partially loaded, P_2 and P_3 are fully loaded.

Cyclic 1-D Mapping

- **Cyclic mapping** can be used to improve load balancing.

- In each iteration, the computations are distributed to all processes.



1	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)	P_0
0	0	0	(4,3)	(4,4)	(4,5)	(4,6)	(4,7)	
0	1	(1,2)	(1,3)	(1,4)	(1,5)	(1,6)	(1,7)	P_1
0	0	0	(5,3)	(5,4)	(5,5)	(5,6)	(5,7)	
0	0	1	(2,3)	(2,4)	(2,5)	(2,6)	(2,7)	P_2
0	0	0	(6,3)	(6,4)	(6,5)	(6,6)	(6,7)	
0	0	0	(3,3)	(3,4)	(3,5)	(3,6)	(3,7)	P_3
0	0	0	(7,3)	(7,4)	(7,5)	(7,6)	(7,7)	

(b) Cyclic 1-D mapping

Source: Figure 8.9 (a) of Ref. [1]

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