Programming Using the Message Passing Paradigm

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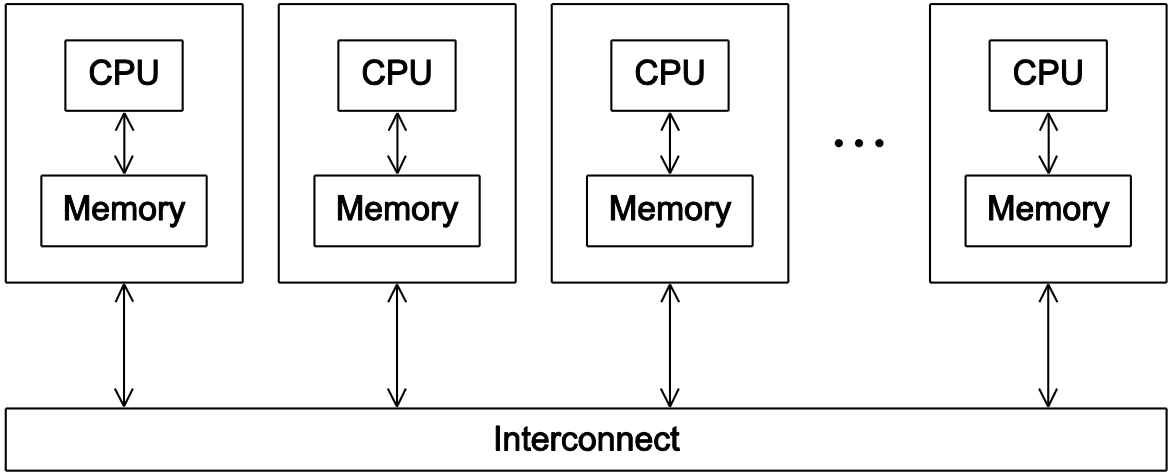
Topics

- **Principles of Message-Passing Programming**
- **Building Blocks**
  - Send and Receive Operations
- **MPI: the Message Passing Interface**
- **Topologies and embedding**
- **Overlapping communication with Computation**
- **Collective communication and computation Operations**
- **Groups and communicators**
- **MPI-derived data types**

A distributed address space system



Principles of Message-Passing

- **The logical view of a message-passing paradigm**
  - p processes
  - Each with its own exclusive address space
- **Data must be explicitly partitioned and placed.**
- **All interactions (read-only or read/write) are two-sided**
  - Process that has the data
  - Process that wants to access the data.
  - Underlying costs are explicit
  - Two-sided interaction can sometimes be awkward
- **Using the *single program multiple data* (SPMD) model**

Send and Receive Operations

- **Prototypes**

```
send(void *sendbuf, int nelems, int dest)
receive(void *recvbuf, int nelems, int source)
```

- **Consider the following code segments:**

```
P0                          P1
a = 100;                    receive(&a, 1, 0)
send(&a, 1, 1);             printf("%d\n", a);
a = 0;
```

- **The semantics of the send**
  - Value received by process P1 must be 100, not 0
  - Motivates the design of the send and receive protocols
    - Non-buffered blocking message passing
    - Buffered blocking message passing
    - Non-blocking message passing

Non-Buffered Blocking Message Passing

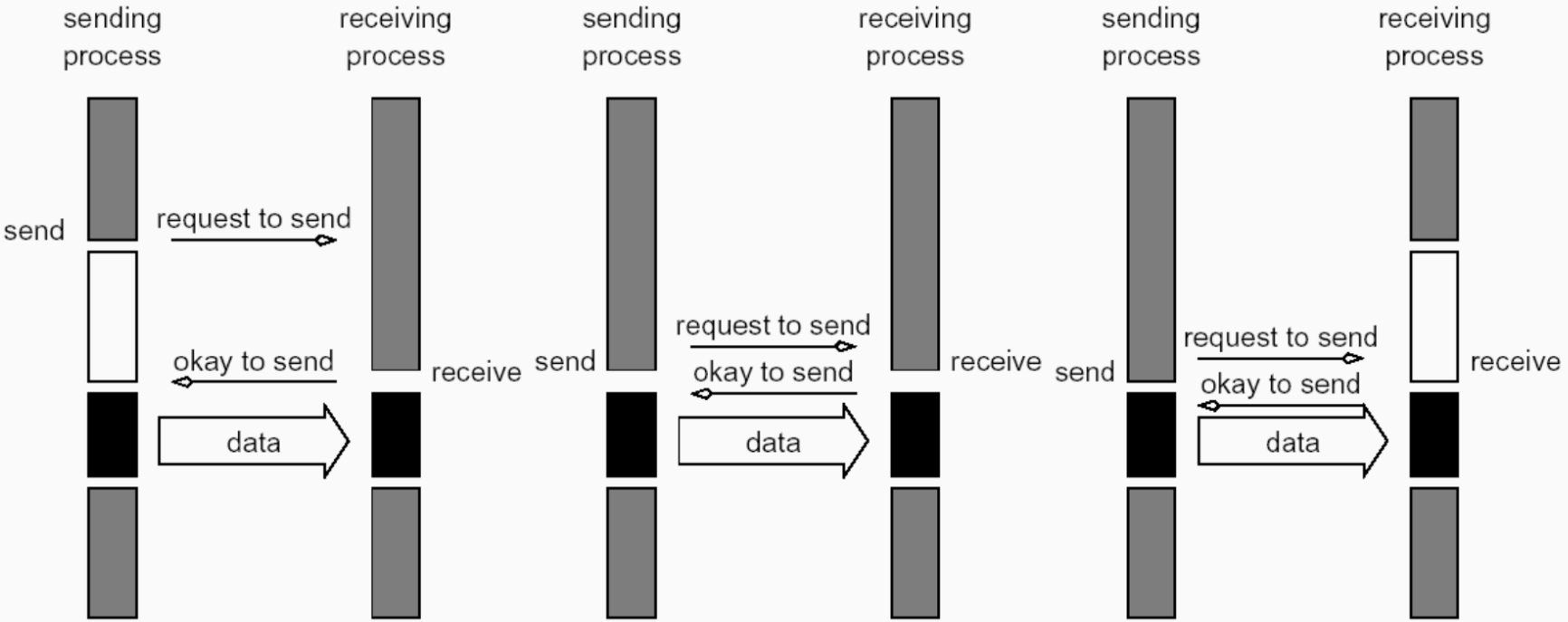
- **A simple method**
  - Send operation to return only when it is safe to do so
  - Send does not return until the matching receive has been encountered
- **Issues**
  - Idling and deadlocks
    - Deadlock example

```
P0:
send(&a, 1, 1);
receive(&b, 1, 1);
```

```
P1:
send(&a, 1, 0);
receive(&b, 1, 0);
```

Non-Buffered Blocking Message Passing

Handshake for a blocking non-buffered send/receive operation



Idling occurs when sender and receiver do not reach communication point at similar times

Buffered Blocking Message Passing

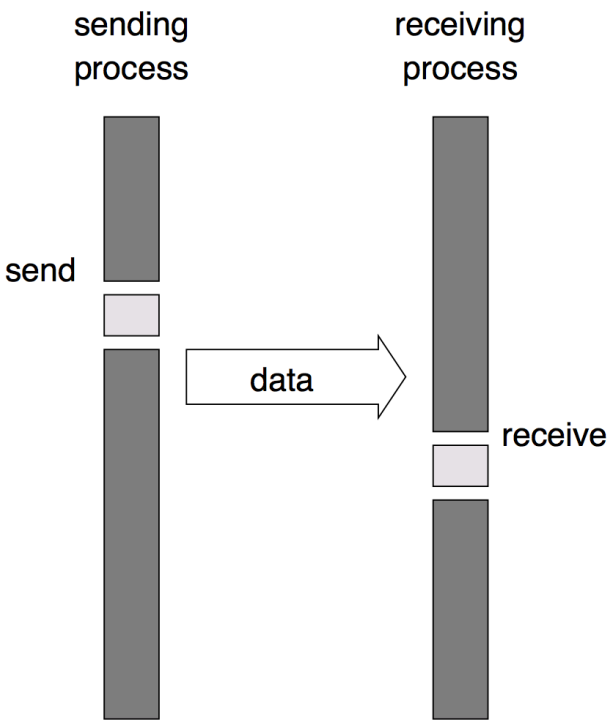
- **Process**
  - Sender copies data into buffer
  - Sender returns after the copy completes
  - Data may be buffered at the receiver
- **A simple solution to idling and deadlock**
- **Trade-off**
  - Buffering trades idling overhead for buffer copying overhead

```
P0:
send(&a, 1, 1);
receive(&b, 1, 1);
```

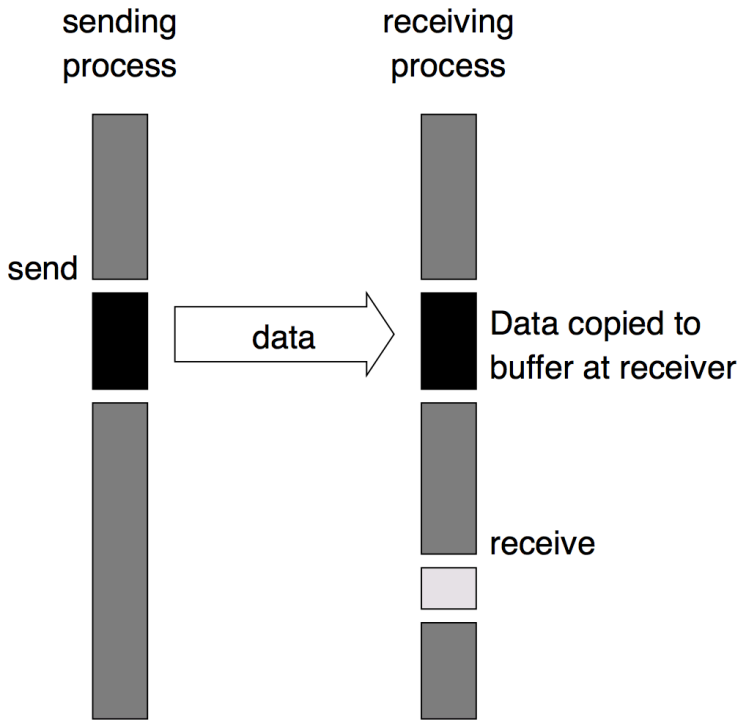
```
P1:
send(&a, 1, 0);
receive(&b, 1, 0);
```

Buffered Blocking Message Passing

Blocking buffered transfer protocols



(a) With communication hardware



(b) w/o communication hardware: sender interrupts receiver and deposits data in buffer at receiver end.

Buffered Blocking Message Passing

Bounded buffer sizes can have significant impact on performance

```
P0:
for (i = 0; i < 1000; i++){
    produce_data(&a);
    send(&a, 1, 1);
  }
```

```
P1:
for (i = 0; i < 1000; i++){
   receive(&a, 1, 0);
   consume_data(&a);
}
```

Buffer overflow leads to blocking sender. Programmers need to be aware of bounded buffer requirements

Buffered Blocking Message Passing

Deadlocks are still possible with buffering since receive operations block.

```
P0:
receive(&a, 1, 1);
send(&b, 1, 1);
```

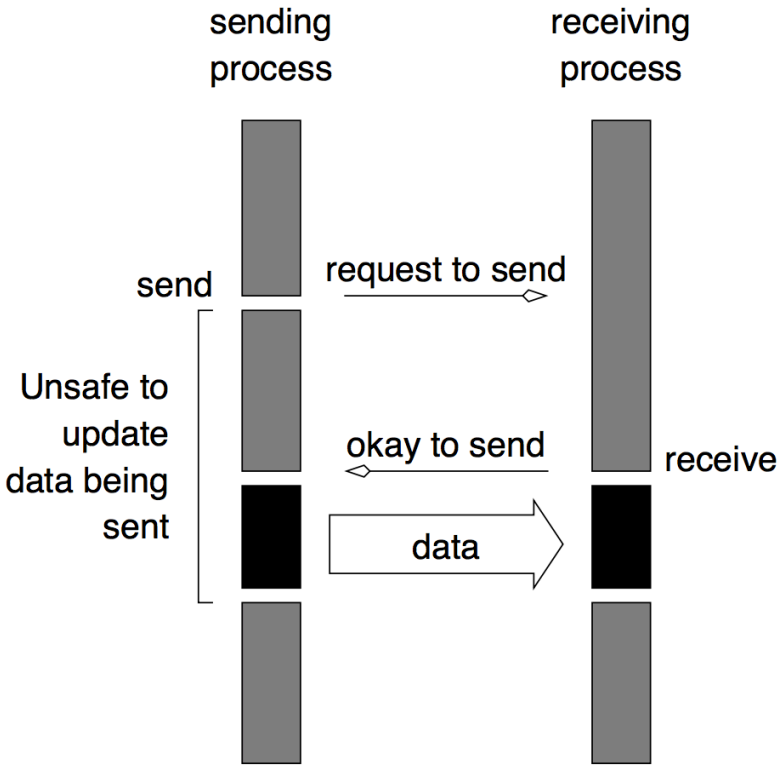
```
P1:
receive(&a, 1, 0);
send(&b, 1, 0);
```

Non-Blocking Message Passing

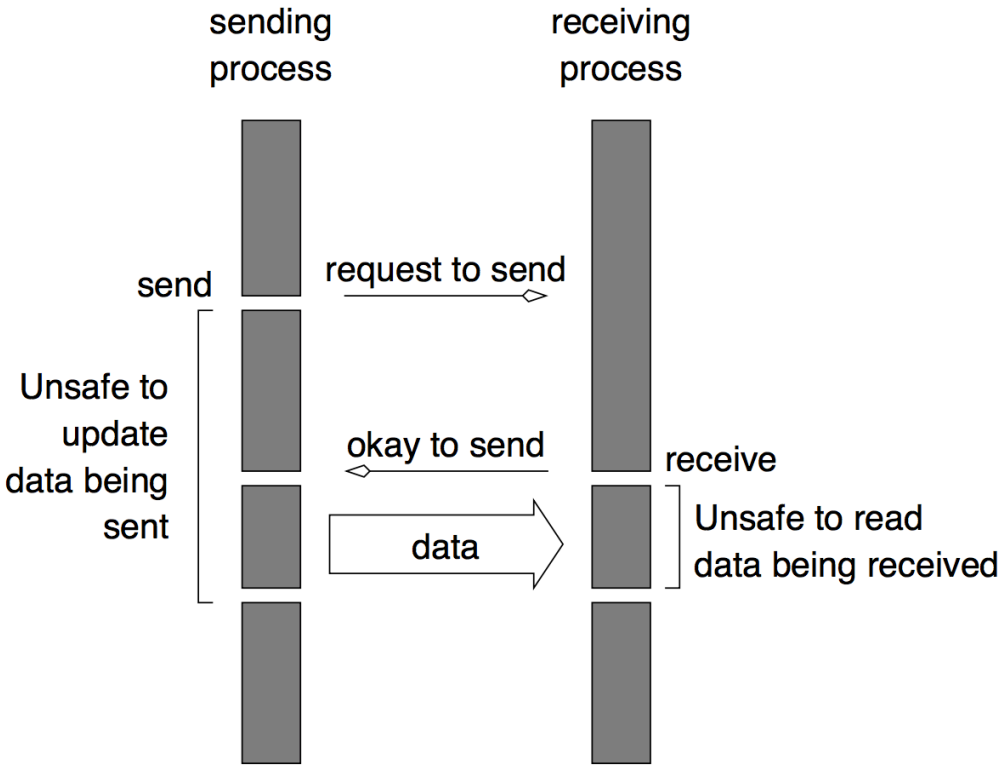
- **Send and receive returns before it is semantically safe**
  - Sender: data can be overwritten before it is sent
  - Receiver: data can be read before it is received
- **Programmer must ensure semantics of the send and receive.**
  - A check-status operation is accompanied
- **Benefit**
  - Capable of overlapping communication overheads with useful computations

- **Message passing libraries typically provide both blocking and non-blocking primitives**

Non-Blocking Message Passing



(a) Without hardware support



(b) With hardware support

MPI: Message Passing Interface

- **Standard library for message-passing**
  - Portable
  - Ubiquitously available
  - High performance
  - C and Fortran APIs
- **MPI standard defines**
  - syntax as well as the semantics of library routines
- **Details**
  - MPI routines, data-types, and constants
  - Prefixed by "MPI_"
- **6 Golden MPI functions**
  - 125 functions but 6 most used functions

MPI: Message Passing Interface

The minimal set of MPI routines.

`MPI_Init`	Initializes MPI.
`MPI_Finalize`	Terminates MPI.
`MPI_Comm_size`	Determines the number of processes.
`MPI_Comm_rank`	Determines the label of calling process.
`MPI_Send`	Sends a message.
`MPI_Recv`	Receives a message.

Starting and Terminating MPI Programs

- **`int MPI_Init(int *argc, char ***argv)`**
  - Initialize the MPI environment
    - strips off any MPI related command-line arguments.
  - Must be called prior to other MPI routines
- **`int MPI_Finalize()`**
  - Must be called at the end of the computation
  - Performs various clean-up tasks to terminate the MPI environment.

- **Return code**
  - MPI_SUCCESS
  - MPI_ERROR

Communicators

- **A communicator defines a *communication domain***
  - A set of processes allowed to communicate with each other
- **Type `MPI_Comm`**
  - Specifies the communication domain
  - Used as arguments to all message transfer MPI routines
- **A process can belong to many different (possibly overlapping) communication domains**
- **`MPI_COMM_WORLD`**
  - Default communicator
  - Includes all the processes

Querying Information in Communicator

- `int MPI_Comm_size(MPI_Comm comm, int *size)`
  - Determine the number of processes
- `int MPI_Comm_rank(MPI_Comm comm, int *rank)`
  - Index of the calling process
  - 0 <= rank < communicator size

Sending and Receiving Messages

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

Hello World using MPI

```
1  #include <stdio.h>
2  #include <string.h>  /* For strlen             */
3  #include <mpi.h>     /* For MPI functions, etc */
4
5  const int MAX_STRING = 100;
6
7  int main(void) {
8     char       greeting[MAX_STRING];
9     int        comm_sz;  /* Number of processes */
10    int        my_rank;  /* My process rank     */
11
12    MPI_Init(NULL, NULL);
13    MPI_Comm_size(MPI_COMM_WORLD, &comm_sz);
14    MPI_Comm_rank(MPI_COMM_WORLD, &my_rank);
15
16    if (my_rank != 0) {
17       sprintf(greeting, "Greetings from process %d of %d!",
18             my_rank, comm_sz);
19       MPI_Send(greeting, strlen(greeting)+1, MPI_CHAR, 0, 0,
20             MPI_COMM_WORLD);
21    } else {
22       printf("Greetings from process %d of %d!\n", my_rank, comm_sz);
23       for (int q = 1; q < comm_sz; q++) {
24          MPI_Recv(greeting, MAX_STRING, MPI_CHAR, q,
25             0, MPI_COMM_WORLD, MPI_STATUS_IGNORE);
26          printf("%s\n", greeting);
27       }
28    }
29
30    MPI_Finalize();
31    return 0;
32 }  /* main */
```

Compilation & Execution

- **Compile**

wrapper script to compile *source file*

```
$ mpicc -g -Wall -o mpi_hello mpi_hello.c
```

- **Execution**

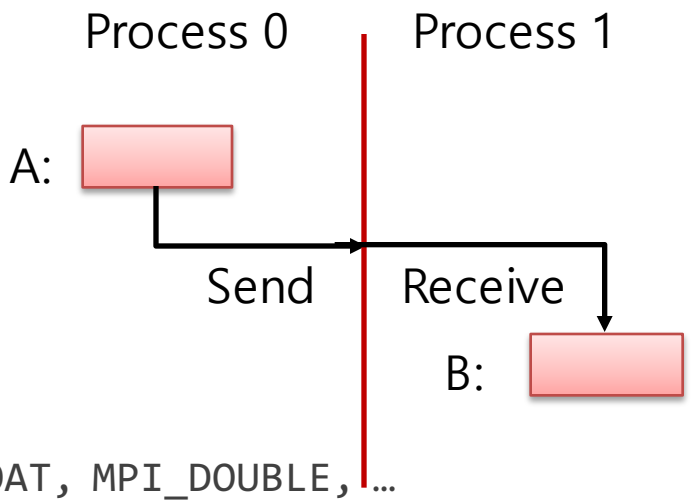
```
$ mpiexec -n <number of processes> <executable>
```

```
$ mpiexec -n 1 ./mpi_hello
Greetings from process 0 of 1 !
```

```
$ mpiexec -n 4 ./mpi_hello
Greetings from process 0 of 4 !
Greetings from process 1 of 4 !
Greetings from process 2 of 4 !
Greetings from process 3 of 4 !
```

Sending and Receiving Messages

- **Point to point communication**



- **Message**
  - Data
    - Buffer: address
    - Count: # of elements
    - Datatype : `MPI_CHAR, MPI_INT, MPI_FLOAT, MPI_DOUBLE, …`
  - Envelope
    - Process ID (source/destination rank)
    - Message tag
    - Communicator

MPI Datatypes

MPI Datatype	C Datatype
MPI_CHAR	signed char
MPI_SHORT	signed short int
MPI_INT	signed int
MPI_LONG	signed long int
MPI_UNSIGNED_CHAR	unsigned char
MPI_UNSIGNED_SHORT	unsigned short int
MPI_UNSIGNED	unsigned int
MPI_UNSIGNED_LONG	unsigned long int
MPI_FLOAT	float
MPI_DOUBLE	double
MPI_LONG_DOUBLE	long double
MPI_BYTE	8 bits
MPI_PACKED	Packed sequence of bytes

Sending and Receiving Messages

- **Message tag**
  - Tags allow programmers to deal with the arrival of messages in an orderly manner
  - Range of tag
    - 0 .. 32767 (2^{15} -1) are guaranteed
    - The upper bound is provided by `MPI_TAG_UB`
    - `MPI_ANY_TAG` can be used as a wildcard value

Message matching

```
MPI_Send(send_buf_p, send_buf_sz, send_type, dest, send_tag,
         send_comm);
```

r

MPI_Send

src = q

MPI_Recv

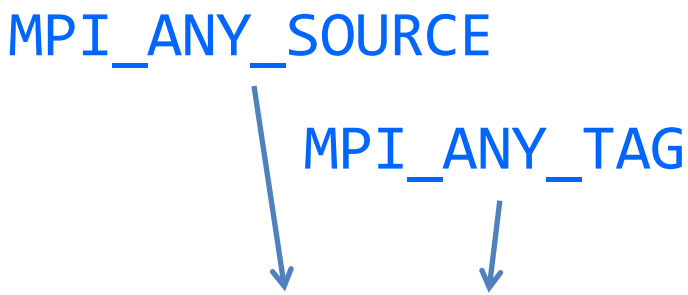
dest = r

```
MPI_Recv(recv_buf_p, recv_buf_sz, recv_type, src, recv_tag,
         recv_comm, &status);
```

q

Receiving Messages

- **Two wildcards of `MPI_recv`**
  - `MPI_ANY_SOURCE`
  - `MPI_ANY_TAG`




```
MPI_Recv(recv_buf_p, recv_buf_sz, recv_type, src, recv_tag,
         recv_comm, &status);
```

- **A receiver can get a message without knowing**
  - The amount of data in the message
  - Sender of the message
  - Tag of the message

Receiving Messages

- **MPI_Status**
  - Stores information about the MPI_Recv operation.
  - Data structure contains:

```
typedef struct MPI_Status {
        int MPI_SOURCE;
        int MPI_TAG;
        int MPI_ERROR; };
```

- **`int MPI_Get_count(MPI_Status *status, MPI_Datatype datatype, int *count)`**
  - Returns the precise count of data items received
  - Not directly accessible

Deadlock Pitfall (1)

```
int a[10], b[10], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
    MPI_Send(a, 10, MPI_INT, 1, 1, MPI_COMM_WORLD);
    MPI_Send(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
    MPI_Recv(b, 10, MPI_INT, 0, 2, MPI_COMM_WORLD);
    MPI_Recv(a, 10, MPI_INT, 0, 1, MPI_COMM_WORLD);
}
...
```

If `MPI_Send` is blocking, there is a deadlock.
MPI standard does not specify
whether the implementation of `MPI_Send` is blocking or not.

Deadlock Pitfall (2)

Circular communication

```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
       MPI_COMM_WORLD);
MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
       MPI_COMM_WORLD);
...
```

Once again, we have a deadlock if `MPI_Send` is blocking.

Avoiding Deadlocks

We can break the circular wait to avoid deadlocks as follows:

```
int a[10], b[10], npes, myrank;
MPI_Status status;
...
MPI_Comm_size(MPI_COMM_WORLD, &npes);
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank%2 == 1) {
        MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
                MPI_COMM_WORLD);
        MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
                MPI_COMM_WORLD);
}
else {
        MPI_Recv(b, 10, MPI_INT, (myrank-1+npes)%npes, 1,
                MPI_COMM_WORLD);
        MPI_Send(a, 10, MPI_INT, (myrank+1)%npes, 1,
                MPI_COMM_WORLD);
}
...
```

Sending and Receiving Messages Simultaneously

- **Exchange messages**

```
int MPI_Sendrecv(void *sendbuf, int sendcount,
    MPI_Datatype senddatatype, int dest, int sendtag,
    void *recvbuf, int recvcount, MPI_Datatype recvdatatype,
    int source, int recvtag, MPI_Comm comm,
    MPI_Status *status)
```

  - Requires both send and receive arguments
  - Avoid the circular deadlock problem

- **Exchange messages using the same buffer**

```
int MPI_Sendrecv_replace(void *buf, int count,
    MPI_Datatype datatype, int dest, int sendtag,
    int source, int recvtag, MPI_Comm comm,
    MPI_Status *status)
```

Non-blocking Sending and Receiving Messages

- **Non-blocking send and receive operations**

```
int MPI_Isend(void *buf, int count, MPI_Datatype datatype,
              int dest, int tag, MPI_Comm comm,
              MPI_Request *request)
int MPI_Irecv(void *buf, int count, MPI_Datatype datatype,
              int source, int tag, MPI_Comm comm,
              MPI_Request *request)
```

- **Tests whether non-blocking operation is finished**

```
int MPI_Test(MPI_Request *request, int *flag,
    MPI_Status *status)
```

- **Waits for the operation to complete**

```
int MPI_Wait(MPI_Request *request, MPI_Status *status)
```

Avoiding Deadlocks

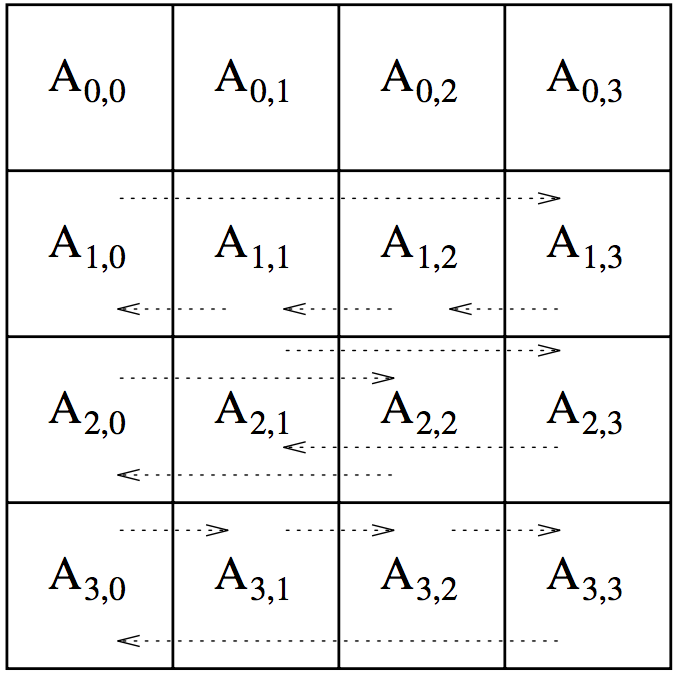
Using non-blocking operations remove most deadlocks

```
int a[10], b[10], myrank;
MPI_Status status;
...
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
if (myrank == 0) {
   MPI_Send(a, 10, MPI_INT, 1, 1, MPI_COMM_WORLD);
   MPI_Send(b, 10, MPI_INT, 1, 2, MPI_COMM_WORLD);
}
else if (myrank == 1) {
   MPI_Recv(b, 10, MPI_INT, 0, 2, &status, MPI_COMM_WORLD);
   MPI_Recv(a, 10, MPI_INT, 0, 1, &status, MPI_COMM_WORLD);
}
...
```

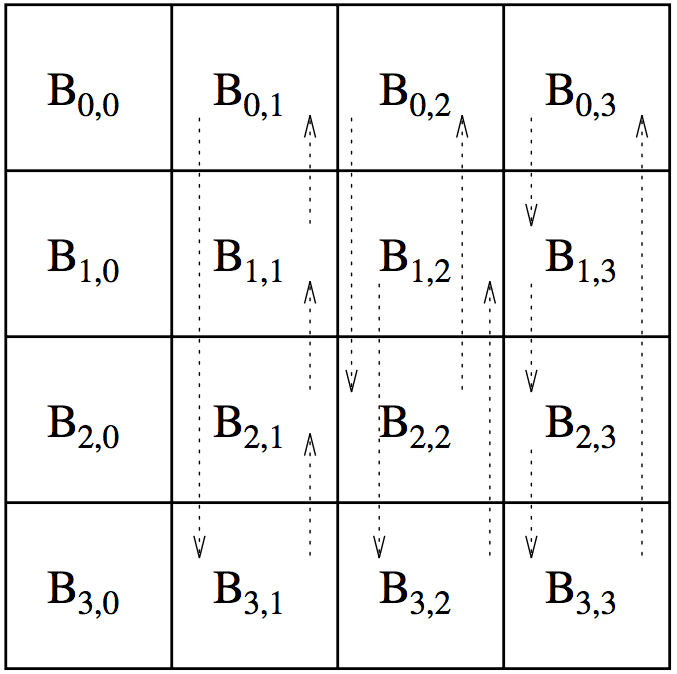
Replacing either the send or the receive operations with non-blocking counterparts fixes this deadlock.

Overlapping Communication with Computation

- Example: Cannon's matrix-matrix multiplication



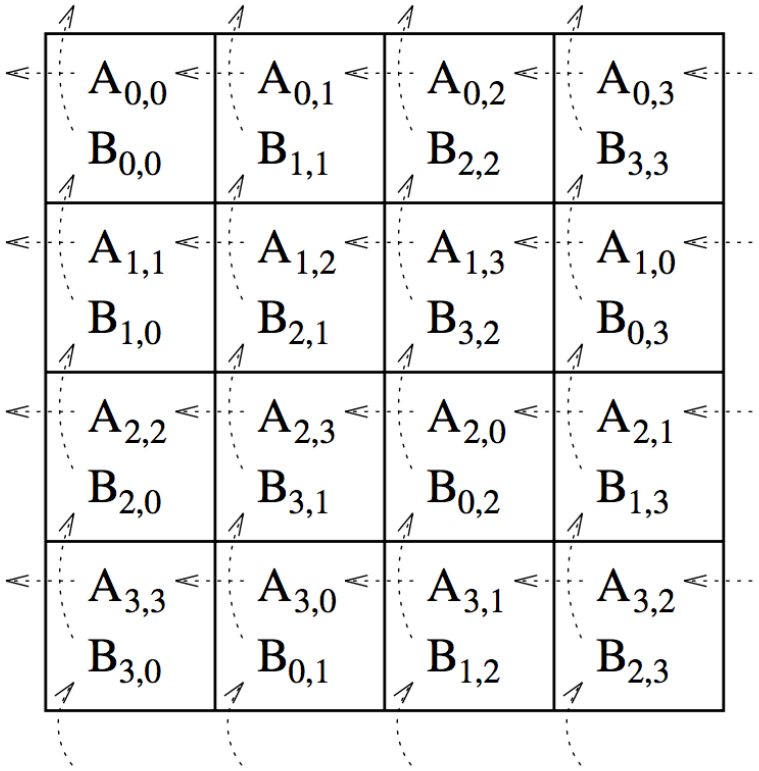
(a) Initial alignment of A



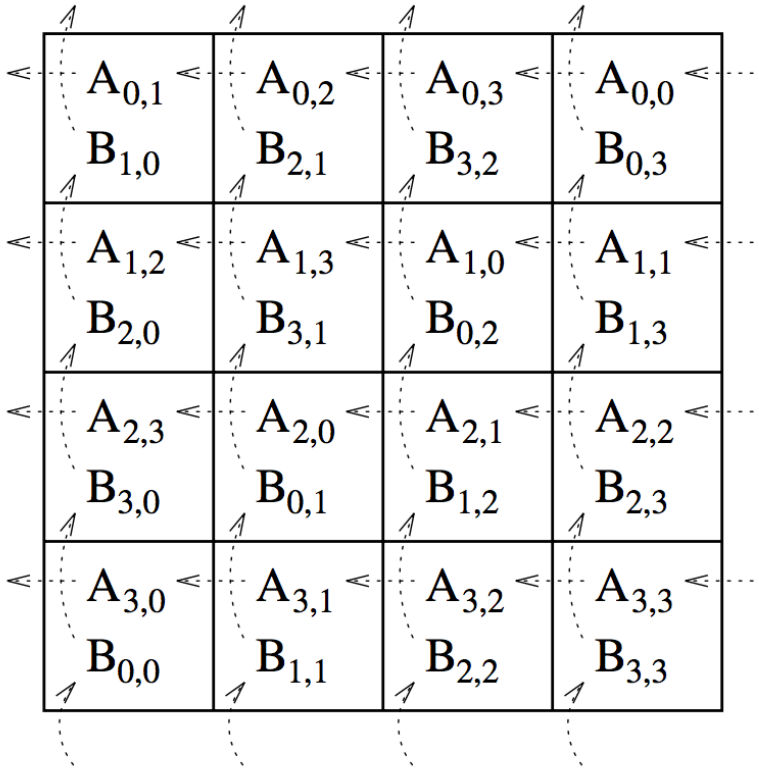
(b) Initial alignment of B

Overlapping Communication with Computation

- Example: Cannon's matrix-matrix multiplication



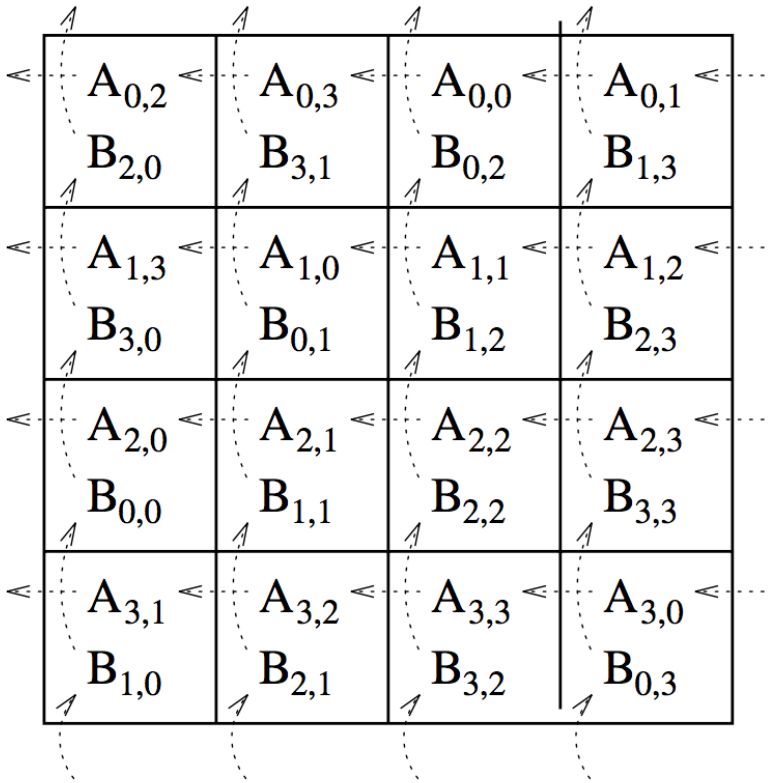
(c) A and B after initial alignment



(d) Submatrix locations after first shift

Overlapping Communication with Computation

- Example: Cannon's matrix-matrix multiplication



(e) Submatrix locations after second shift

$A_{0,3}$ $B_{3,0}$	$A_{0,0}$ $B_{0,1}$	$A_{0,1}$ $B_{1,2}$	$A_{0,2}$ $B_{2,3}$
$A_{1,0}$ $B_{0,0}$	$A_{1,1}$ $B_{1,1}$	$A_{1,2}$ $B_{2,2}$	$A_{1,3}$ $B_{3,3}$
$A_{2,1}$ $B_{1,0}$	$A_{2,2}$ $B_{2,1}$	$A_{2,3}$ $B_{3,2}$	$A_{2,0}$ $B_{0,3}$
$A_{3,2}$ $B_{2,0}$	$A_{3,3}$ $B_{3,1}$	$A_{3,0}$ $B_{0,2}$	$A_{3,1}$ $B_{1,3}$

(f) Submatrix locations after third shift

Overlapping Communication with Computation

- Using blocking communications

```
/* Get into the main computation loop */
for (i=0; i<dims[0]; i++) {
  MatrixMultiply(nlocal, a, b, c); /*c=c+a*b*/

  /* Shift matrix a left by one */
  MPI_Sendrecv_replace(a, nlocal*nlocal, MPI_DOUBLE,
      leftrank, 1, rightrank, 1, comm_2d, &status);

  /* Shift matrix b up by one */
  MPI_Sendrecv_replace(b, nlocal*nlocal, MPI_DOUBLE,
      uprank, 1, downrank, 1, comm_2d, &status);
}
```

Code snippet of Cannon's matrix-matrix multiplication

Overlapping Communication with Computation

- Using non-blocking communications

```
/* Get into the main computation loop */
for (i=0; i<dims[0]; i++) {
  MPI_Isend(a_buffers[i%2], nlocal*nlocal, MPI_DOUBLE,
      leftrank, 1, comm_2d, &reqs[0]);
  MPI_Isend(b_buffers[i%2], nlocal*nlocal, MPI_DOUBLE,
      uprank, 1, comm_2d, &reqs[1]);
  MPI_Irecv(a_buffers[(i+1)%2], nlocal*nlocal, MPI_DOUBLE,
      rightrank, 1, comm_2d, &reqs[2]);
  MPI_Irecv(b_buffers[(i+1)%2], nlocal*nlocal, MPI_DOUBLE,
      downrank, 1, comm_2d, &reqs[3]);

  /* c = c + a*b */
   MatrixMultiply(nlocal, a_buffers[i%2], b_buffers[i%2], c);

  for (j=0; j<4; j++)
    MPI_Wait(&reqs[j], &status);
}
```

Code snippet of Cannon's matrix-matrix multiplication

Collective Communication

- MPI provides an extensive set of functions of collective communication operations
- Operations are defined over a group corresponding to the communicator
- All processors in a communicator must call these operations

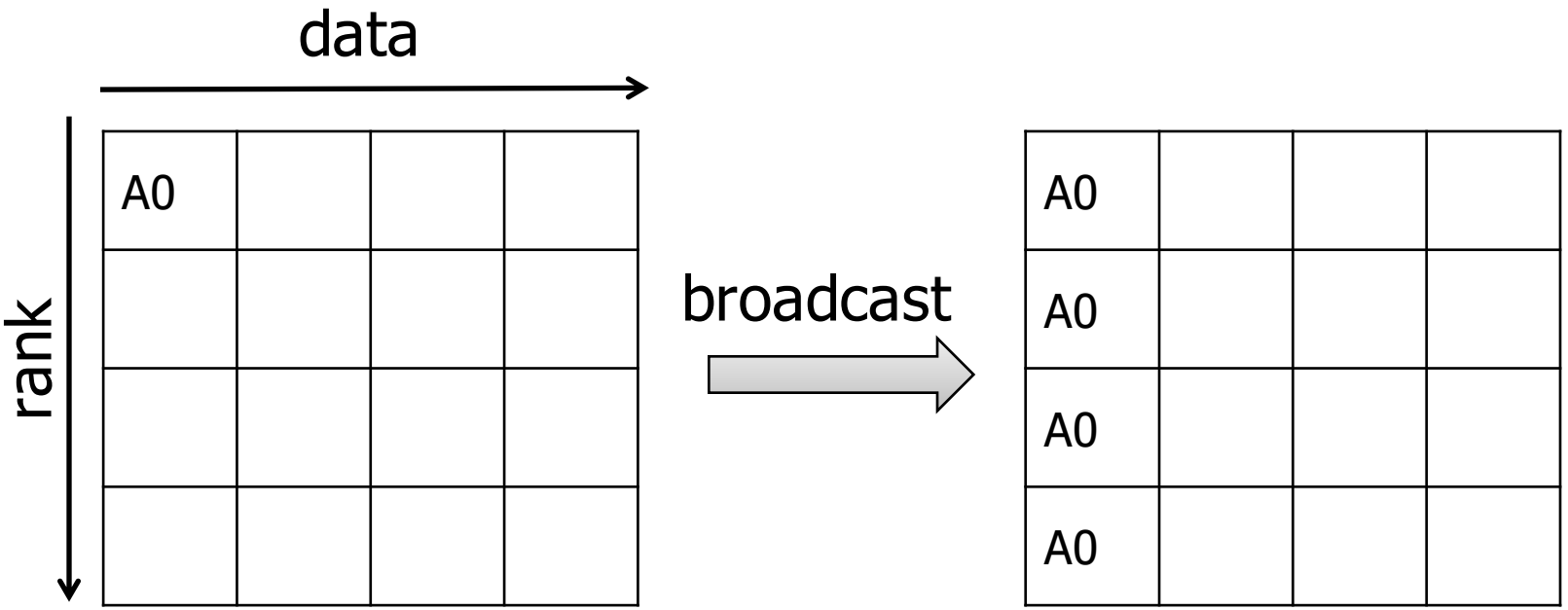
- Simple collective communication: barrier

```
int MPI_Barrier(MPI_Comm comm)
```

  - Waits until all processes arrive

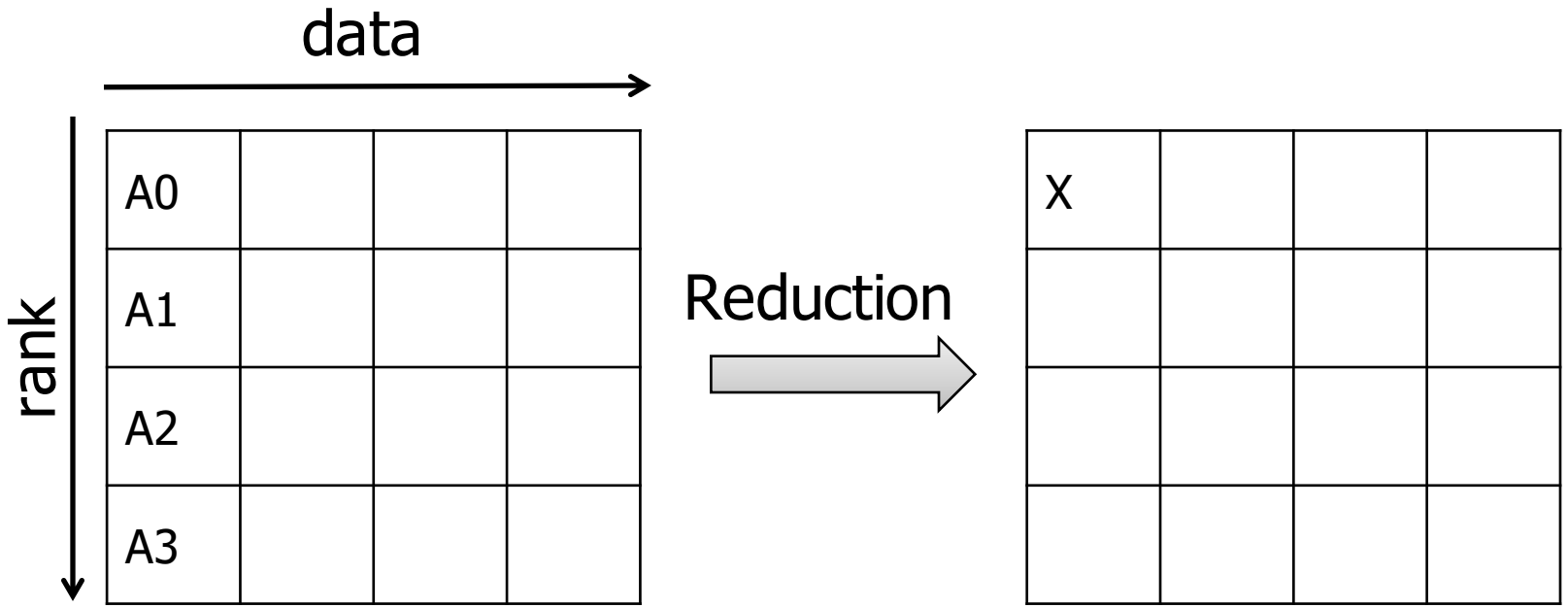
One-to-All Broadcast

```
int MPI_Bcast(void *buf, int count, MPI_Datatype datatype,
              int source, MPI_Comm comm)
```



All-to-One Reduction

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



X = A0 op A1 op A2 op A3

Predefined Reduction Operations

Operation	Meaning	Datatypes
MPI_MAX	Maximum	C integers and floating point
MPI_MIN	Minimum	C integers and floating point
MPI_SUM	Sum	C integers and floating point
MPI_PROD	Product	C integers and floating point
MPI_LAND	Logical AND	C integers
MPI_BAND	Bit-wise AND	C integers and byte
MPI_LOR	Logical OR	C integers
MPI_BOR	Bit-wise OR	C integers and byte
MPI_LXOR	Logical XOR	C integers
MPI_BXOR	Bit-wise XOR	C integers and byte
MPI_MAXLOC	max-min value-location	Data-pairs
MPI_MINLOC	min-min value-location	Data-pairs

Collective Communications (1)

- **All processes must call the same collective function.**
  - Ex. `MPI_Recv()` in P0 + `MPI_Reduce()` in P1 (X)
- **The arguments must be compatible to each other**
  - Ex.

Process 0

```
MPI_Reduce(in_buf,
        out_buf,
        1,
        MPI_CHAR,
        MPI_SUM,
        0,
        MPI_COMM_WORLD);
```

Mismatch!!

Process 1

```
MPI_Reduce(in_buf,
        out_buf,
        1,
        MPI_CHAR,
        MPI_SUM,
        1,
        MPI_COMM_WORLD);
```

Collective Communications (2)

- **Output argument is only used in the destination process**
  - But, other processes should provide destination argument, even if it is NULL
  - Ex.

Process 0

```
MPI_Reduce(in_buf,
        out_buf,
        1,
        MPI_CHAR,
        MPI_SUM,
        0,
        MPI_COMM_WORLD);
```

Process 1

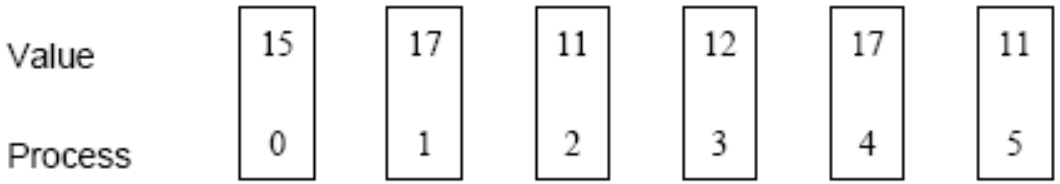
```
MPI_Reduce(in_buf,
        NULL,
        1,
        MPI_CHAR,
        MPI_SUM,
        0,
        MPI_COMM_WORLD);
```

Collective vs. Point-to-Point Comm.

- **Point-to-point communication**
  - MPI_Send/Recv are matched on the basis of tags and ranks
- **Collective communication**
  - Do NOT use tags
  - They're matched solely on the basis of receiver's rank and order

MPI_MAXLOC and MPI_MINLOC

- **MPI_MAXLOC**
  - Combines pairs of values (v_i, l_i)
  - Returns the pair (v, l)
    - v is the maximum among all v_i 's
    - l is the corresponding l_i
      - » (if there are more than one, it is the smallest among all these l_i 's).
- **MPI_MINLOC does the same, except for minimum value of v_i.**




```
MinLoc(Value, Process) = (11, 2)
MaxLoc(Value, Process) = (17, 1)
```

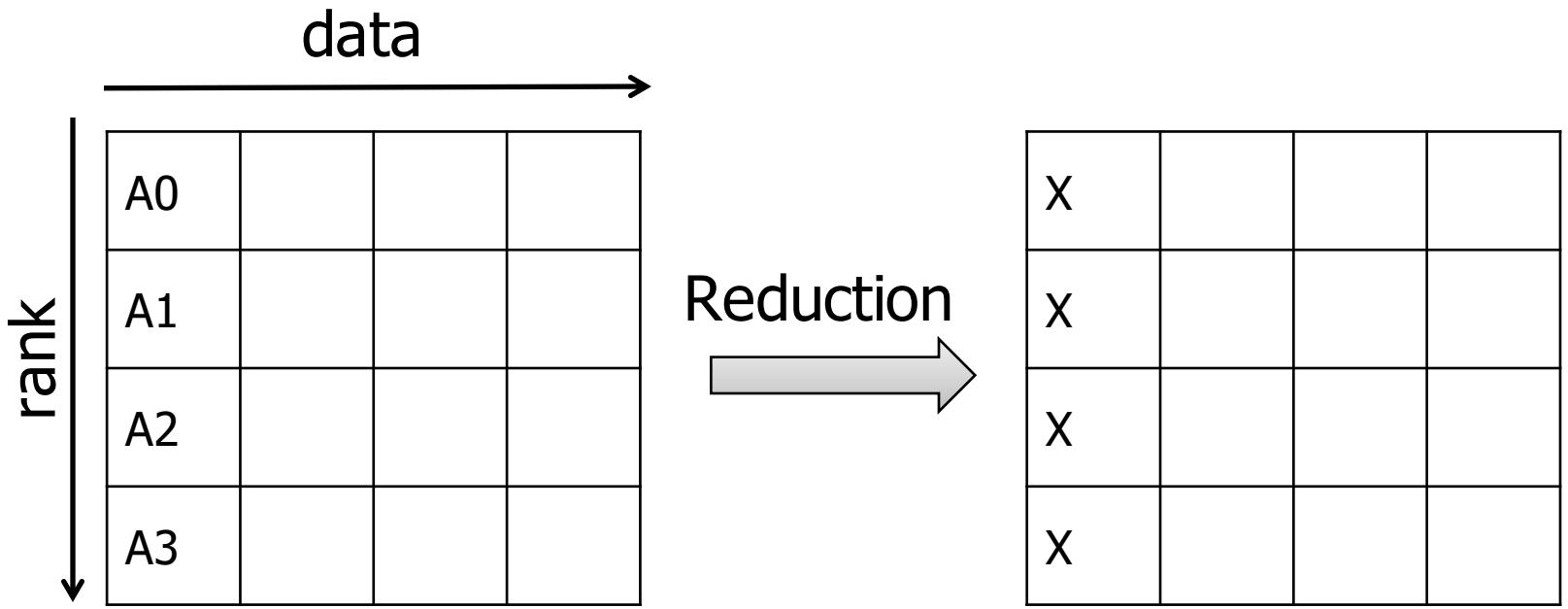
MPI_MAXLOC and MPI_MINLOC

MPI datatypes for data-pairs used with the MPI_MAXLOC and MPI_MINLOC reduction operations.

MPI Datatype	C Datatype
`MPI_2INT`	pair of ints
`MPI_SHORT_INT`	short and int
`MPI_LONG_INT`	long and int
`MPI_LONG_DOUBLE_INT`	long double and int
`MPI_FLOAT_INT`	float and int
`MPI_DOUBLE_INT`	double and int

All-to-All Reduction

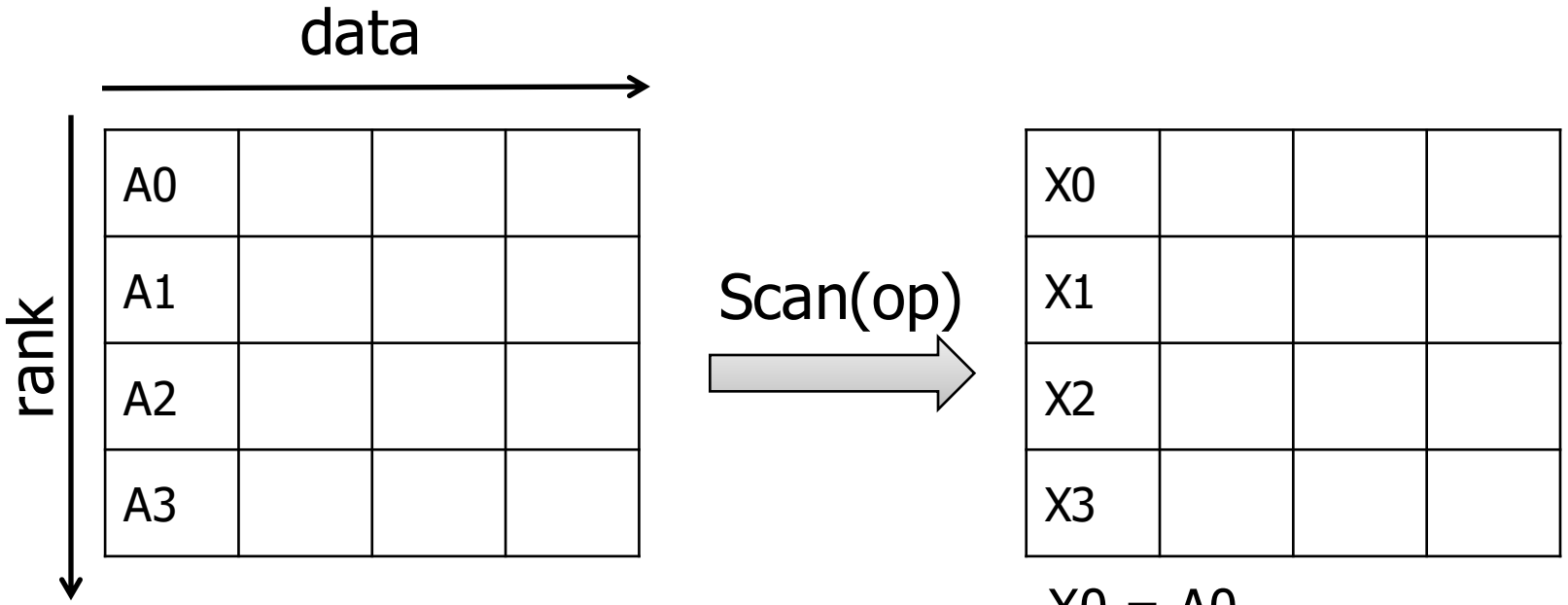
```
int MPI_Allreduce(void *sendbuf, void *recvbuf,
  int count, MPI_Datatype datatype, MPI_Op op,
  MPI_Comm comm)
```



X = A0 op A1 op A2 op A3

Prefix Operation (Inclusive)

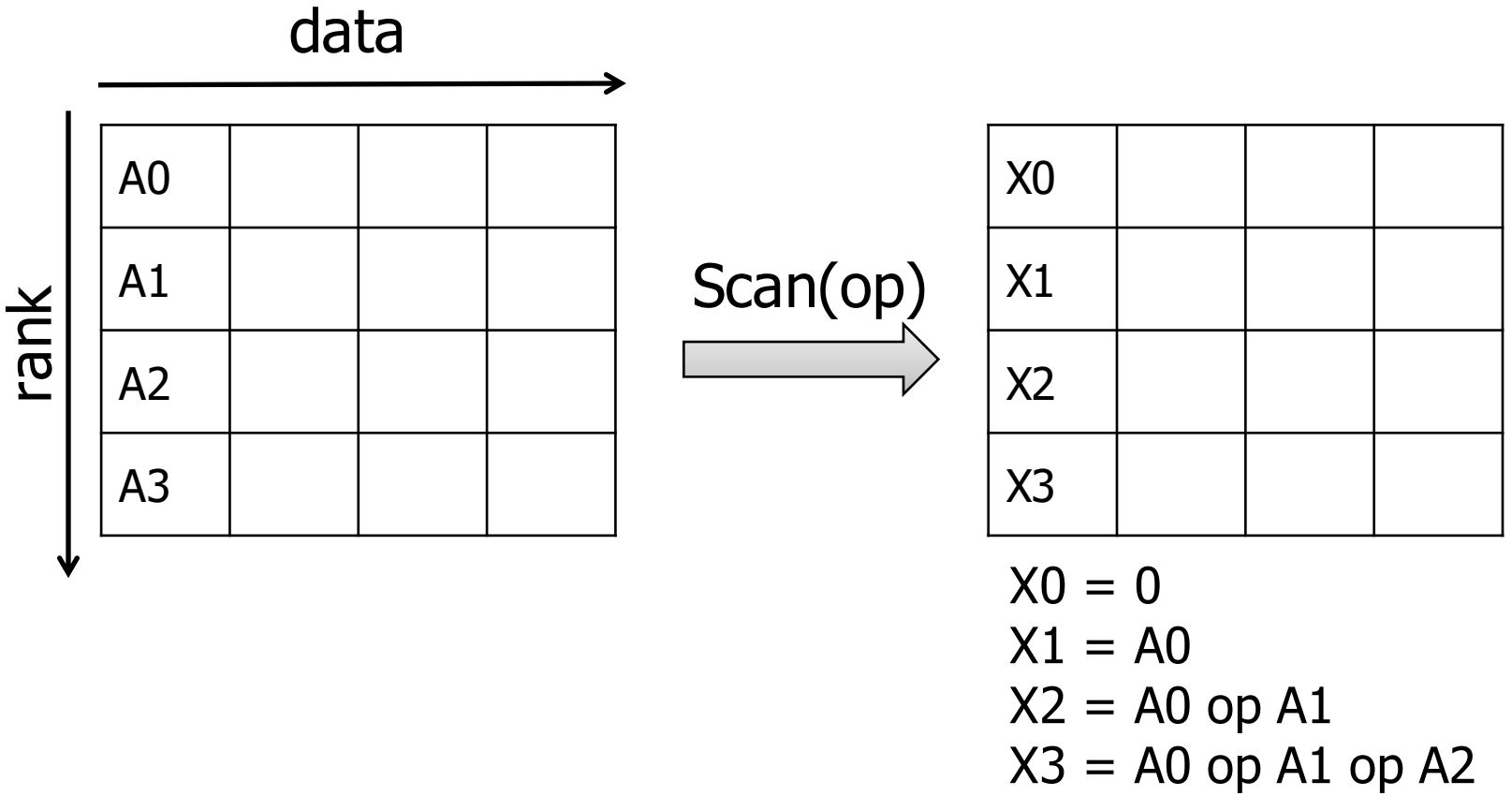
```
int MPI_Scan(void *sendbuf, void *recvbuf, int count,
             MPI_Datatype datatype, MPI_Op op,
             MPI_Comm comm)
```



X0 = A0,
X1 = A0 op A1,
X2 = A0 op A1 op A2,
X3 = A0 op A1 op A2 op A3

Prefix Operation (Exclusive)

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



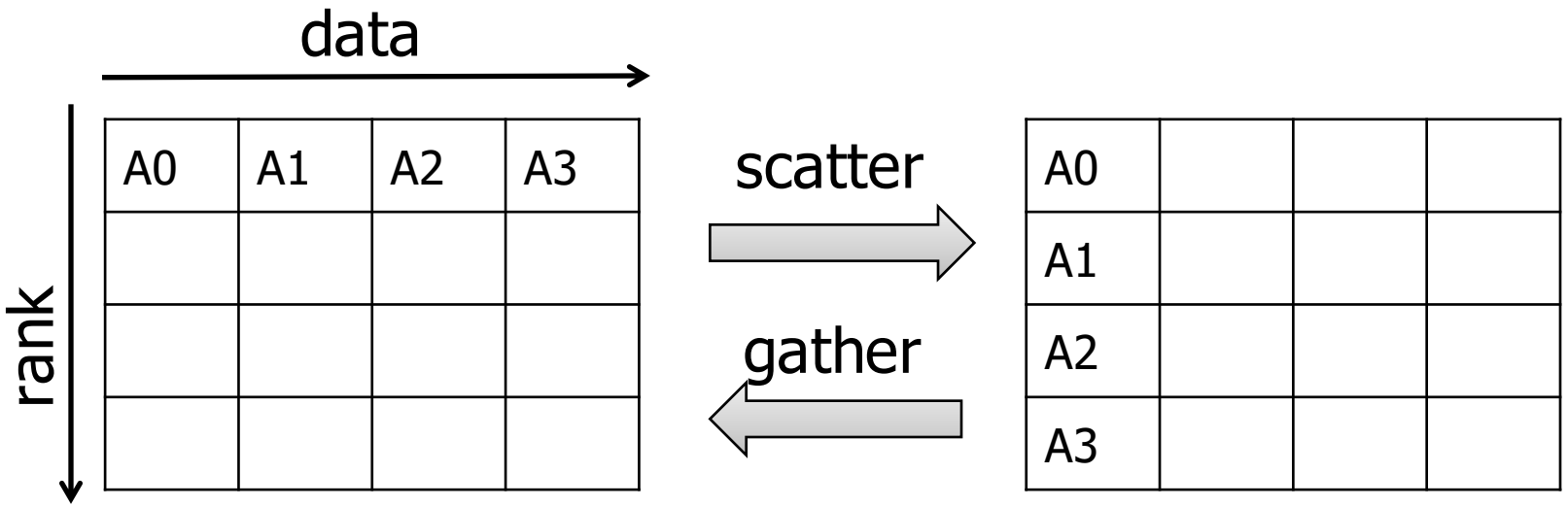
Scatter and Gather

- **Gather data at one process**

```
int MPI_Gather(void *sendbuf, int sendcount,
          MPI_Datatype senddatatype, void *recvbuf,
          int recvcount, MPI_Datatype recvdatatype,
          int target, MPI_Comm comm)
```

- **Scatter data from source to all processes**

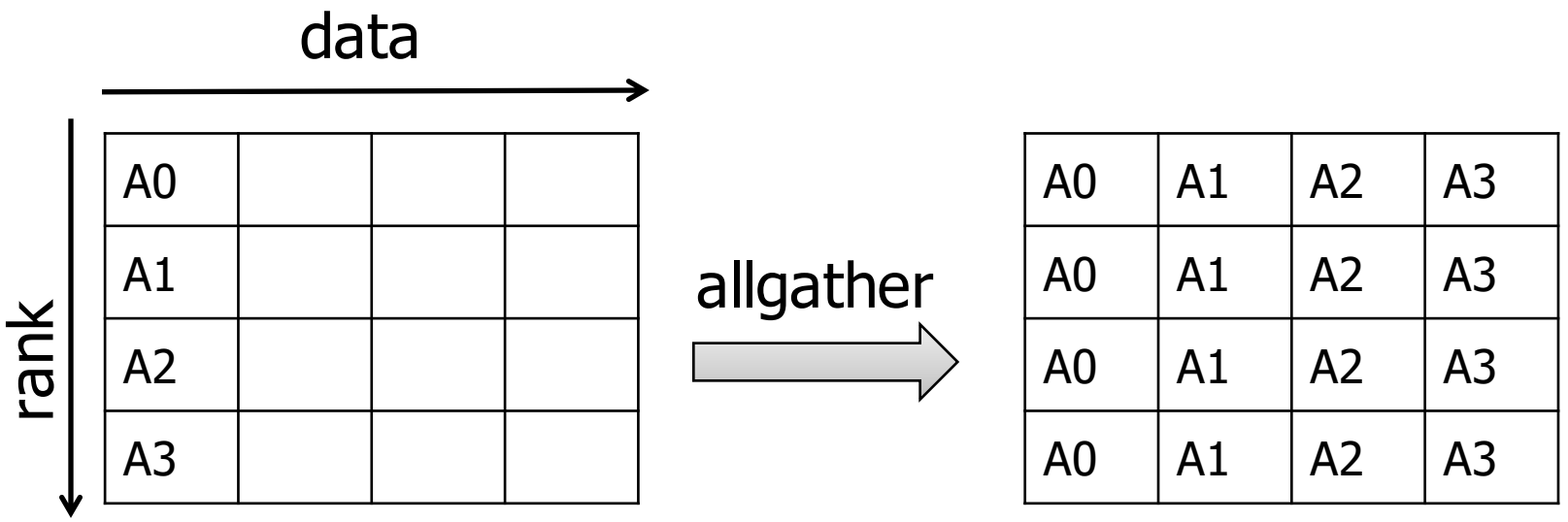
```
int MPI_Scatter(void *sendbuf, int sendcount,
          MPI_Datatype senddatatype, void *recvbuf,
          int recvcount, MPI_Datatype recvdatatype,
          int source, MPI_Comm comm)
```



Allgather

- **Gather and scatter them to all processes**

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

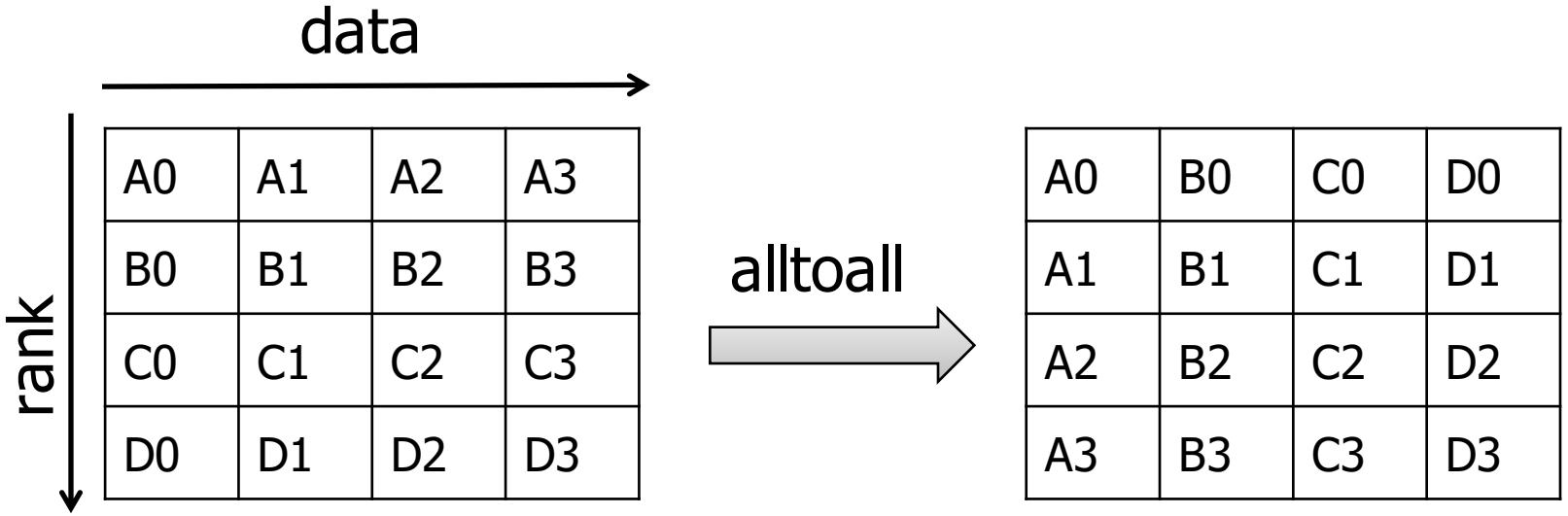


All-to-All

- **The all-to-all personalized communication**

```
int MPI_Alltoall(void *sendbuf, int sendcount,
 MPI_Datatype senddatatype, void *recvbuf,
                    int recvcount, MPI_Datatype recvdatatype,
          MPI_Comm comm)
```

  - Analogous to a matrix transpose



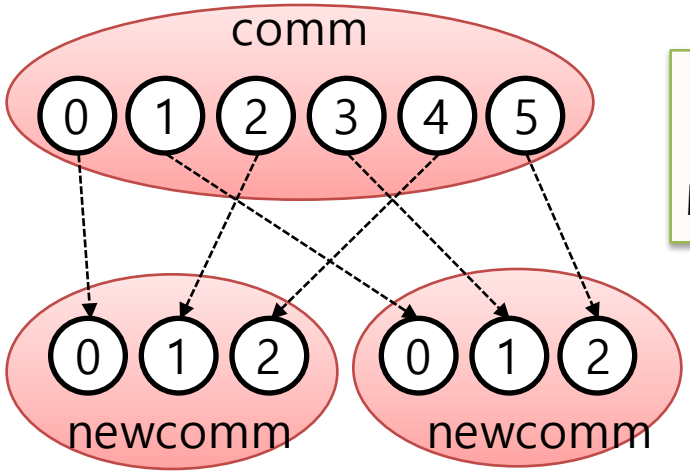
Communicators

- **All MPI communication is based on a communicator which contains a context and a group**
  - Contexts define a safe communication space for message-passing – viewed as system-managed tags
  - Contexts allow different libraries to co-exist
  - Group is just a set of processes
  - Processes are always referred to by the unique rank in a group

- **Pre-defined communicators**
  - MPI_COMM_WORLD
  - MPI_COMM_NULL // initial value, cannot be used as for comm
  - MPI_COMM_SELF // contains only the local process

Communicator Manipulation

- **Duplicate communicator**
  - `MPI_Comm_dup(comm, newcomm)`
  - Create a new context with similar structure
- **Partition the group into disjoint subgroups**
  - `MPI_Comm_split(comm, color, key, newcomm)`
  - Each sub-communicator contains the processes with the same *color*
  - The rank in the sub-communicator is defined by the *key*



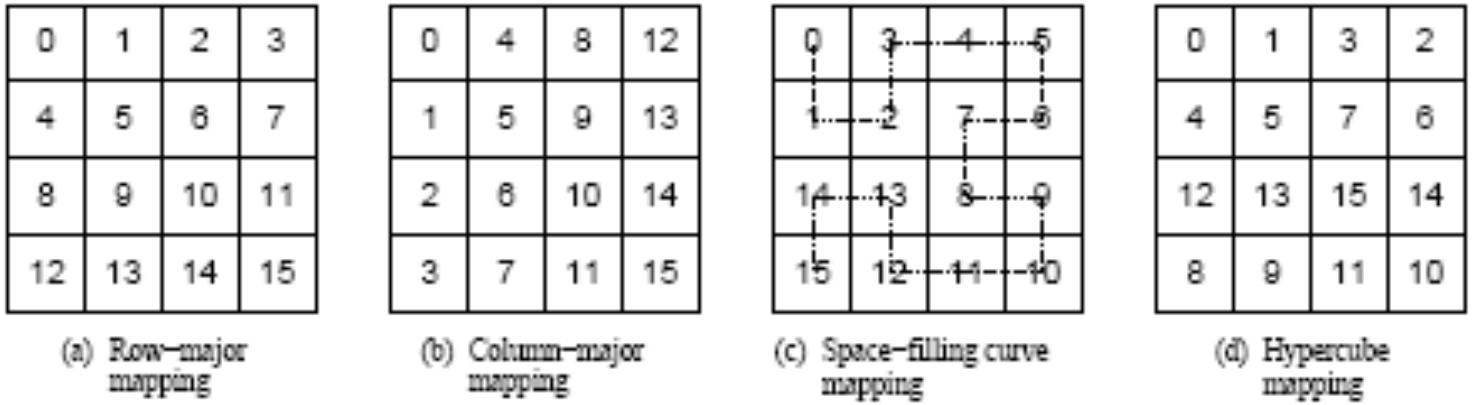

```
color = (rank % 2 == 0)? 0 : 1;
key   = rank / 2;
MPI_Comm_split(comm, color, key, &newcomm);
```

Communicator Manipulation – con't

- **Obtain an existing group and free a group**
  - `MPI_Comm_group(comm, group)` – create a group having processes in the specified communicator
  - `MPI_Group_free(group)` – free a group
- **New group can be created by specifying members**
  - `MPI_Group_incl(), MPI_Group_excl()`
  - `MPI_Group_range_incl(), MPI_Group_range_excl()`
  - `MPI_Group_union(), MPI_Group_intersect()`
  - `MPI_Group_compare(), MPI_Group_translate_ranks()`
- **Subdivide a communicator**
  - `MPI_Comm_create(comm, group, newcomm)`

Topologies and Embeddings

- **Process ids in `MPI_COMM_WORLD` can be mapped**
  - Higher dimensional meshes
  - Or other topologies



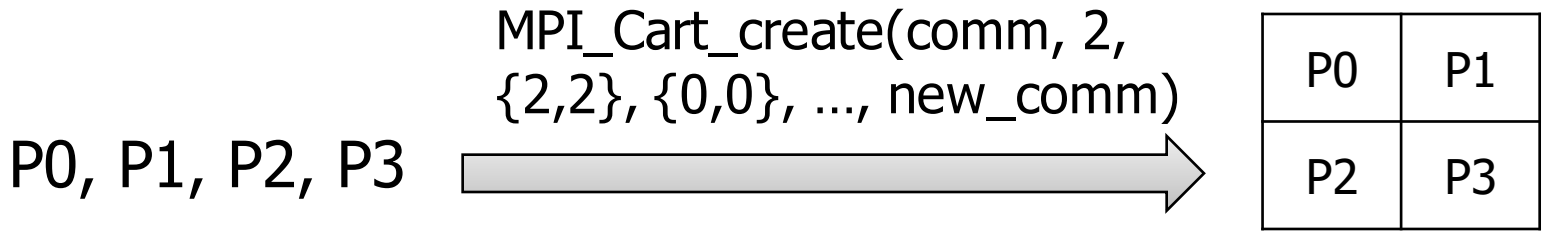
- **The goodness of any mapping**
  - Determined by the interaction pattern of a program or topology of the machine
  - MPI does not provide the programmer any control over these mappings

Creating Cartesian Topologies

- **Creates cartesian topologies**

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

  - Creates a new communicator with dims dimensions.
    - ndims = number of dimensions
    - dims = vector of length of each dimension
    - periods = vector indicates which dims are periodic (wrap-around link)
    - Reorder = flag – ranking may be reordered



Using Cartesian Topologies

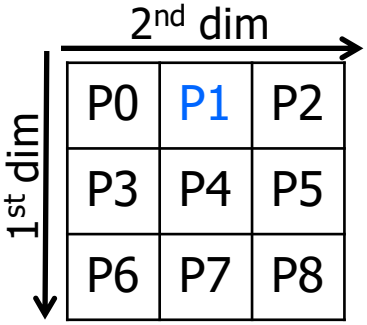
- Sending and receiving messages still require ranks (or process IDs)
- Convert ranks to cartesian coordinates and vice-versa

```
int MPI_Cart_coord(MPI_Comm comm_cart, int rank, int maxdims,
                   int *coords)

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

- The most common operation on cartesian topologies is a shift

```
int MPI_Cart_shift(MPI_Comm comm_cart, int dir, int s_step,
    int *rank_source, int *rank_dest)
```



Examples:

P1 calls MPI_Cart_coord() → (0, 1)
MPI_Cart_rank({0, 1}) → 1 (P1)
MPI_Cart_shift(0 (direction), 2 (step)) → src:P2, dst:P0
(assuming all dims are periodic)

Splitting Cartesian Topologies

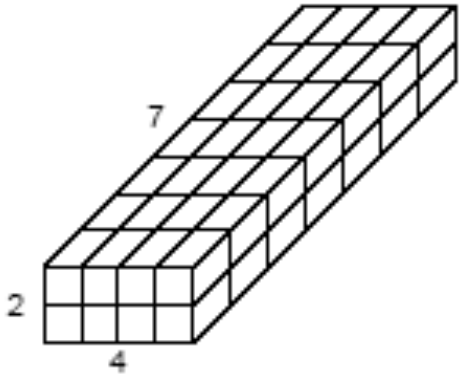
- **Partition a Cartesian topology to form lower-dimensional grids:**

```
int MPI_Cart_sub(MPI_Comm comm_cart, int *keep_dims,
        MPI_Comm *comm_subcart)
```

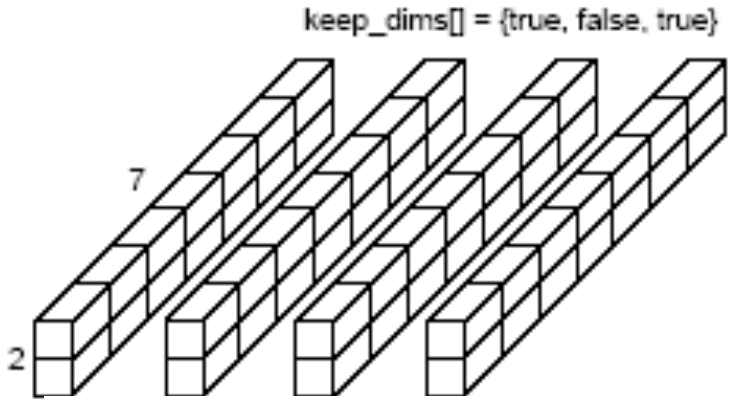
  - `keep_dims[i]` determines whether to split or not the `i`th dimension

- **The coordinate of a process in a sub-topology**
  - Derived from its coordinate in the original topology
  - Disregarding the coordinates that correspond to the dimensions that were not retained
  - Example: (2, 3) → (2) if dims = {true, false}

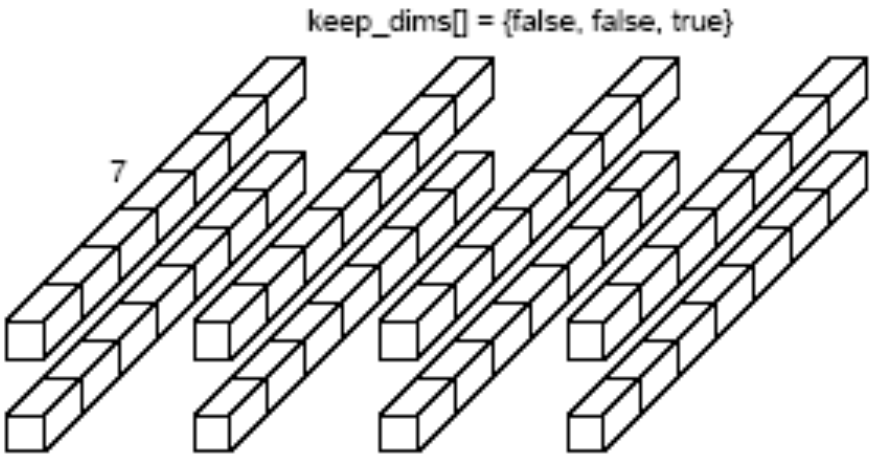
Splitting Cartesian Topologies



2 x 4 x 7



four 2 x 1 x 7



eight 1 x 1 x 7

Limitations of MPI Data Types

- **Only primitive data types can be exchanged through `MPI_Send/Recv`**

- **Many programs use more complex data structures**
  - Ex. `struct` in C

MPI datatype	C datatype
MPI_CHAR	signed **char**
MPI_SHORT	signed **short int**
MPI_INT	signed **int**
MPI_LONG	signed **long int**
MPI_LONG_LONG	signed **long long int**
MPI_UNSIGNED_CHAR	**unsigned char**
MPI_UNSIGNED_SHORT	**unsigned short int**
MPI_UNSIGNED	**unsigned int**
MPI_UNSIGNED_LONG	**unsigned long int**
MPI_FLOAT	**float**
MPI_DOUBLE	**double**
MPI_LONG_DOUBLE	**long double**
MPI_BYTE	
MPI_PACKED	

Basic data types in MPI

MPI Derived Data Types

- **To make more complex data types to be exchanged through MPI communication methods**
  - MPI should know the size of a data structure
  - MPI should know the members within the data structure
    - Location
    - Size of each member

```
struct a {
    MPI_DOUBLE x[2];
    MPI_DOUBLE y[2];
    MPI_LONG value[2];
};
```

Member	Offset in bytes
x	0
y	16
value	32

MPI_Type create_struct

- **Builds a derived datatype consisting of individual elements**

```
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 */);
```

- `array_of_block_lengths`
  - Each member can be either a variable or an array
  - Ex. {2, 2, 2};
- `array_of_displacements`
  - Offsets of each member from start address
  - Ex. {0, 16, 32}
- `array_of_types`
  - Types of each member
  - Ex. {MPI_DOUBLE, MPI_DOUBLE, MPI_LONG}

```
struct a {
    MPI_DOUBLE x[2];
    MPI_DOUBLE y[2];
    MPI_LONG value[2];
};
```

MPI_Get_address

- To know the address of the memory location referenced by `location_p`
- The address is stored in an integer variable of type `MPI_Aint`

```
int MPI_Get_address(
      void*      location_p  /* in  */,
      MPI_Aint*  address_p   /* out */);
```

```
struct a {
    MPI_DOUBLE x[2];
    MPI_DOUBLE y[2];
    MPI_LONG value[2];
};
```

```
struct a a;
MPI_Get_address(&a.x, &x_addr);
MPI_Get_address(&a.y, &y_addr);
MPI_Get_address(&a.value, &value_addr);
array_of_displacements[0] = x_addr - &a;
array_of_displacements[1] = y_addr - &a;
array_of_dispalcements[2] = value_addr - &a;
```

Other methods

- **MPI_Type_commit**
  - To let MPI know the new data type
  - After calling this function, the new data type can be used in MPI communication methods

```
int MPI_Type_commit(MPI_Datatype*  new_mpi_t_p  /* in/out */);
```

- **MPI_Type_free**
  - When the new data type is no longer used, this function frees any additional storages used for the new data type

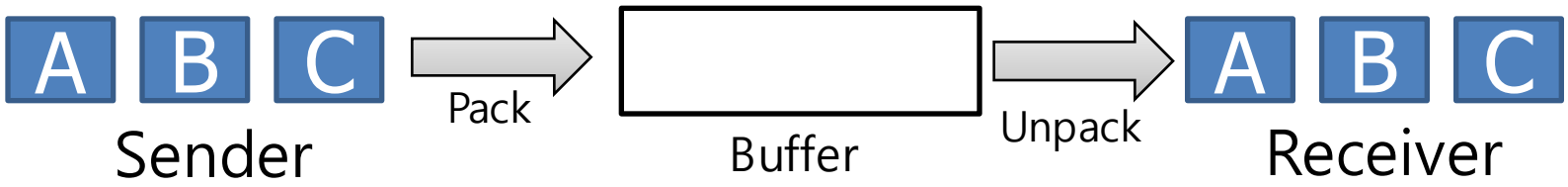
```
int MPI_Type_free(MPI_Datatype*  old_mpi_t_p  /* in/out */);
```

MPI_Pack/Unpack

- An alternative method to send/receive a complex data structure
- Pack multiple data types into a single buffer
- One pair of MPI_Send & MPI_Recv
- Sender and receiver have to know which data types are packed in the single buffer

```
buffer = malloc()
MPI_Pack(A)
MPI_Pack(B)
MPI_Pack(C)
MPI_Send(buffer, MPI_PACKED)
```

```
buffer = malloc()
MPI_Recv(buffer, MPI_PACKED)
MPI_Unpack(A)
MPI_Unpack(B)
MPI_Unpack(C)
```



Concluding Remarks

- **MPI or the Message-Passing Interface**
  - An interface of parallel programming in distributed memory system
  - Supports C, C++, and Fortran
  - Many MPI implementations
    - Ex, MPICH2
- **SPMD program**
- **Message passing**
  - Communicator
  - Point-to-point communication
  - Collective communication
  - Safe use of communication is important
    - Ex. MPI_Sendrecv()

References

- COMP422: Parallel Computing by Prof. John Mellor-Crummey at Rice Univ., 2015.
- Ananth Grama, Anshul Gupta, George Karypis, and Vipin Kumar. "Introduction to Parallel Computing," Chapter 6. Addison Wesley, 2003.