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Barcelona Supercomputing Center
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Introduction to the MPI programming model
Session 2

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PATC Parallel Programming Workshop October 2013

MPI Specifics

- Communicators: Scope of communication operations
- Structure of messages: complex data types
- Data transfer:
  - Synchronous/asynchronous
  - Blocking/non-blocking
- Message tags/identifiers
- Communication partners:
  - Point-to-point
  - Wild card process and message tags

Scope of processes

- Communicator group processes
- A group defines the set of processes, that can communicate with each other
- Used in point-to-point and collective communication
- After starting a program, its processes subscribe to the "Universe" ==> `MPI_COMM_WORLD`
- Each program has its own "Universe"

Usage of Communicators

- Fence off communication environment
- Example: Communication in library
  What happens, if a program uses a parallel library that uses MPI itself?
- 2 Kinds of communicators:
  - Intra-communicator: inside a group
  - Inter-communicator: between groups
- Processes in each group are always numbered *0* to *m-1* for *m* processes in a group

MPI Specifics

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  - Point-to-point
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Structure of Messages

- Standard data types:
  - Integer, Float, Character, Byte, ...
  - (Continuous) arrays
- Complex data types:
  - Messages including different data: counter + elements
  - Non-continuous data types: sparse matrices
- Solutions:
  - Pack/unpack functions
  - Special (common) data types:
    - Array of data types
    - Array of memory displacements
  - Managed by the message-passing library

Point-to-Point Communication

MPI:

- Data types for message contents:
  - Standard types:
    - `MPI_INT`
    - `MPI_FLOAT`
    - `MPI_CHAR`
    - `MPI_DOUBLE`
    - ...
  - User defined types: derived from standard types

Data Transfer

Blocking:

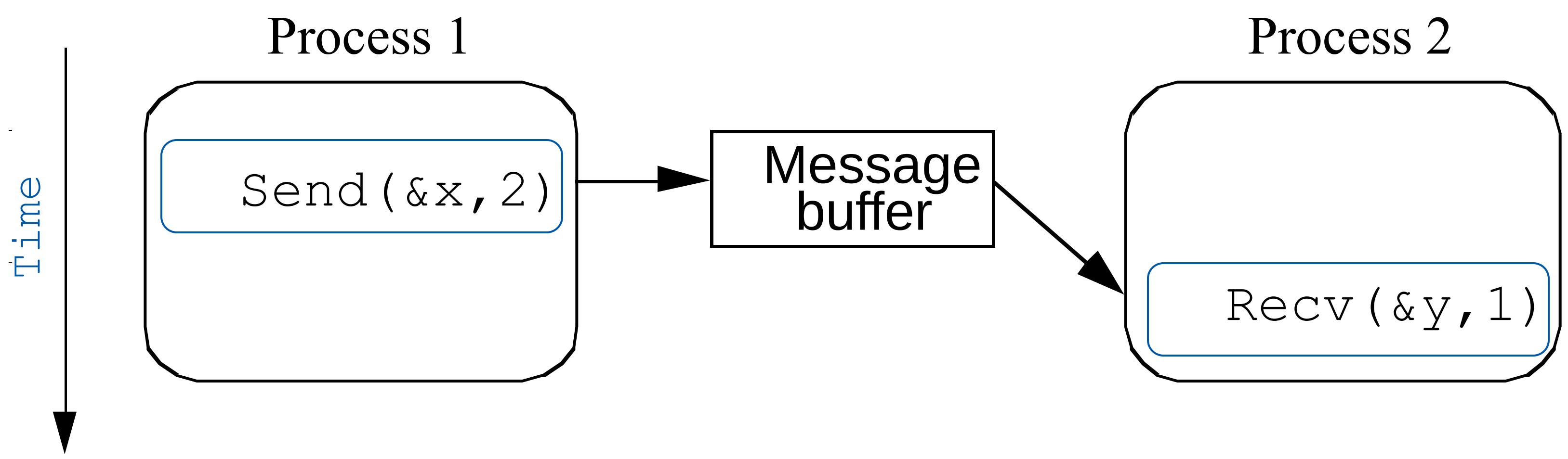
- Function does not return,
  before message can be accessed again
- Process is „blocked“

Non-blocking:

- Function returns, whether data transfer is finished or not
- Requires function to query the status of the data transfer
- Message buffers are needed
  - Length of message is limited
- Overlapping of communication and computation is possible
  - ⇨ Reduction of execution time

Data Transfer with Message Buffer

Non-blocking send:



MPI Viewpoint

Concepts for blocking:

- *Locally blocking:*
  - Function is blocked, until messages has been copied into buffer
  - Transfer needs not be completed

- *Locally non-blocking:*
  - Function returns immediately, whether message has been copied or not
  - User is responsible for message

Standard Send/Receive

- **`MPI_Send`**:
  - Is locally complete as soon as the message is free for further processing
  - The message needs not be received
    ⇨ most likely it will have been transferred to communication buffer

- **`MPI_Recv`**:
  - Is locally complete, as soon as the message has been received

Pitfall: Deadlock

Cyclic message exchange in a ring:

```
if (rank == 0) {
  MPI_Send(buffer,length,MPI_CHAR,1,…);
  MPI_Recv(buffer,length,MPI_CHAR,1,…);
} else if (rank == 1) {
  MPI_Send(buffer,length,MPI_CHAR,0,…);
  MPI_Recv(buffer,length,MPI_CHAR,0,…);
}
```

- Problem: both processes are blocked, since each process is waiting on receive to complete send.
- Cyclic resource-dependencies

Deadlock Solution

No cyclic dependencies:

```
if (rank == 0) {
  MPI_Send(buffer,length,MPI_CHAR,1,…);
  MPI_Recv(buffer,length,MPI_CHAR,1,…);
} else if (rank == 1) {
  MPI_Recv(buffer,length,MPI_CHAR,0,…);
  MPI_Send(buffer,length,MPI_CHAR,0,…);
}
```

Blocking Test

```
int MPI_Probe (int source, int tag
 MPI_Comm comm, MPI_Status *status)
```

- `source` Origin process of message
- `tag` Generic message tag
- `comm` Communication handler
- `status` Status information

- Is locally complete,
  as soon as a message has been received
- Does not return the message,
  but provides only status information about it

MPI_Sendrecv

Performs send and receive in one single function call:

```
MPI_Sendrecv (
 pointer to send buffer                        void *sendbuf,
 size of send message (in elements)            int sendcount,
 datatype of element                MPI_Datatype sendtype,
 destination                        int dest,
 tag                                int sendtag,
 pointer to receive buffer          void *recvbuf,
 size of receive message (in elem.)            int recvcount,
 datatype of element                MPI_Datatype recvtype,
 source                             int source,
 tag                                int recvtag,
 communicator                                  MPI_Comm communicator,
 return status                      MPI_Status *status);
```

MPI_Sendrecv_replace

Performs send and receive in one single function call and operates only one one single buffer:

	MPI_Sendrecv_replace (
pointer to buffer	**void *buf,**
size of message (in elements)	**int count,**
datatype of element	**MPI_Datatype type,**
destination	**int dest,**
tag	**int sendtag,**
source	**int source,**
tag	**int recvtag,**
communicator	**MPI_Comm communicator,**
return status	**MPI_Status *status);**

Non-blocking Functions

- **`MPI_Isend`**:
  - Returns immediately,
    whether function is locally complete or not
  - Message has not been copied
    ⇨ Changes may affect contents of message

- **`MPI_Irecv`**:
  - Returns immediately,
    whether a message has arrived or not

- **`MPI_Iprobe`**:
  - Non-blocking test for a message

Auxiliary Functions

Is an operation completed or not?

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

- Waits until operation is completed

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

- Returns immediately.
  `flag` contains status of request (true/false).

Additional Wait-Functions

```
int MPI_Waitany(int count,
MPI_Request *array_of_requests, int *index, MPI_Status *status)

int MPI_Waitall(int count,
MPI_Request *array_of_requests,
MPI_Status *status)

int MPI_Waitsome(int incount,
MPI_Request *array_of_requests, int *outcount, int *array_of_indices,
MPI_Status *array_of_statuses)
```

Additional Test-Functions

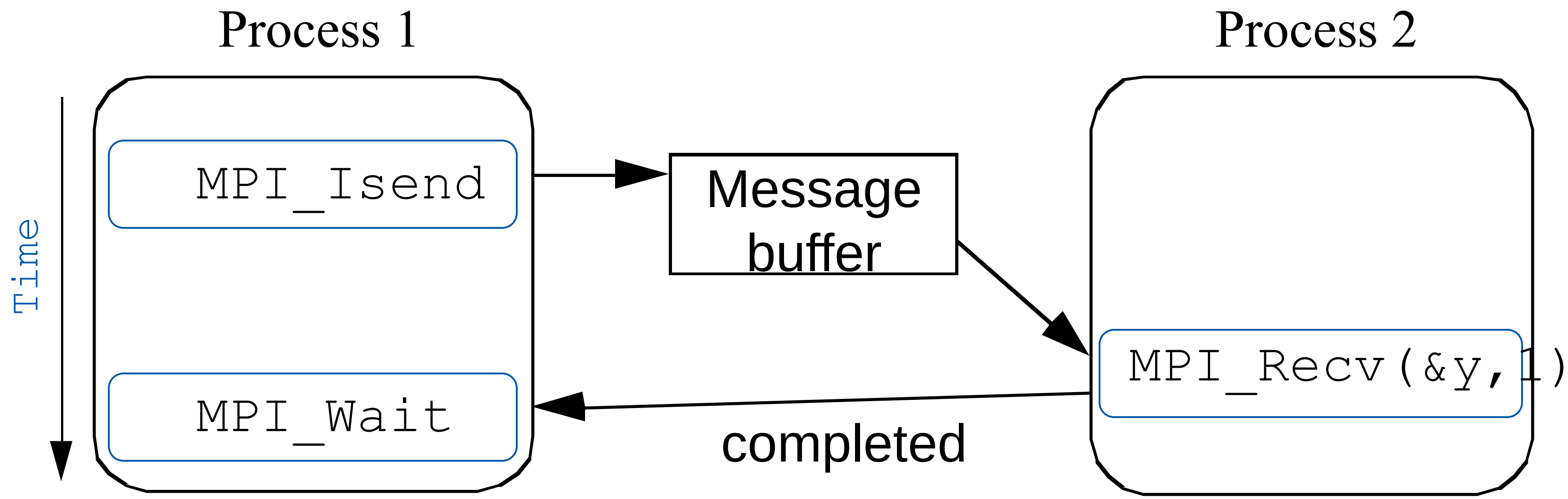
```
int MPI_Testany(int count,
MPI_Request *array_of_requests, int *index,
int *flag, MPI_Status *status)

int MPI_Testall(int count,
MPI_Request *array_of_requests,
int *flag, MPI_Status *status)

int MPI_Testsome(int incount,
MPI_Request *array_of_requests, int *outcount, int
*array_of_indices,
MPI_Status *array_of_statuses)
```

Non-Blocking Functions

Example: Overlapping of Computation and Communication



Example: *Overlapping*

```
if (myrank == 0) {
    int x;
    MPI_Isend(&x,1,MPI_INT,1,3,MPI_COMM_WORLD,
                    req)
    compute();
    MPI_Wait(req,status);
    }
else {
    int x;
    MPI_Recv(&x,1,MPI_INT,0,3,MPI_COMM_WORLD,
                    stat)
    }
```

Additional Send-Modes

Possibilities:

	Blocking	*Non-blocking*
Standard	`MPI_Send`	`MPI_Isend`
Synchronous	`MPI_Ssend`	`MPI_Issend`
Buffered	`MPI_Bsend`	`MPI_Ibsend`
Ready	`MPI_Rsend`	`MPI_Irsend`

Additional Send-Modes

All functions are available blocking & non-blocking

- **Standard Mode**:
  - No assumption about corresponding receive function
  - Buffers depend on implementation
- **Synchronous Mode**:
  - Send/Receive can be started independently but must finish together

Data Transfer

Synchronous communication: *Rendezvous*

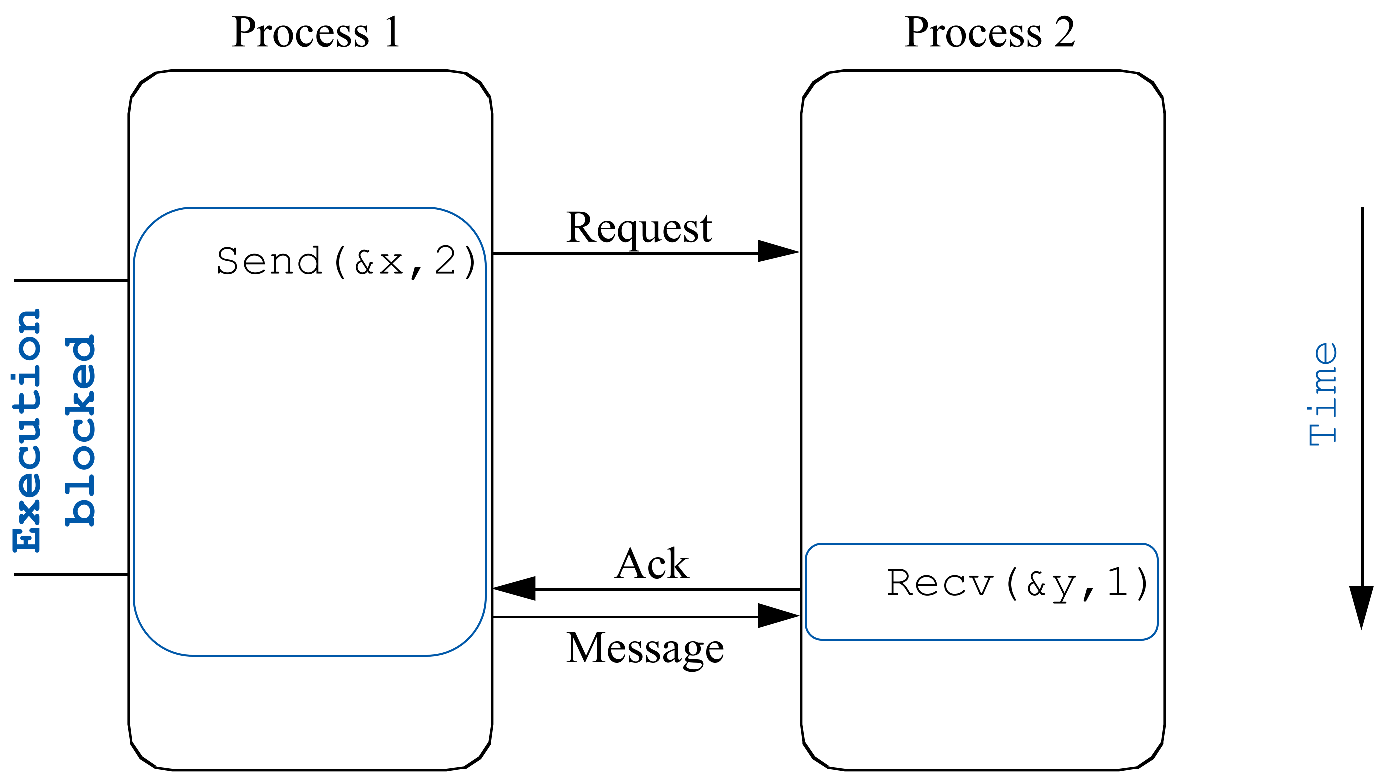
- Return from function represents end of transfer
- Message buffers are not required
- `Send` function waits until receive finished
- `Recv` function waits until message arrives
- Side effect: synchronization of processes

Data Transfer

Asynchronous Communication:

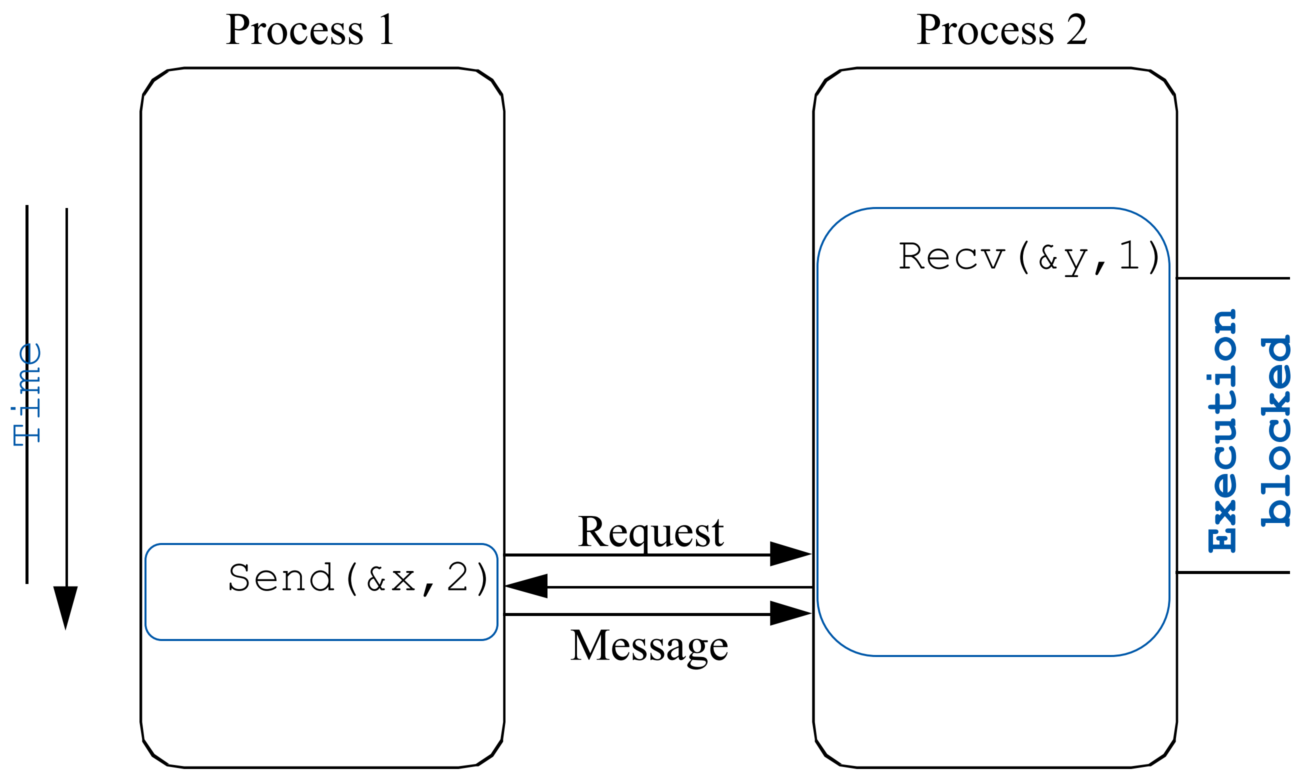
- Send and receive have no temporal connection
- Message buffers are required
- Buffers located at sender or receiver
- Send process does not know,
  whether message actually arrived or not
- Target process may not receive a message

Case 1: Send is called before receive



Synchronous Data Transfer

Case 2: Recv is called before send



Additional Send-Modes

Possibilities:

	Blocking	*Non-blocking*
Standard	`MPI_Send`	`MPI_Isend`
Synchronous	`MPI_Ssend`	`MPI_Issend`
Buffered	`MPI_Bsend`	`MPI_Ibsend`
Ready	`MPI_Rsend`	`MPI_Irsend`

Message Tags

Additional Parameter:

- Identifier for message contents
- Supports distinction of different messages (e.g. commands, data, ...)
- Increases flexibility
- *msgtag* is usually arbitrarily chosen integer

Example:

```
send(&x,2,5) → recv(&y,1,5)
```

Wildcard-Identifiers

Receive-Function:

- Defines message origin and and message tag
- Only corresponding messages are accepted
- All other messages are ignored

Wild card == *Joker*

- Permits messages from arbitrary origin
- Permits messages with arbitrary tag

Wild Card

`recv(&y,a,b)`	origin = a tag = b
`recv(&y,?,b)`	arbitrary origin tag = b
`recv(&y,a,?)`	origin = a arbitrary tag
`recv(&y,?,?)`	arbitrary origin arbitrary tag

MPI Specifics:

- *Wild Card* at receive operation:
  - for message origin: `MPI_ANY_SOURCE`
  - for message tag: `MPI_ANY_TAG`

Problem:

Race Conditions/Nondeterminism

Collective Operations

Until now:

- Point-to-point operations ==> 1 Sender, 1 Receiver

Now:

- Functions and operations involving multiple processes

Collective Operations

Possibilities:

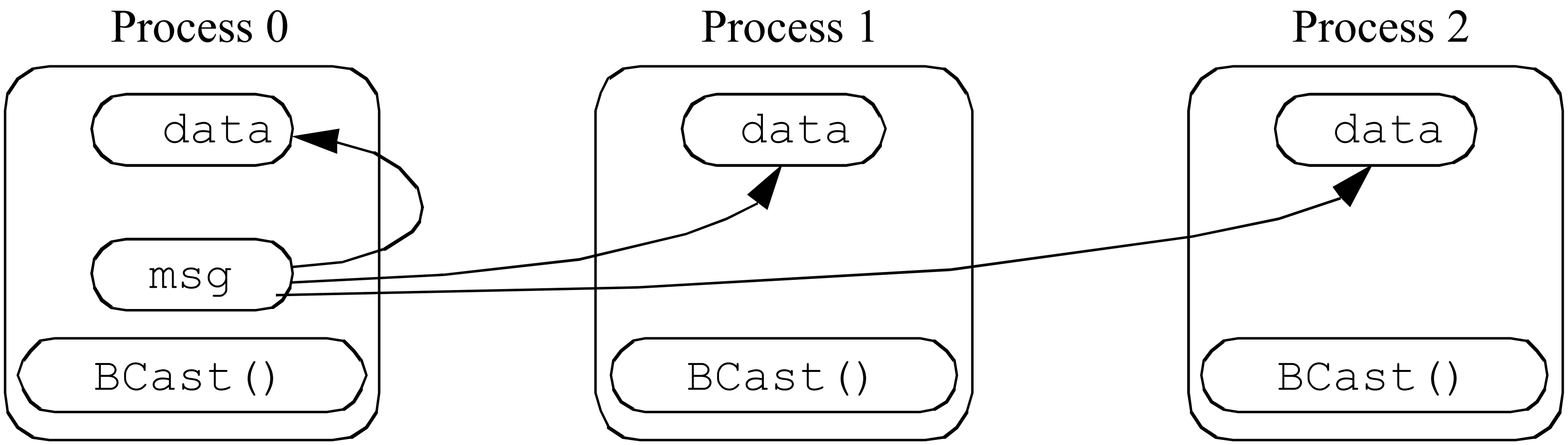
- `MPI_Barrier`: has to be passed by all processes
- `MPI_Bcast`: one process to all others
- `MPI_Gather`: collect data of other processes
- `MPI_Scatter`: distribute data onto other processes
- `MPI_Reduce`: combine data of other processes
- `MPI_Reduce_scatter`: combine and distribute
- ...

Barrier Synchronization

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

- Communicator *comm* defines a group of processes, that has to wait
  until each process has arrived at the barrier

Broadcast/Multicast



MPI Broadcast

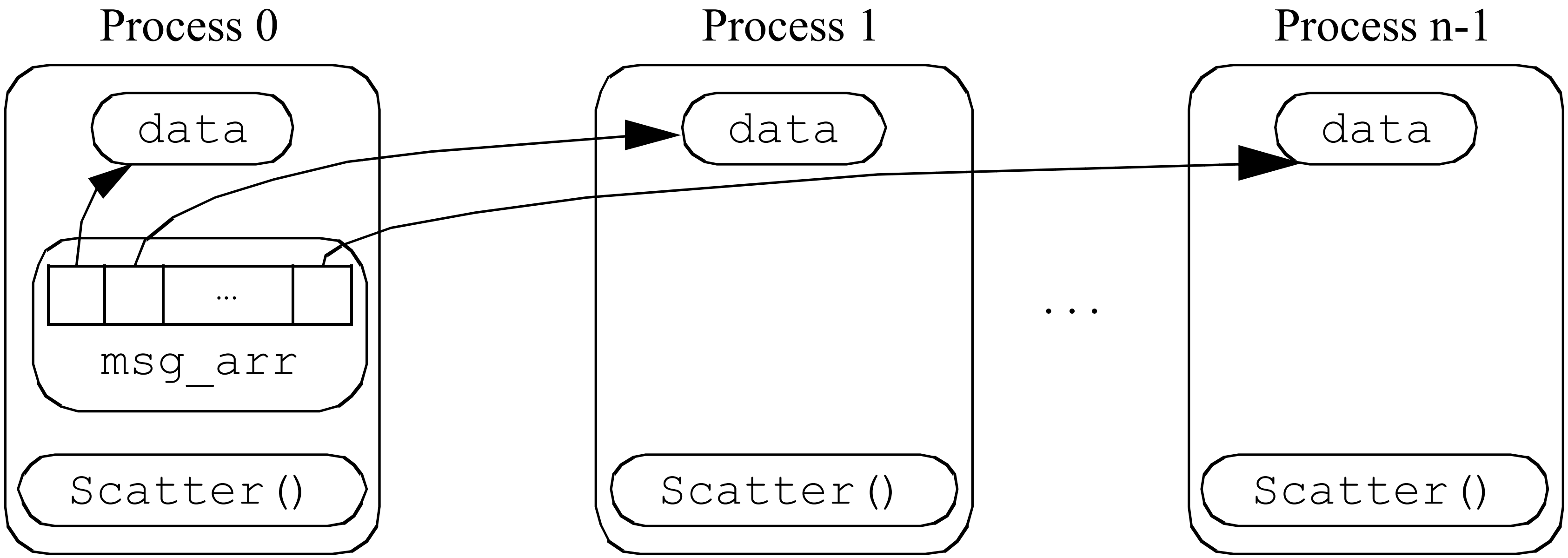
```
int MPI_Bcast(
void *buffer, int count,
MPI_Datatype datatype,
int root, MPI_Comm comm)
```

- Message *buf* of process *root* is distributed to all processes within communicator *comm*

Scatter

- Distribute the array *msg_arr* of process *root* to all other processes
  - Contents at index i is sent to process i
  - Different implementations possible: Data may be returned to *root*, ...
  - Widely used in SPMD Model

Scatter


Process 0
Process 1
Process n-1
data
data
data
...
msg_arr
Scatter()
Scatter()
Scatter()
. . .

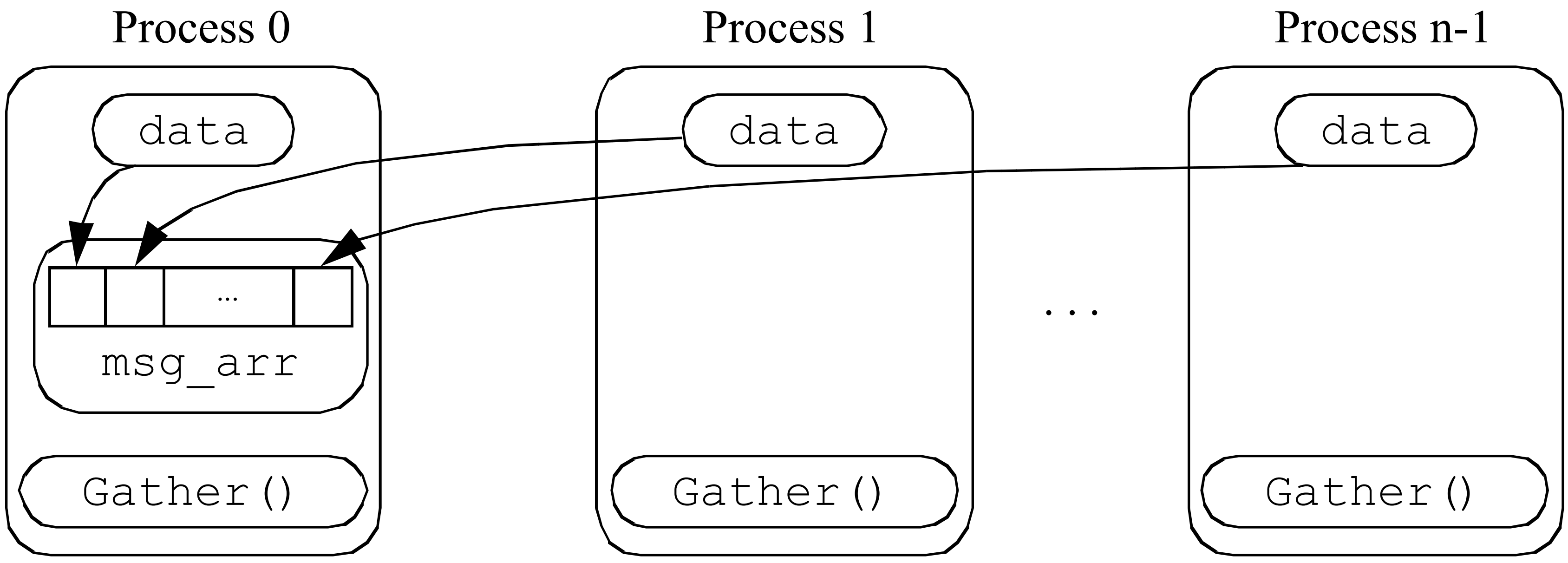
MPI Scatter

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

Gather

- Collect data of all processes on process *root* in array *msg_arr*
  - Data of process i is stored at index i
  - Opposite of Scatter-Operation
  - Usually at the end of a distributed computation
  - Different implementations possible

Gather



Process 0
Process 1
Process n-1
data
data
data
...
msg_arr
. . .
Gather()
Gather()
Gather()

MPI Gather

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

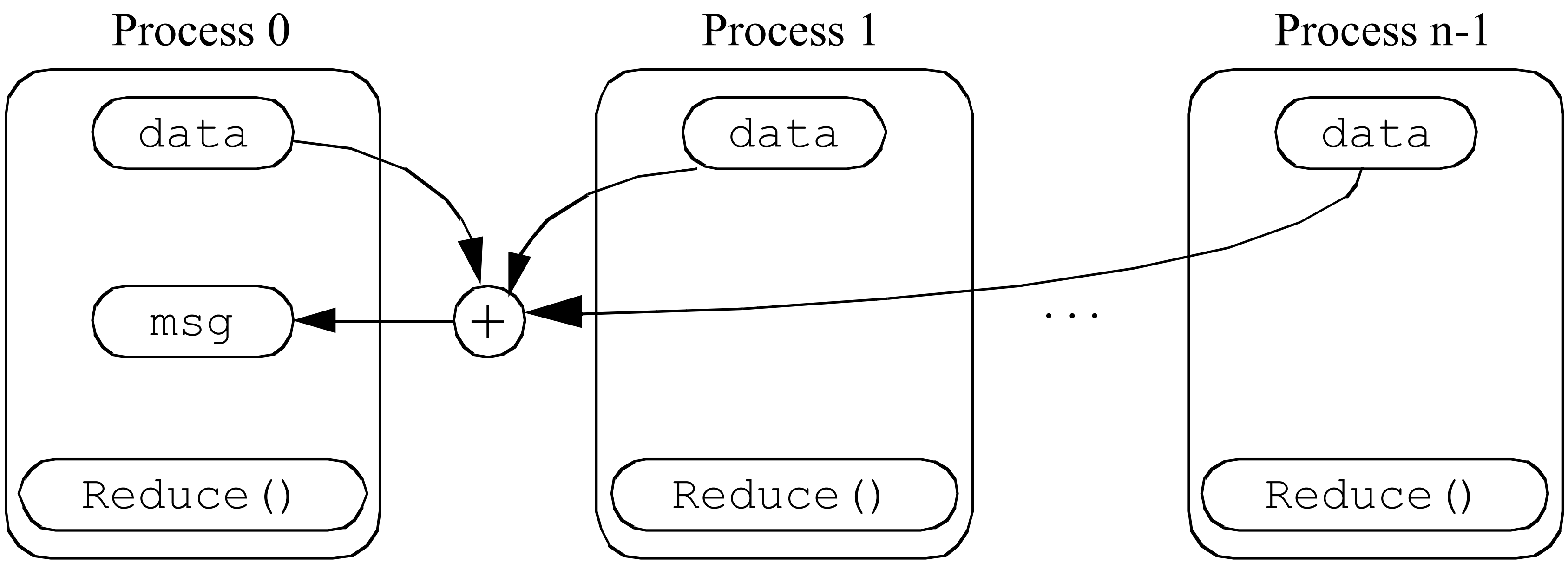
Example: *Data Collection*

```
int data[10];
...
MPI_Comm_rank(MPI_COMM_WORLD,&myrank);
if (myrank == 0) {
   MPI_Comm_size(MPI_COMM_WORLD,&grp_size);
   buf = (int*)malloc(grpsize*10*sizeof(int));
   }
MPI_Gather(data,10,MPI_INT,
   buf,grpsize*10,MPI_INT,0,MPI_COMM_WORLD);
```

Reduce

- Global operation on process *root* during data collection
  - Combination of **Gather** + global operation
  - logical or arithmetic operation possible
  - Different implementations possible:
    operation on *root*,
    partial, distributed operations, ...

Reduce



Process 0
Process 1
Process n-1
data
data
data
msg
+
. . .
Reduce ()
Reduce ()
Reduce ()

MPI Reduce

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

Operations:

`MPI_MAX, MPI_MIN, MPI_SUM, MPI_PROD, …`

Selected Features

- Communicators:
  How to create process groups?
- Topologies:
  How to create virtual topolgies?
- General data types:
  How to use your own data types?

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Communicators

Standard intra-communicator:

- MPI_COMM_WORLD =
  All processes of a program

Functions:

- MPI_Comm_group (comm, group)
- MPI_Group_excl (group, n, ranks, newgroup)
- MPI_Comm_create (comm, group, comm_out)
- MPI_Comm_free (comm)
- ...

Example: Communicator

```
#include <mpi.h>

int main(int argc, char *argv[])
{
    int rank,size;
    int array[8] = {2,3,0,0,0,0,0,0};
    int i,subrank;
    MPI_Status status;
    MPI_Group group;
    MPI_Comm  comm;

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

Example: Communicator

```
...

    MPI_Comm_group(MPI_COMM_WORLD,&group);
    MPI_Group_excl(group,2,array,&group);
    MPI_Group_rank(group,&subrank);
    MPI_Group_size(group,&size);

    MPI_Comm_create(MPI_COMM_WORLD,group,&comm);
    if(subrank != MPI_UNDEFINED) {
       MPI_Gather(&rank,1,MPI_INT,&array,1,
                  MPI_INT,0,comm);
       MPI_Comm_free(&comm);
    }
```

Example: Communicator

```
...

    if(rank == 0) {
       for(i=0;i<size;i++) printf("%d ",array[i]);
       printf("\n");
       }
    MPI_Finalize();
}
```

```
mpirun -np 8 group
0 1 4 5 6 7
```

Selected Features

- Communicators:
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- Topologies:
  How to create virtual topolgies?
- General data types:
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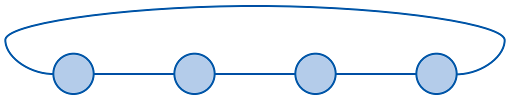
Topologies

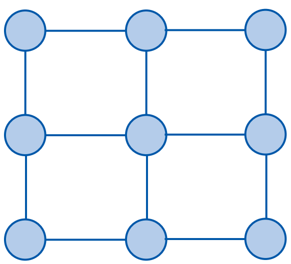
- Topology:
  A graph with the processes as nodes and connections between them as edges.
  - A topology is an attribute stored (*cached*) with a communicator.
  - General graph topology and as special case: grid-topology (Cartesian topology)
  - Topologies are **virtual** and are mapped to the underlying hardware topology
- Topologies add semantics to the program
- Topologies can simplify the code

- Line

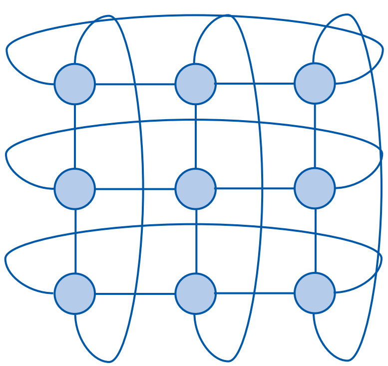
- Ring



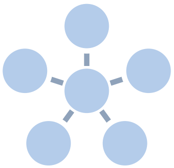
- Mesh



- Torus



- Star



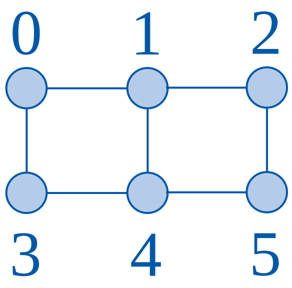
Name	Dimension	Connected?
Line	1	no
Ring	1	yes
Cube	2+	no
Torus	2+	yes
(Hypercube)	4+	no

Note that star is not a grid topology

Grid Topology in MPI

- ```
  MPI_Cart_Create (MPI_Comm old_comm,
                   int number_of_dims,
                   int dim_sizes[],
                   int connected[],
                   int reorder,
                   MPI_Comm *cart_comm)
  ```
- **reorder** determines whether processes in the new communicator can have ranks different to ranks in the old communicator.
  Reordering may have performance advantages.
- Collective operation
  ```

Grid Topology in MPI (2)



- Example:

```
int dims[2], connected[2];
MPI_Comm grid_comm;
dims[0] = 2;
dims[1] = 3;
connected[0] = 0; /* no wrap-around */
connected[1] = 0;
MPI_Cart_create(MPI_COMM_WORLD,2,dims,
                connected, TRUE, &grid_comm);
```

Grid Topology in MPI (3)

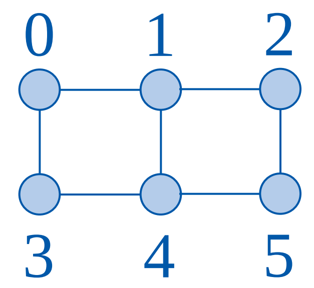
- Processes are numbered in row-major order (2d grids).
- Translation of rank to coordinates by

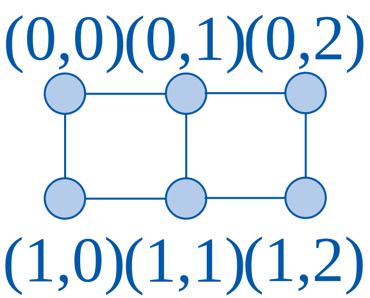
```
MPI_Cart_coords(
        MPI_Comm comm,
        int rank,
        int number_of_dims,
        int coordinates[])
```

- Translation of coordinates to rank by

```
MPI_Cart_rank(
        MPI_Comm comm,
        int coordinates[],
        int *rank)
```

- Local operations



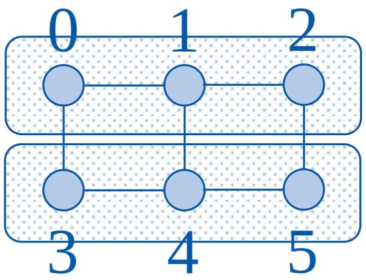


Grid Topology in MPI (4)

- Sub-grid-topologies

```
int free_coords[2];
MPI_comm row_comm;
free_coords[0] = 0;
free_coords[1] = 1;

MPI_Cart_sub (grid_comm,free_coords,
              &row_comm);
```

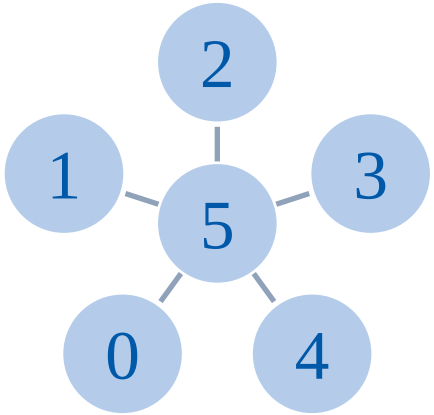


- Creates for each row a new communicator, because the second coordinate (the columns) is declared as *free*. A free coordinate varies, a while a non-free coordinate is fixed for each communicator.
- Collective operation

General Topologies in MPI

- Sparse representation of a graph with one integer and two sets

process	neighbours
0	5
1	5
2	5
3	5
4	5
5	0,1,2,3,4



nnodes = 6;

index = {1,2,3,4,5,9}

edges = {5,5,5,5,5,0,1,2,3,4}

index[0] == degree of node 0

index[i] – index[i-1] == degree of node i, i > 0

- Topologies ease the understanding of a program for humans
  - Better maintainability
  - Lower number of errors
  - “Code is written once but read very often.”

- Performance implications unclear
  - Benefits / penalties of using topologies depends on
    - MPI implementation
    - Underlying network
    - Current actual network partition assigned to user MPI program

Selected Features

- Communicators:
  How to create process groups?
- Topologies:
  How to create virtual topologies?
- General data types:
  How to use your own data types?

General MPI Data Types

- Specification:
  - Array of data types (Type signatures)
  - Array of memory displacements (Type map)

- Message construction:
  - buf ... Start address in memory
  - Typemap = $\{(type_0,disp_0),..., (type_{n-1},disp_{n-1})$
  - Typesig = $\{type_0,..., type_{n-1}\}$
- i^{th} Element:
  - Address = buf + $disp_i$, Data type: $type_i$

MPI Data Types

Functions for creation of data types:

- MPI_Type_contiguous
- MPI_Type_vector
- MPI_Type_hvector
- MPI_Type_indexed
- MPI_Type_hindexed
- MPI_Type_struct

Additional functions:

- MPI_Address
- MPI_Type_extent
- MPI_Type_size

Minimum Set of Functions?

For an arbitrary MPI program,
*only **6 Functions** are needed*

- `MPI_Init(...)`
- `MPI_Finalize(...)`
- `MPI_Comm_rank(...)`
- `MPI_Comm_size(...)`
- `MPI_Send(...)`
- `MPI_Recv(...)`