An Introduction to MPI

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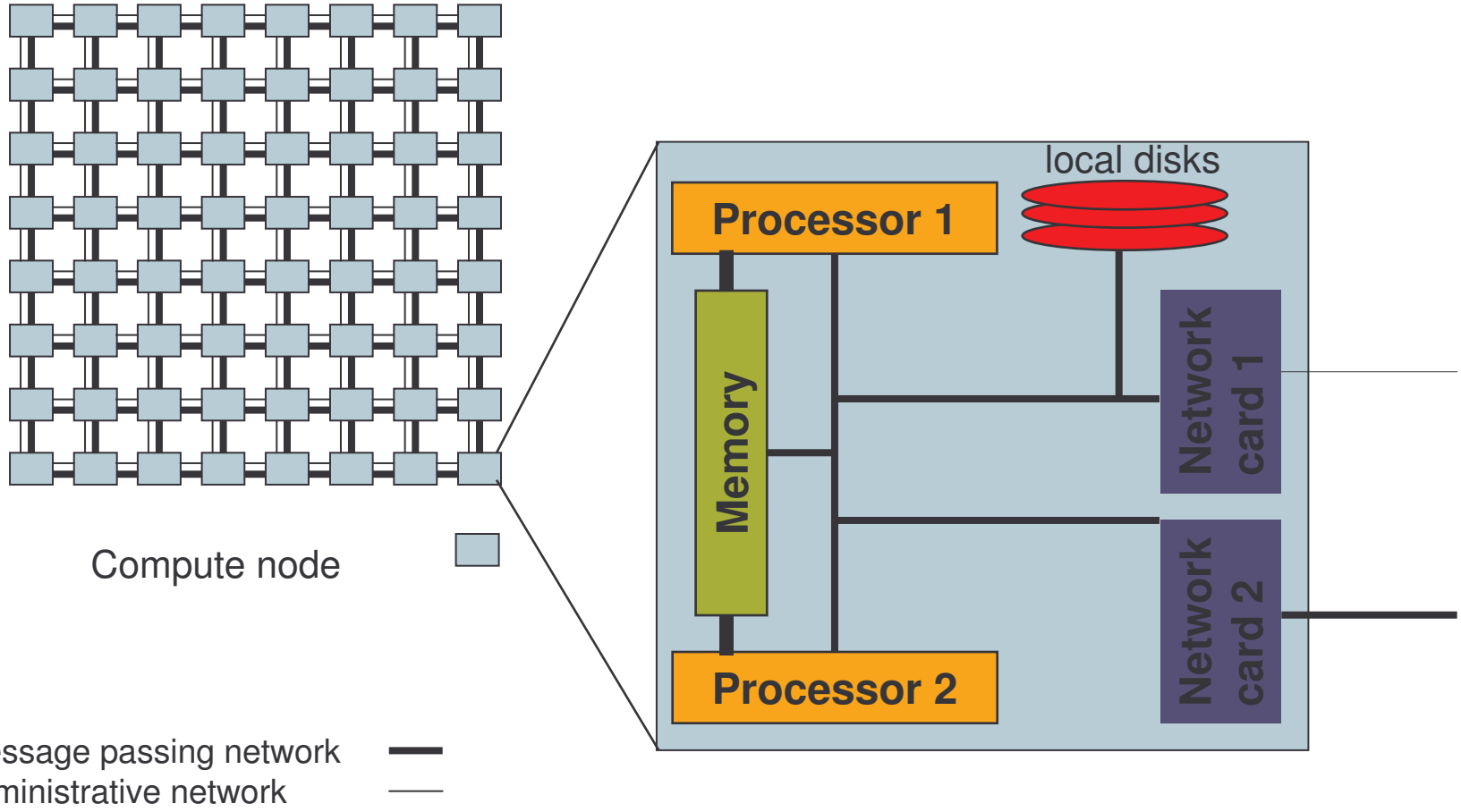
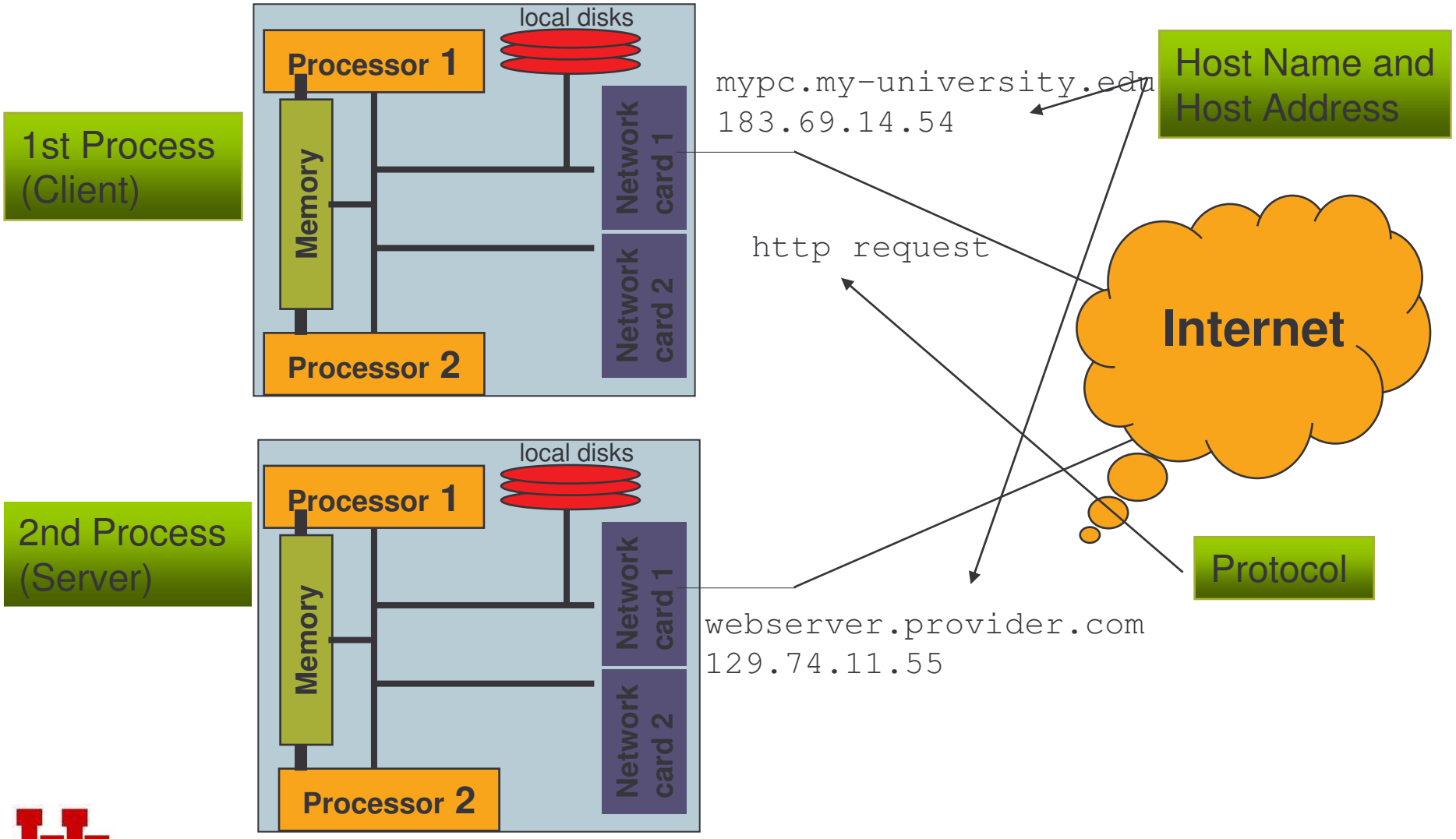
Overview

- Distributed memory machines
- Basic principles of the Message Passing Interface (MPI)
  - addressing
  - startup
  - data exchange
  - process management
  - communication

Distributed memory machines



Communication between different machines



Communication between different machines on the Internet

- Addressing:
  - hostname and/or IP Address
- Communication:
  - based on protocols, e.g. http or TCP/IP
- Process start-up:
  - every process (= application) has to be started separately

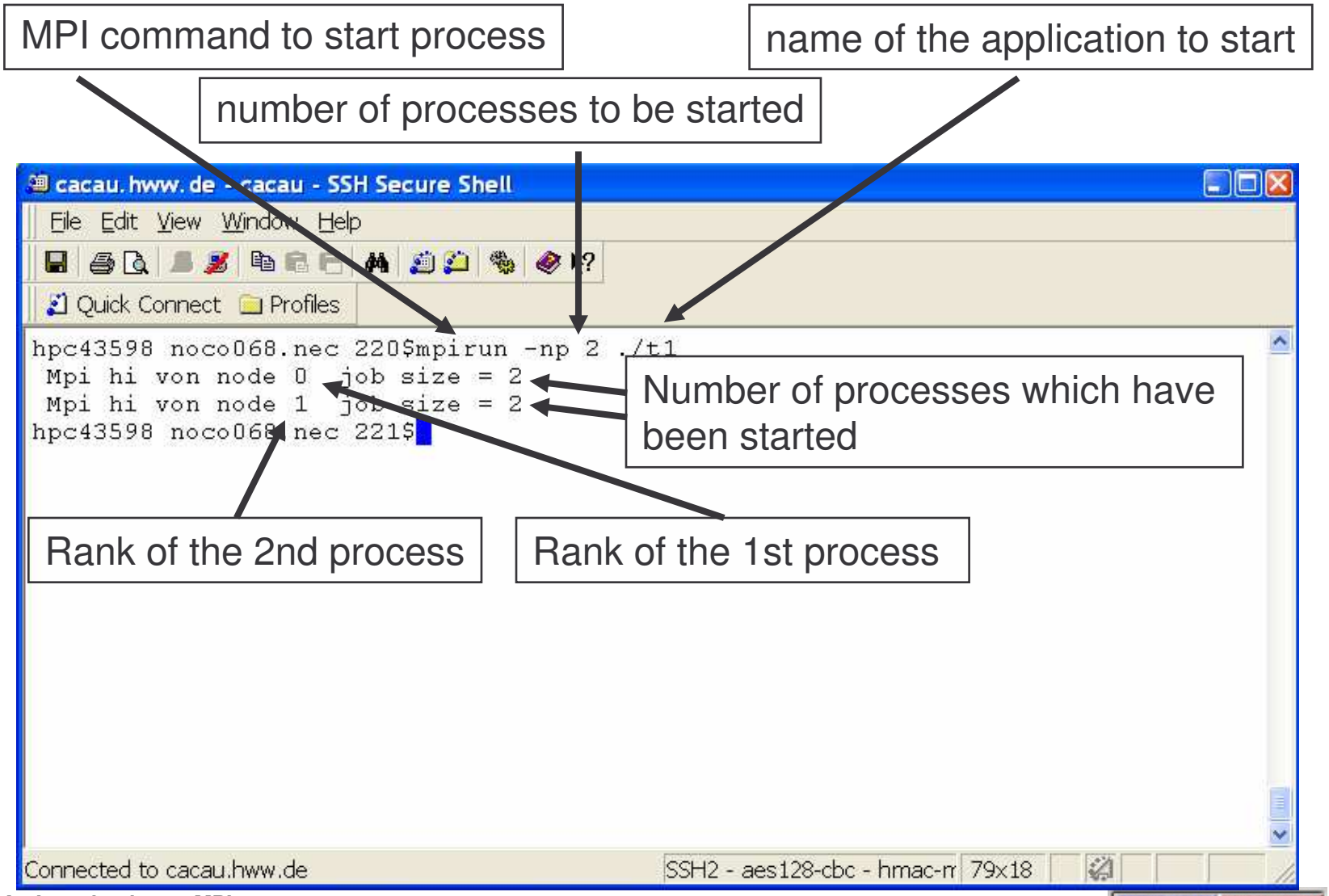
The Message Passing universe

- Process start-up:
  - Want to start *n*-processes which shall work on the same problem
  - mechanisms to start n-processes provided by MPI library
- Addressing:
  - Every process has a unique identifier. The value of the rank is between *0* and *n-1.*
- Communication:
  - MPI defines interfaces/routines how to send data to a process and how to receive data from a process. It does not specify a protocol.

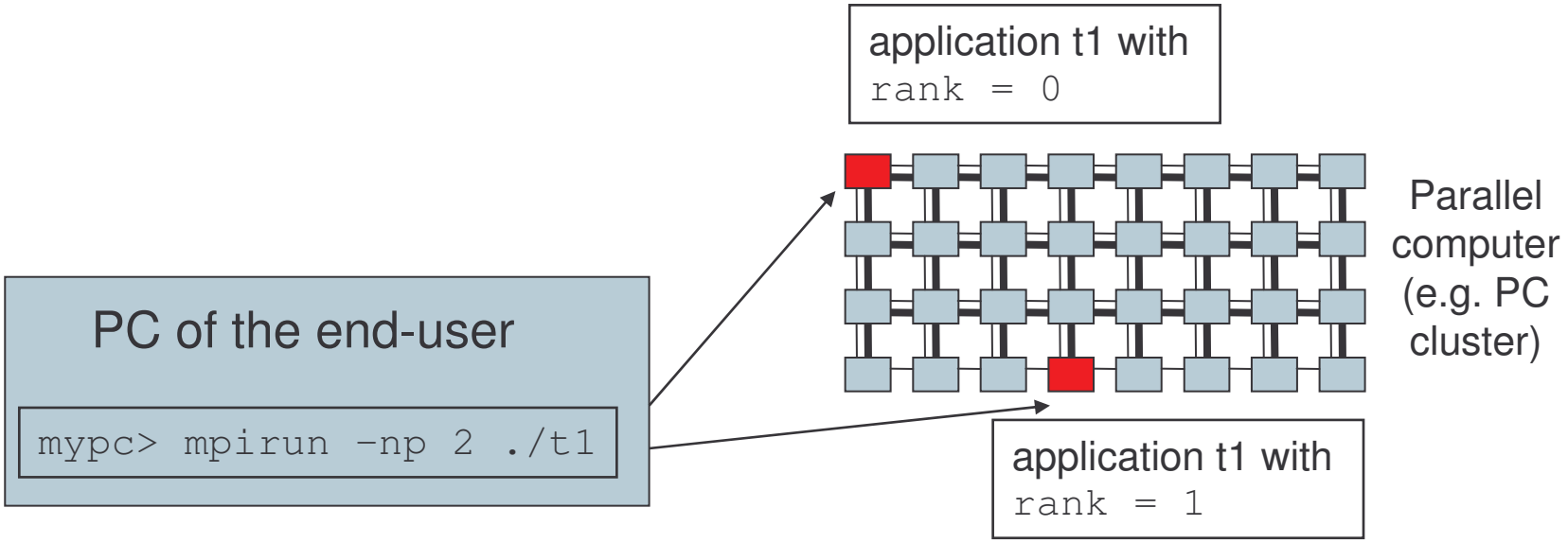
History of MPI

- Until the early 90's:
  - all vendors of parallel hardware had their own message passing library
  - Some public domain message passing libraries available
  - all of them being incompatible to each other
  - High efforts for end-users to move code from one architecture to another
- June 1994: Version 1.0 of MPI presented by the MPI Forum
- June 1995: Version 1.1 (errata of MPI 1.0)
- 1997: MPI 2.0 – adding new functionality to MPI

Simple Example (I)



Simple example (II)



`mpirun` starts the application `t1`

- two times (as specified with the –np argument)
- on two currently available processors of the parallel machine
- telling one process that his `rank` is 0
- and the other that his `rank` is 1

Simple Example (III)

```
#include "mpi.h"

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

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

  printf ("Mpi hi von node %d job size %d\n",
           rank, size);

  MPI_Finalize ();
  return (0);
}
```

MPI basics

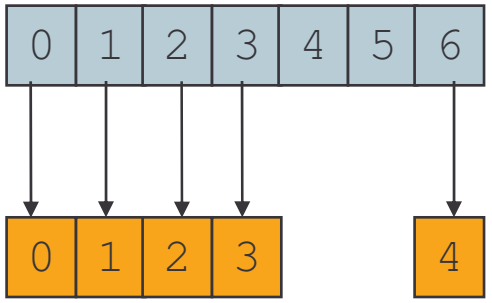
- `mpirun` starts the required number of processes
- every process has a unique identifier (`rank`) which is between `0` and `n-1`
  - no identifiers are duplicate, no identifiers are left out
- all processes which have been started by `mpirun` are organized in a process group (`communicator`) called `MPI_COMM_WORLD`
- `MPI_COMM_WORLD` is static
  - number of processes can not change
  - participating processes can not change

MPI basics (II)

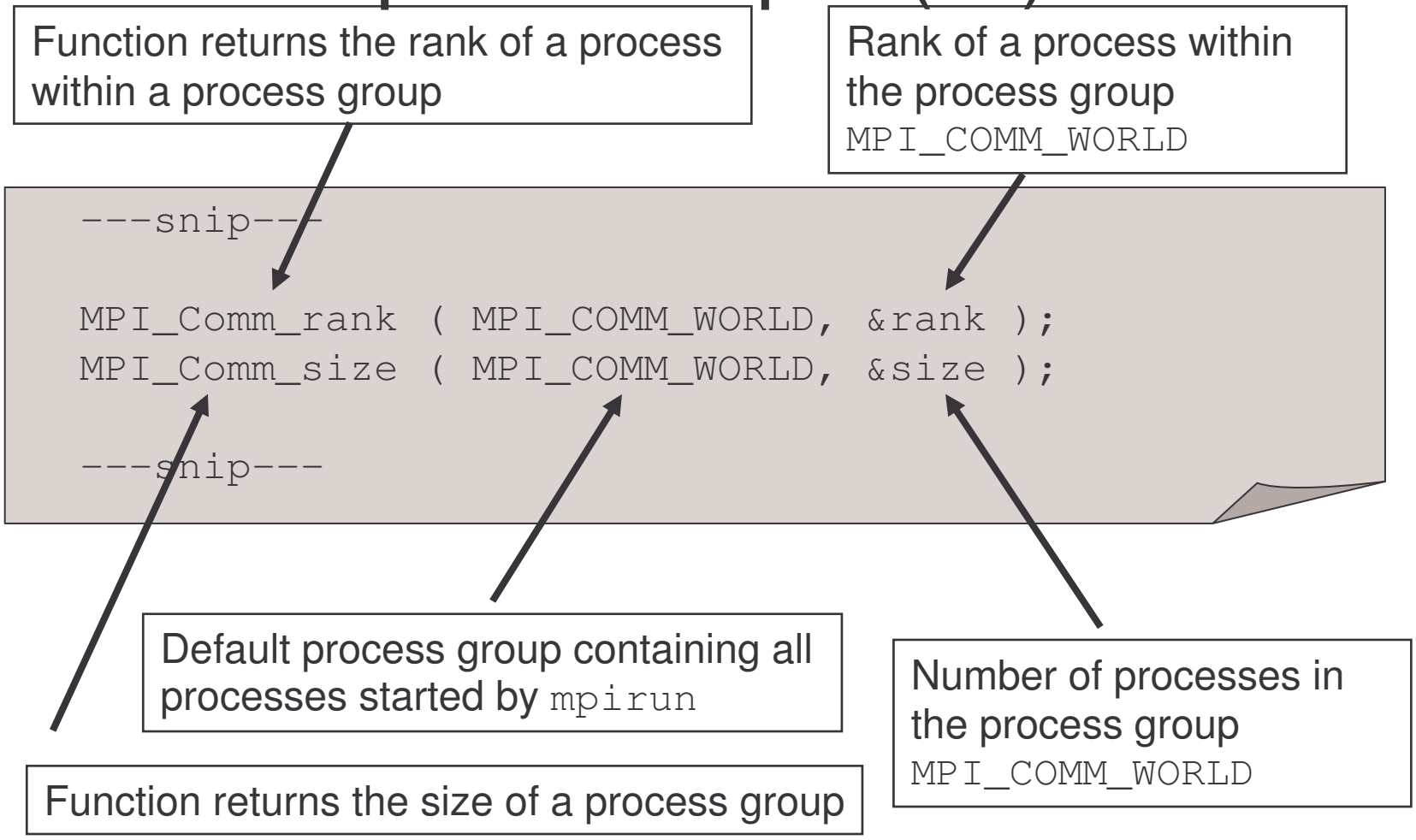
- The rank of a process is always related to the process group
  - e.g. a process is uniquely identified by a tuple (`rank, process group`)
- A process can be part of the several groups
  - i.e. a process has in each group a rank

`MPI_COMM_WORLD, size=7`

`new process group, size = 5`



Simple Example (IV)



Simple Example (V)

Function sets up parallel environment:

- processes set up network connection to each other
- default process group (`MPI_COMM_WORLD`) is set up
- should be the first function executed in the application

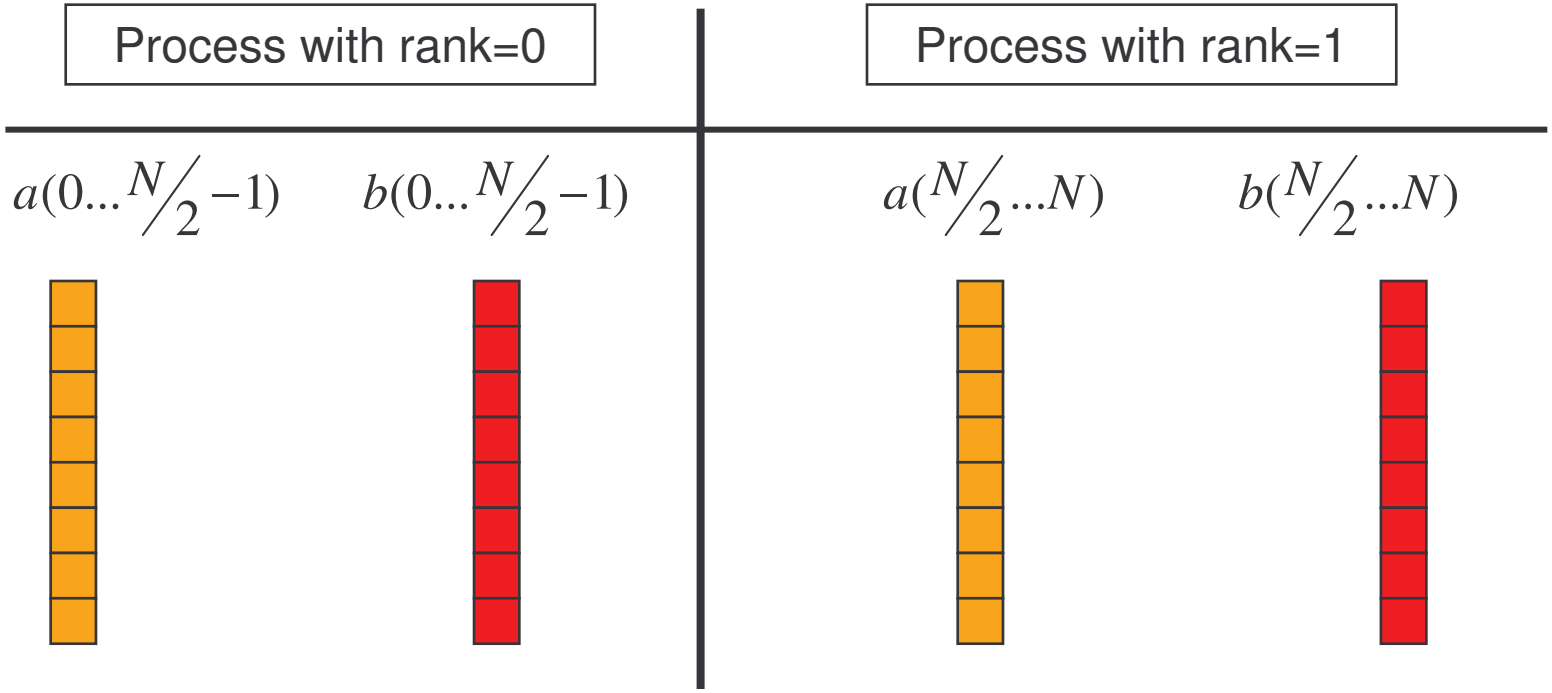
```
---snip---
MPI_Init (&argc, &argv );
---snip---
MPI_Finalize ();
---snip---
```

Function closes the parallel environment

- should be the last function called in the application
- might stop all processes

Second example – scalar product of two vectors

- two vectors are distributed on two processors
  - each process holds half of the original vector



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Second example (II)

- Logical/Global view of the data compared to local view of the data

Process with rank=0	Process with rank=1
$a(0...N/2-1)$	$a(N/2...N)$
$a_{local}(0) \Rightarrow a(0)$	$a_{local}(0) \Rightarrow a(N/2)$
$a_{local}(1) \Rightarrow a(1)$	$a_{local}(1) \Rightarrow a(N/2+1)$
$a_{local}(2) \Rightarrow a(2)$	$a_{local}(2) \Rightarrow a(N/2+2)$
$\vdots$	$\vdots$
$a_{local}(n) \Rightarrow a(N/2-1)$	$a_{local}(n) \Rightarrow a(N-1)$

Second example (III)

- Scalar product:

$$s = \sum_{i=0}^{N-1} a[i] * b[i]$$

- Parallel algorithm

$$s = \sum_{i=0}^{N/2-1} (a[i] * b[i]) + \sum_{i=N/2}^{N-1} (a[i] * b[i])$$

$$= \underbrace{\sum_{i=0}^{N/2-1} (a_{local}[i] * b_{local}[i])}_{rank=0} + \underbrace{\sum_{i=0}^{N/2-1} (a_{local}[i] * b_{local}[i])}_{rank=1}$$

  - requires communication between the processes

Second example (IV)

```
#include "mpi.h"

int main ( int argc, char **argv )
{
  int i, rank, size;
  double a_local[N/2], b_local[N/2];
  double s_local, s;

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

  s_local = 0;
  for ( i=0; i<N/2; i++ ) {
    s_local = s_local + a_local[i] * b_local[i];
  }
```

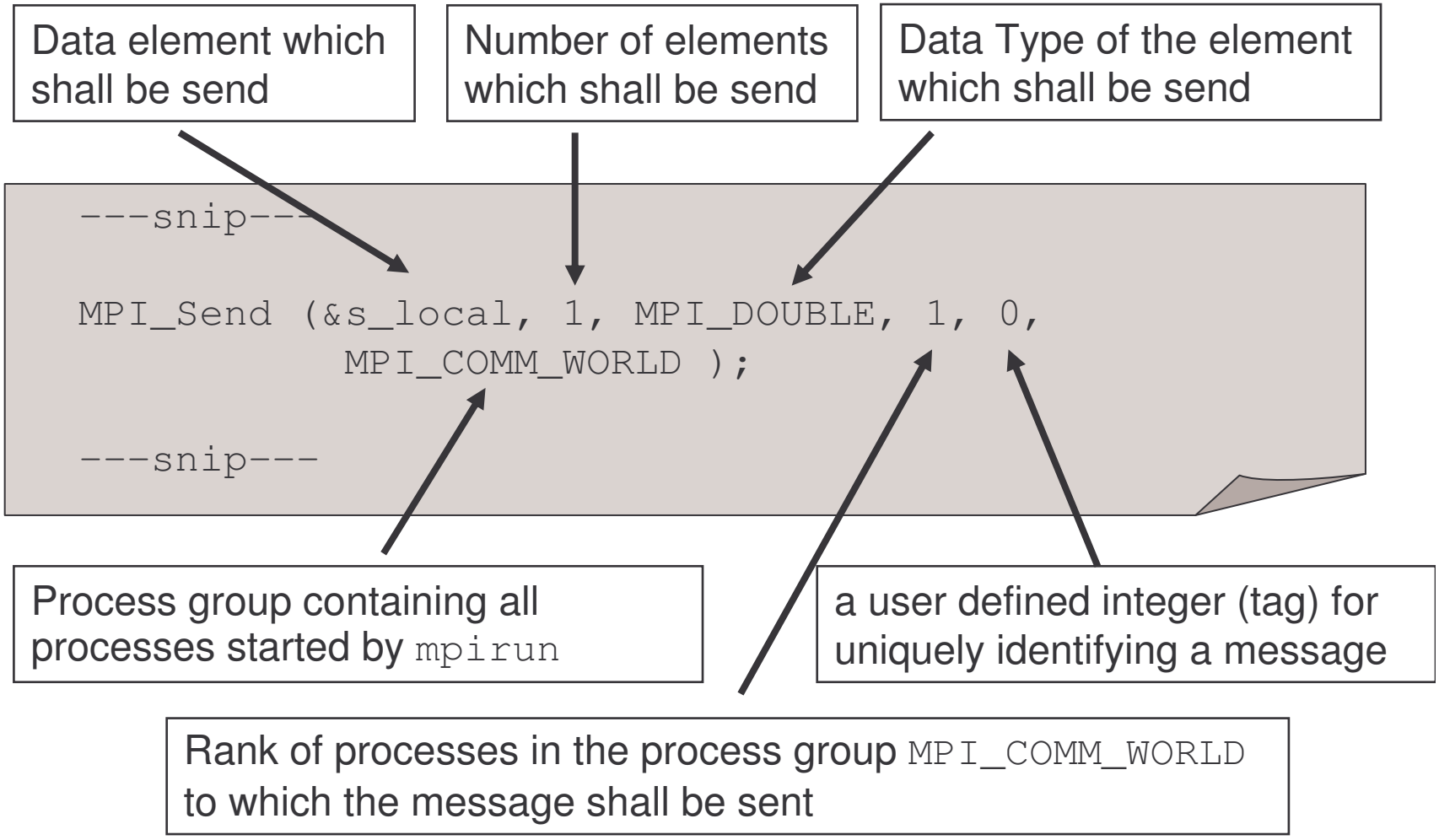
Second example (V)

```
  if ( rank == 0 ) {
    /* Send the local result to rank 1 */
    MPI_Send ( &s_local, 1, MPI_DOUBLE, 1, 0,
               MPI_COMM_WORLD);
}
  if ( rank == 1 ) {
    MPI_Recv ( &s, 1, MPI_DOUBLE, 0, 0,
               MPI_COMM_WORLD, &status );

    /* Calculate global result */
    s = s + s_local;
  }
```

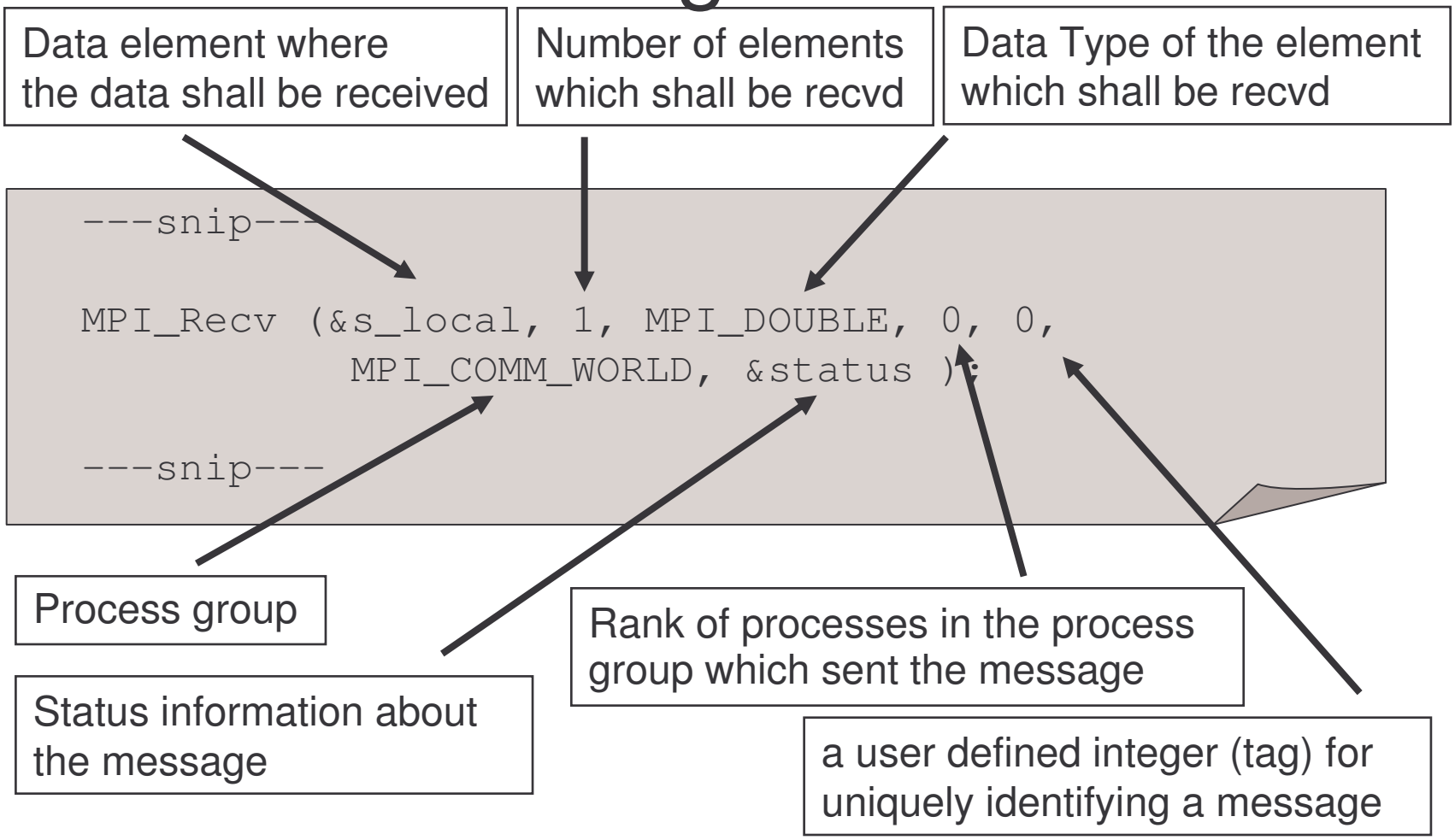
Second example (VI)

```
  /* Rank 1 holds the global result and sends it now
     to rank 0 */
  if ( rank == 0 ) {
    MPI_Recv (&s, 1, MPI_DOUBLE, 1, 1, MPI_COMM_WORLD,
              &status );
  }
  if ( rank == 1 ) {
    MPI_Send (&s, 1, MPI_DOUBLE, 0, 1, MPI_COMM_WORLD);
  }

  /* Close the parallel environment */
  MPI_Finalize ();
  return (0);
}
```

Sending Data



Receiving Data



Faulty examples (I)

- Sender mismatch:
  - if rank does not exist (e.g. `rank > size` of `MPI_COMM_WORLD`), the MPI library can recognize it and return an error
  - if rank does exist (`0<rank<size` of `MPI_COMM_WORLD`) but does not send a message => `MPI_Recv` waits forever => deadlock

```
  if ( rank == 0 ) {
    /* Send the local result to rank 1 */
    MPI_Send ( &s_local, 1, MPI_DOUBLE, 1, 0,
               MPI_COMM_WORLD);
}
  if ( rank == 1 ) {
    MPI_Recv ( &s, 1, MPI_DOUBLE, 5, 0,
               MPI_COMM_WORLD, &status );

}
```

Faulty examples (II)

- Tag mismatch:
  - if tag outside of the allowed range (e.g. `0<tag<MPI_TAG_UB`) the MPI library can recognize it and return an error
  - if tag in `MPI_Recv` then the tag specified in `MPI_Send` => `MPI_Recv` waits forever => deadlock

```
  if ( rank == 0 ) {
    /* Send the local result to rank 1 */
    MPI_Send ( &s_local, 1, MPI_DOUBLE, 1, 0,
               MPI_COMM_WORLD);
}
  if ( rank == 1 ) {
    MPI_Recv ( &s, 1, MPI_DOUBLE, 0, 18,
               MPI_COMM_WORLD, &status );

}
```

What you've learned so far

- Six MPI functions are sufficient for programming a distributed system memory machine

```
MPI_Init(int *argc, char ***argv);
MPI_Finalize ();

MPI_Comm_rank (MPI_Comm comm, int *rank);
MPI_Comm_size (MPI_Comm comm, int *size);

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

So, why not stop here?

- Performance
  - need functions which can fully exploit the capabilities of the hardware
  - need functions to abstract typical communication patterns
- Usability
  - need functions to simplify often recurring tasks
  - need functions to simplify the management of parallel applications

So, why not stop here?

- Performance
  - asynchronous point-to-point operations
  - one-sided operations
  - collective operations
  - derived data-types
  - parallel I/O
  - hints
- Usability
  - process grouping functions
  - environmental and process management
  - error handling
  - object attributes
  - language bindings

Collective operation

- all process of a process group have to participate in the same operation
  - process group is defined by a communicator
  - all processes have to provide the same arguments
  - for each communicator, you can have one collective operation ongoing at a time
- collective operations are abstractions for often occurring communication patterns
  - eases programming
  - enables low-level optimizations and adaptations to the hardware infrastructure

MPI collective operations

```
MPI_Barrier
MPI_Bcast
MPI_Scatter
MPI_Scatterv
MPI_Gather
MPI_Gatherv
MPI_Allgather
MPI_Allgatherv
MPI_Alltoall
MPI_Alltoallv
MPI_Reduce
MPI_Allreduce
MPI_Reduce_scatter
MPI_Scan
```

```
MPI_Exscan
MPI_Alltoallw
```

More MPI collective operations

- Creating and freeing a communicator is considered a collective operation
  - e.g. `MPI_Comm_create`
  - e.g. `MPI_Comm_spawn`

- Collective I/O operations
  - e.g. `MPI_Write_all`

- Window synchronization calls are collective operations
  - e.g. `MPI_Win_fence`

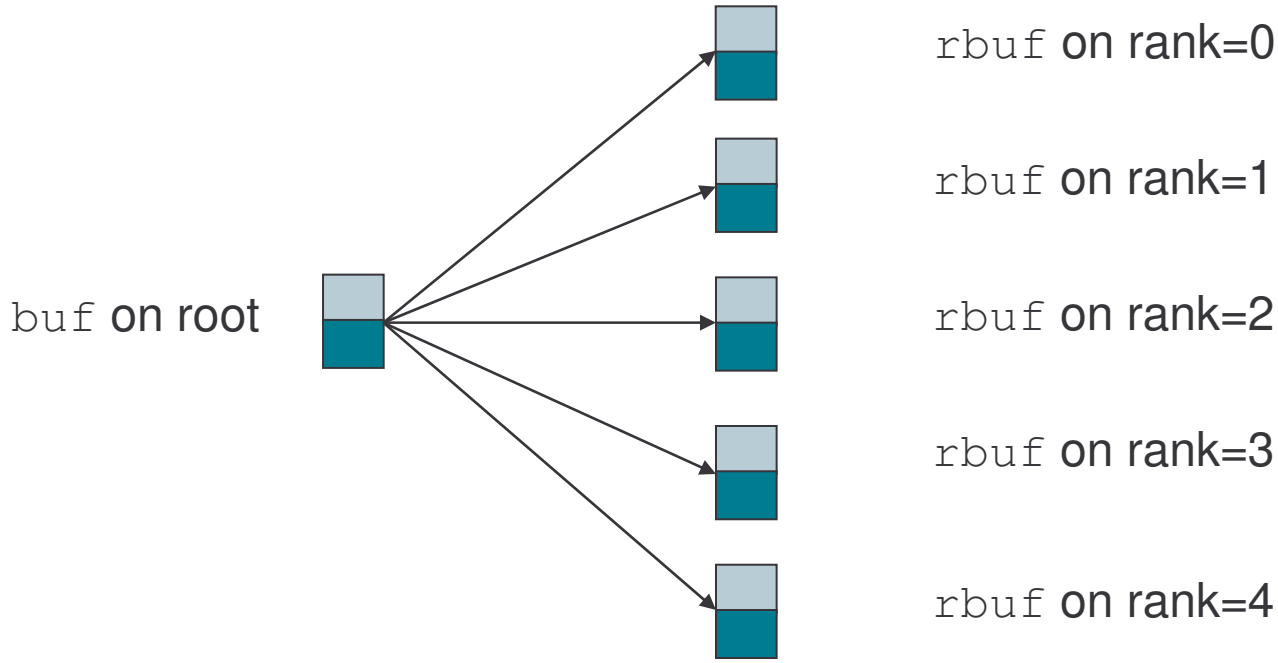
MPI_Bcast

```
MPI_Bcast (void *buf, int cnt, MPI_Datatype dat,
           int root, MPI_Comm comm);
```

- The process with the rank `root` distributes the data stored in `buf` to all other processes in the communicator `comm`.
- Data in `buf` is identical on all processes after the bcast
- Compared to point-to-point operations no `tag`, since you cannot have several ongoing collective operations

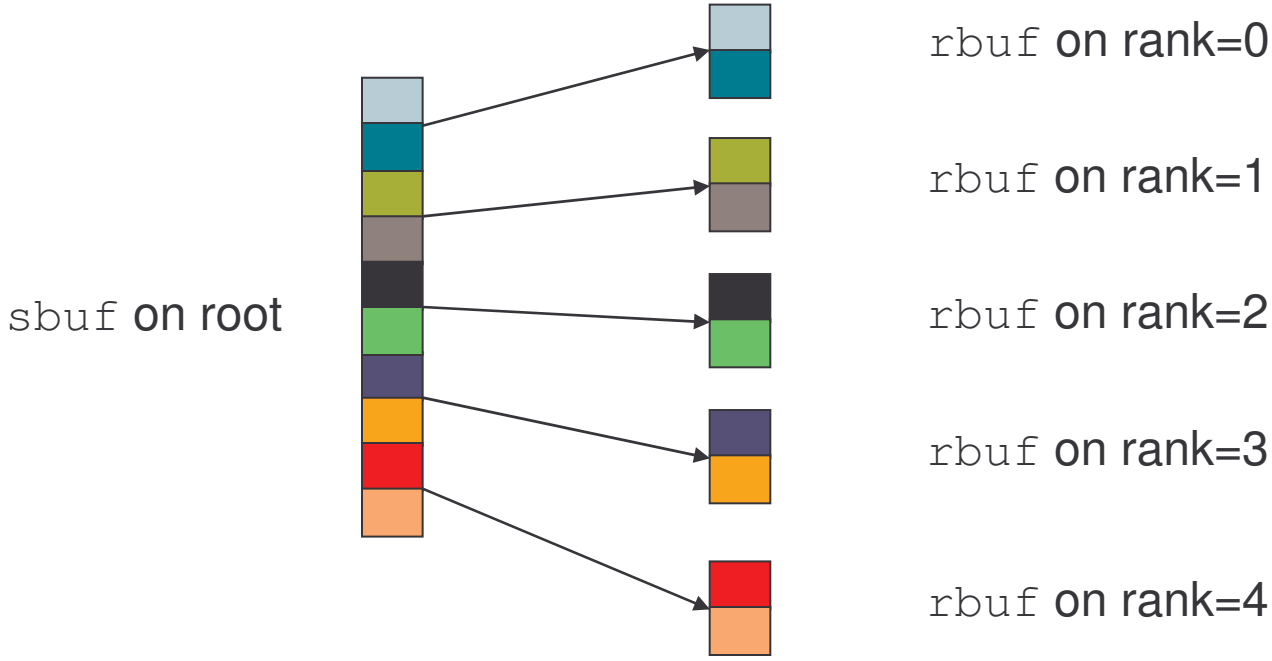
MPI_Bcast (II)

```
MPI_Bcast (buf, 2, MPI_INT, 0, comm);
```



MPI_Scatter (II)

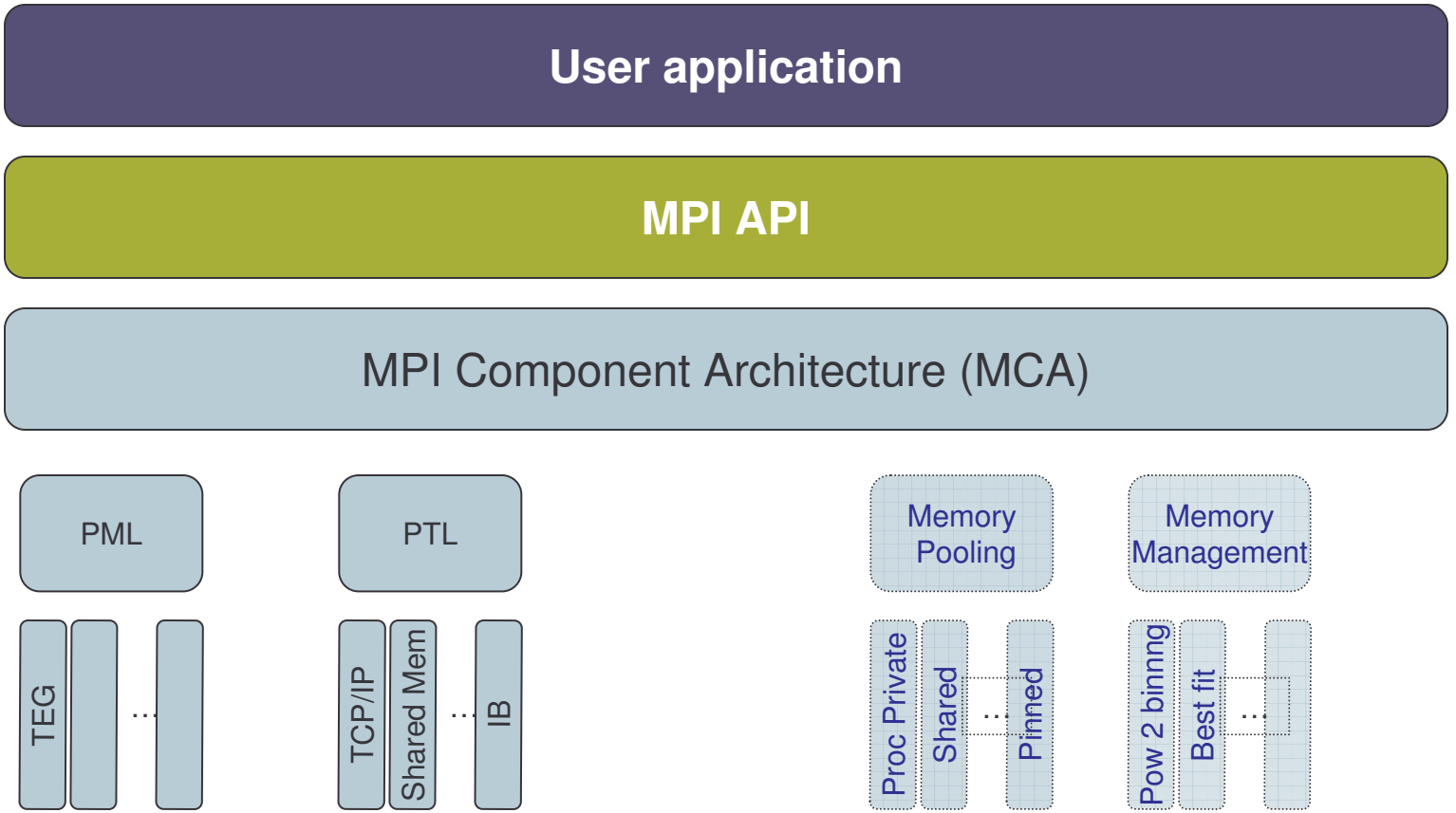
```
MPI_Scatter (sbuf, 2, MPI_INT, rbuf, 2, MPI_INT, 0, comm);
```



MPI Error handlers

- An error handler is a function which is called by the MPI library in case an error occurs
  - Wrong input parameters
  - Network or process failures
- MPI defines two predefined error handlers:
  - MPI_ERRORS_ARE_FATAL (Default): Abort the application on the first error
  - MPI_ERRORS_RETURN: Return error-code to user
    - State of MPI undefined
    - does *not* necessarily allow the user to continue to use MPI after an error is detected
- User can register its own error handler functions

Some implementation aspects: Open MPI



Some Links

- MPI Forum:
  - http://www.mpi-forum.org
- My personal MPI home page:
  - http://www.cs.uh.edu/~gabriel/mpihome.html

- Open MPI:
  - http://www.open-mpi.org
- MPICH:
  - http://www-unix.mcs.anl.gov/mpi/mpich/