Introduction to MPI

Introduction to the HPC System of the University Oldenburg
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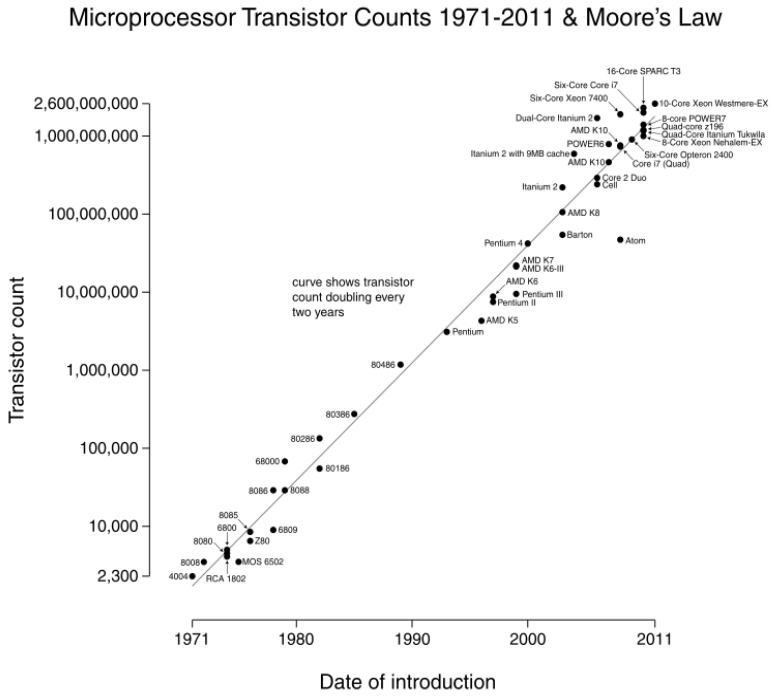
- Motivation for Parallel Computing
- Overview of Parallel Hardware Architectures and Programming Models
- Introduction to MPI
- Examples and Exercises using MPI

Why Parallel Computing?

- Moore's Law
  - the number of transistors in a dense integrated circuit doubles every 12 to 24 months
  - often interpreted as computing speed doubles every ~18 months
  - empirical law and self-fulfilling prophecy
  - Moore's Law must eventually break down

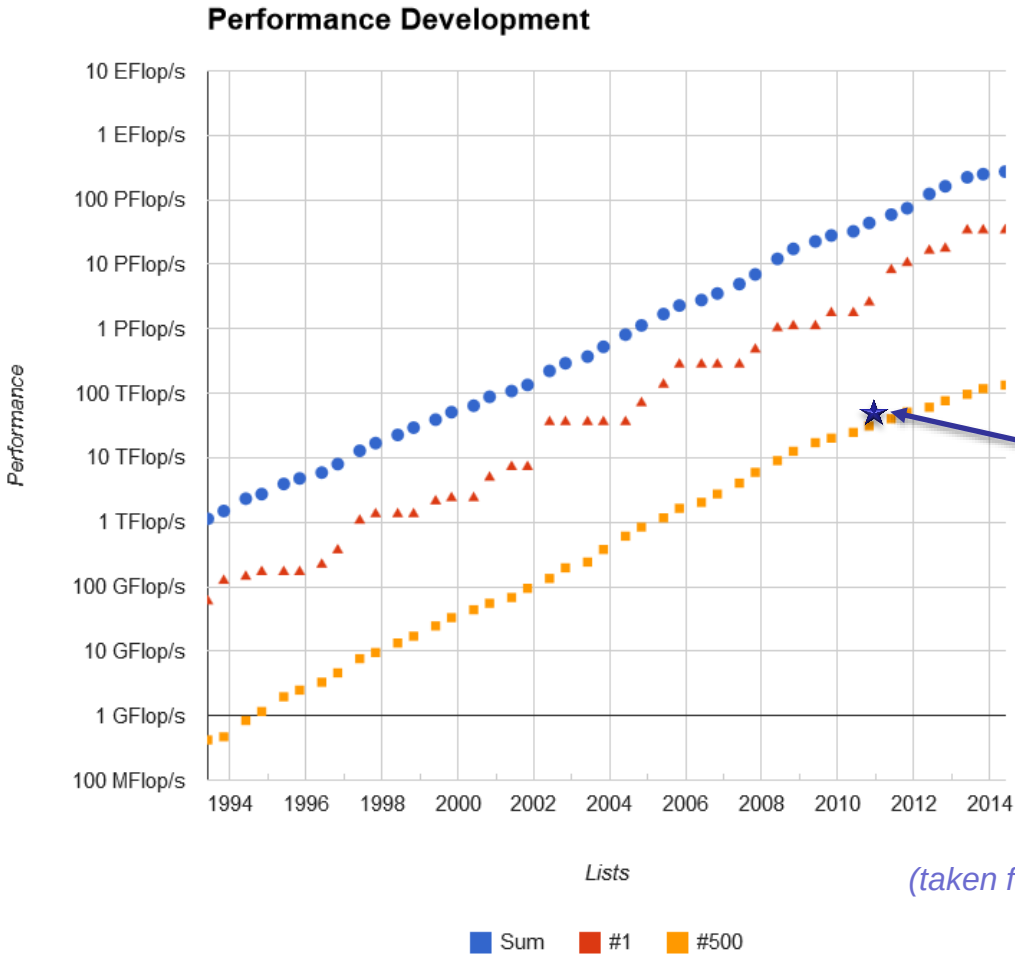


(taken from Wikipedia)

Why Parallel Computing?

- laws of physics set limit of how fast computers can become
  - speed of light, quantum scale, … *(see Lloyd, 2000, Nature, **406,** 1047)*
- of course before that there technical limitations
  - e.g. heat from CPU power dissipation → limits the cycle frequency
- what is the solution to the problem?
  1. develop more efficient algorithms
  2. parallel computing

The Fastest Computers on Earth



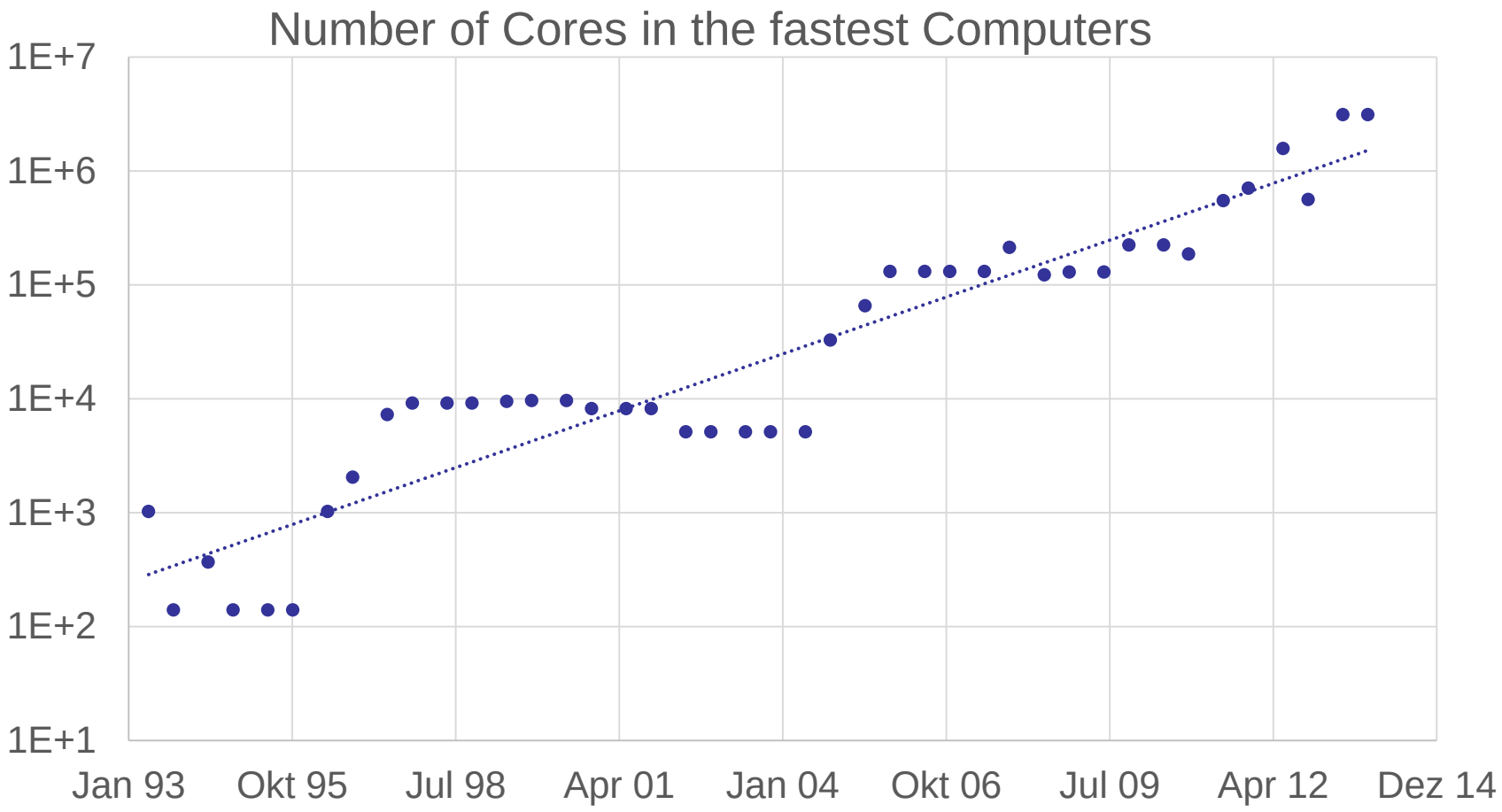
Theoretical Peak Performance

FLOW/HERO/UV100 ≈ 45 Tflop/s

(plot shows measured performance)

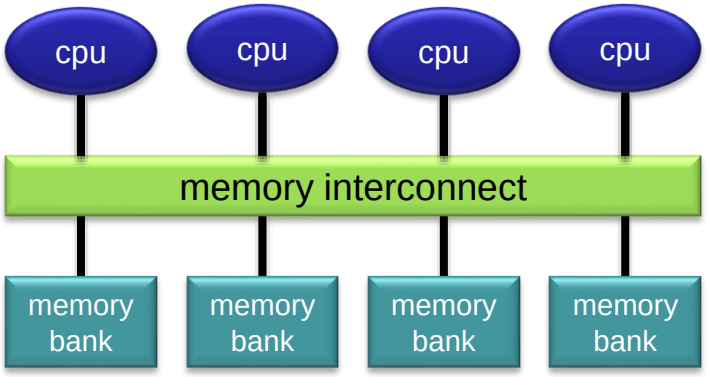
(taken from top500.org)

Why Parallel Computing?

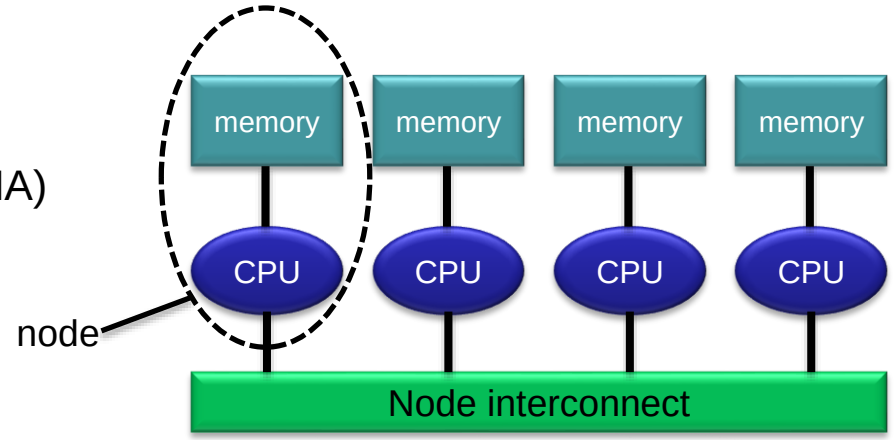


Parallel Hardware Architectures

- multiprocessor
  - shared memory
  - cores are connected to memory with the same speed
  - **U**niform **M**emory **A**ccess (UMA)
  - **S**ymmetric **M**ulti-**P**rocessing (SMP)

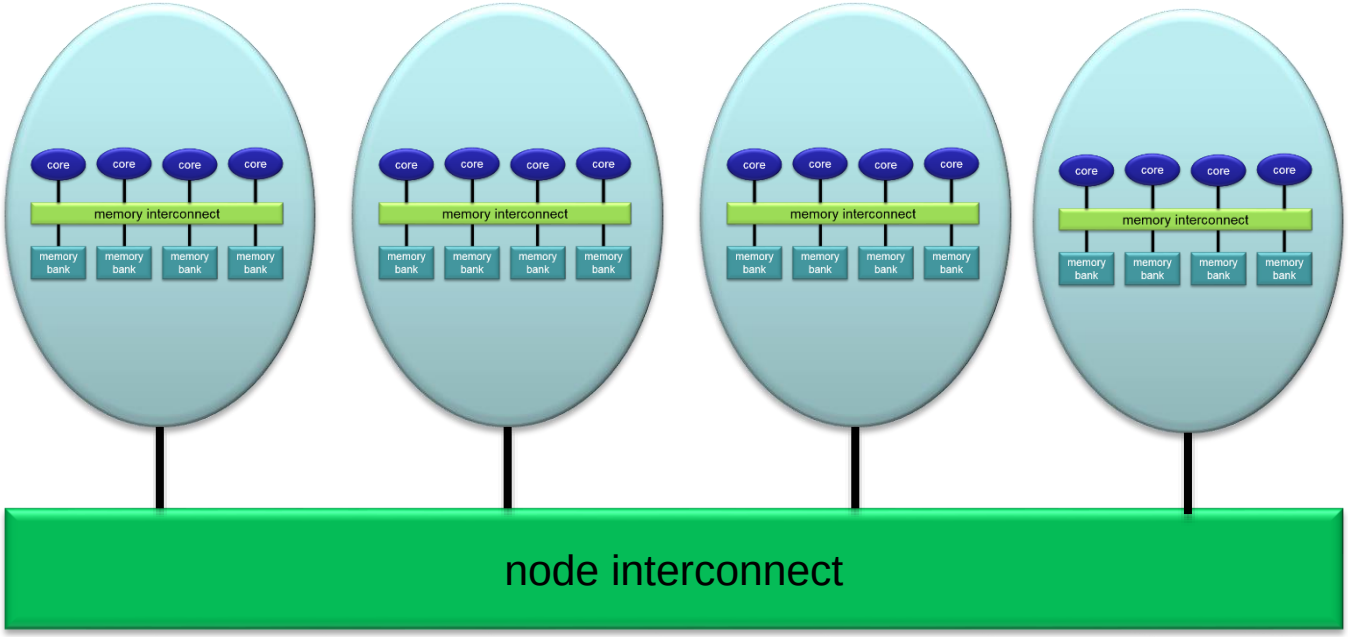


- multicomputer
  - distributed memory
  - **N**on-**U**niform **M**emory **A**ccess (NUMA)
  - nodes are connected by node-interconnect
  - different network topologies



Parallel Hardware Architectures

- most modern HPC systems (e.g. FLOW and HERO) are clusters of SMP/ccNUMA nodes



Parallelization Strategies

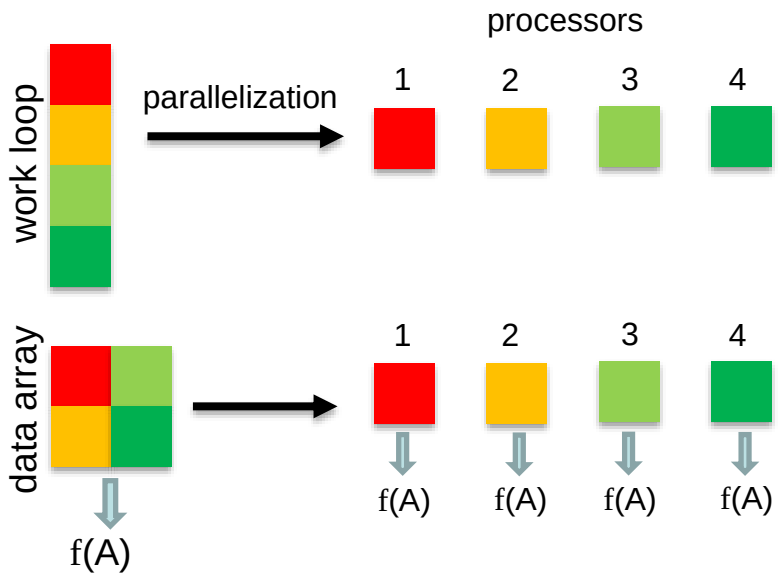
- two major resources for computations
  - processor
  - memory

- parallelization means
  - distributing the work
  - distributing the data (on distributed memory machines)
  - synchronization of work
  - communication of data (on distributed memory machines)

- parallel programming models provide the methods to achieve the above goals

Distributing Work and Data

- Work decomposition
  - based on loop decomposition
- Data decomposition
  - all the work for a local chunk of the data is done by the local processor
- Domain decomposition
  - work and data are distributed according to a higher model, e.g. reality



Parallel Programming Models

- two dominating programming models:
  - OpenMP: uses directives to define work decomposition
  - MPI: standardized message-passing interface
- other programming models
  - HPF (high-performance Fortran)
  - PGAS (Partitioned Global Address Space), e.g. Co-Array Fortran UPC (Unified Parallel C)
- programming models for compute devices
  - CUDA
  - OpenCL
  - OpenACC

Overview MPI

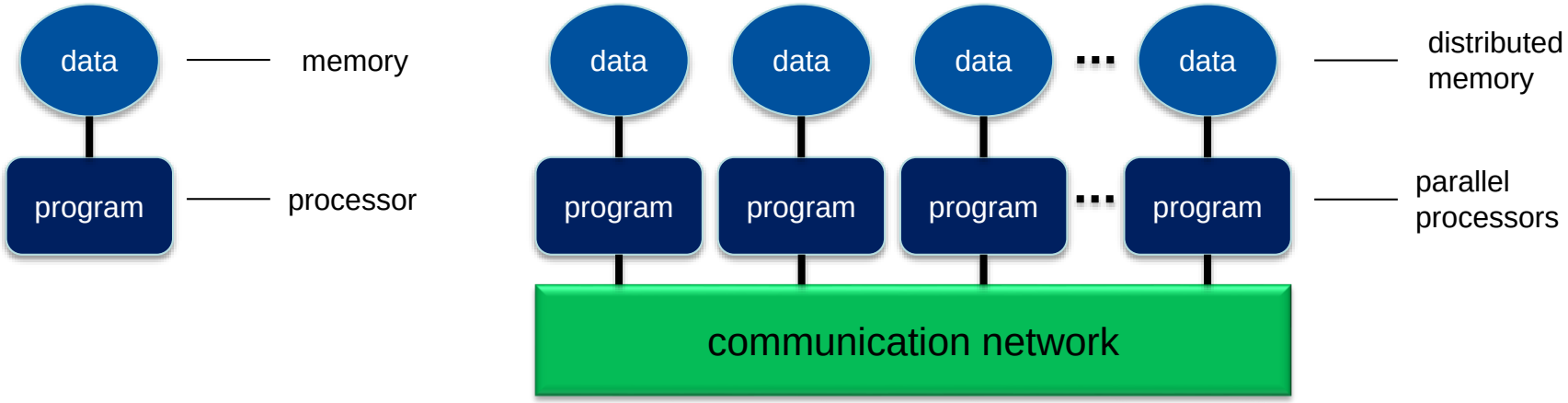
- Introduction to the Message Passing Interface
- Point-to-Point Communication
- Collective Communication
- Other and New Features of MPI
  - Derived Datatypes
  - Virtual Topologies
  - Process Creation and Management
  - One-sided Communication and Shared Memory
  - MPI and Threads
  - Parallel File I/O

History of MPI

- MPI is a standard with the prime goals
  - to provide a message-passing interface
  - to provide source-code portability
  - to allow efficient implementations
- MPI exists for more than 20 years
  - MPI-1.0 was released in June, 1994
  - MPI-2.0 was released in July, 1997 and provided additional functionality
  - MPI-3.0, the current standard, was released in October, 2012 and was developed for better platform and application support (in particular clusters of SMP nodes)

A Message-Passing Interface

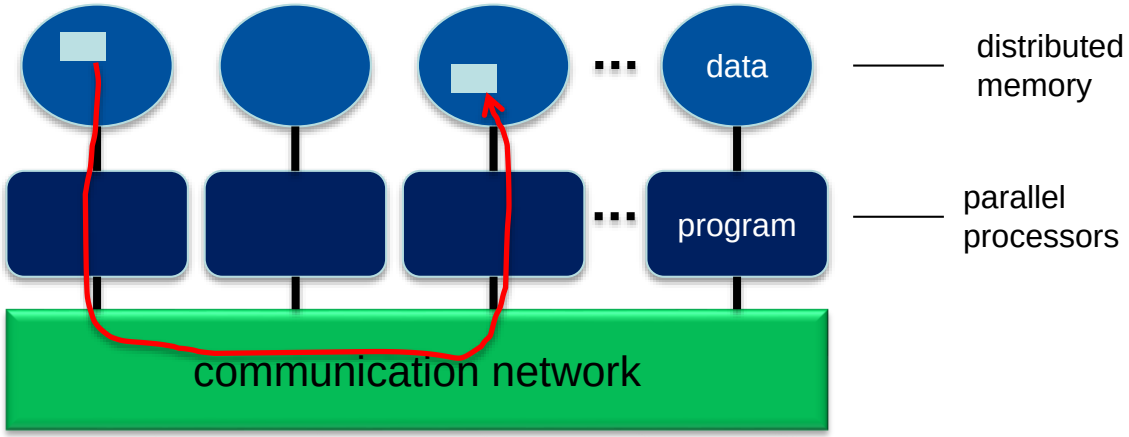
- sequential program vs. message-passing program



- message-passing programming paradigm:
  - each processor runs a (sub)program, typically the same (SPMD)
  - variables of subprograms have the same name but different (distributed) data
  - communication by special library routines ➔ message passing

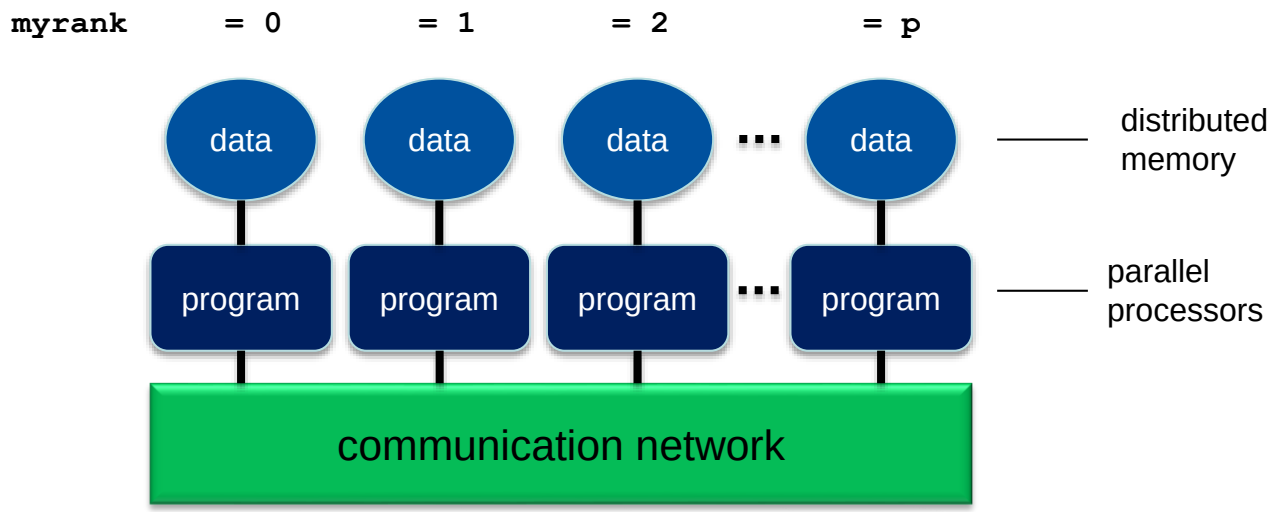
Message Passing

- messages are passed through the communication network
- messages require the following information:
  - sending and receiving process
  - data location
  - data type
  - data size



- in order to use the message-passing interface the program must be
  - connected to the MPI library (at compile time)
  - started with the MPI startup tool (mpirun or mpiexec)
  - at runtime MPI is initialized with special library calls (MPI_Init())

Process Identification



- processes in MPI are identified by their rank
  - determined by calling a library function
  - rank is used for addressing when sending messages
  - rank is used for making decisions, e.g. when distributing the data and work

Example: MPI_HelloWorld

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

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

   MPI_Init(&argc, &argv);

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

   if (my_rank == 0)
   {
     printf ("Hello world!\n");
   }

   printf("I am process %i out of %i.\n", my_rank, size);

   MPI_Finalize();
}
```

MPI Header and Module Files

- C/C++: `#include <mpi.h>`
- Fortran:
  ```
  include "mpif.h"
  ```
  or
  ```
  use mpi
  ```
  or
  ```
  use mpi_f08
  ```
  - the use of the old style include-statement is strongly discouraged as no compile-time argument checking can be done
  - recommended is the use of mpi_f08

MPI Library Calls

- in general an MPI library call has the form

C/C++:
```
error = MPI_Xxxxx(parameter, …);
MPI_Xxxxx(parameter, …);
```

Fortran:
```
CALL MPI_Xxxxx(parameter, …, ierror)
```

  - in Fortran the use of ierror has change with MPI-3.0:
    if (and only if!) you are using the module file mpi_f08, ierror is an optional argument. In any other case ierror cannot be omitted otherwise terrible unforeseen things may happen.
  - refer to the MPI-3.0 standard document to look up the definitions and argument list of available MPI functions
    http://www.mpi-forum.org/docs/

MPI_Init() and MPI_Finalize()

- MPI is initialized with
  - C/C++: `MPI_Init(&argc, &argv);`
  - Fortran: `CALL MPI_Init(ierror)`

  - must be the first MPI-routine that is called (few exceptions)
  - call as early as possible in your program
  - in C/C++ argv and argc are passed by reference (possibly cleans argv from unwanted MPI arguments)

- MPI is finalized with
  - C/C++: `MPI_Finalize();`
  - Fortran: `CALL MPI_Finalize(ierror)`

  - must be the last MPI-routine that is called (few exceptions)

MPI Communicators

- all MPI processes (subprograms) are combined in the communicator MPI_COMM_WORLD
  - MPI_COMM_WORLD is a handle predefined in the header files
  - each process in a communicator has its own rank starting from 0 until (size-1)
  - the size of a communicator and the rank of a process within the communicator can be determined with special library calls
  - it is possible to define your own communicators (e.g. for a subset of processes) and handles

MPI_Comm_size() and MPI_Comm_rank()

- to determine the size of a communicator use

```
MPI_Comm_size(MPI_COMM_WORLD, &size);
```

- to determine the rank of a process within a communicator use

```
MPI_Comm_rank(MPI_COMM_WORLD, &myrank);
```

  - note that **`size`** is the same on every process whereas **`myrank`** is different

Example: MPI_HelloWorld

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#include <mpi.h>

int main(int argc, char *argv[])
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   MPI_Init(&argc, &argv);

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   }

   printf("I am process %i out of %i.\n", my_rank, size);

   MPI_Finalize();
}
```

Example: MPI_HelloWorld

```
PROGRAM MPI_HelloWorld
  USE mpi_f08
  IMPLICIT NONE

  INTEGER rank, size

  CALL MPI_Init()

  CALL MPI_Comm_rank(MPI_COMM_WORLD, rank)
  CALL MPI_Comm_size(MPI_COMM_WORLD, size)

  IF (rank .EQ. 0) THEN
     WRITE(*,*) 'Hello world!'
  END IF

  WRITE(*,*) 'I am process', rank, ' out of', size

  CALL MPI_Finalize()

END PROGRAM MPI_HelloWorld
```

Compiling an MPI Program

- programs are compiled using a wrapper command:

C: `$ mpicc [options] <source.c> -o <executable>`
C++: `$ mpic++ [options] <source.cpp> -o <executable>`
Fortran: `$ mpifort [options] <source.f90> -o <executable>`

  - uses the standard compiler (GCC, ICS) with some extra options

- example on HERO:

```
[abcd1234@hero02 ~]$ module load ics/2013_sp1.3.174/64
[abcd1234@hero02 ~]$ module load openmpi/1.8.2/intel
[abcd1234@hero02 ~]$ mpicc MPI_HelloWorld.c -o MPI_HelloWorld
```

Running an MPI Program

- programs are executed using the MPI startup tool

  $ **mpirun –np <N> [options] <executable>**

  or $ **mpiexec –np <N> [options] <executable>**

- example on HERO:
  - note: do not normally run programs on the head nodes

```
[abcd1234@hero02 ~]$ mpirun -np 4 --mca btl ^openib MPI_HelloWorld
I am process 2 out of 4.
I am process 3 out of 4.
I am process 1 out of 4.
Hello world!
I am process 0 out of 4.
```

Running an OpenMPI Program with SGE

```
#!/bin/bash
####### SGE settings
#$ -cwd
#$ -N MPI_HelloWorld

####### parallel environment
#$ -l cluster=hero
#$ -pe openmpi 4
#$ -R y

####### requesting resources
#$ -l h_rt=0:10:0
#$ -l h_vmem=1000M
#$ -l h_fsize=100M

# loading modules
module load intel intel/ics/2013_sp1.3.174/64
module load openmpi/1.8.1/ics

# the --mca options tells MPI not to use Infiniband (prevents warning)
mpirun -np $NSLOTS -machinefile $TMPDIR/machines --mca btl ^openib MPI_HelloWorld
```

Sending and Receiving Messages

- the MPI library provides functions to send and receive messages:
  - sending: MPI_Send(…)
  - receiving: MPI_Recv(…)

  - any message sent must be received, otherwise → deadlock
  - function prototypes (here C/C++, Fortran is analogous)

```
MPI_Send(void* data, int count, MPI_Datatype datatype, int destination,
         int tag, MPI_Comm communicator)

MPI_Recv(void* data, int count, MPI_Datatype datatype, int source,
         int tag, MPI_Comm communicator, MPI_Status* status)
```

MPI Data Types

- MPI needs to know the type of data that is send
- predefined handles are provided for standard data types, e.g.:
  - **`MPI_INT, MPI_FLOAT, MPI_DOUBLE, MPI_CHAR,`** …
- you can also define handles for your own data types

MPI Send and Receive Example

```
...
int number;
if (my_rank == 0) {
       number = 42;
    MPI_Send(&number, 1, MPI_INT, 1, 0, MPI_COMM_WORLD);
} else if (my_rank == 1) {
    MPI_Recv(&number, 1, MPI_INT, 0, 0, MPI_COMM_WORLD,
             MPI_STATUS_IGNORE);
    printf("Process 1 received number %d from process 0\n",
            number);
}
...
```

Sending and Receiving Messages

- message can be sent in different ways
  - synchronous vs. asynchronous:
    sender receives a confirmation receiving of the message is initiated
  - unbuffered vs. buffered:
    the message can be buffered so the sender can continue using the sent variable, requires additional memory
  - blocking vs. non-blocking:
    send or receive functions return immediately allowing to overlap communication and computation

for details refer to the MPI-3.0 standard

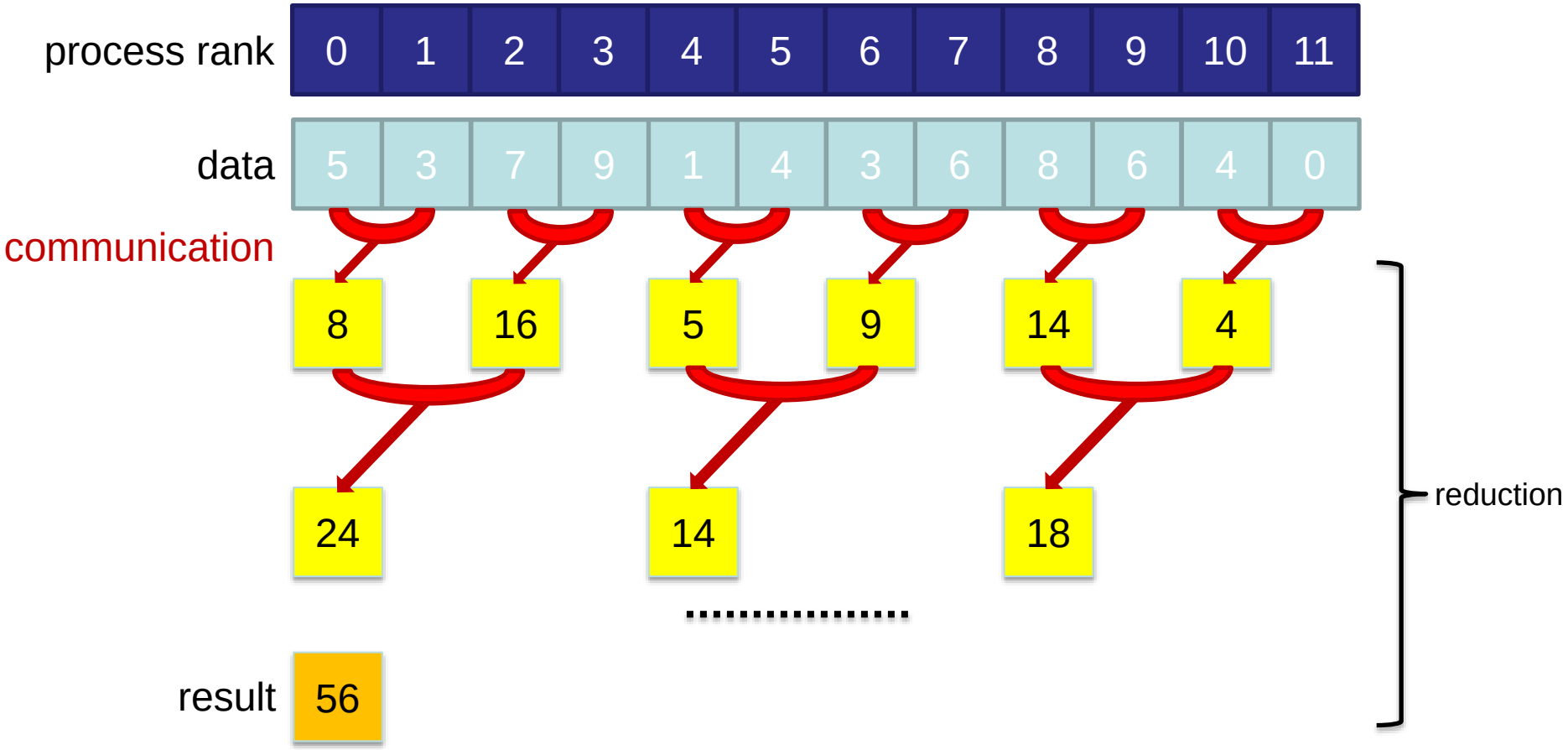
Collective Communication

- so far we have looked at point-to-point communication
- MPI allows knows
  - one-to-all
  - all-to-one
  - all-to-all

  } communication

- example: calculate the sum of the elements of an array

Collective Communication



Collective Communication

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- MPI allows knows
  - one-to-all
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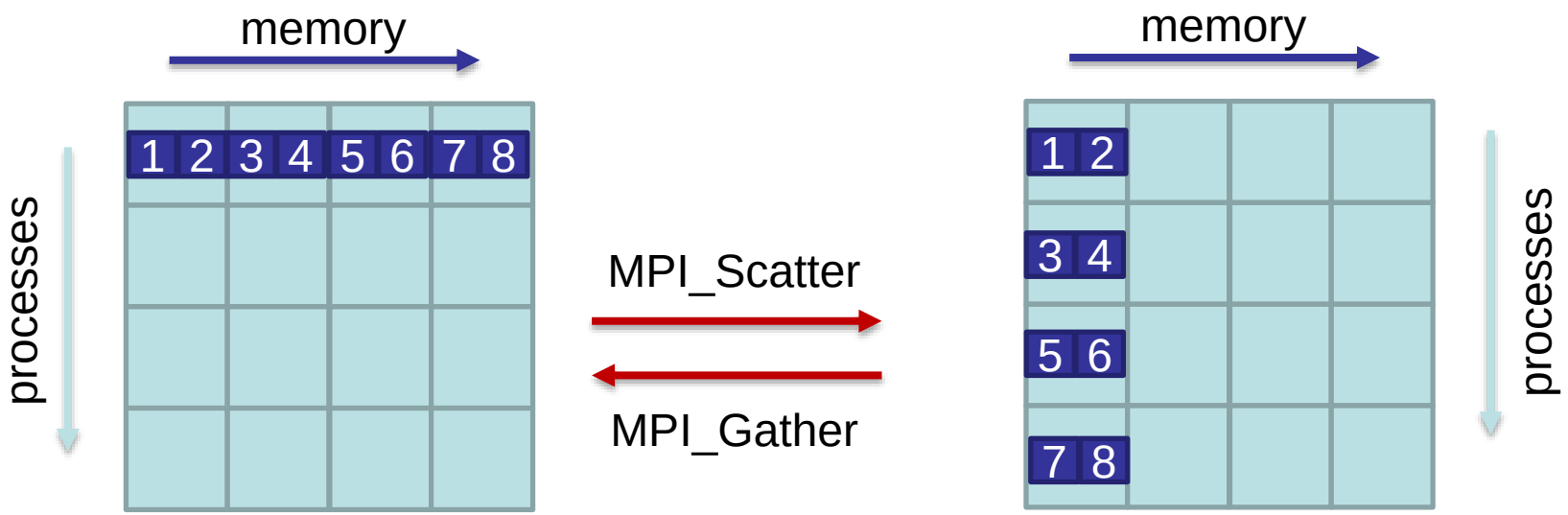
  } communication

- example: calculate the sum of the elements of an array
- MPI collective communication is very efficient due to tree-based communication
- collective communication can still be very expensive, in particular all-to-all

Collective Communication

- a selection of collective MPI communications:
  - MPI_Bcast(…) sending data from one process to all others
  - MPI_Scatter(…) distributing an array of data from one to all
  - MPI_Gather(…) collecting an array of data from all to one
  - MPI_Reduce(…) reduction operation defined by a handle, e.g. MPI_SUM
  - MPI_Barrier(…) used to synchronize all processes
  - …
- some also have all-to-all variant, e.g. MPI_Allreduce
- since MPI-3.0 also non-blocking calls

Example: MPI_Scatter and MPI_Gather



Summary

- MPI allows the parallelization of programs by distribution data and work through the passing of messages
  - MPI is a platform-independent standard
  - very flexible but also more time-consuming to program
  - read the standard document for more details
    → http://www.mpi-forum.org/docs/
- MPI library calls can be used to send and receive messages
  - whenever needed use higher-level functions for collective communication for efficiency
- with MPI you can introduce new types of errors in your program, e.g. deadlocks
  - however, many errors in parallel programs stem from error in the serial code

MPI Exercises and Examples

- Programming Exercises include
  - MPI_HelloWorld
  - MPI_PingPong
  - MPI_RingSend
  - Timing MPI_Send()

- Do as many exercises as you can or like
  - Solutions are provided
    but do not look at solutions until you completed the exercise!

Exercise 1: MPI_HelloWorld

- Write an MPI_HelloWorld program following the example given before
  - compile and run the program on the cluster
  - what do you notice when you run the program several times? Can you explain the behavior?

Exercise 2: MPI_PingPong

- Write an MPI_PingPong program to run with two processes doing the following:
  - initialize a counter
  - one process increments the counter and sends it to the other
  - the other process receives the message and then increments the counter and sends it back
  - repeat until n messages have been sent

Exercise 3: MPI_RingSend

- Write an MPI_RingSend program to run with any number of processes computing on all processes the sum of all ranks:
  - each process receives the current sum from its left neighbor (rank-1)
  - each process adds its own rank to the current sum
  - each process sends the new current sum to its right neighbor
  - the ring is terminated after one round
  - note: the left/right neighbor for rank 0/(size-1) is (size-1)/0

  - is MPI_RingSend a truly parallel program when using MPI_Send() and MPI_Recv()?

Exercise 4: Timing MPI_Send()

- Write an MPI program that sends an array of doubles from one process to another
  - using MPI_Wtime() measure the time it takes to complete the MPI_Send() call
  - determine this time as function of N where N is the size of the array
  - plot the result and explain