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EMCL

Heidelberg Institute for Theoretical Studies

HITS

- Part 2 -
Parallel Programming

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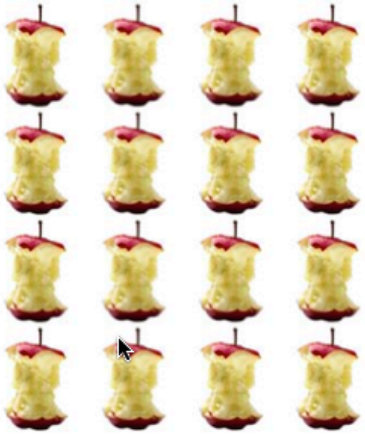
The Challenge

- Make your algorithms ready for
  - Fine-grained parallelism
  - Scalability with respect to thousands of threads
  - Data locality

Single-core

Multi-core



Many-core

But how?

The big picture

Hardware evolution

- Memory wall: Data movement cost prohibitively expensive
- Power wall: Nuclear power plant for each machine (in the cloud)?
- ILP wall: 'Automagic' maximum resource utilisation?
- Memory wall + power wall + ILP wall = brick wall

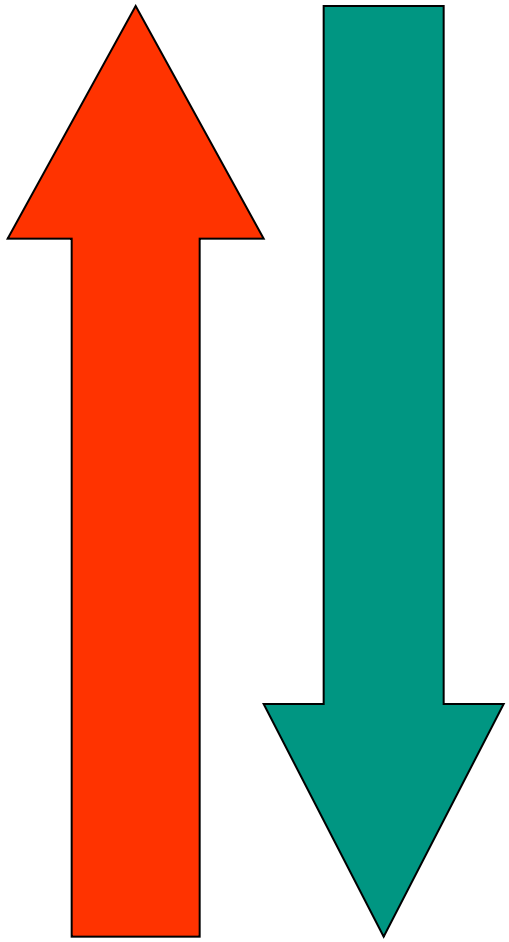
Inevitable paradigm shift: Parallelism and heterogeneity

- In a single chip: singlecore → multicore, manycore, ...
- In a workstation (cluster node): NUMA, CPUs and GPUs, ...
- In a big cluster: different nodes, communication characteristics, ...

This is our problem as applied mathematicians

- Affects all machines we use, including workstations and laptops

Conflicting developments



Complexity of cores

Heterogeneous Platforms

Easy living
+
Limited performance

Responsibility of programmer

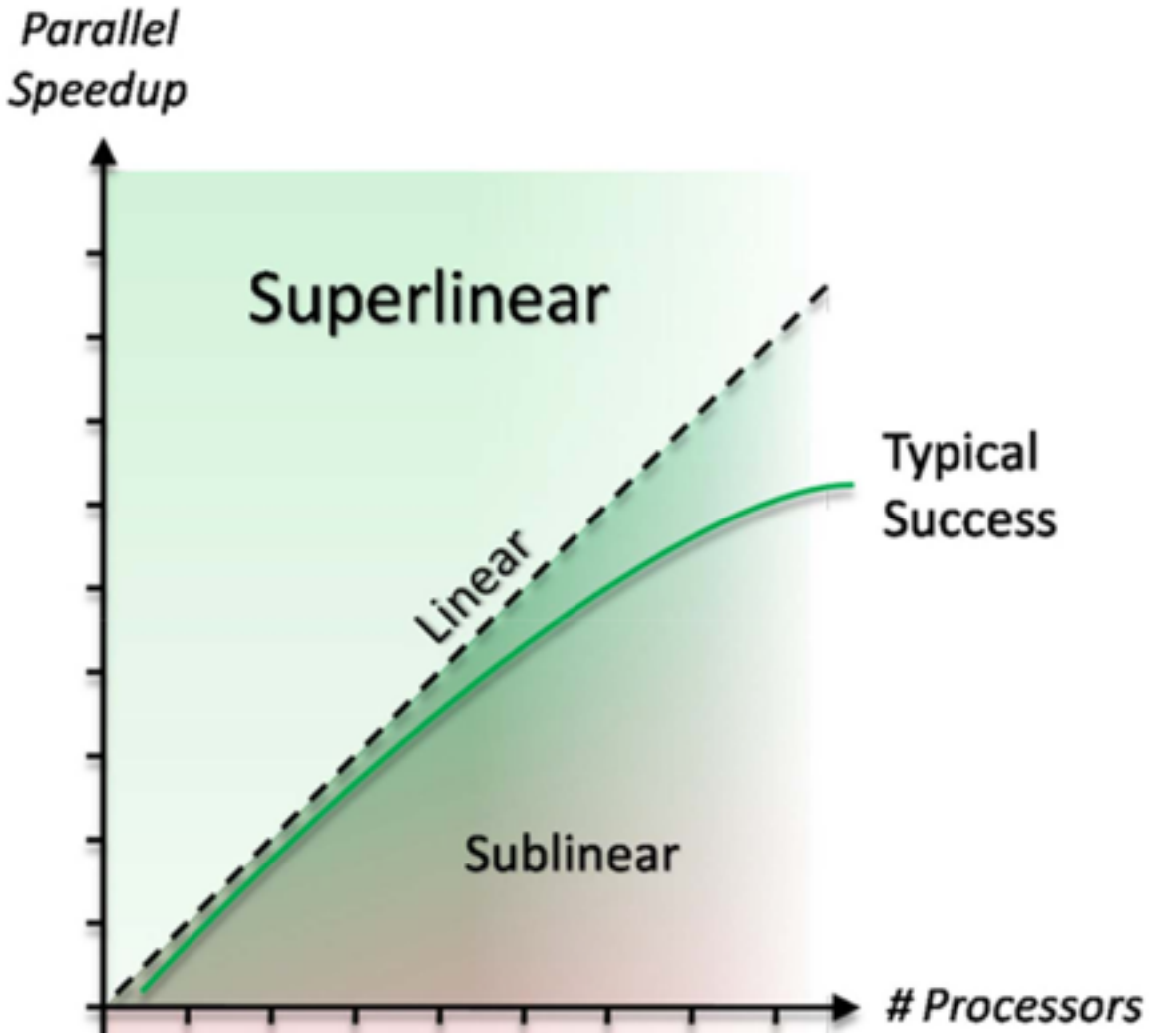
Scalability
+
Performance increase

Speedup in parallel computing

The **speedup** is defined as the ratio of the serial runtime of the best sequential algorithm for solving a problem to the time taken by the parallel algorithm to solve the same problem on *p* processors.

$$S = \frac{T_S}{T_P}$$

Speedup in parallel computing



Efficiency in parallel computing

The efficiency is defined as the ratio of speedup to the number of processors. Efficiency measures the fraction of time for which a processor is usefully utilized.

$$E = \frac{S}{p} = \frac{T_S}{pT_p}$$

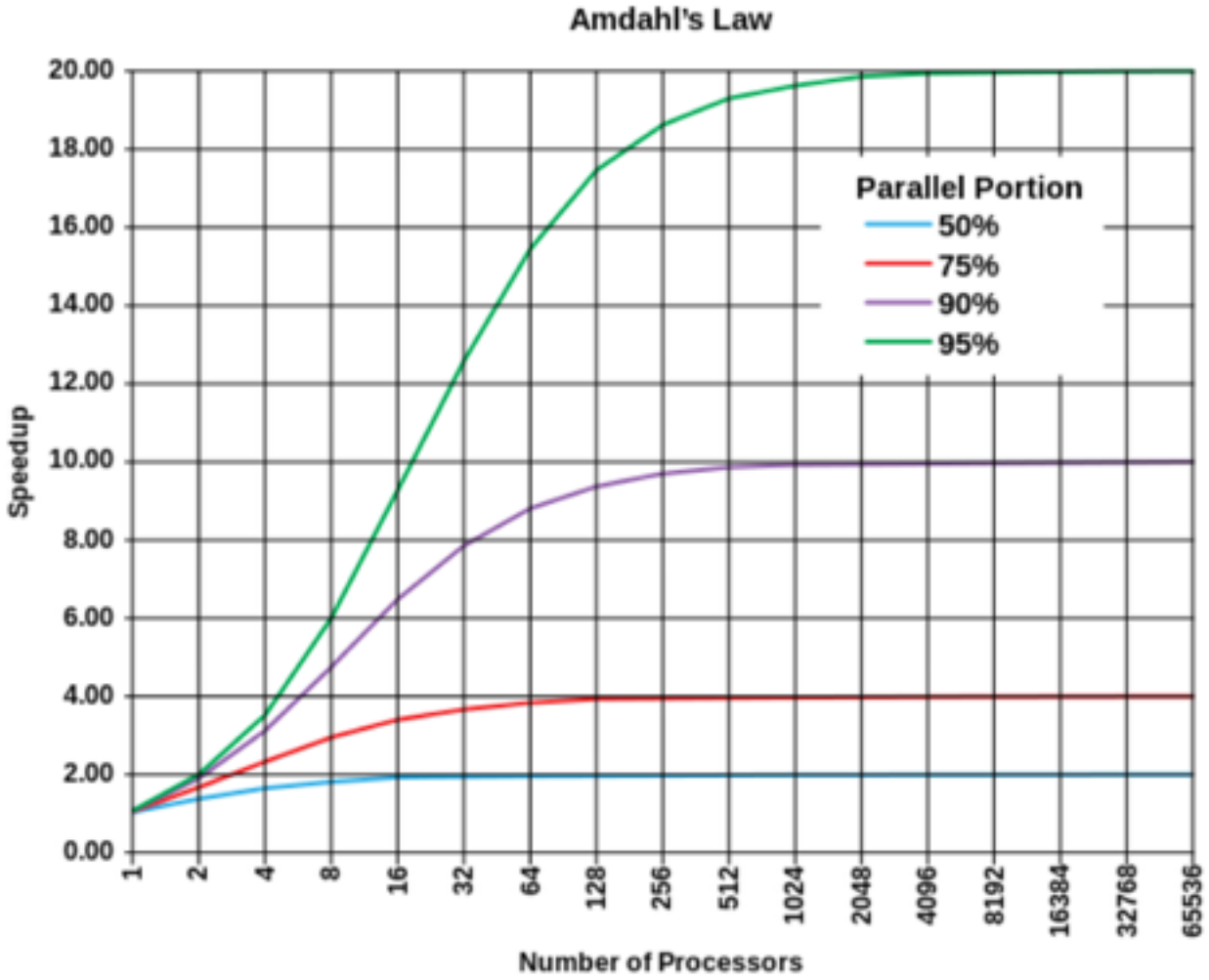
Amdahl´s law

$$T = (1 - p)T + pT$$

$$T(s) = (1 - p)T + \frac{p}{s}T$$

$$\frac{T}{T(s)} = \frac{1}{1 - p + \frac{p}{s}}$$

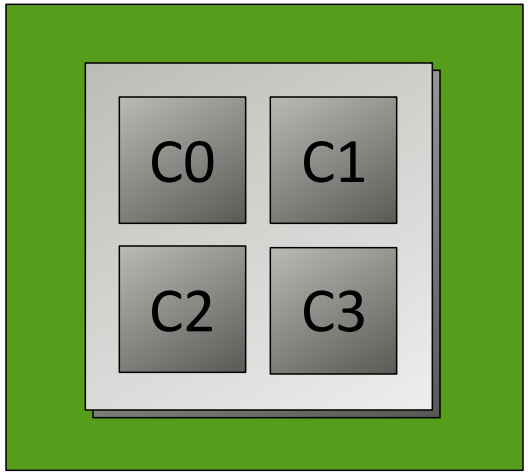
Amdahl´s law



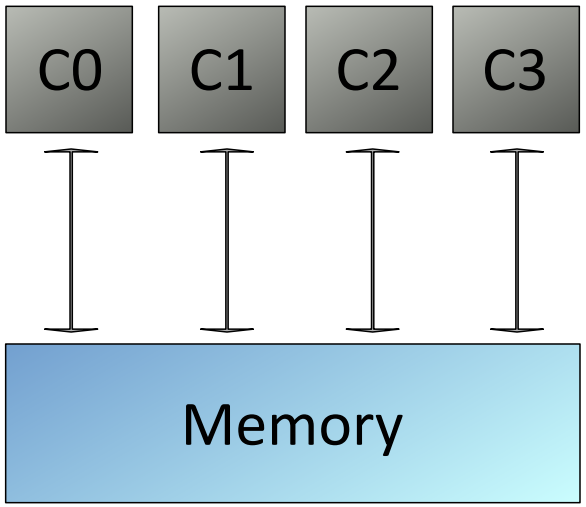
Source: Wikipedia

Parallelism on the Chip Level

- Parallelism on the Chip-Level
  - Multi-Core CPUs
  - GPUs
  - ...



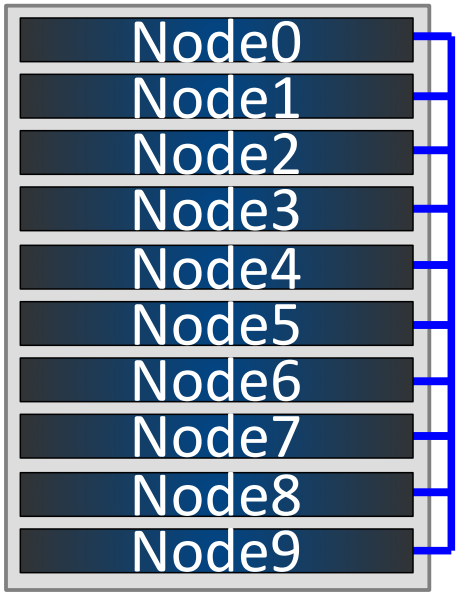
- Memory shared over the cores



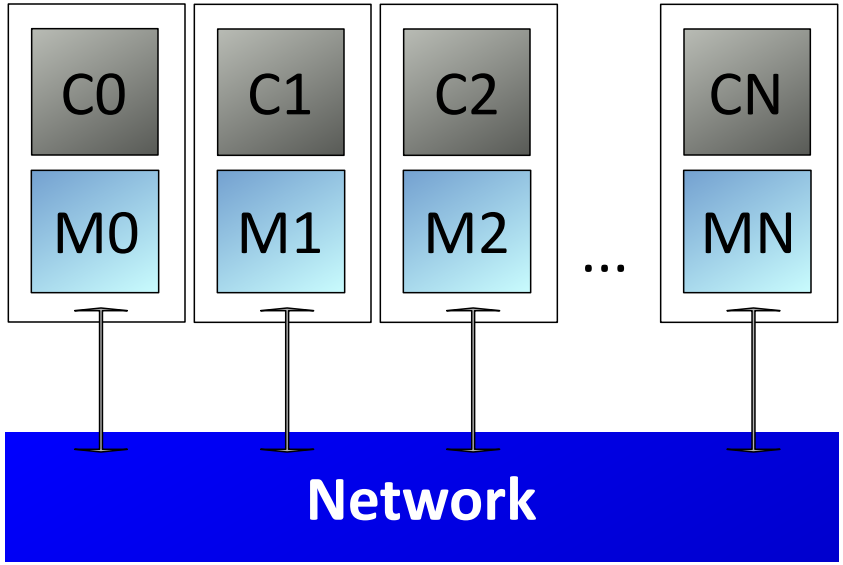
=> direct memory accesses possible!

Parallelism on the Cluster Level

- HPC-Cluster consists of several nodes, each of which has
  - Computing instance
  - Memory instances



- Memory distributed within the cluster



=> direct memory accesses only locally
=> beyond: network communication

Paradigms of Parallel Programming

- **Shared memory**
  - Different processors/threads share main memory

- **Distributed memory (message passing)**
  - Each processor has its own memory

- Hybrid approach

PGAS (Partitioned Global Address Space)

Global memory address space, but portions of the memory space may have an affinity for particular processes/threads

Paradigms of Parallel Programming

- **Shared memory**
  - Different processors/threads share main memory
- => **OpenMP** (Open Multi-Processing) → C/C++/Fortran API for shared memory multiprocessing

- **Distributed memory (message passing)**
  - Each processor has its own memory
- => **MPI (Message Passing Interface)** → Standard for library routines for message-passing programs (C/C++/Fortran/Java/…)

- Hybrid approach

PGAS (Partitioned Global Address Space)

Global memory address space, but portions of the memory space may have an affinity for particular processes/threads

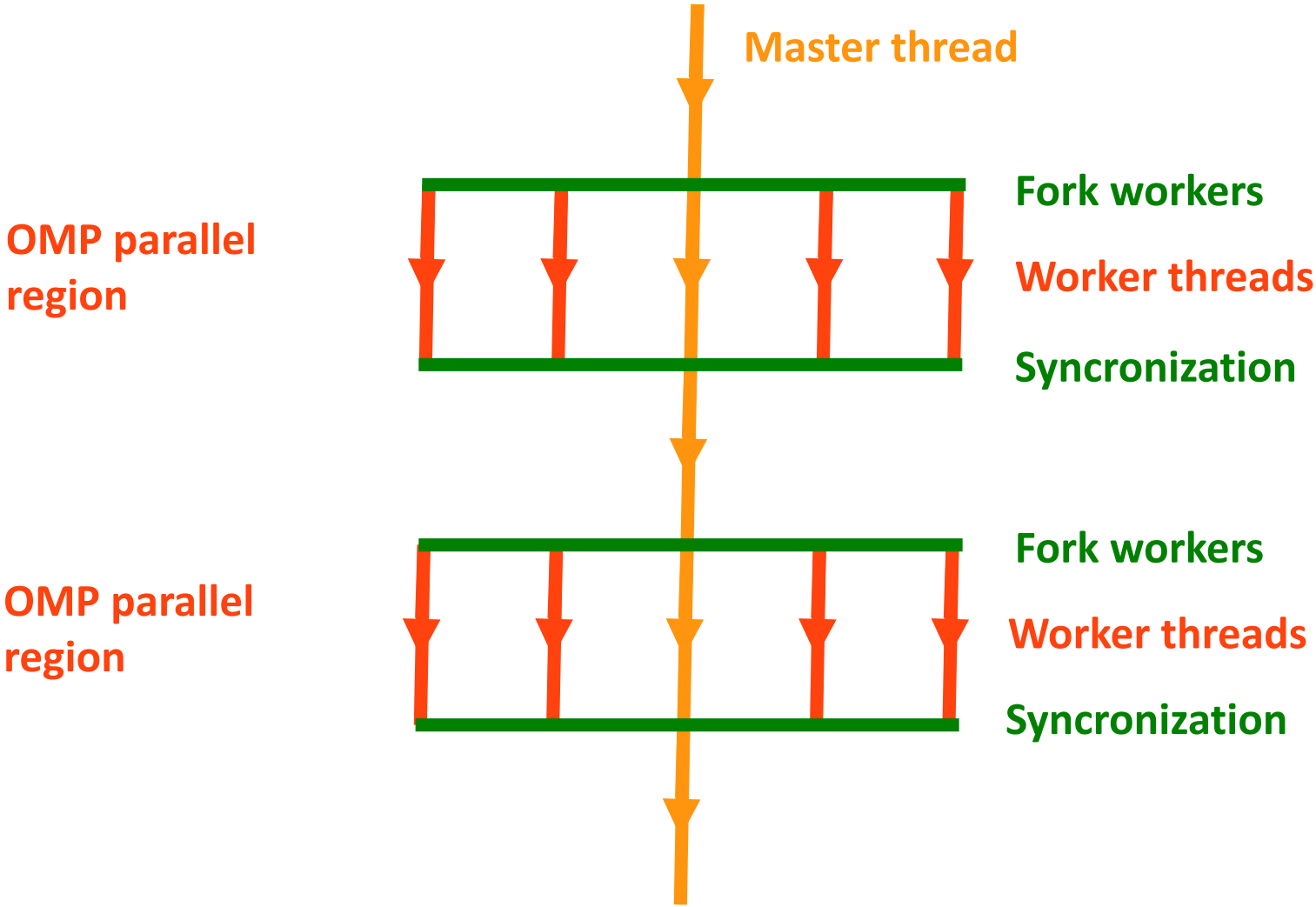
OpenMP: Overview

- OpenMP is an **easy, portable specification** for node-level parallelisation
- Thread-based, shared memory, **single-node** (in contrast to MPI)

- How does it work?
  - Annotate the C/C++/FORTRAN source code with pragmas
  - The compiler transparently generates the necessary code
  - Fork and join model
    - Non-parallel blocks are only executed by the main (or master) thread
    - Parallel blocks are executed in parallel by a team-of-threads

- OpenMP pragmas are ignored of not activated

OpenMP: Fork and join model



SC14 OpenMP tutorial, C. Terboven et al

OpenMP: Core syntax

- Most OpenMP pragmas apply to a „structured block“ or „parallel region“

```
#pragma omp parallel
{
  // statements
}
```

- Only statements inside a block marked with the „parallel“ clause will be executed in parallel

OpenMP: Core syntax / Compiling

- Most OpenMP pragmas apply to a „structured block“ or „parallel region“

```
#pragma omp parallel
{
  // statements
}
```

- Only statements inside a block marked with the „parallel“ clause will be executed in parallel

- GCC

```
gcc -fopenmp -o example example.c
```

- Intel

```
icc -openmp -o example example.c
```

OpenMP: Hello world example

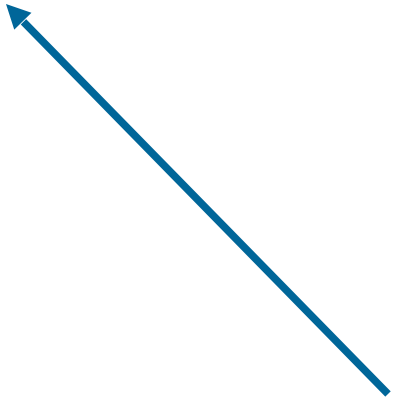
```
#include <omp.h>
#include <iostream>


using namespace std;


int main(int argc, char **argv)
{
  // fork threads
  #pragma omp parallel
  {
    cout << "Thread "
         << omp_get_thread_num() << endl;
    }
  } // join threads

  cout << „All done!“ << endl;
  return 0;
}
```

```
$ export OMP_NUM_THREADS=4
$ ./main
Thread 0
Thread 3
Thread 2
Thread 1
All done!
```



?

no order guaranteed

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MPI: Overview

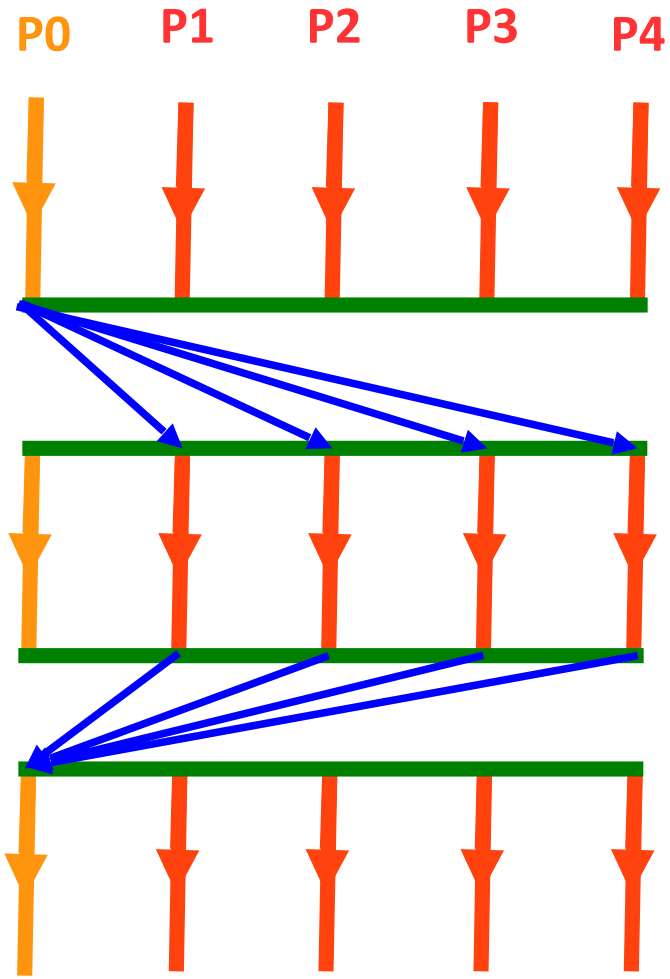
- MPI is a **standardized** and **portable message-passing system** which defines the syntax and the semantics of **core library routines**
- Several implementations of MPI exist, e.g. for C, C++, Fortran, Java

- How does it work?
  - Message-passing between several processes through calls of MPI functions
    - Communicators (defines groups of processes)
    - Point-to-point communication, e.g. MPI_Send or MPI_Receive
    - Collective functions, e.g. all-to-one or one-to-all communication
  - Linking against a MPI library necessary
  - Parallel program is typically started using mpirun/mpiexec (agent)
  - → assignment of processes and CPUs

  By default, full code is executed by every process

MPI: Message passing approach

Process 0 often treated as special process (not necessary)



One-to-all communication

All-to-one communication

MPI: Core syntax (1)

- The library header has to be included, e.g. in C/C++

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

- The MPI execution environment has to be initialized at the beginning and terminated at the end of a program, e.g. in C/C++

```
int main(int argc, char **argv)
{
  MPI_Init(&argc, &argv);

  // statements

  MPI_Finalize();
}
```

- All processes run the same code

MPI: Core syntax (2)

- One-to-one communication

```
int MPI_Send(const 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)
```

Explanation of parameters

Parameter	Comment
buf	initial address of send/receive buffer (choice)
count	number of elements in send/receive buffer (nonnegative integer)
datatype	datatype of each send/receive buffer element (handle)
dest / source	rank of destination/source (integer)
tag	message tag (integer)
comm	communicator (handle)
status	status object (Status)

MPI: Hello world example

```
#include <iostream>
#include <mpi.h>


using namespace std;


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

  // initialize the MPI execution environment
  MPI_Init(&argc, &argv);

  // determine rank and size
  MPI_Comm_size(MPI_COMM_WORLD, &size);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);

  cout << "Hello world from rank " << rank << endl;
  if (rank == 0)
    cout << "Size = " << size << endl;

  // terminate MPI execution environment
  MPI_Finalize();

  return 0;
}
```

```
$ mpirun -np 2 ./main
Hello world from rank 0
Size = 2
Hello world from rank 1
```

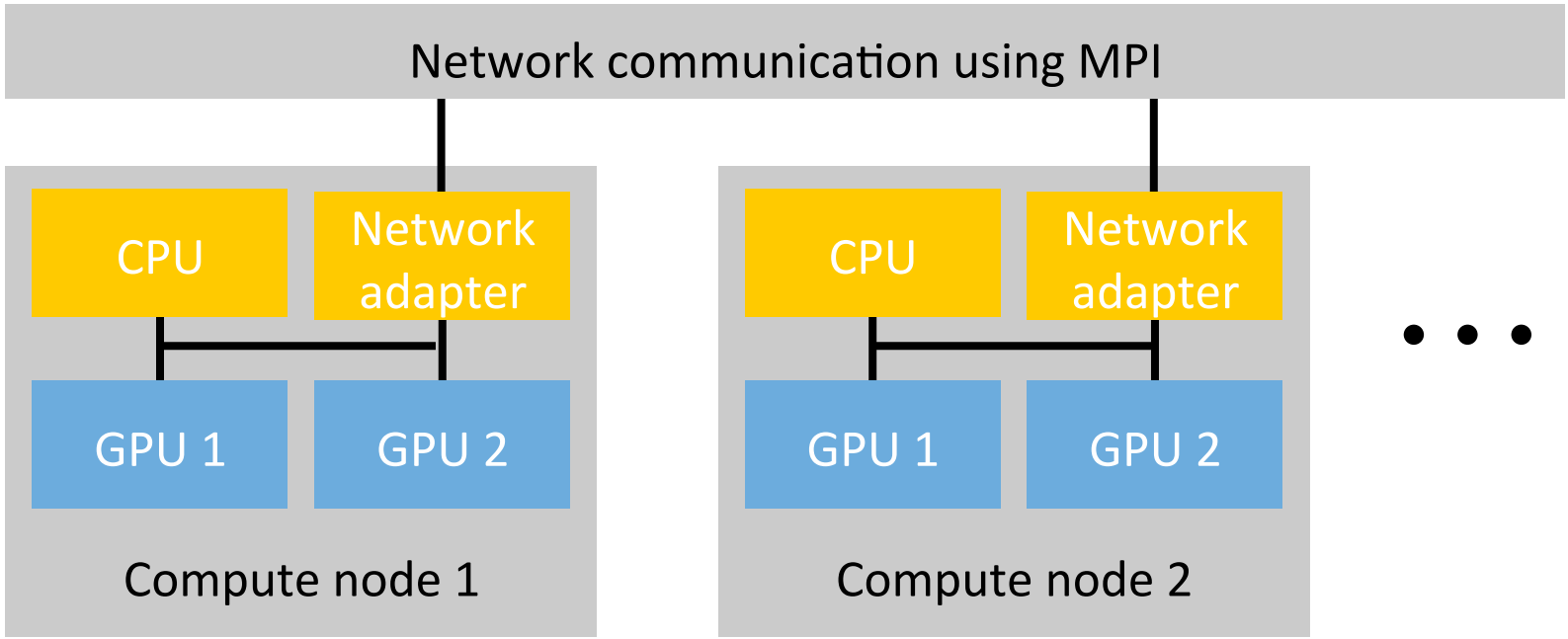
Debugging: Approaches and Tools

- New problems due to parallelism, e.g.
  - Deadlocks
  - Race conditions
  - Irreproducibility

- Approaches and Tools, e.g.
  - Valgrind (Memory Tracing Tools)
  - Marmot (MPI-Analysis Tool)
  - Total View (Debugger)
  - DDT (Debugger)

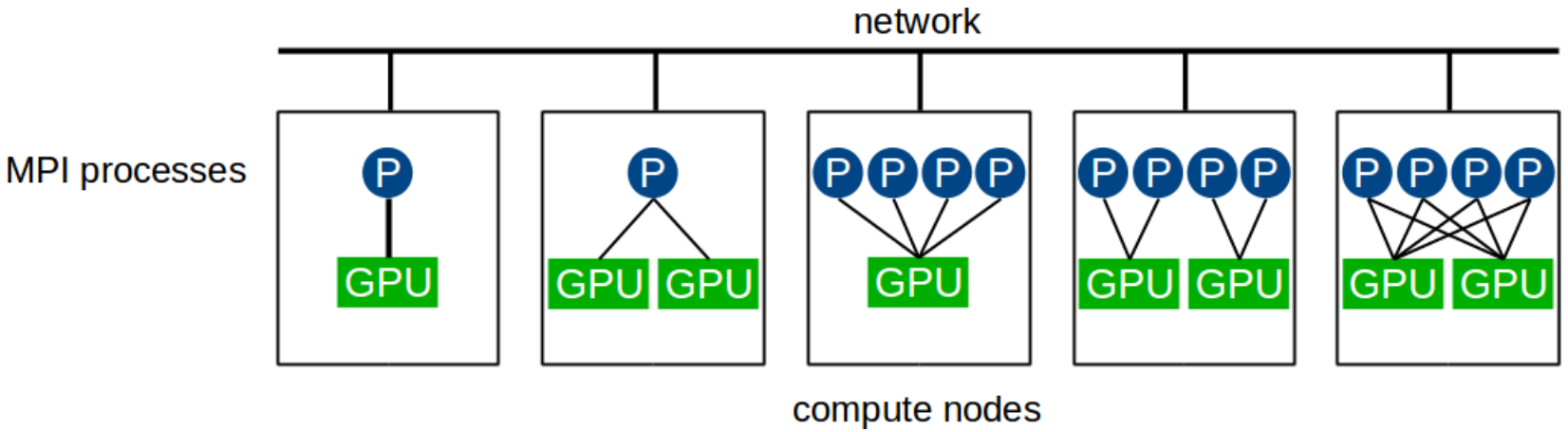
Multi-GPU implementation for multiple compute nodes

- Multiple compute nodes, each equipped with GPUs, are connected over the network using MPI
- An additional layer of asynchronism is added to the algorithm



Hybrid parallel configurations

- MPI, OpenMP & CUDA



- from Kepler on: HyperQ feature, 32 concurrent CUDA streams
- must use Multi-Process Service to share one GPU

Thank you