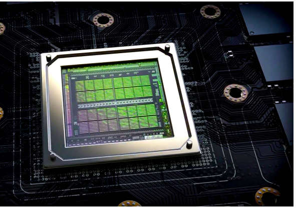
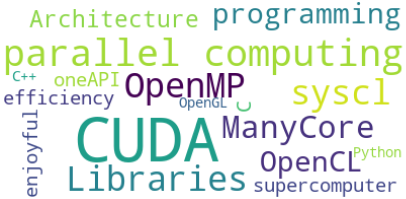
GEORG-AUGUST-UNIVERSITÄT GÖTTINGEN IN PUBLICA COMMODA SEIT 1737

Julian Kunkel

Welcome to the Practical Course on High-Performance Computing





Recording!

- This broadcast channel will be recorded via BBB
  - This includes your video, audio (if shared) and chat messages
  - We can start/stop video recording if necessary
- Recordings will be available 1-2 days later
- We **may publish** selected trainings on our YouTube channel
  - Will include video, audio if shared
  - Feel free to use the chat in broadcast if you have questions to lectures
    It won't be rendered for the YouTube video

Outline

Learning Objectives of the Module

- Construct parallel processing schemes from sequential code using MPI and OpenMP
- Justify performance expectations for code snippets
- Sketch a typical cluster system and the execution of an application
- Characterize the scalability of a parallel app based on observed performance
- Analyze the performance of a parallel application using performance analysis tools
- Describe the development and executions models of MPI and OpenMP
- Construct small parallel apps that demonstrate features of parallel apps
- Demonstrate the usage of an HPC system to load existing software packages and to execute parallel apps and workflows
- Demonstrate the application of software engineering concepts

Role of learning objectives

- The LOs describe what you should be **able to do** after completing the course

Organization of the Module

- Attendees
  - GWDG academy users
    - Researchers, PhD students, users of HPC systems in the NHR and local
  - University students
    - Need to develop a software after the course to obtain their credits
    - Details will be explained at the end of the week
- Webpage `https://hps.vi4io.org/teaching/summer_term_2023/pchpc` provides
  - Links to Slides, exercise sheets and more
- Communication via two BBB channels
  - Broadcast: you should listen to this one the whole week
    - The trainer will present slides, walk through exercises, share suggestions
    - Do not share video, note that we record this channel
  - Breakout: room for group work and general support requests during sessions
- For university attendees: may use StudIP for asynchronous communication
  - We use it for announcements
  - Please use it for any purpose around the topic!

Organization of the Module

- Block course: 1 week of training (this week)
  - Mix of lecture, hands-on tutorials and guided exercises
  - May contain introductory and harder tasks
  - You can take a break anytime as necessary (particularly during guided exercises)
- Group work and community (30 min)
  - Learning in a virtual environment is difficult, therefore, we form groups!
  - Imagine you sit in a room with 4 people to share ideas and work together
  - The group *should* stick together in a breakout room the whole week
  - We will **now** organize teams of 5 attendees
    1. Join the Breakout BBB session
    2. Room 1-9 are reserved for GWDG-Academy attendees
    3. Room 10-11 are for DLR attendees
    4. Room 12+ are for University attendees
    5. Join a random room with <5 attendees - or with peers you know
    6. Work on the "Welcome" groupwork (next slide)

Group Work: Welcome

- Tasks:
  1. Introduce yourself to your peers and describe with one sentence why you join this course
  2. Have one of you share the screen of the course
- Time: 25 min
- Organization: breakout groups - please use your mic and chat

Support Structure

- Support request takes place primarily in the Breakout BBB
  - This channel will never be recorded
  - Ask questions to colleagues and to us
  - We will support your learning journey but **YOU** are responsible for it
- Utilize screen sharing (similarly as we would if in the same room)
- L1: Try to resolve issues in your breakout group with your peers
  - Please use your microphone, share screen and work together (on issues)
  - It is beneficial for learning
- L2: Ask questions in the global breakout chat
  - We have trainers that will reply to you, maybe other peers will reply too!
- L3: If breakout chat doesn't help, a trainer will connect to your breakout group
- If we realize that the issue should be given to all, the trainer will use the broadcast channel to demonstrate how the issue can be resolved

A Typical Session

1. Trainer gives an introduction to the topic
   - May include some short/small group works (for your breakout group)
2. Trainer may give a tutorial to overcome introductory obstacles
   - Step-by-step walkthrough
   - We provide an exercise sheet describing the steps and giving an introduction
3. Attendees work on tasks individually and in their breakout group
   - We provide an exercise sheet
   - Attendees should store their results (e.g. in a Git repository)
4. At the end of the session volunteers may share results on broadcast channel

Feedback

- While we are experienced in training/teaching, some aspects are new to us:
  - The block course format
  - The online learning format
  - The joint organization GWDG academy and University
  - Some new material and composition too
- Hence, there may be minor hickups in the delivery...
- Please be open and patient with us
- Our goal: Improving your skill with a pleasant learning journey
- Please speak up if you are unsatisfied with some aspects
- Feel free to share feedback (to us/me) if you see room for improvement

Learning Outcomes

After the session, a participant should be able to:

- Characterize distributed, parallel computing and HPC
- Describe how the scientific method relies on HPC
- Sketch generic parallel/distributed system architectures
- Sketch a simple program for vector addition using pseudocode

Outline

Scientific Method

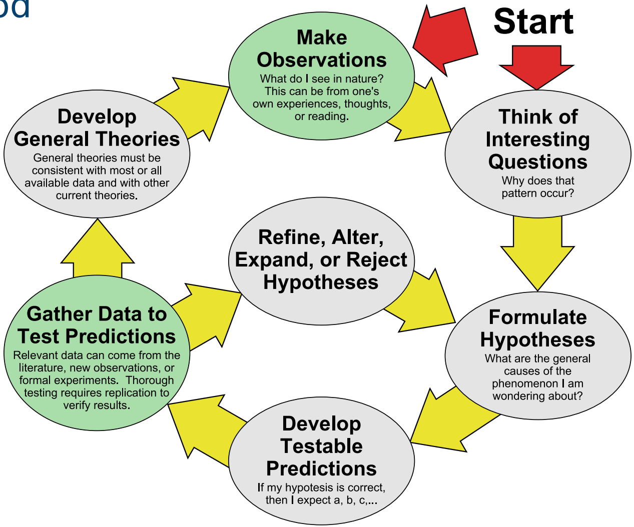
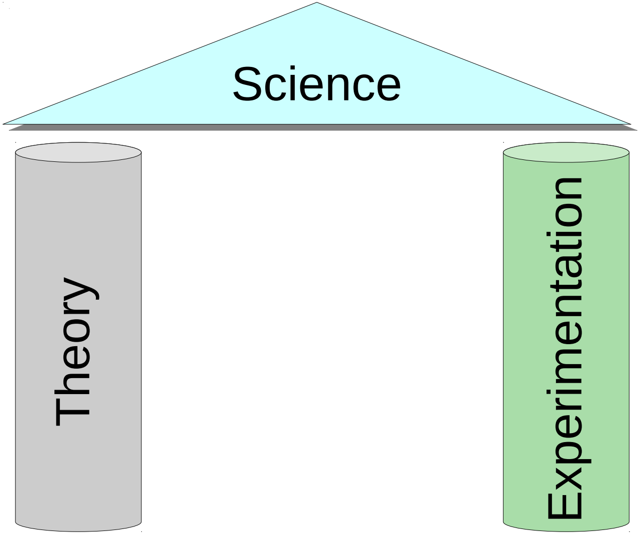
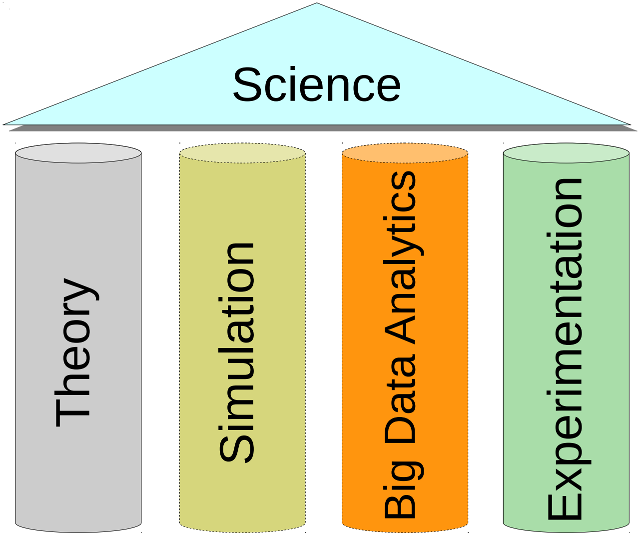


Figure: Based on “The Scientific Method as an Ongoing Process”, ArchonMagnus
https://en.wikipedia.org/wiki/Scientific_method

Pillars of the Scientific Method



Pillars of Science: **Modern Perspective**



Computer-Aided Simulation

Modelling and Simulation of the world replaces traditional experiment

Computer simulation is an instrument empowering scientists with

- arbitrary temporary and spatial resolutions
- manipulation of arbitrary (model) parameters
- reproducability
- conducting experiments that are infeasible due to ethics, risks or costs
  - Impact of explosion of nuclear power plant
  - Impact of poison to humans
  - Influence of brain neurons
- Prediction of the future
  - Weather forecast, climate
  - COVID19 infection progression ...

Simulation is Compute and Memory-Intense

Examples

- Simulation of billions of neurons requires certain memory
- Modelling of plane engines consist of billions of "elements"
- AI-Models compute with 1000s of GPUs
- Deadline of simulations
  - Weather prediction requires high resolutions but must complete faster than 24h

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How can we cope with the huge demand for compute/storage resources?

- A single PC/server/workstation is not able to solve compute task

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How can we cope with the huge demand for compute/storage resources?

- A single PC/server/workstation is not able to solve compute task
- We need more performance ... High performance ...

High-Performance Computation

Relation of the Scientific Method to Simulation

Simulation models real systems to gain new insight

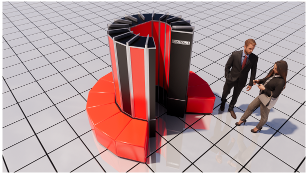
- Instrument to make observations, e.g., high-resolution and fast timescale
- Typically used to validate/refine theories, identify new phenomen
- Classical computational science: hard facts (based on models)
- The frontier of science needs massive computing resources on supercomputers
- Data-intensive sciences like climate imposes challenges to data handling, too

Outline

High-Performance Computing

Definitions

- HPC: Field providing massive compute resources for a computational task
  - Task needs too much memory or time for a normal computer
  - ⇒ Enabler of complex challenging simulations
- Supercomputer: aggregates power of many compute devices
  - In the past large monolithic computers such as the Cray
  - Nowadays: 100-1,000s of servers that are clustered together
  - Comparison: Car is to Formula-1 like Computer to Supercomputer



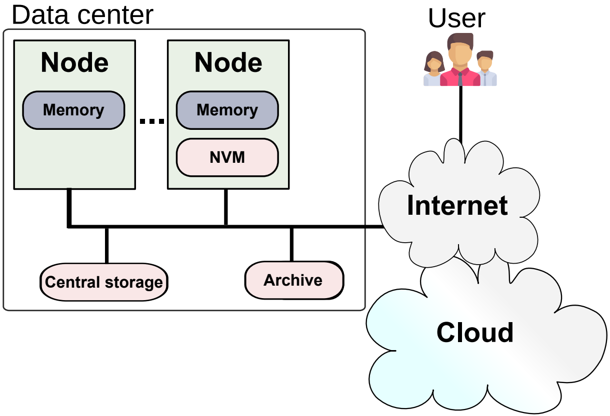
Introducing: One of the Fastest Supercomputers of the World

FUGAKU at RIKEN Center for Computational Science

- Nodes/Servers: 158,978
  7.6 Million CPU Cores
- Compute Peak: 540 Petaflop/s (10^{15})
- Memory: 5 Petabyte
- Storage: 150 Petabyte HDDs
- Energy Consumption: 30 Megawatt
- Costs: 1 Billion (program) $

The Top500 is a list of the most performant supercomputers

Supercomputers & Data Centers



Credits: STFC

JASMIN Cluster at RAL / STFC

Used for data analysis of the Centre for Environmental Data Analysis (CEDA)

HPC in Göttingen

GWDG: unversity data center and providing innovative technology solutions

- HPC sytems for local scientists, German wide and for DLR
- Integrates research for HPC systems and services

Outline

Distributed Computing

Field in computer science that studies **distributed systems**[1]

Definition

- System which components[2] are located on different networked computers
- Components communicate and coordinate actions by passing messages
- Components interact to achieve a common goal
- *In the wider sense*: autonomous processes coordinated by passing messages

Characteristics

- Distributed memory: components have their own (private) memory
- Concurrency of components: different components compute at the same time
- Lack of a global clock: clocks may diverge
- Independent failure of components, e.g., due to power outage

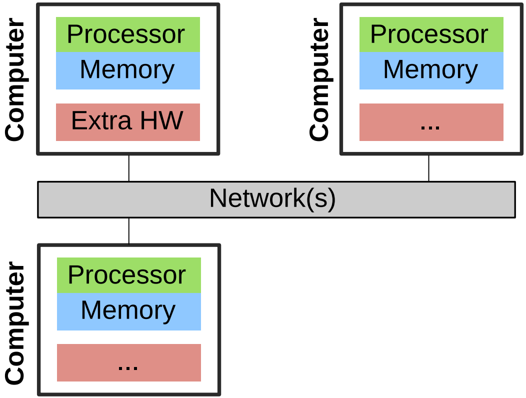
[1] https://en.wikipedia.org/wiki/Distributed_computing

[2] In this context, means a component from a software architecture.

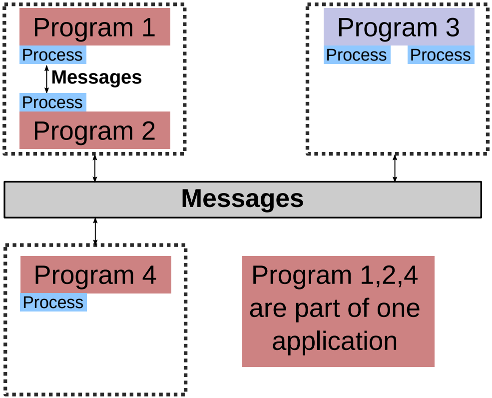
Example Distributed System and Distributed Program

- A **distributed program** (DP) runs on a distributed system
  - Processes are instances of one program running on one computer
- A **distributed applications/algorithm** may involve various DPs/different vendors

Hardware perspective



Software perspective (mapped to hw)



Example Distributed Applications and Algorithms

Applications

- The Internet and telecommunication networks
- Cloud computing
- Wireless sensor networks
- The Internet of Things (IoT) – "everything is connected to the Internet"

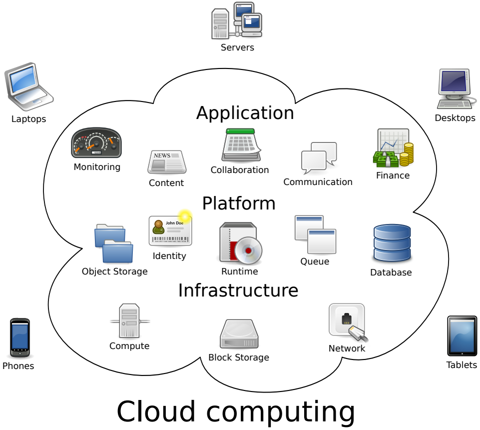
Algorithms (selection from real world examples)

- Consensus: reliable agreement on a decision (malicious participants?)
- Leader election
- Reliable broadcast (of a message)
- Replication

Cloud Computing

Definition

- On-demand availability of computer system resources (data storage and computing)
  - Without direct active management by the user
- Typically relates to distributed resources
  - provided by data centers
  - to many users
  - over the Internet
- Fog/Edge Computing: brings cloud closer to user



Examples

- Applications: Dropbox, Google Mail, Office 365
- Infrastructure: Amazon, Google, Microsoft, Oracle

Challenges using Distributed Systems

- Programming: concurrency introduces new types of programming mistakes
  - It is difficult to think about all cases of concurrency
  - Must coordinate between programs
  - No global view and debugging
- Resource sharing: system shares resources between all users
- Scalability: system must be able to grow with the requirements
  - numbers of users/data volume/compute demand
  - retain performance level (response time)
  - requires to add hardware, though
- Fault handling: detect, mask, and recover from failures
  - Failures are innevitable and the normal mode of operation
- Heterogenity: system consists of different hardware/software
- Transparency: Users do not care about how/where code/data is
- Security: Availability of services, confidentiality of data

Outline

Definition: Parallel Computing

Many calculations **or** the execution of processes are carried out simultaneously[3]

Characteristics

- Goal is to improve performance for an application
  - Either allowing to solve problems within a deadline or increased accuracy
- Application/System must coordinate the otherwise independent parallel processing
  - There are various programming models for parallel applications
- Different architectures to speed up computation: **may use** distributed systems

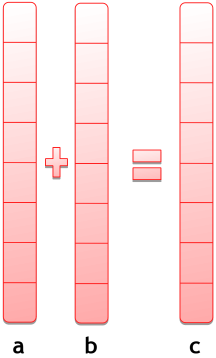
Levels of parallelism (from hardware perspective)

- Bit-level: process multiple bits concurrently (e.g., in an ALU)
- Instruction-level: process multiple instructions concurrently on a CPU
- Data: run the same computation on **different data**
- Task: run **different** computations concurrently

[3] `https://en.wikipedia.org/wiki/Parallel_computing`

Bit-Level Parallelism: Vector Parallelism with SIMD

- SIMD = Single instruction multiple data
  - Apply the same operation on multiple data
- Example: Vector addition: a = b + c
  - $c_i = a_i + b_i$ for all vector elements i

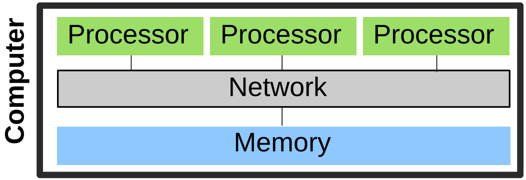


- AVX-512 works on 8x 64-bit elements in parallel, i.e., run same operation on all

Parallel Architectures

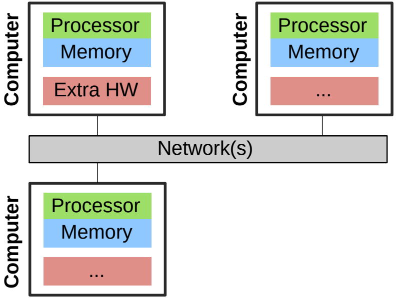
In practice, systems are a mix of two paradigms:

Shared memory



- Processors can access a joint memory
  - Enables communication/coordination
- Cannot be scaled up to any size
- Very expensive to build one big system
- Programming with **OpenMP**

Distributed memory systems (again!)

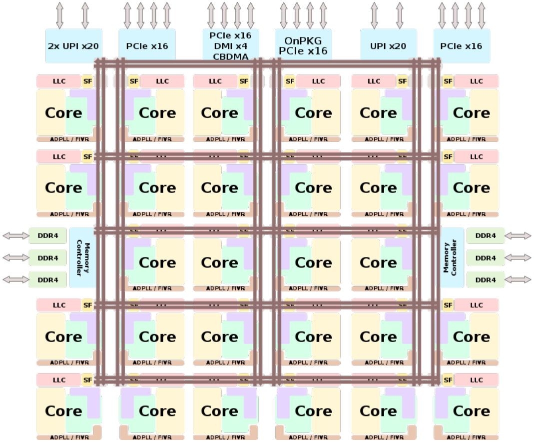


- Processor can only see own memory
- Performance of the network is key
- Programming with **Message Passing**

Multicore CPU: Xeon Platinum 8280M Cascade Lake-SP

Performance

- FLOPs: 32 · frequency · cores
  - ▶ 28 cores, 2.7 GHz (1.8 GHz AVX512)
  - ⇒ 2.2 TFLOPs
- 6 Channel DDR4, max 2.933 GHz
  - ▶ Throughput 131 GB/s
- Power: 205 Watt



Architecture

- Each core executes code independently
  - ▶ Feature rich: speculative execution, ...
- Each core has two AVX-512 units
  - ▶ Vector parallelism on 512 bits
- Summary: complex architecture, heavy cores, optimized for latency

Manycore GPU: NVIDIA A100

Accelerated computing is outside of this course, concepts are transferrable

Performance

- FLOPs: 9.7 TFLOPs FP64
  - 312 TFLOPs Tensor (FP16)
  - 1.41 GHz
- 40 GByte HBM2 memory
  - 10 memory channels
  - Throughput 1600 GB/sec
- Power: 400 Watt

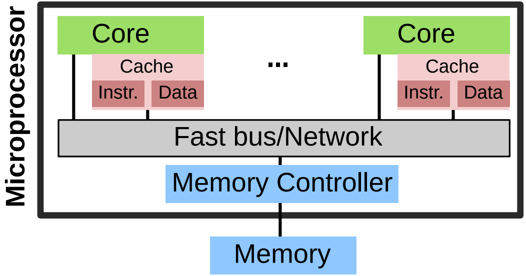
Architecture

- 128 Streaming multiprocessors
  - Each with 32 FP64 cores
  - ⇒ 4096 cores per GPU
- Summary: Simple cores, optimized for throughput
- Problem: deep pipeline, higher latency, costly startup time of program

Parallel Programs

- A **parallel program** runs on parallel hardware
  In the strict sense: A parallel application coordinates concurrent processing

Schema of a multicore processor



Processor provides all levels of parallelism

- Multiple ALU/other units
- Pipelining of processing stages
- SIMD: Single Instruction - Multiple Data
  - Same operation on multiple data
  - Instruction set: SSE, AVX
- Multiple cores
  - Each with own instruction pointer
- May use (GPU) accelerators
  - CPU in charge for processing

Group Work

- Think about an application of parallel computation - describe the use case briefly
- What computation is performed in parallel?
- Which architecture / hardware presented would you like to use for it?
- Time: 5 min
- Organization: breakout groups - please use your mic or chat

Challenges

- Programming: imports errors from distributed computed +
  - Low-level APIs and code-optimization to achieve performance
  - Performance-optimized code is difficult to maintain
  - Expensive and challenging to debug 1'000 concurrently running processes
  - Utilizing all compute resources efficiently (load balancing)
  - Grand challenges are difficult to test, as nobody knows the true answer
- Performance engineering: Optimizing code is main agenda for HPC
  - Covered in this course
- Scalability: stricter than distributed systems
  - Strong-scaling: same problem, more parallelism shall improve performance
  - Weak-scaling: data scales with processors, retain time-to-solution
- Environment: bleeding edge and varying hardware/software systems
  - Obscure special-purpose hardware (FPGA/ASIC Application-Specific Integrated Circuit)
  - Limited knowledge to administrate, use, and to compare performance

Outline

Programming

- Let's investigate how to create a "parallel" program

Abstractions and examples

- Sequential code to compute vector addition
- Automatically parallelizable code for shared memory using OpenMP
  - Parallelizes code based on user-provided directives
- Manual parallelization for distributed memory using Message passing

Vector Addition: Sequential CPU Code

Compute function = "kernel"

```
void vecAdd(int * restrict a, int * restrict b, int * restrict c, int n){
  for(int i=0; i < n; i++){
    c[i] = a[i] + b[i];
  }
}
```

Execution

```
  int a[8];
  int b[8];
  int c[8];
  // fill a and b somehow
  vecAdd(a, b, c, 8);
```

- Both codes may be placed in the same file ⇒ we call this a "single source"

Directive-Based Parallelism using OpenMP: CPU Code

Compute function = "kernel"

```
void vecAdd(int * restrict a, int * restrict b, int * restrict c, int n){
// A preprocessor directive telling the compiler to parallelize the for loop
#pragma OMP parallel for
  for(int i=0; i < n; i++){
    c[i] = a[i] + b[i];
  }
}
```

Execution

- The same code as before, just compile with -fopenmp...

```
  int a[8];
  int b[8];
  int c[8];
  // fill a and b with values ...
  vecAdd(a, b, c, 8);
```

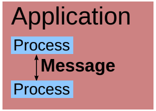
Message Passing

Definition

- Message passing is the sending of a message to a process[4]
- What: any data from the memory of the sender
- How: Programmer explicitly requests send/recv

Content of a message

- Header (Sender, receiver, type[5])
- Data (from memory)



Addressing

- How to define to whom I sent, from whom to receive?
  - Addressing via "process number": Rank 0 - (N-1)
  - Processes are enumerated upon start

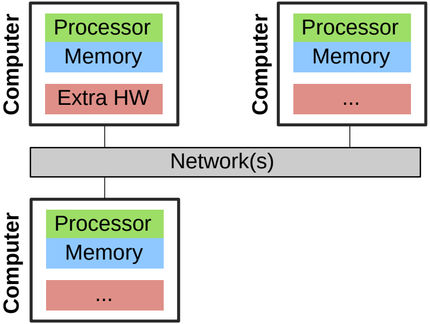
[4] The general definition in distributed systems is more generic

[5] Distinguishs different messages

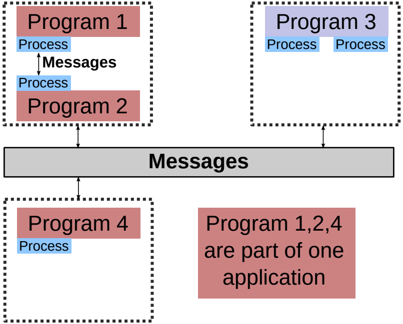
Example Execution of an Message Processing Program

- Processes are instances of an application
  - Executed on different computers
  - May execute the same or different code
  - Addressing via enumeration of the processes
- Different applications can be executed concurrently

Hardware perspective



Software perspective



Programming with Message Passing

- Code of processes of the program define how they cooperate
- Important standard: The Message Passing Interface (MPI)
  - MPI implementations are a library with communication functions

Single Program Multiple Data (SPMD)

- SPMD: A single binary program created from one source code
- Every process of a program runs on different data
- Example message passing inside one code:

```
int Rank = getRank(); // Determine my rank
if(Rank == 0){
  // Send message (18 bytes to Rank 1)
  send(1, 18, "Hello from rank 0");
}else if(Rank == 1){
  char data[100];
  // Receive message from Rank 0
  receive(0, 18, data);
  printf("%s\n", data);
}
```

Concurrent Execution

- Assumption: our example program is executed with two processes
  - Instructions of both processes are executed concurrently and independent

Executed code

Prozess 0

```
int rang = getRank();  // returns 0
if(rang == 0){
  send(1, 18, "Hello from rank 0");
}else...

}
```

Message

Prozess 1

```
int rang = getRank();  // returns 1
if(rang == 0){

}else if(rang == 1){
  char data[100];
  receive(0, 18, data);
  printf("%s\n", data);
}
```

- Semantics of message exchange is defined by operation/function
  - Receive must block until a suitable message is received
  - Sending might complete before message is actually received/processed
- Program code is **parallelizable** if any paralell and concurrent execution path leads to the **same solution**

Outline

Computational Science

- When we talked about computer-aided simulation, we meant computational science

Definitions

- Multidiciplinary field using advanced computing capabilities to understand and solve complex problems
  - Typically using mathematical models and computer simulation
  - Problems are motivated by industrial or societal challenges
- May utilize single computer, distributed systems, or supercomputers

Examples utilizing distributed computing

- Finding the higgs boson (CERN)
- Bioinformatics applications, e.g., gene sequencing

Examples utilizing high-performance computing

- Computing the weather forecast for tomorrow / next week
- Simulating a tokamak fusion reactor

Summary

- HPC and supercomputers are enablers for scientific computing
- Supercomputers are relevant for data science
- Parallel computing is the simultaneous calculation/execution
- Shared-memory, distributed-memory and GPU-Architectures differ
- GPUs are accelerating CPUs for massively parallel workloads
- Programming can be challenging
- Programming paradigms
  - Auto-parallelization with compiler-directives (OpenMP, shared mem)
  - Paralellization with Message Passing (distributed computing)
- Simple example: Vector addition