# Introduction

## Parallel Programming

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# Outline

- Introduction
  - Organization
  - Lecture
  - Exercises
  - Outlook
  - Summary

# Survey

- How familiar are you with C?
  1. Expert
  2. Advanced
  3. Beginner
  4. Not at all

# Survey

- How familiar are you with Linux?
    1. Expert
    2. Advanced
    3. Beginner
    4. Not at all

# Survey

- How familiar are you with Git?
    1. Expert
    2. Advanced
    3. Beginner
    4. Not at all

# Lecture and Exercises

- Lecture: Wednesdays, 17:15–18:45
  - Foundation and background of parallel programming
  - Lecture will be recorded for later viewing
  - We will also use this time slot to clear up questions etc.
- Exercises: Wednesdays, 11:15–12:45
  - Practical exercises about parallel programming
  - We will discuss solutions and take a look at the next exercise sheet
- Exam: Written

# Communication

- Please sign up for the Mattermost team
  - If there are questions about the lecture or exercises, please ask them there
  - Feel free to use it for discussion and communication with your fellow students
    - You can also use it to find people for your exercise group
  - You can of course also send us e-mails:
    - `michael.kuhn@ovgu.de` (lecture and general)
    - `michael.blesel@ovgu.de` (exercises)
- Slides, exercise sheets etc. will be available on the website

# Literature

- High Performance Computing: Modern Systems and Practices (Thomas Sterling, Matthew Anderson and Maciej Brodowicz)
- Parallel Programming: for Multicore and Cluster Systems (Thomas Rauber and Gudula Rünger) (e-book at UB)
- Parallel Programming: Concepts and Practice (Dr. Bertil Schmidt, Dr. Jorge Gonzalez-Dominguez, Christian Hundt and Moritz Schlarb) (book at UB)

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# Topics

- Introduction (10 April – today ☺)
    - A brief overview of some topics we will cover in the lecture
    - This is an outlook, no need to understand everything immediately
- Performance Analysis and Optimization (17 April)
    - How to measure performance correctly and identify relevant components
    - Math, code and compiler optimizations
- Hardware Architectures (24 April)
    - Differences between shared and distributed memory
    - Non-uniform memory access
- Parallel Programming (8 May)
    - How to parallelize problems
    - Potential problems and new kinds of errors

# Topics…

- Programming with OpenMP (22 May)
    - High-level parallelization using compiler annotations
    - Loops, tasks, synchronization etc.
- Operating System Concepts (29 May)
    - Differences between processes and threads
    - Shared memory regions, I/O, scheduling etc.
- Programming with POSIX Threads (5 June)
    - Low-level parallelization using library functions
    - Thread creation, joining, synchronization, condition variables etc.
- Programming with MPI (12 June)
    - Parallelization using the Message Passing Interface
    - Communication, I/O, collective operations etc.

# Topics…

- Networking and Scalability (19 June)
    - Performance metrics for network technologies and topologies
    - Scalability considerations for large systems
- Advanced MPI and Debugging (26 June)
    - Advanced concepts for message passing applications (such as RMA)
    - How to debug parallel programs using multiple threads and processes
- Parallel I/O (3 July)
    - Why parallel I/O is needed in parallel applications
    - Architecture of parallel distributed file systems
- Research Talks (10 July)
    - Research topics currently investigated in our group

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# Overview

- Exercises will consist of parallel programming in C
    - Trying out the concepts taught in the lecture
- You should have experience in a programming language
    - Experience in C is not necessary (but helps)
- We will work mostly on our cluster via SSH
    - Logging in and setting everything up will be part of the first exercise

# Topics

- Introduction and setup (10 April)
  - Log in to cluster, set up software environment etc.
- Debugging (22 April)
  - Using GDB, Valgrind etc.
- Performance optimization (29 April)
  - Optimizing a serial application
- Parallelizing with OpenMP and parallelization schema (20 May)
  - Preparing a parallelization schema for the serial application
  - Parallelizing the optimized application with OpenMP

# Topics…

- Parallelizing with POSIX Threads (3 June)
    - Parallelizing the optimized application with POSIX Threads
- Introduction to MPI (10 June)
    - Getting familiar with the Message Passing Interface
- Parallelizing with MPI (Jacobi) (17 June)
    - Parallelizing the optimized application with MPI

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# Motivation

- Parallel programming is an important skill
    - Processors feature an increasing amount of cores
    - Even current phones have eight cores
- Serial applications will not be able to fully utilize a machine
    - Except for cases we call trivial parallelization
    - Sometimes possible to run multiple serial applications in parallel
- Parallelization is very important in science
    - Many problems can only be solved on supercomputers
    - High-performance computing (HPC)

# Performance Analysis and Optimization

- It is difficult to measure performance correctly
    - There are many factors and components to consider
    - Performance is influenced by caching, network, input/output (I/O) etc.
    - Errors can influence or even invalidate all results
- Optimization requires deep knowledge of the hardware
    - How do the different levels of caches interact?
    - Can we reach the main memory from all cores with the same speed?
    - How does our application behave with more cores?

# Performance Analysis and Optimization…

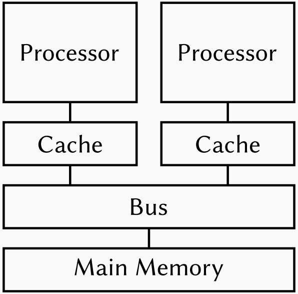
- There are also technical issues to take into account
  - HPC applications are typically run via a batch scheduler
  - Operating system services can influence performance
- Measuring performance can be hard
  - Which components are involved and have to be measured?
  - Which performance can we expect on a given system?

# Hardware Architectures

- Until ca. 2005: Performance increase via clock rate
    - Going from n GHz to 2n GHz will usually double application performance
- Since ca. 2005: Performance increase via core count
    - Clock rate cannot be increased further
    - Power consumption/heat depends on clock rate
    - Biggest supercomputers on TOP500 list have more than 10,000,000 cores
- Important classification: Memory access model
    - Shared and distributed memory
    - In reality, typically hybrid systems

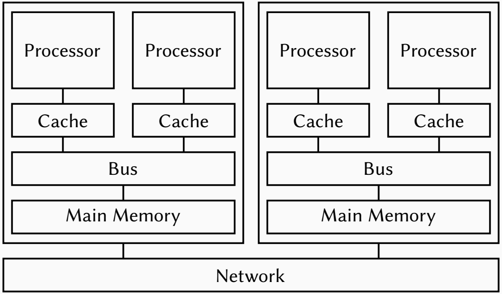
# Hardware Architectures...

- All processors have access to shared memory
    - There might be speed differences due to NUMA
- Typically refers to single machines
    - Shared memory can also be virtual
- Processors consist of multiple cores
    - Each core has its own caches
    - Shared cache for the whole processor
- Access to shared memory via a bus
    - This also limits scalability of shared memory



# Hardware Architectures. . .

- Processors only have access to own memory
    - Typically with shared memory architecture
- Typically refers to a cluster of machines
    - Could theoretically be used inside machine
- Machines are connected via a network
    - Determines scalability and performance
    - Different network technologies and topologies

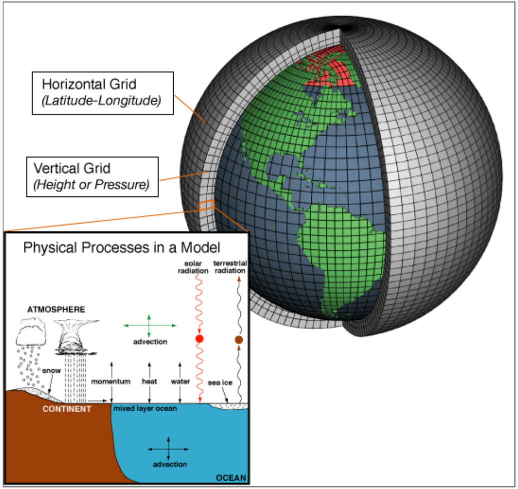


# Parallel Programming

- Parallel programming is used to increase application performance
    - In HPC, OpenMP and MPI are often used together
- OpenMP is an interface for shared memory
    - Applications run as multiple threads within a single process
    - OpenMP features thread management, task scheduling, synchronization and more
- MPI (Message Passing Interface) is an interface for distributed memory
    - Applications run distributed over multiple compute nodes
    - MPI features message passing, input/output and other functions
- Both approaches are available for multiple programming languages

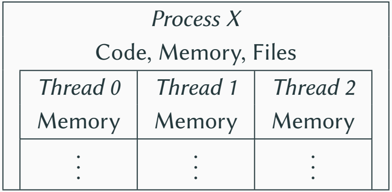
# Parallel Programming…

- Numerical problems are mostly iterative
  - Simulations often performed in time steps
- Global conditions for termination
  - Run for a specified number of time steps
- Data structures are often regular
  - Data often stored in one or more matrices
- Many phenomena are highly parallel
  - Galaxies, planets, climate and weather
- Parallel computing is well-suited
  - Data and components can be distributed



[NOAA, 2007]

# Parallel Programming…



*Process X*

Code, Memory, Files

| *Thread 0* | *Thread 1* | *Thread 2* |
|---|---|---|
| Memory | Memory | Memory |
| ⋮ | ⋮ | ⋮ |

- We will only take a look at threads for now
    - Message passing will be covered later
- Processes are instances of an application
    - Applications can be started multiple times
    - Processes are isolated from each other by the operating system
    - Resources like allocated memory, opened files etc. are managed per-process
- Threads are lightweight processes
    - Threads have their own stacks but share all other resources
    - Shared access to resources has to be synchronized
    - Uncoordinated access can lead to errors very easily

# Parallel Programming…

- Threads share a common address space
  - Communication is often done via shared variables
  - Threads are processed independently, that is, in parallel
  - If one thread crashes, the process crashes with all threads
- Processes have their own address spaces
  - Typically have to start multiple processes for distributed memory
  - Overhead is normally higher than with shared memory
  - There are also concepts for distributed shared memory
- In practice, hybrid approaches are used
  - A few processes per node (e. g., one per socket)
  - Many threads per process (e. g., one per core)

# Parallelization with OpenMP

- Numerical applications often deal with matrices
  - Matrices are as big as the main memory allows
  - We want to calculate the sum of all elements
- Have to go through all rows and columns
  - Process one element after the other

| | | | | |
|---|---|---|---|---|
| (0,0) | (0,1) | ... | (0,n-1) | (0,n) |
| ... | ... | ... | ... | ... |
| (m,0) | (m,1) | ... | (m,n-1) | (m,n) |

```
for (int i = 0; i < m; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
```

# Parallelization with OpenMP…

- OpenMP allows parallelization using compiler pragmas
    - Very convenient for developers, no internal knowledge necessary
    - Reduced functionality when compared to system-level approaches

```
#pragma omp parallel for
for (int i = 0; i < m; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
```

# Parallelization with OpenMP…

```
for (int i = 0; i < m/2; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
```

```
for (int i = m/2; i < m; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
```

- First for loop is split up across multiple threads
  - Usually as many threads as there are cores
  - OpenMP can also do dynamic distributions and further scheduling
- Example: Laptop with two cores
  - First core calculates `0` to `(m/2)-1`
  - Second core calculates `m/2` to `m-1`

# Parallelization with OpenMP...

- This solution was very easy but also wrong ☺
    - Instead of the correct sum, we get weird values
    - Every time we run the application, the result changes

```
$ ./openmp
sum=3773725
$ ./openmp
sum=4012997
$ ./openmp
sum=12325088
$ ./openmp
sum=2456866
$ ./openmp
sum=11970989
$ ./openmp
sum=2818054
$ ./openmp
sum=3979092
```

# Parallelization with OpenMP...

- This solution was very easy but also wrong ☺
  - Instead of the correct sum, we get weird values
  - Every time we run the application, the result changes
- Shared memory makes it easy to access the sum variable
  - Access has to be synchronized, otherwise errors occur
  - We have produced a so-called race condition
- There are several possibilities to solve the problem
  - Add a lock around the operation (slow)
  - Use atomic instructions (fast)

```
$ ./openmp
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```

# Debugging

- Parallel programming has at least two new error classes
    1. Deadlocks
    2. Race conditions
- A race condition has resulted in a wrong result in our example
    - Incrementing a variable consists of three operations
        1. Loading the variable
        2. Modifying the variable
        3. Storing the variable
    - Operations have to be performed atomically

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| T0 | T1 | V |
|---|---|---|
| Load 0 | | 0 |
| Inc 1 | | 0 |
| Store 1 | | 1 |
| | Load 1 | 1 |
| | Inc 2 | 1 |
| | Store 2 | 2 |

# Debugging

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    1. Loading the variable
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    3. Storing the variable
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| T0 | T1 | V |
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| Load 0 | | 0 |
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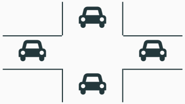
| | Load 1 | 1 |
| | Inc 2 | 1 |
| | Store 2 | 2 |

| T0 | T1 | V |
|---|---|---|
| Load 0 | | 0 |
| Inc 1 | Load 0 | 0 |
| Store 1 | Inc 1 | 1 |
| | Store 1 | 1 |

# Debugging...

- Deadlocks cause parallel applications to stop progressing
  - Can have different causes, most often due to locking
  - May not be reproducible if there is time-dependent behavior
- Error condition can be difficult to find
  - Trying to lock an already acquired lock results in a deadlock
  - Erroneous communication patterns (everyone waits for the right neighbor)
- Error effect is typically easy to spot
  - Spinlocks or livelocks can look like computation, though



# Debugging…

- Race conditions can lead to differing results
    - Debugging often hides race conditions
- Error condition is often very hard to find
    - Can be observed at runtime or be found by static analysis
    - Modern programming languages like Rust can detect data races
- Error effect is sometimes not observable
    - Slight variations in the results are not obvious
    - The correct result cannot be determined for complex applications
    - Repeating a calculation can be too costly

# Networking Aspects

- Scalability of shared memory systems is limited
    - Current processors feature up to 64 cores with 128 threads
    - Typically two, at most four processors per node
- Computation is only one part of parallel applications
    - They need to store data in main memory and persist it to storage
    - Amount of main memory and storage per node is also limited
- To solve the biggest problems, we need distributed memory systems
    - These typically consist of a cluster of shared memory systems
    - Multiple nodes are connected via a so-called interconnect

# Networking Aspects…

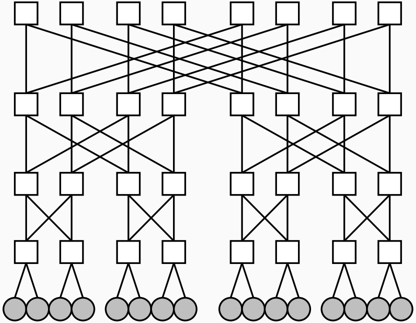
- Processors require data fast
    - 3 GHz equals three operations per nanosecond
    - Even accessing the main memory is too slow
    - Multiple cache levels hide main memory latency
- Network and I/O extremely slow in comparison
    - Waiting for an HDD ruins performance
    - SSDs have alleviated the problem a bit

| Level | Latency |
|---:|---:|
| L1 cache | ≈ 1 ns |
| L2 cache | ≈ 5 ns |
| L3 cache | ≈ 10 ns |
| RAM | ≈ 100 ns |
| InfiniBand | ≈ 500 ns |
| Ethernet | ≈ 100,000 ns |
| SSD | ≈ 100,000 ns |
| HDD | ≈ 10,000,000 ns |

[Bonér, 2012] [Huang et al., 2014]

# Networking Aspects…

- Network topologies can get quite complex
  - Easy: All nodes are connected to a single switch
- Larger systems use hierarchical topologies
  - A fat tree has different throughputs depending on the tree level
- Fat trees can also have blocking factor (2:1)
  - Nodes in enclosure can communicate at 100 %
  - Enclosures in rack can communicate at 50 %
  - Racks can communicate at 25 %



[A5b, 2010]

## Networking Aspects…

- Current network technologies feature high throughputs
  - InfiniBand can do up to 600 GBit/s
  - Ethernet can do up to 400 GBit/s
  - There are more technologies like Intel's Omni-Path
- Sophisticated approaches required to reach these high speeds
  - Kernel bypass to save context switches
  - Zero copy to avoid exhausting bus speeds

# Programming with MPI

- Parallel applications can be run across multiple nodes
    - Typically as separate processes, requires message passing
    - MPI is the de-facto standard
- MPI offers operations for communication and more
    - Process groups and synchronization
    - Sending, receiving, reduction etc.
    - Point-to-point, collective or one-sided communication
- MPI also supports parallel I/O
    - Concurrent access to shared files

# Programming with MPI…

- Parallel application now runs as two independent processes
  - Processes can only see their own results, no shared memory
  - There is no risk of overwriting other values as in the OpenMP example
  - However, results have to be communicated between processes somehow

```
for (int i = 0; i < m/2; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
```

```
for (int i = m/2; i < m; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
```

# Programming with MPI...

- MPI allows us to perform efficient reduction operations
    - A predefined reduction operation is the sum

```c
MPI_Init(NULL, NULL);
for (int i = 0; i < m/2; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
MPI_Allreduce(&sum, &allsum, 1,
              MPI_INT, MPI_SUM,
              MPI_COMM_WORLD);
MPI_Finalize();
```

```c
MPI_Init(NULL, NULL);
for (int i = m/2; i < m; i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
MPI_Allreduce(&sum, &allsum, 1,
              MPI_INT, MPI_SUM,
              MPI_COMM_WORLD);
MPI_Finalize();
```

# Programming with MPI…

- Application code is typically still contained in one file
    - MPI allows us to write a generic version of the application
    - We can determine our rank and the number of processes

```c
MPI_Init(NULL, NULL);
MPI_Comm_rank(MPI_COMM_WORLD, &rank);
MPI_Comm_size(MPI_COMM_WORLD, &size);
for (int i = (m/size) * rank; i < (m/size) * (rank + 1); i++) {
    for (int j = 0; j < n; j++) {
        sum += arr[i][j];
    }
}
MPI_Allreduce(&sum, &allsum, 1, MPI_INT, MPI_SUM, MPI_COMM_WORLD);
MPI_Finalize();
```

# Scalability

- When writing parallel applications, we must consider scalability
    - Scalability describes how an application behaves with increasing parallelism
- HPC systems are usually very expensive and should be used accordingly
    - Procurement costs can reach up to € 250,000,000
- To determine scalability, we have to analyze performance
    - HPC systems are complex, performance yield is often not optimal
    - Many different components interact with each other
        - Processors, caches, main memory, network, storage system etc.

# Scalability…

- In addition to procurement costs, operating is also quite expensive
    - 1. Frontier (USA): 1.2 EFLOPS at 22.7 MW ≈ € 52,700,000/a (in Germany)
    - 5. LUMI (Finland): 380 PFLOPS at 7.1 MW ≈ € 16,500,000/a (in Germany)
    - 74. Levante (Germany): 10 PFLOPS at 2 MW ≈ € 4,600,000/a
- Communication and I/O are often responsible for performance problems
    - High latency, which causes excessive waiting times for processors
    - Communication and I/O typically happen synchronously

# Scalability…

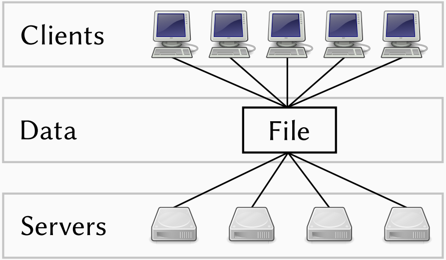
- The performance improvement we get is called speedup
  - In the best case, the speedup is equal to the number of threads
  - In reality, the speedup is usually lower due to overhead
- Speedup can sometimes be higher than the number of threads
  - This is called a superlinear speedup and usually points at a problem
  - For example, each thread’s data suddenly fits into the cache
    - This means that the measured problem became too small
    - Larger problems will not fit and therefore have a lower speedup

# Parallel I/O

- Applications typically need input data and produce output data
  - I/O is an important aspect and can be relevant for overall performance
  - Without I/O, the results of a scientific application would be lost
- Applications often run for multiple days or weeks
  - To cope with crashes, it is necessary to write checkpoints
  - Jobs are often only allowed to run for a few hours at a time
- As mentioned before, storage devices have high latencies
  - Waiting for I/O usually impacts performance negatively
  - File systems try to cache data aggressively to hide latency

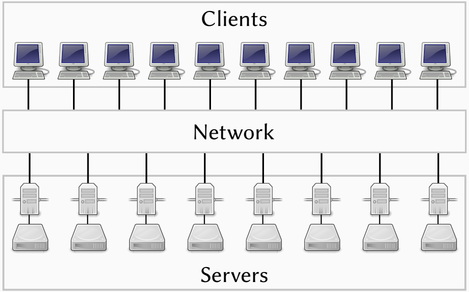
# Parallel I/O…

- Access via parallel distributed file systems
  - Allow concurrent access from clients
  - Distribute data across servers
- Clients can access a shared file
  - Everyone can read input and write results
  - Necessary for parallel applications
- Servers share the load
  - Files are split up and distributed
  - Use capacity and throughput of many servers



# Parallel I/O…

- Computation and storage usually separated
    - Can be optimized for respective workloads
    - No interference of other components
- Clients run parallel applications
    - Small local storage for OS and caching
    - Access to the file system via the network
    - No direct access to file system's devices
- Servers store data and metadata
    - Typically servers with many HDDs and SSDs



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- Parallel programming is an important skill
    - Current computers always have multiple cores or processors
- Parallelization is used to improve performance
    - It is necessary to understand the hardware and keep scalability in mind
- Shared memory and distributed memory are the two main architectures
    - Threads can be used for shared memory systems
    - Message passing is often used for distributed memory systems
- Parallel applications can have deadlocks and race conditions
    - These errors can be hard to find and non-deterministic

# References

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[Bonér, 2012] Bonér, J. (2012). **Latency Numbers Every Programmer Should Know.** https://gist.github.com/jboner/2841832.

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