

Introduction

Parallel Programming

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OTTO VON GUERICKE
UNIVERSITÄT
MAGDEBURG

Dr. Georgiana Mania, Dr. Jannek Squar, Prof. Dr. Michael Kuhn

mania@dkrz.de, jannek.square@uni-hamburg.de, michael.kuhn@ovgu.de

Parallel Computing and I/O

Institute for Intelligent Cooperating Systems

Faculty of Computer Science

Otto von Guericke University Magdeburg

<https://parcio.ovgu.de>

Outline

Introduction

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Lecture

Exercises

Outlook

Summary

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

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

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

- Lecture: Thursdays, 11:15–12:45
 - Foundation and background of parallel programming
 - We will also use this time slot to clear up questions etc.
- Exercises: Wednesdays, 09:15–10:45; Thursdays, 13:15–14:45
 - Practical exercises about parallel programming
 - We will discuss solutions and take a look at the next exercise sheet
- Exam: Written

- 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:
 - mania@dkrz.de, jannek.squar@uni-hamburg.de (lecture)
 - michael.blesel@ovgu.de (exercises and general)
- Slides, exercise sheets etc. will be available on the website

- 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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- Introduction (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
 - How to measure performance correctly and identify relevant components
 - Math, code and compiler optimizations
- Hardware Architectures
 - Differences between shared and distributed memory
 - Non-uniform memory access

- Parallel Programming
 - How to parallelize problems
 - Potential problems and new kinds of errors
- Programming with OpenMP
 - High-level parallelization using compiler annotations
 - Loops, tasks, synchronization etc.
- Operating System Concepts
 - Differences between processes and threads
 - Shared memory regions, I/O, scheduling etc.

- Programming with POSIX Threads
 - Low-level parallelization using library functions
 - Thread creation, joining, synchronization, condition variables etc.
- Programming with MPI
 - Parallelization using the Message Passing Interface
 - Communication, I/O, collective operations etc.
- Networking and Scalability
 - Performance metrics for network technologies and topologies
 - Scalability considerations for large systems

- Advanced MPI and Debugging
 - Advanced concepts for message passing applications (such as RMA)
 - How to debug parallel programs using multiple threads and processes
- ICON – a Large Parallel Scientific Application
 - How parallelism is used in real-world applications
- Research Talks
 - Research topics currently investigated in our group

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- 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

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

- Parallelizing with POSIX Threads
 - Parallelizing the optimized application with POSIX Threads
- Introduction to MPI
 - Getting familiar with the Message Passing Interface
- Parallelizing with MPI (Jacobi)
 - Parallelizing the optimized application with MPI
- Parallelizing with MPI (Gauß-Seidel)
 - Parallelizing the optimized application with MPI

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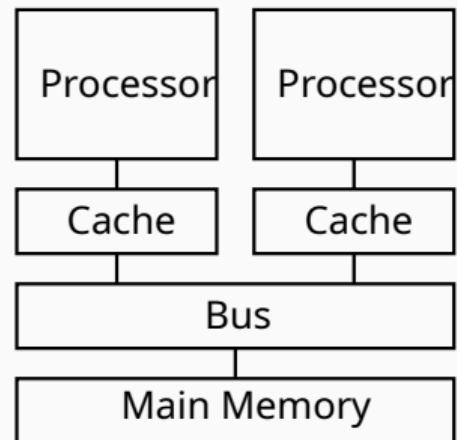
- Parallel programming is an important skill
 - Processors feature an increasing amount of cores
 - Even current phones have eight cores
- Serial applications will not be able to fully utilize a machine
 - Except for cases we call trivial parallelization
 - Sometimes possible to run multiple serial applications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

- 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?

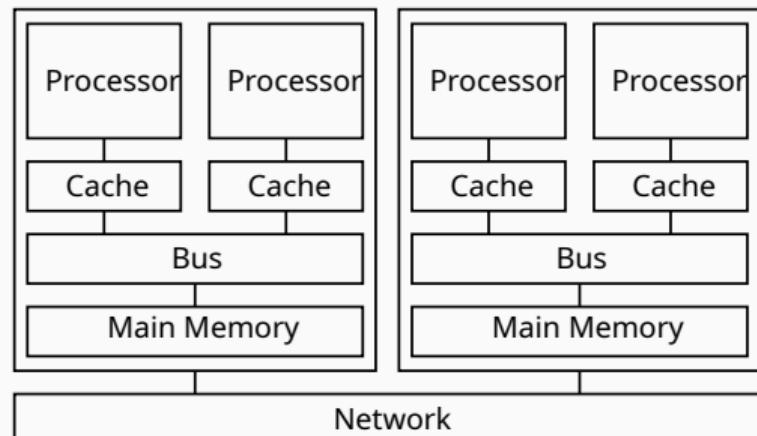
- There are also technical issues to take into account
 - HPC applications are typically run via a batch scheduler
 - Operating system services can influence performance
- Measuring performance can be hard
 - Which components are involved and have to be measured?
 - Which performance can we expect on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

- 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

- 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

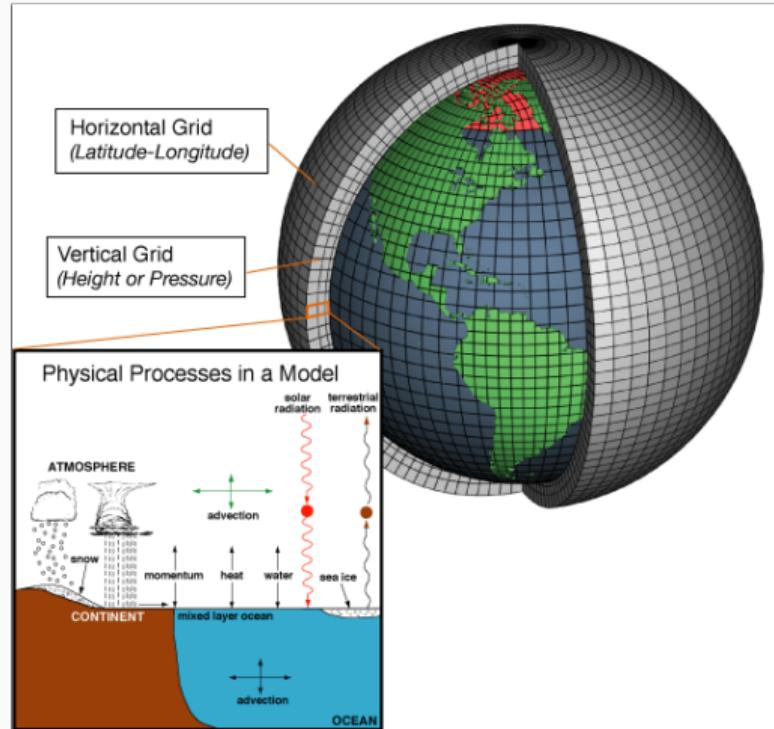


- Processors only have access to own memory
 - Typically with shared memory architecture
- Typically refers to a cluster of machines
 - Could theoretically be used inside machine
- Machines are connected via a network
 - Determines scalability and performance
 - Different network technologies and topologies



- Parallel programming 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

- 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]

- 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

Process X		
Code, Memory, Files		
Thread 0 Memory	Thread 1 Memory	Thread 2 Memory
:	:	:

- 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)

- 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

```
1 for (int i = 0; i < m; i++) {  
2     for (int j = 0; j < n; j++) {  
3         sum += arr[i][j];  
4     }  
5 }
```

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

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

```
1 #pragma omp parallel for
2 for (int i = 0; i < m; i++) {
3     for (int j = 0; j < n; j++) {
4         sum += arr[i][j];
5     }
6 }
```

```
1 for (int i = 0; i < m/2; i++) {  
2     for (int j = 0; j < n; j++) {  
3         sum += arr[i][j];  
4     }  
5 }
```

```
1 for (int i = m/2; i < m; i++) {  
2     for (int j = 0; j < n; j++) {  
3         sum += arr[i][j];  
4     }  
5 }
```

- 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 $m-1$

- 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

```
1 $ ./openmp  
2 sum=3773725  
3 $ ./openmp  
4 sum=4012997  
5 $ ./openmp  
6 sum=12325088  
7 $ ./openmp  
8 sum=2456866  
9 $ ./openmp  
10 sum=11970989  
11 $ ./openmp  
12 sum=2818054  
13 $ ./openmp  
14 sum=3979092
```

- 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)

```
1 $ ./openmp  
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```

- 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

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 - Incrementing a variable consists of three operations
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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

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

- 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



- 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

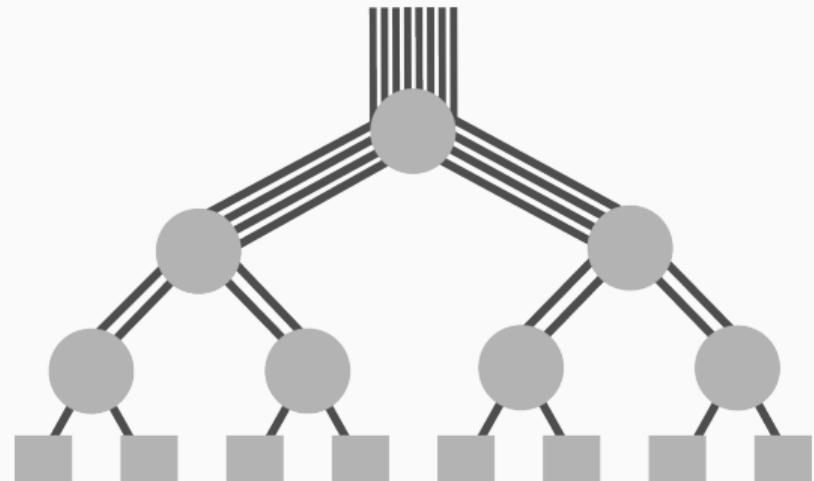
- Scalability of shared memory systems is limited
 - Current processors feature up to 64 cores with 128 threads
 - Typically two, at most four processors per node
- Computation is only one part of parallel applications
 - They need to store data in main memory and persist it to storage
 - Amount of main 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

- 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]

- Network topologies can get quite complex
 - Easy: All nodes are connected to one 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 communicate at 100 %
 - Enclosures in rack communicate at 50 %
 - Racks communicate at 25 %



[Solnushkin, 2012]

- 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

- 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

- 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

```
1 for (int i = 0; i < m/2; i++) {  
2     for (int j = 0; j < n; j++) {  
3         sum += arr[i][j];  
4     }  
5 }
```

```
1 for (int i = m/2; i < m; i++) {  
2     for (int j = 0; j < n; j++) {  
3         sum += arr[i][j];  
4     }  
5 }
```

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

```
1 MPI_Init(NULL, NULL);
2 for (int i = 0; i < m/2; i++) {
3     for (int j = 0; j < n; j++) {
4         sum += arr[i][j];
5     }
6 }
7 MPI_Allreduce(&sum, &allsum, 1,
8                 MPI_INT, MPI_SUM,
9                 MPI_COMM_WORLD);
10 MPI_Finalize();
```

```
1 MPI_Init(NULL, NULL);
2 for (int i = m/2; i < m; i++) {
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7 MPI_Allreduce(&sum, &allsum, 1,
8                 MPI_INT, MPI_SUM,
9                 MPI_COMM_WORLD);
10 MPI_Finalize();
```

- 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

```
1 MPI_Init(NULL, NULL);
2 MPI_Comm_rank(MPI_COMM_WORLD, &rank);
3 MPI_Comm_size(MPI_COMM_WORLD, &size);
4 for (int i = (m/size) * rank; i < (m/size) * (rank + 1); i++) {
5     for (int j = 0; j < n; j++) {
6         sum += arr[i][j];
7     }
8 }
9 MPI_Allreduce(&sum, &allsum, 1, MPI_INT, MPI_SUM, MPI_COMM_WORLD);
10 MPI_Finalize();
```

- 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.

- In addition to procurement costs, operating is also quite expensive
 - 1. Frontier (USA): 1.2 EFLOPS at 22.7 MW \approx € 52,700,000/a (in Germany)
 - 5. LUMI (Finland): 380 PFLOPS at 7.1 MW \approx € 16,500,000/a (in Germany)
 - 74. Levante (Germany): 10 PFLOPS at 2 MW \approx € 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

- 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

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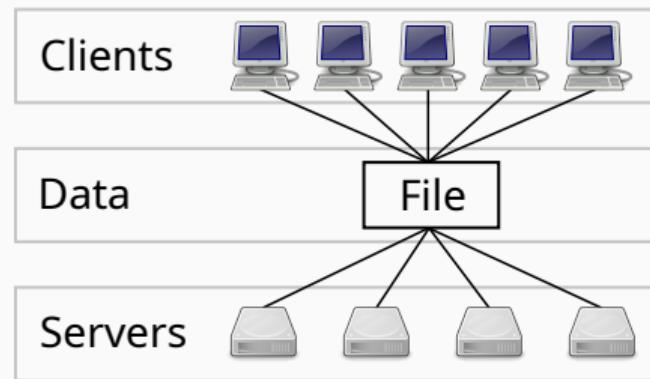
- Parallel programming is an important skill
 - Current computers always have multiple cores or processors
- Parallelization is used to improve performance
 - It is necessary to understand the hardware and keep scalability in mind
- Shared memory and distributed memory are the two main architectures
 - 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

- [Bonér, 2012] Bonér, J. (2012). **Latency Numbers Every Programmer Should Know.**
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- [Solnushkin, 2012] Solnushkin, K. S. (2012). **Fat tree varying ports.**
https://clusterdesign.org/fat-trees/fat_tree_varying_ports/.

- 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

- 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



- 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

