Networking and Scalability

Parallel Programming

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Outline

- Which MPI thread mode is the default?
  1. MPI_THREAD_SINGLE
  2. MPI_THREAD_FUNNELED
  3. MPI_THREAD_SERIALIZED
  4. MPI_THREAD_MULTIPLE

- Which behavior does `MPI_Ssend` have?
    1. Blocking local
    2. Non-blocking local
    3. Blocking non-local
    4. Non-blocking non-local

- Which function buffers data while sending?
    1. `MPI_Send`
    2. `MPI_Bsend`
    3. `MPI_Isend`
    4. `MPI_Rsend`

- What is the difference between MPI_Reduce and MPI_Allreduce?
    1. MPI_Reduce performs a local operation, MPI_Allreduce across all ranks
    2. MPI_Reduce collects the value at the root rank, MPI_Allreduce at every rank
    3. MPI_Allreduce performs a barrier before, MPI_Reduce does not
    4. MPI_Allreduce performs a barrier afterwards, MPI_Reduce does not

Outline

Motivation

- Shared memory systems have limited scalability
  - Machines usually have two to four processors with a few dozen cores
  - OpenMP is a convenient and high-level programming concept
- Complex problems require more resources than available on a single node
  - Simulations require more computational power and main memory
  - Multiple nodes are connected via a so-called interconnect
- Distributed memory can be scaled almost arbitrarily
  - These typically consist of a cluster of shared memory systems
  - The largest machines have up to 10,000,000 cores in several thousand nodes

Motivation…

- Network connections are required to connect multiple nodes
  - Compute nodes have to communicate with each other
  - Storage nodes offer services via the network
- Necessary for inter-process communication across nodes
  - Shared memory objects enable communication on one node
  - Message passing is a programming concept for distributed memory
- Network can be designed using a variety of topologies
  - Bus, ring, star, fully connected mesh, fat tree etc.

Motivation…

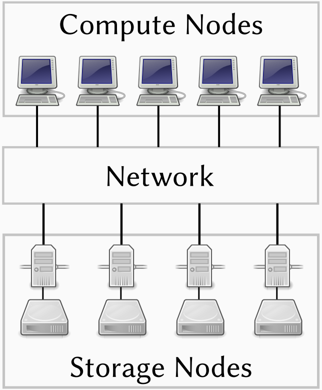
- Processors require data fast
  - 3 GHz equals three operations per nanosecond
  - Even accessing the main memory is too slow
  - Cache levels hide main memory latency
- Network and I/O extremely slow in comparison
  - Waiting for an HDD ruins performance
  - SSDs have alleviated the problem a bit
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

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]

Motivation...

- Computation is only one part of parallel applications
  - Store data in main memory and persist it to storage
  - Main memory and storage per node is also limited
- Storage nodes are usually separate
  - Exclude influence on each other
  - Nodes can be tuned for their respective workloads
- Data has to be transferred for each I/O operation
  - I/O typically also includes network latency
  - Node-local buffers can be used as a workaround



Outline

Overview

- Several components are necessary to build a network
  - Network interface cards (NIC)
    - Each node is equipped with one or more of them
  - Network cables
    - Supercomputers need hundreds to thousands of kilometers of cables
    - Fiber cables offer high frequencies and less loss than copper cables
  - Network switches
    - Multiple switches can be required depending on the network topology
- Network is often split into multiple sub-networks
  - Separate communication, storage and management networks

Overview…

- Have to consider both the hardware and software perspective
- Network technology should be adaptable to different environments
  - Allow using different network topologies depending on requirements
- Different network technologies typically have different interfaces
  - For convenience reasons, a high level of abstraction is preferred
  - High performance might require breaking the high level of abstraction
- Data should be transferred as efficiently as possible
  - High numbers of system calls can have a negative performance impact
  - Some network technologies use kernel bypass to improve performance

Performance

- Performance characteristics are especially important in HPC
  - Network should introduce as little additional overhead as possible
- Bandwidth (in GBit/s or GB/s)
  - Actual throughput might be less due to protocol overhead etc.
- Latency (in ns)
  - Highly dependent on software overheads
  - Depending on distance, physics also becomes important ($\approx$ 1 ms per 100 km)
- Robustness and error rate
  - Network should handle faults in single cables or switches
  - Other factors might cause errors that should be detected and corrected
- TCP/IP support
  - TCP usage is almost ubiquitous and some applications support nothing else

Performance...

- Use case: Sending data to another process
    1. Data is produced by application and resides in its address space

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  5. Target NIC copies received data to kernel space

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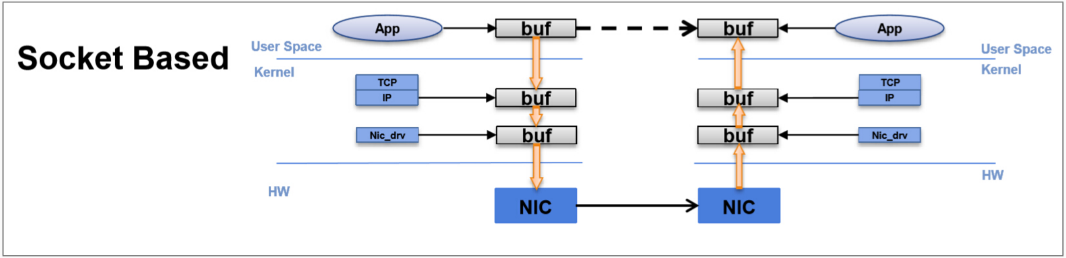
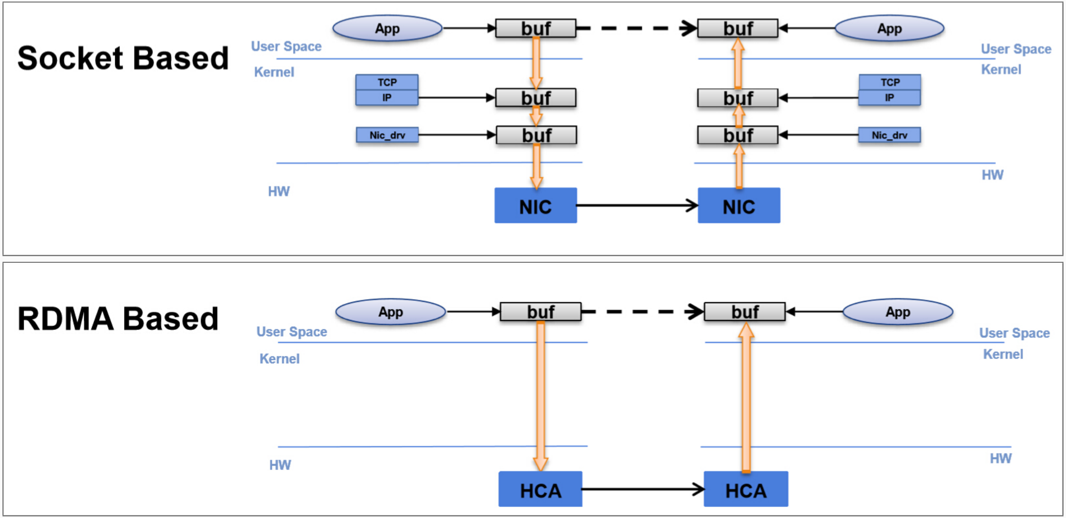
- Different terminology depending on network technology
  - Ethernet uses a network interface card (NIC)
  - InfiniBand uses a host channel adapter (HCA)



[Chenfan, 2016]

RDMA and Zero Copy



[Chenfan, 2016]

RDMA and Zero Copy...

- Remote direct memory access (RDMA)
  - Target's memory can be accessed directly without interruption
  - Memory might have to be registered and/or locked
- Zero copy
  - Avoid copies between user space and kernel space
  - Potential copies within the kernel (kernel buffer and driver buffer)
  - Additional copies between kernel space and device
- Copying is expensive from performance and energy perspectives
  - Copying data once reduces maximum throughput by a factor of two etc.

Offloading

- Network stacks have been designed for different requirements
  - High latencies, low throughputs and potentially high error rates
  - TCP/IP includes support for retransmissions etc.
- Packets are typically small
  - Ethernet normally uses 1,500 bytes frames, TCP up to 64 KiB
  - Worst case: One interrupt per packet
- Operating systems implement their own network stacks
  - Operations have to be performed in software
  - Software overheads can be problematic for high-speed interconnects

Offloading…

- Interrupts can quickly accumulate for high packet rates
  - Interrupts prevent applications from performing computations
- Polling requires processor time to check for new packets
  - Can be more efficient if many packets can be retrieved at once
- Parts of network protocols can be provided in hardware
  - TCP Offload Engine is widely used to improve TCP performance
- DMA allows data to be copied without involving processor
  - Otherwise, processor would have to copy data actively

Kernel Bypass

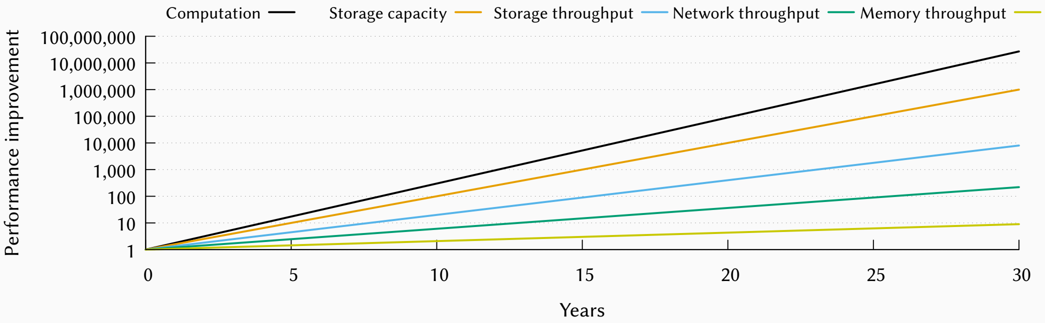
- Traditionally, talking to the network card requires the kernel
  - Kernel manages and talks to the NIC via a driver
  - Applications talk to kernel via system calls
- Context switches and interrupts cause high overhead
  - Kernel bypass allows applications to talk to the NIC directly
- Different approaches exist already [Majkowski, 2015]
  - Many require special hardware support or dedicated NICs
  - For instance, specialized network API that manages queues on NIC

Quiz

- How many additional memory buffers does zero copy require?
    1. One memory buffer in kernel space
    2. One memory buffer in user space
    3. No additional memory buffers

Outline

Performance Development



- Hardware improves exponentially, but at different rates
  - Storage capacity and throughput are lagging behind computation
- Network and memory throughput are even further behind
  - Transferring data has become a very costly operation

Performance Development…

- Network bandwidth has increased steadily over the years
- Two main competitors in HPC
  1. Ethernet
  2. InfiniBand
- InfiniBand supports multiple links
  - x1 is base performance
  - x4, x8 and x12 are faster

Technology	Bandwidth	Year
Ethernet	10 Mbit/s	1980
Fast Ethernet	100 Mbit/s	1995
Gigabit Ethernet	1 Gbit/s	1998
InfiniBand SDR x1	2 Gbit/s	2001
InfiniBand SDR x12	24 Gbit/s	2001
10 Gigabit Ethernet	10 Gbit/s	2002
InfiniBand DDR x12	48 Gbit/s	2005
InfiniBand QDR x12	96 Gbit/s	2007
100 Gigabit Ethernet	100 Gbit/s	2010
InfiniBand FDR x12	163.64 Gbit/s	2011
InfiniBand EDR x12	300 Gbit/s	2014
Omni-Path	100 Gbit/s	2015
400 Gigabit Ethernet	400 Gbit/s	2017
InfiniBand HDR x12	600 Gbit/s	2017

[Wikipedia, 2020]

InfiniBand

- InfiniBand is a networking standard
  - Promoted by the InfiniBand Trade Association
  - Mellanox is the major vendor for InfiniBand (now part of Nvidia)
- Mostly used in HPC due to high throughput and low latency
  - Throughputs up to 600 GBit/s
  - Latencies of less than 500 ns
- InfiniBand provides support for RDMA
  - Used by MPI's own RDMA support

InfiniBand…

- No standard API
    - Standard only has a list of verbs such as `ibv_open_device`
    - De-facto standard software stack by OpenFabrics Alliance
    - libibverbs for Linux, kernel support since 2005
- Packets of up to 4 KB for messages
    - RDMA read or write
    - Send or receive
    - Transaction operation
    - Multicast operation
    - Atomic operation

Quiz

- How much throughput can we typically expect from Gigabit Ethernet?
  1. 10 MB/s
  2. 12 MB/s
  3. 100 MB/s
  4. 120 MB/s
  5. 1 GB/s
  6. 1.2 GB/s

Outline

Overview

- Reminder: Scalability is ambiguous and can apply to different components
  - We have taken a look at the scalability of hardware architectures before
- How big we can scale something while keeping the benefits
  - How easy it is to increasing a network's size
  - How well invested money correlates with improved performance
  - How well an application can run on more cores/nodes
- We will now take a look at the scalability of parallel applications

Motivation

- 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.

Motivation…

- In addition to procurement costs, operating costs are also quite high
  - 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

Speedup

- The performance improvement we get is called speedup
  - In the best case, the speedup is equal to the number of tasks
  - In reality, the speedup is usually lower due to overhead (communication, I/O etc.)
- Speedup can sometimes be higher than the number of tasks
  - This is called a superlinear speedup and usually points at a problem
  - For example, each task'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

Speedup...

- Speedup: $S(n) = \frac{T(1)}{T(n)}$
  - $T(1)$: Runtime of one task
  - $T(n)$: Runtime of n tasks

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- Efficiency: $E(n) = \frac{S(n)}{n}$
  - Normalizes the speedup to the $[0, 1]$ range

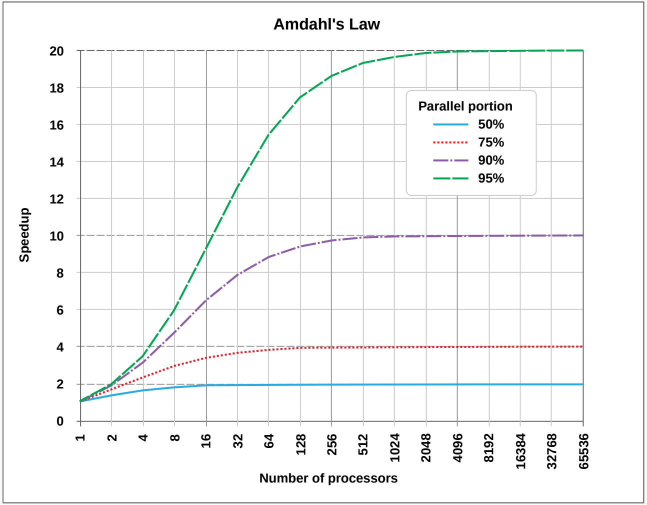
Amdahl's Law

- Amdahl's law describes an upper limit for the speedup
  - Every application contains a serial portion that limits the speedup
- f is the serial portion ($\in [0, 1]$)

$$S(n) = \frac{1}{f + \frac{1-f}{n}} \Rightarrow S_{max} = \frac{1}{f}$$

- Even seemingly small serial portions have a large impact
  - $f = 0.01 \Rightarrow S_{max} = 100$
  - Try to keep serial portion as small as possible
- Problem: Only applies if problem size is fixed
  - It usually makes sense to increase the problem size if more nodes are available

- Examples
  - 5 % serial portion
    - $S_{max} = 20$
  - 50 % serial portion
    - $S_{max} = 2$
- Parallelization might sometimes not be worth it
  - Weigh up required effort against potential speedup



[Daniels220, 2008]

Gustafson's Law

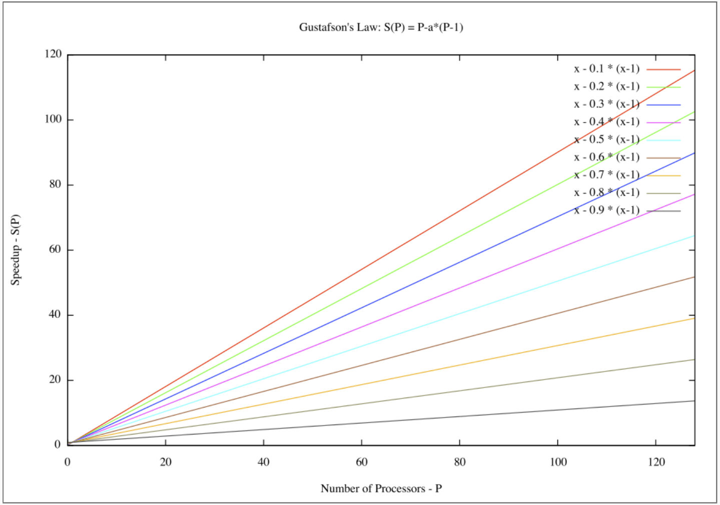
- Gustafson's law also describes an upper limit for the speedup
  - In contrast to Amdahl's law, problem size can be increased
  - However, time has to be fixed (problem size has to be chosen appropriately)
  - Every application contains a serial portion
- f is the serial portion ($\in [0, 1]$)

$$S(n) = n + f(1 - n) = n + f - fn = n - fn + f = n - f(n - 1)$$

- Also does not apply to all kinds of applications
  - Problem sizes cannot always be scaled up arbitrarily

Gustafson's Law...

- Examples
  - 5 % serial portion
    - $S(120) = 114$
  - 50 % serial portion
    - $S(120) = 60$
- Much better than with Amdahl's law
  - Increasing problem size compensates overhead



[Peahihawaii, 2011]

Strong and Weak Scaling

- Scaling behavior can be generalized based on problem size
  - Increasing speedup with constant problem size is harder
  - Algorithms can be judged and compared based on their scaling behavior

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  - Algorithms can be judged and compared based on their scaling behavior
- Weak scaling
  - Increase problem size together with task count (related to Gustafson's law)
- Strong scaling
  - Increase task count with constant problem size (related to Amdahl's law)
- Example: Matrix calculation
  - Matrix contains $1{,}000 \times 1{,}000$ elements
  - Calculation for one element requires elements from neighbors

Strong Scaling

- Parallelization with 5 tasks
  - Each task has a sub-matrix of $200 \times 1{,}000$ elements
  - Each task has to communicate $2 \times 1{,}000$ elements with others
  - Communication-to-computation ratio is 1:100

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- Parallelization with 10 tasks
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- Parallelization with 100 tasks
  - Each task has a sub-matrix of $10 \times 1{,}000$ elements
  - Each task has to communicate $2 \times 1{,}000$ elements with others
  - Communication-to-computation ratio is 1:5

Weak Scaling

- Parallelization with 10 tasks and doubled matrix size
  - Each task has a sub-matrix of $141 \times 1{,}414$ elements
  - Each task has to communicate $2 \times 1{,}414$ elements with others
  - Communication-to-computation ratio is 1:70

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  - Each task has a sub-matrix of $141 \times 1{,}414$ elements
  - Each task has to communicate $2 \times 1{,}414$ elements with others
  - Communication-to-computation ratio is 1:70
- Parallelization with 10 tasks and tenfold matrix size
  - Each task has a sub-matrix of $316 \times 3{,}162$ elements
  - Each task has to communicate $2 \times 3{,}162$ elements with others
  - Communication-to-computation ratio is 1:158

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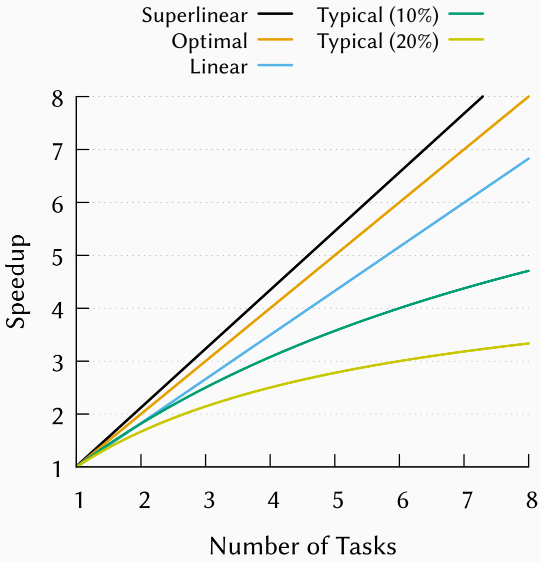
  - Each task has a sub-matrix of $316 \times 3{,}162$ elements
  - Each task has to communicate $2 \times 3{,}162$ elements with others
  - Communication-to-computation ratio is 1:158
- Parallelization with 100 tasks and hundredfold matrix size
  - Each task has a sub-matrix of $100 \times 10{,}000$ elements
  - Each task has to communicate $2 \times 10{,}000$ elements with others
  - Communication-to-computation ratio is 1:50

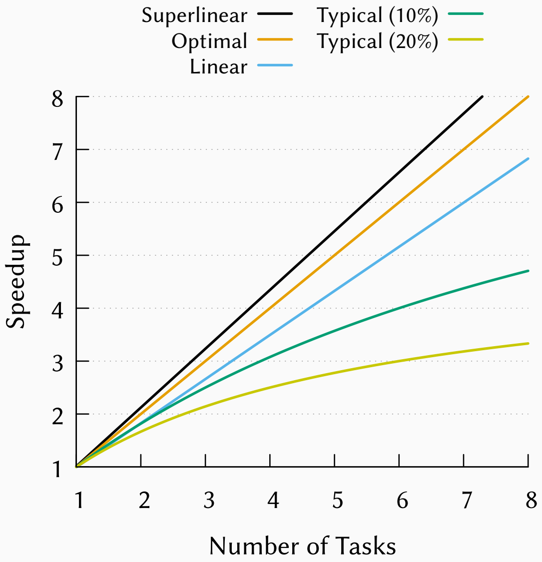
Speedup

- Speedup graphs visualize performance



Speedup

- Speedup graphs visualize performance
- Optimal speedup
  - Perfect scaling, no overhead



Speedup

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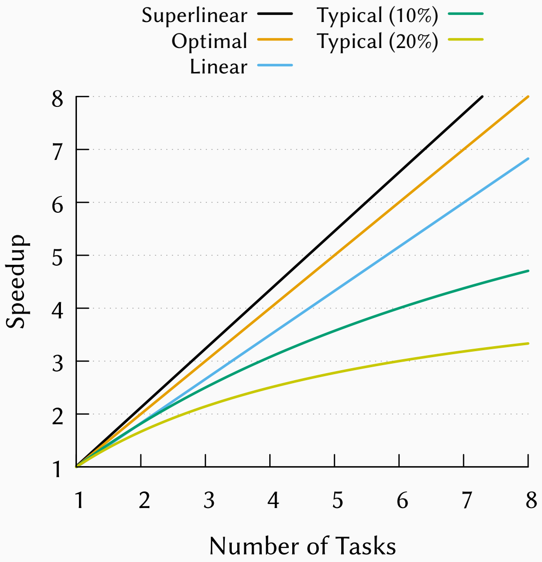
- Linear speedup
  - Constant overhead



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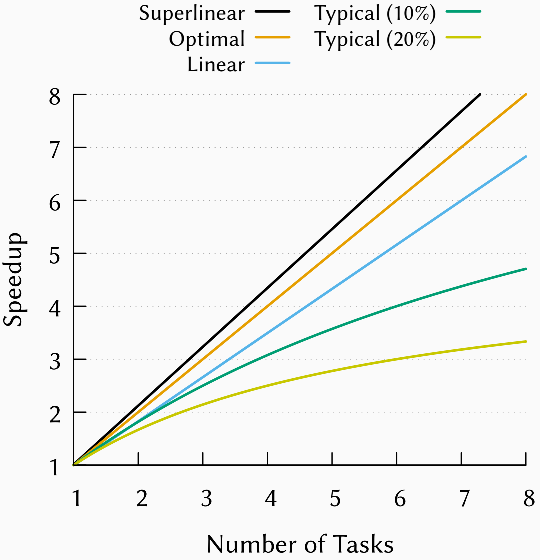
- Typical speedup
  - Overhead keeps growing
  - With 10 or 20 % serial portion according to Amdahl's law



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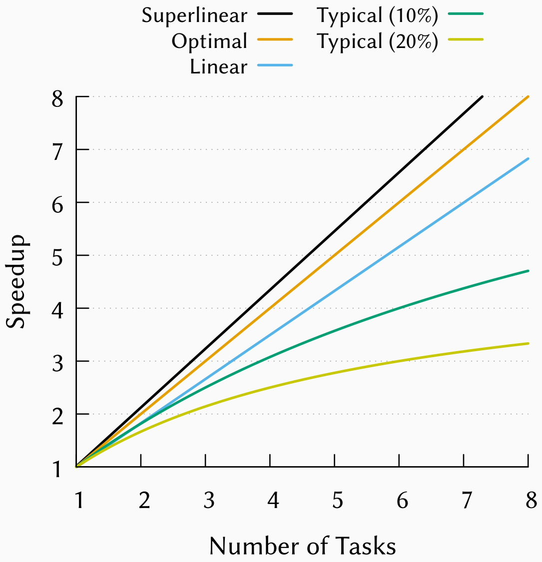
- Superlinear speedup
  - Negative overhead?



Superlinear Speedup

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  - We have n search algorithms with runtimes t_i
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- Serial version
  1. Set $t_{min} = \infty$
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     2.2 Otherwise, set $t_{min} = t_i$
- The serial version has a runtime of $t_{serial} \geq t_{min} \times n$
  - $t_{serial} > t_{min} \times n$ if we do not run the fastest algorithm first

- Parallel version
  1. Run each algorithm i on its own core
     1.1 As soon as the first one finishes, set $t_{min} = t_i$ and terminate all other algorithms

Superlinear Speedup...

- Parallel version
  1. Run each algorithm i on its own core
     1.1 As soon as the first one finishes, set $t_{min} = t_i$ and terminate all other algorithms
- The parallel version has a runtime of $t_{parallel} = t_{min}$

$$S = \frac{t_{serial}}{t_{parallel}} \Rightarrow S \geq \frac{t_{min} \times n}{t_{min}} \Rightarrow S \geq n$$

Quiz

- What mistake did we make to achieve a superlinear speedup?
    1. We did not make a mistake
    2. We did not choose the fastest serial algorithm
    3. We cannot run each algorithm on its own core

- Improved serial version
  1. Run each algorithm *i* for a time slice *t*
     1.1 As soon as the first one finishes, set $t_{min} = t_i$ and terminate all other algorithms

Superlinear Speedup...

- Improved serial version
  1. Run each algorithm i for a time slice t
     1.1 As soon as the first one finishes, set $t_{min} = t_i$ and terminate all other algorithms
- The improved version has a runtime of $t_{serial} \approx t_{min} \times n$
  - Overhead depends on length of the time slice
  - This gets rid of the superlinear speedup

Outline

Summary

- Networking is necessary to build distributed memory systems
    - Shared memory systems have limited scalability
- Network technologies have different performance characteristics
    - The two major competitors are Ethernet and InfiniBand
- High-performance networking requires optimizations
    - RDMA, zero copy, offloading and kernel bypass help reduce overhead
- Scalability can be measured using speedup and efficiency
    - There are limits to scalability, demonstrated by Amdahl and Gustafson's laws

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