Introduction to Parallel Computing

National Tsing Hua University
Instructor: Jerry Chou
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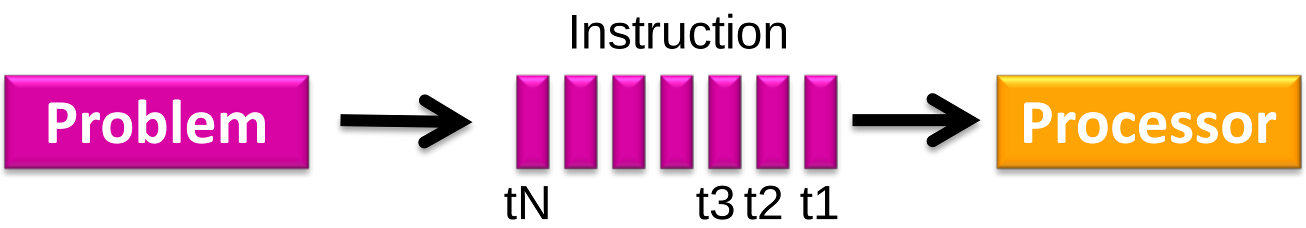
Outline

- Parallel Computing Introduction
  - What is parallel computing
  - Why need parallel computing
- Classifications of Parallel Computers & Programming Models
- Supercomputer & Latest technologies
- Parallel Program Analysis

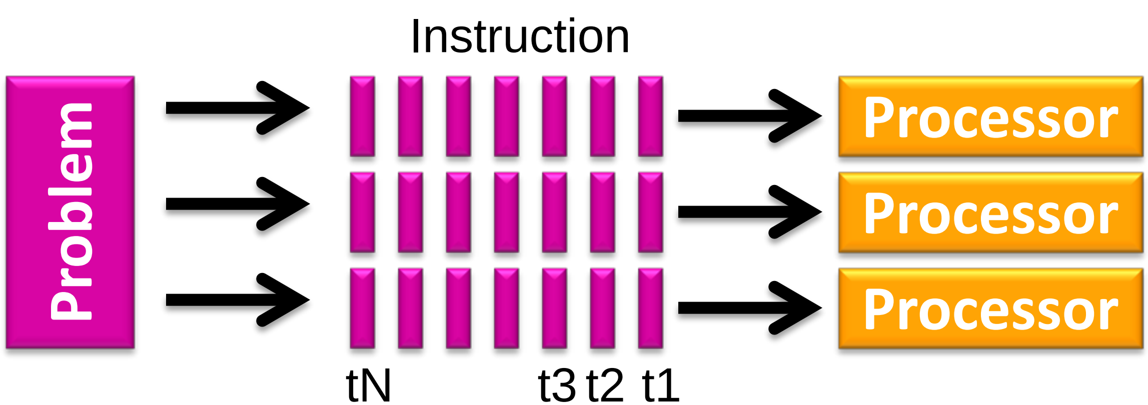
What is Parallel Computing?

"Solve a *single problem* by using *multiple processors* (i.e. *core*) working together"

- Traditionally, program has been written for serial computation



- In parallel computing, use multiple computer resources to solve a computational problem



Difference between parallel computing & distributed computing

The two terminologies are very closely related.

But come from ***different backgrounds***

- Parallel computing …
  - Means different activities happen at the same time
  - Spread out a single application over many cores/ processors/processes to get it done bigger or faster
  - Mostly used in scientific computing
- Distributed computing…
  - Activities across systems or distanced servers
  - Focus more on concurrency and resource sharing
  - From the business/commercial world

The Universe is Parallel

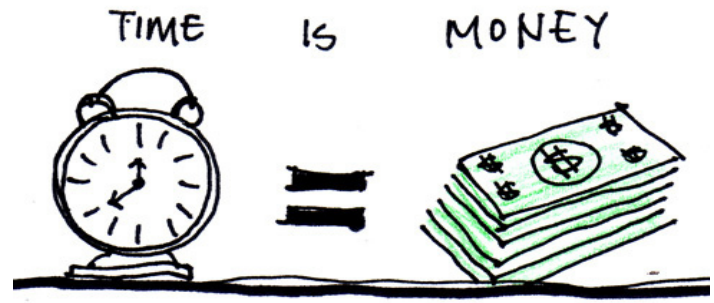
- Parallel computing is an evolution of serial computing that attempts to emulate what has always been the state of affairs in the natural world

Why need Parallel Computing

- Save time
  - Use more resources to shorten execution with potential cost saving

4 hours of work

Finish in 1 hour!!!

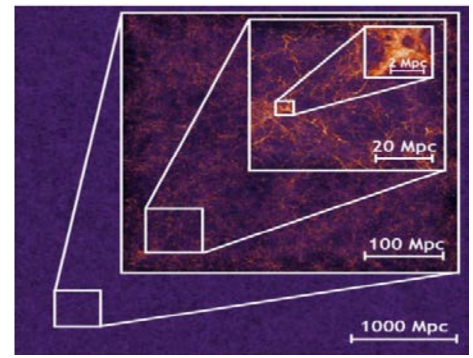


  - Shorter execution time allows more runs or more tuning opportunity

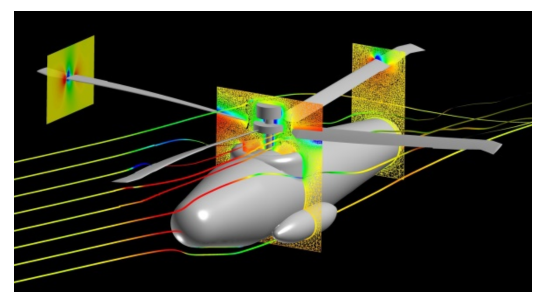
	DUAL XEON CPU server	DGX-1 GPU server (8 GPUs)
FLOPS	3TF	**170TF**
Node Mem BW	76GB/s	768GB/s
Alexnet Train Time	150 Hr	**2Hr**
Train in 2Hr	**>250Nodes**	1Node

Why need Parallel Computing

- Solve larger problem
  - Impossible or impractical to solve on a single computer
  - **Scientific computing**:
    - Trillion particles
    - Tens and hundreds of parameters
    - TBs of data to be processed/analyzed
    - Several hours of execution using millions of cores (PetaFLOPS)



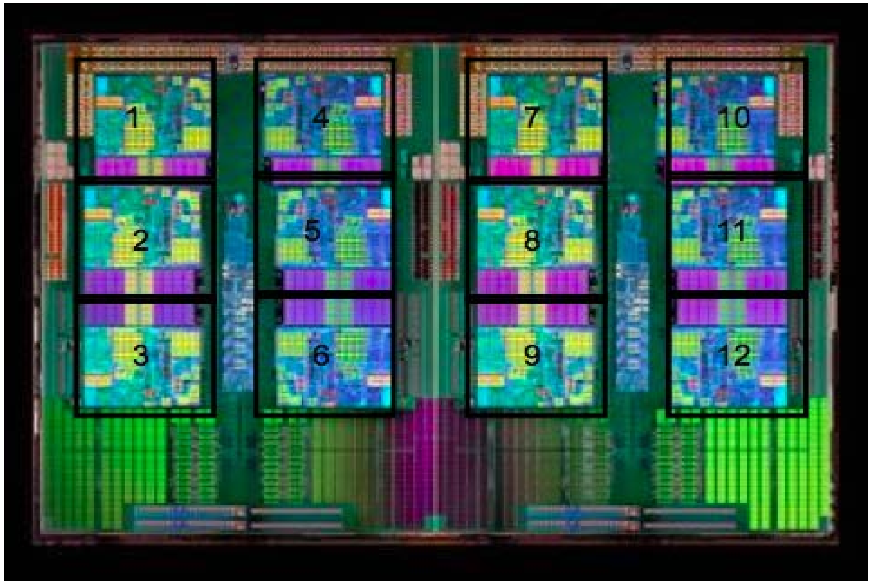
1 trillion particles, 4.225 Gpc box-size simulation, and 6 kpc force resolution.



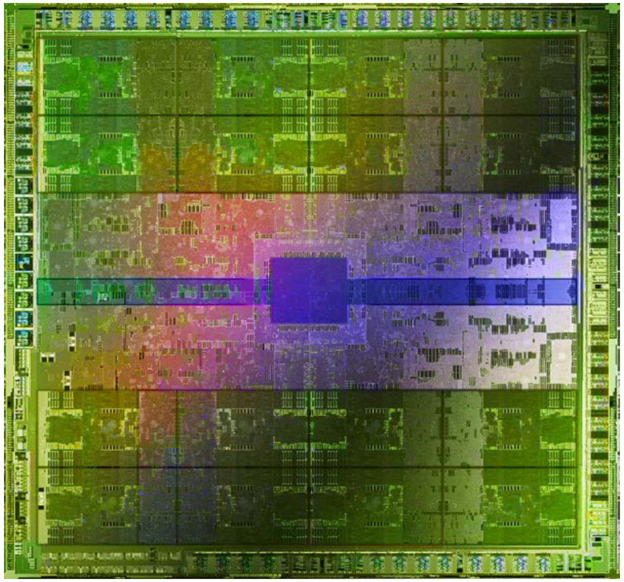
The world has been driven by science research!

Why need Parallel Computing

- Make better use of the underlying parallel hardware
  - Advance in computer architecture



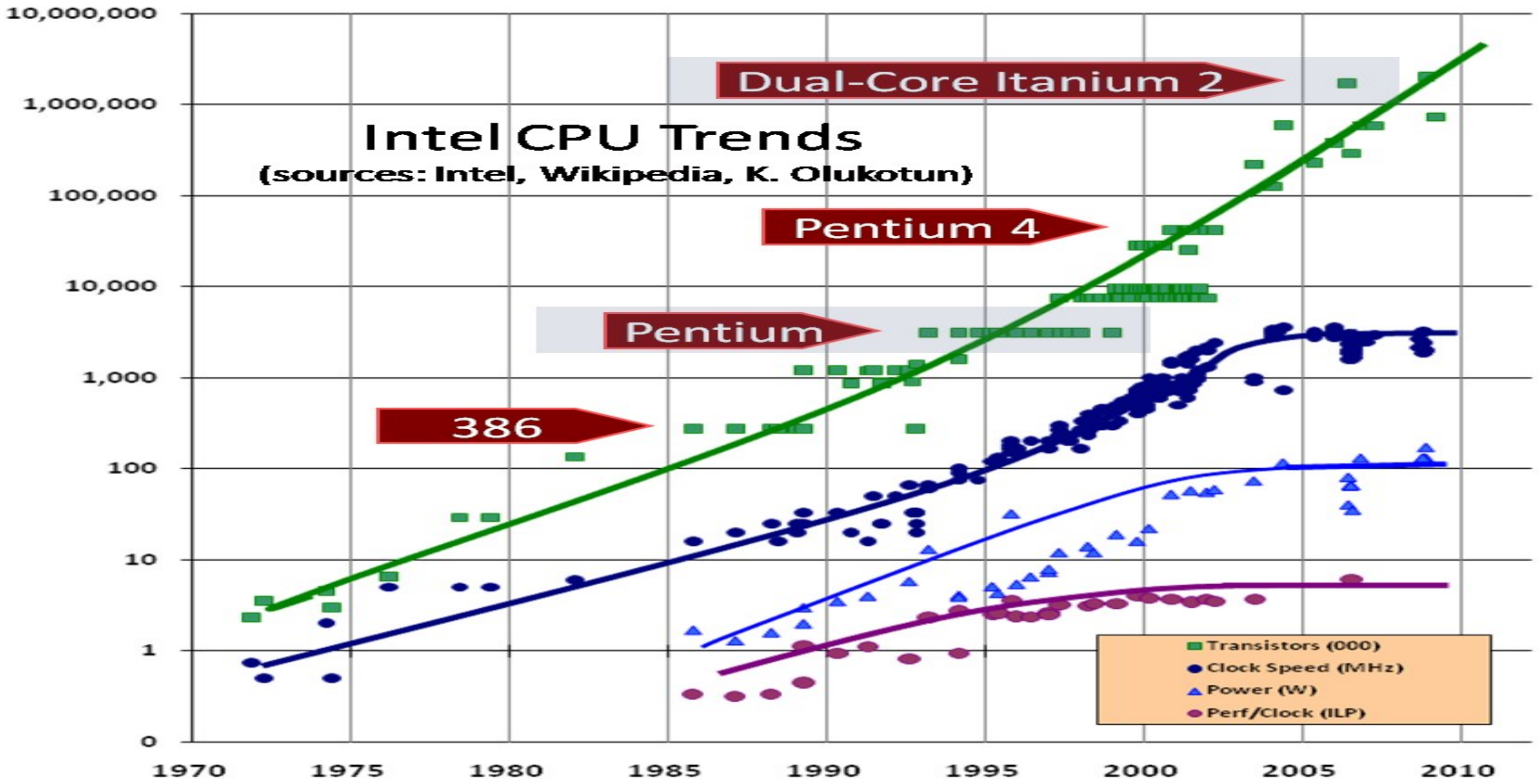
12 Cores IBM Blade Multi-core CPU



512 Cores NVIDIA Fermi GPU

The Death of CPU Scaling

- Increase of transistor density ≠ performance
  - The power and clock speed improvements collapsed



"Parallel Computing is a *trend* and *essential tools* in today's world!"

Trend of Parallel Computing

Single-Core Era

Enabled by:
- Moore's Law
- Voltage Scaling

Constraint by:
- Power
- Complexity

Assembly → C/C++ → Java …

Muti-Core Era

Enabled by:
- Moore's Law
- SMP

Constraint by:
- Power
- Parallel SW
- Scalability

Pthread → OpenMP …

Distributed System Era

Enabled by:
- Networking

Constraint by:
- Synchronization
- Comm. overhead

MPI → MapReduce …

Heterogeneous Systems Era

Enabled by:
- Abundant data parallelism
- Power efficient GPUs

Constraint by:
- Programming models
- Comm. overhead

Shader → CUDA → OpenCL …

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- Classifications of Parallel Computers & Programming Models
  - Flynn’s classic taxonomy
  - Memory architecture classification
  - Programming model classification
- Supercomputer & Latest technologies
- Parallel Program Analysis

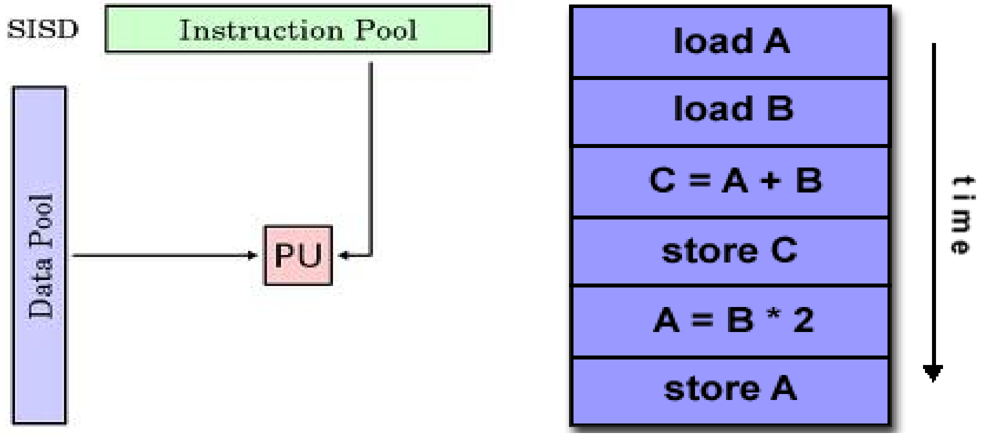
Parallel Computer Classification

- **Flynn's classic taxonomy**
  - Since **1966** (50 years ago …)
  - From the process unit prospective: Classify computer architecture based two independent dimensions: Instruction & Data

SISD **Single Instruction** **Single Data**	**SIMD** **Single Instruction** **Multiple Data**
MISD **Multiple Instruction** **Single Data**	**MIMD** **Multiple Instruction** **Multiple Data**

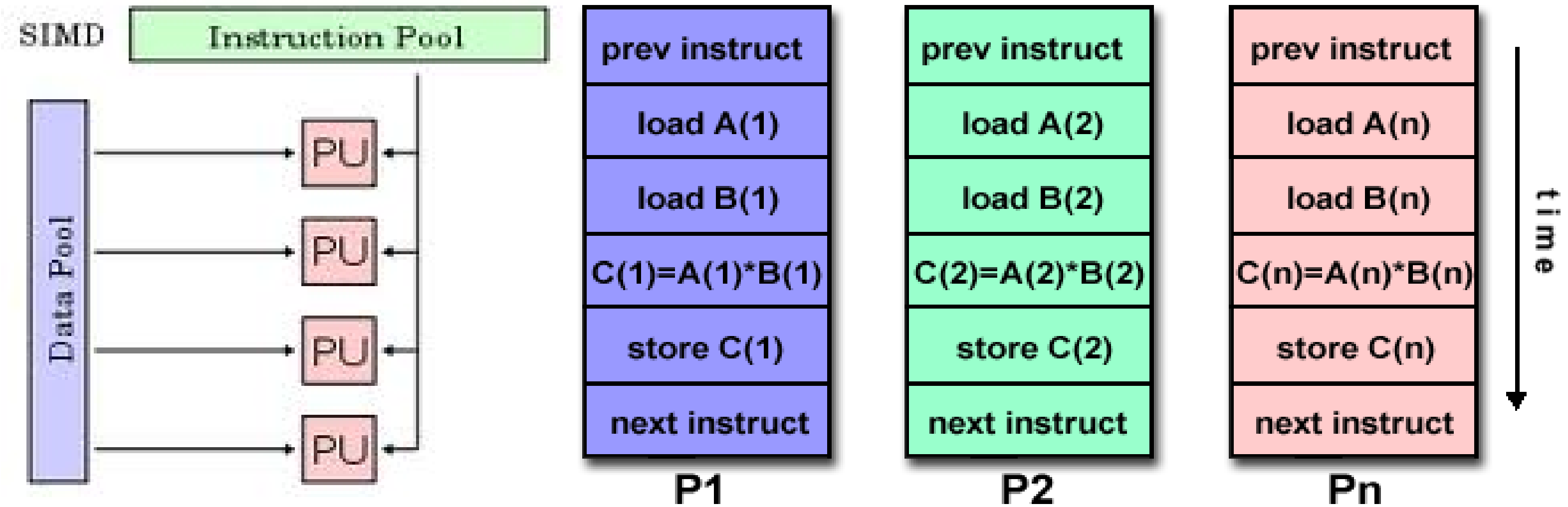
Flynn’s classic taxonomy: SISD

- Single Instruction, Single Data (SISD):
  - A serial (non-parallel) computer
  - **Single Instruction:** Only one instruction stream is being acted on by the CPU during any one clock cycle
  - **Single Data:** Only one data stream is being used as input during any one clock cycle
  - Example: Old mainframes, **single-core** processor



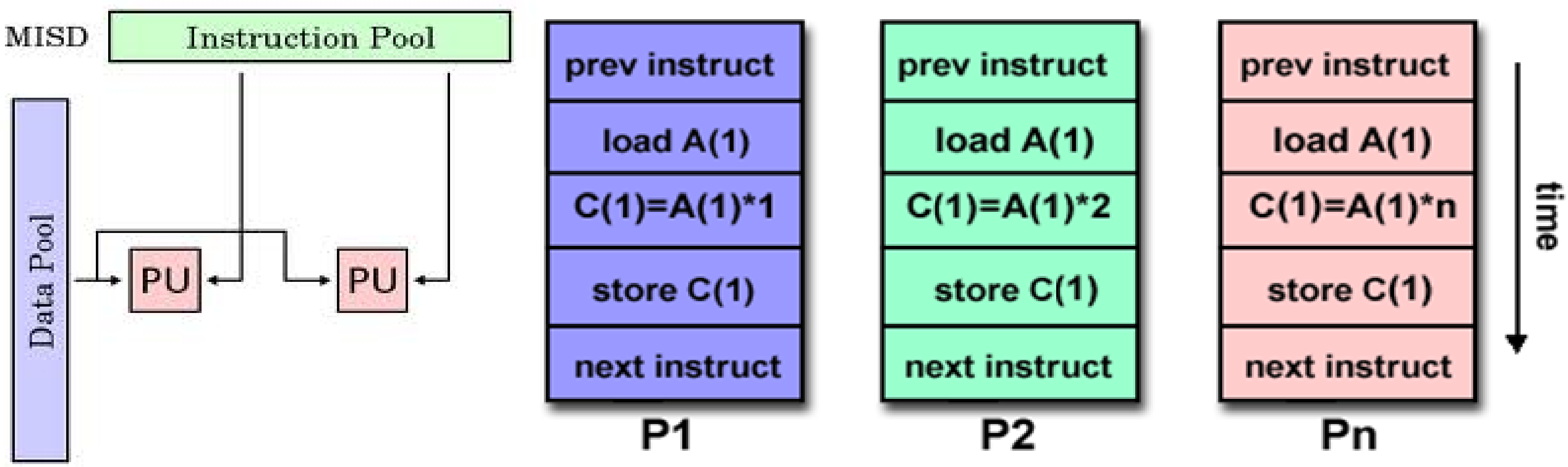
Flynn’s classic taxonomy: SIMD

- Single Instruction, Multiple Data (SIMD):
  - **Single Instruction:** All processing units execute the same instruction at any given clock cycle
  - **Multiple Data:** Each processing unit can operate on a different data element
  - Example: GPU, vector processor (X86 AVX instruction)



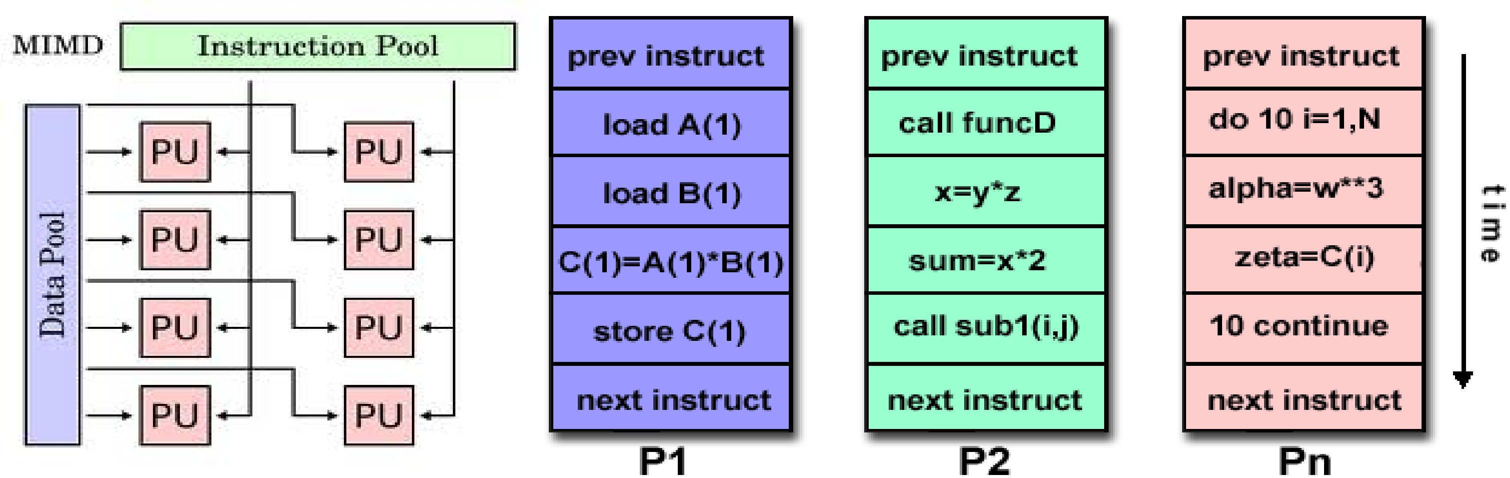
Flynn's classic taxonomy: MISD

- Multiple Instruction, Single Data (MISD):
  - **Multiple Instruction:** Each processing unit operates on the data independently via separate instruction streams.
  - **Single Data:** A single data stream is fed into multiple processing units.
  - Example: Only experiment by CMU in 1971; Could be used for **fault tolerance**



Flynn's classic taxonomy: MIMD

- Multiple Instruction, Multiple Data (MIMD):
  - **Multiple Instruction:** Every processor may be executing a different instruction stream
  - **Multiple Data:** Every processor may be working with a different data stream
  - Example: Most modern computers, such as **multi-core CPU**



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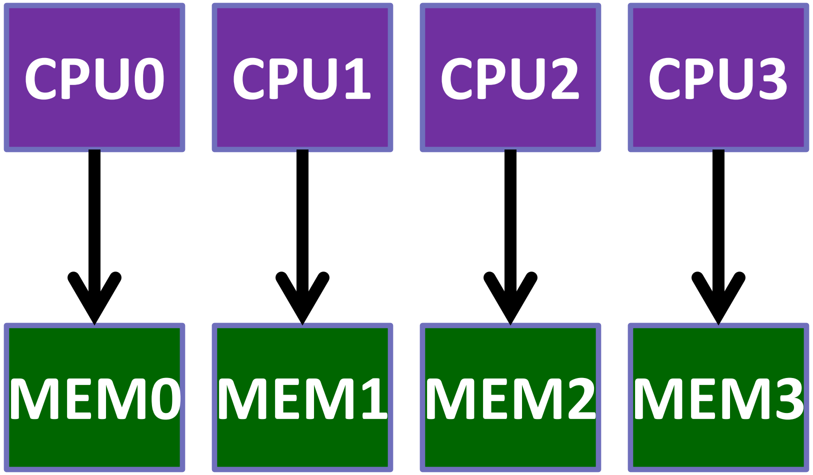
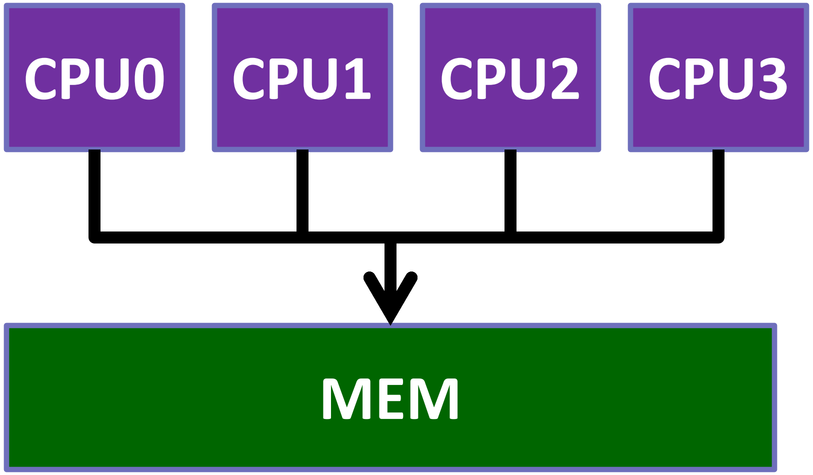
Shared Memory vs. Distributed Memory Computer Architecture



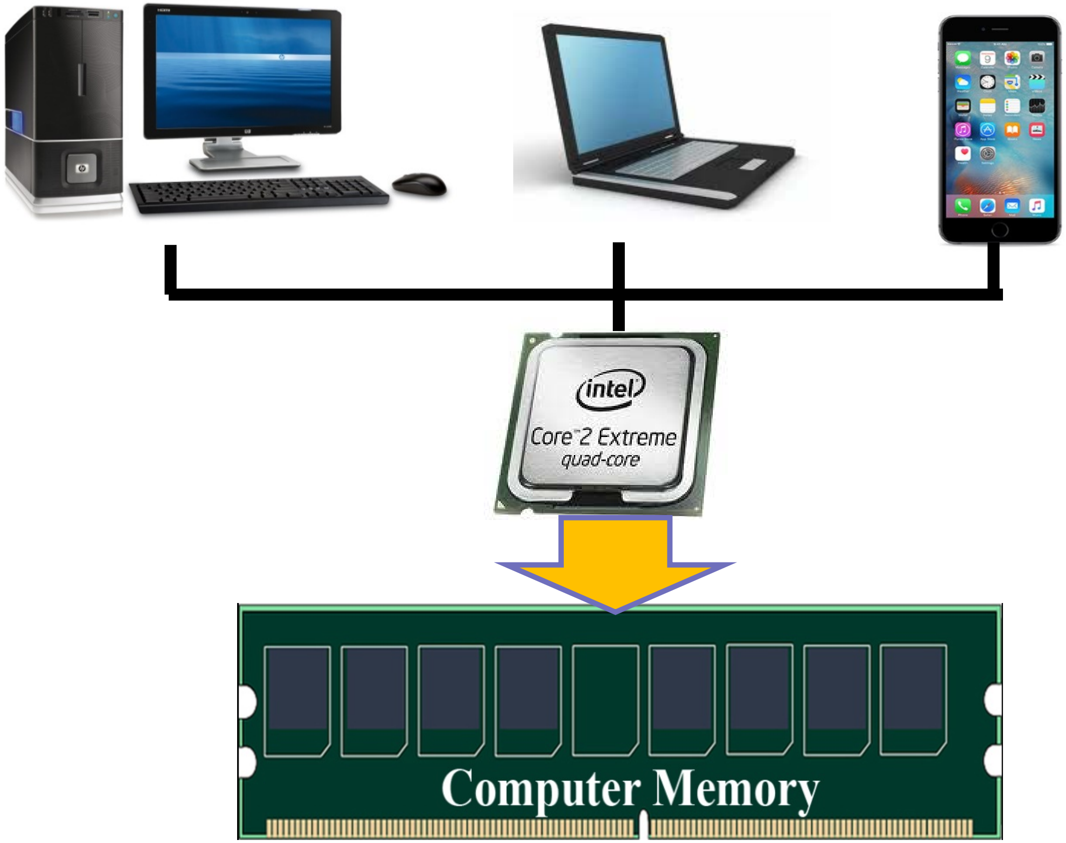
Distributed memory



Shared memory

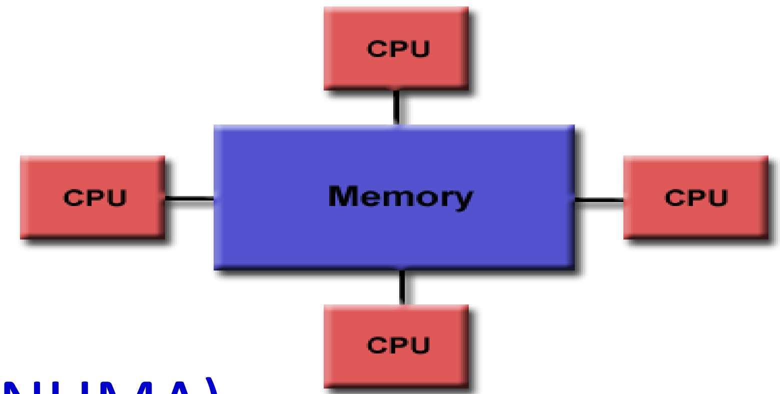
Shared Memory Multiprocessor Computer System

- Single computer with multiple internal multi-core processors

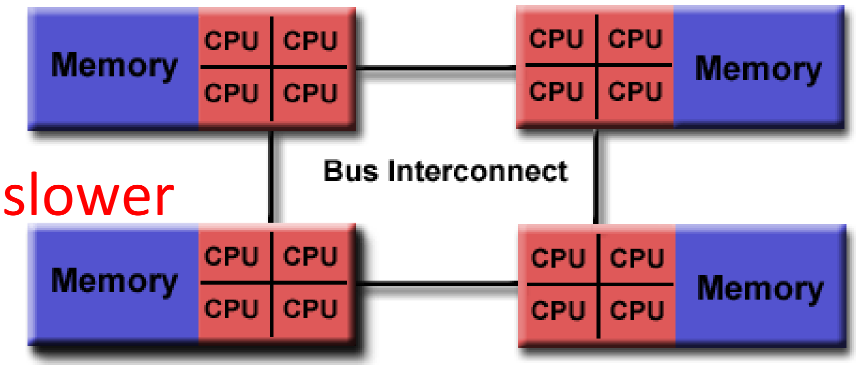


Shared Memory Computer Architecture

- Uniform Memory Access (UMA):
  - Most commonly represented today by Symmetric Multiprocessor (SMP) machines
  - Identical processors
  - Equal access times to memory
  - Example: commercial servers



- Non-Uniform Memory Access (NUMA):
  - Often made by physically linking two or more SMPs
  - One SMP can directly access memory of another SMP
  - Memory access across link is slower
  - Example: HPC server



Distributed Memory Multicomputer

- Connect multiple computers to form a computing platform without sharing memory

Cluster: tens of servers

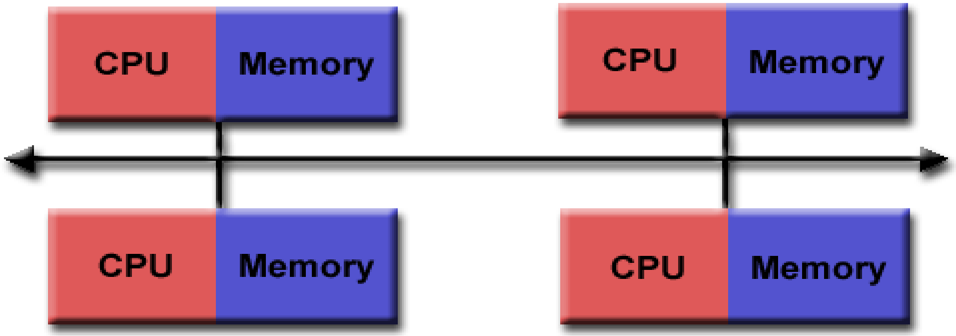
Supercomputer: hundreds of servers

Datacenter: thousands of servers

Distributed Memory Multicomputer

- Require a communication network (i.e. not bus) to connect inter-processor memory
- Processors have their own memory & **address space**
- Memory change made by a processor has **NO effect** on the memory of other processors
- Programmers or programming tools are responsible to explicitly define how and when data is communicated between processors

Network fabric: Ethernet, InfiniBand



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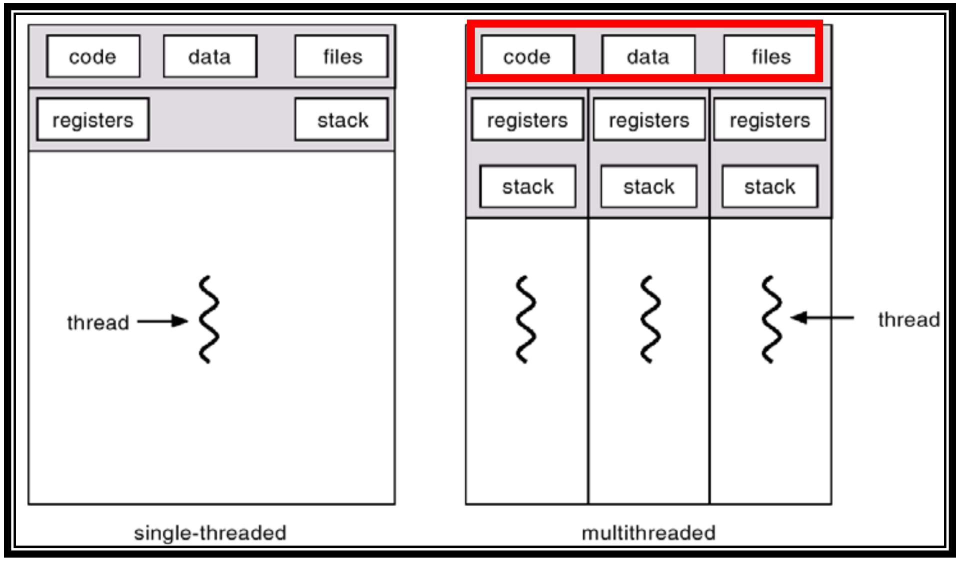
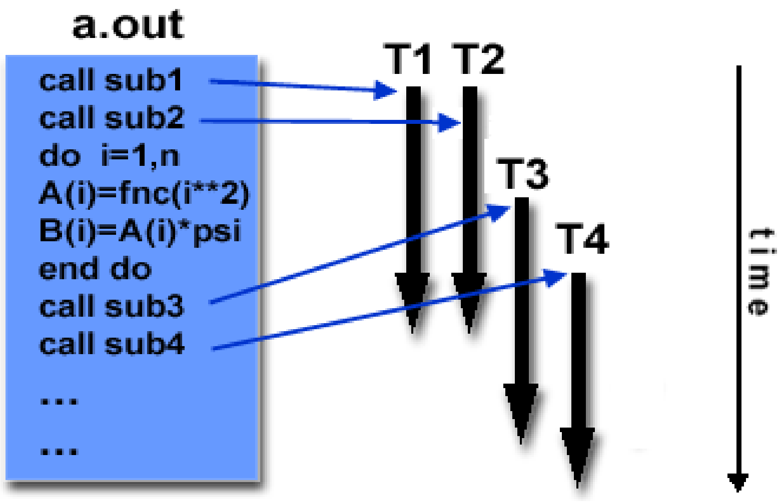
Parallel Programming Model

- **Parallel programming models exist as an abstraction above hardware & memory architectures**
- In general programming models are designed to match the computer architecture
  - Shared memory prog. model for shared memory machine
  - Message passing prog. model for distributed memory machine
- But programming models are **NOT** restricted by the machine or memory architecture
  - Message passing model can be supported on SHARED memory machine: e.g., MPI on a single server
  - Shared memory model on DISTRIBUTED memory machine: e.g., Partitioned Global Address Space

Shared Memory Programming Model

- A single process can have multiple, **concurrent execution paths**
- Threads have **local data**, but also, **shares resources**
- Threads communicate with each other through **global memory**
- Threads can come and go, but the main program remains
  - to provide the necessary shared resources until the application has completed





Shared Memory Programming Model

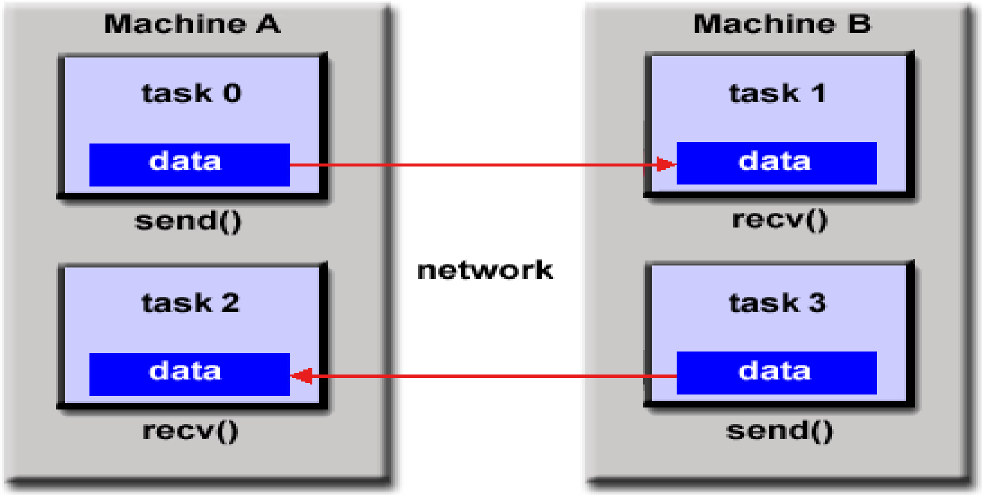
- Implementation
  - A library of subroutines called from parallel source code
    - E.g.: **POSIX Thread (Pthread)**
  - A set of compiler directives imbedded in either serial or parallel source code
    - E.g.: **OpenMP**

```
#include <pthread.h>
void print_message_function ( void *ptr ) {
  printf("Hello, world.\n");
}
int main() {
  pthread_t thread;
  pthread_create (&thread, NULL, (void *)
            &print_message_function, NULL);
  pthread_join(thread, NULL);
}
```

```
#include <omp.h>
int main() {
    #pragma omp parallel
    {
        printf("Hello, world.\n");
    }
}
```

Message Passing Programming Model

- A set of tasks that use their own local memory during computation
  - Multiple tasks can reside on the same physical machine and/or across an arbitrary number of machines
- Tasks exchange data through communications by sending and receiving **messages** (Memory copy)
- MPI API:
  - Send, Recv, Bcast, Gather, Scatter, etc.



Shared Memory vs. Message Passing

Shared Memory

- Convenient:
  - Can share data structures
  - Just annotate loops
  - Closer to serial code
- Disadvantages
  - No locality control
  - Does not scale
  - Race conditions

Message Passing

- Scalable
  - Locality control
  - Communication is all explicit in code (cost transparency)
- Disadvantage
  - Need to rethink entire application/ data structures
  - Lots of tedious pack/unpack code
  - Don’t know when to say “receive” for some problems

Summary

- The designs and popularity of **programming model** and **parallel systems** are highly influenced by each other
- **openMP, MPI, Pthreads, CUDA** are just some of the parallel languages for users to do **parallel programming**
- In reality, knowing what is **parallel computing** is more **IMPORTANT** than knowing how to do **parallel programming**, because that's how you can…
  - Learn a new parallel programming tools quickly
  - Understand the performance of your program
  - Optimize the performance of your program

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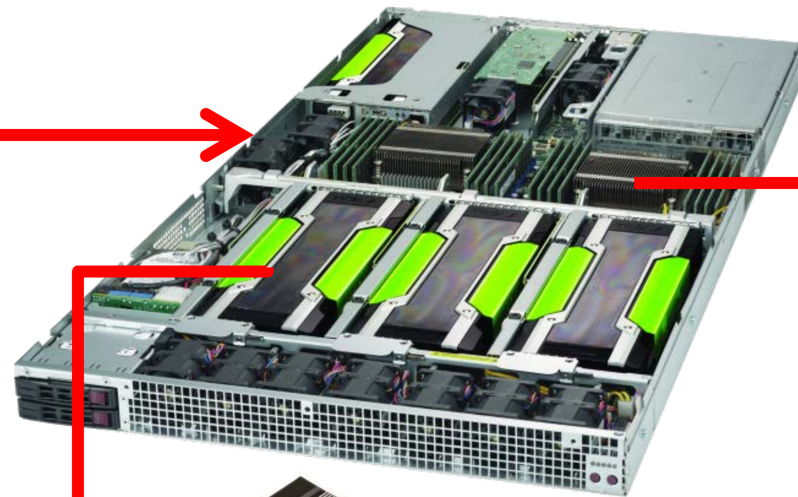
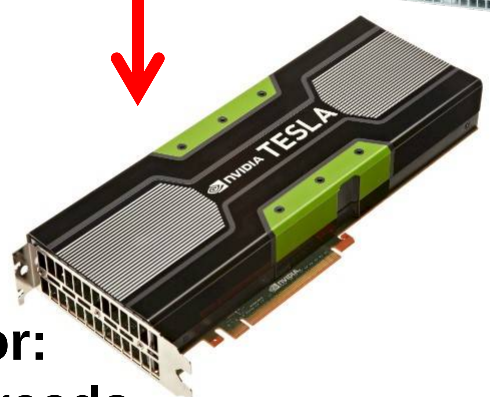
Today’s Typical Parallel Computers

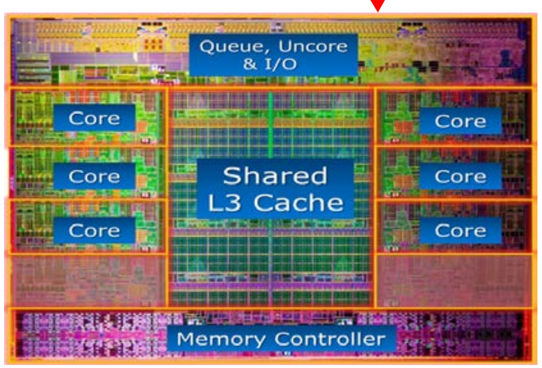
Racks: 16~42U

Node/Server: 1~4U





Multi-core Processor:
100x cores/1000xthreads



Co-Processor: 4~12 cores

Supercomputers

- Definition: A computer with a high-level computational capacity compared to a general-purpose computer
- Its performance is measured in floating-point operations per second (FLOPS) instead of million instructions per second (MIPS)
- Ranked by the TOP500 list since 1993
  - According to the HPL benchmark results
  - Announced twice a year at ISC and SC conferences

HPL Benchmark

- A parallel implementation of Linpack library
  - Measure **floating point rate of execution**

What uses such benchmark?

- Computation:
  - To solve **linear matrix equation**

$$Ax = b; \quad A \in \mathbf{R}^{n \times n}; \; x, b \in \mathbf{R}^n$$

  - LU factorization by Panel factorization.
  - Divide a matrix into many pieces.
  - All parameters must be determined by user.

What makes it a supercomputer

- What makes it a supercomputer?
  - All the latest hardware technologies
  - Customized system configurations
  - Optimized software and libraries
  - Huge amount of cost in money and **energy**
- It represents a competition of technology and wealth among a countries ……

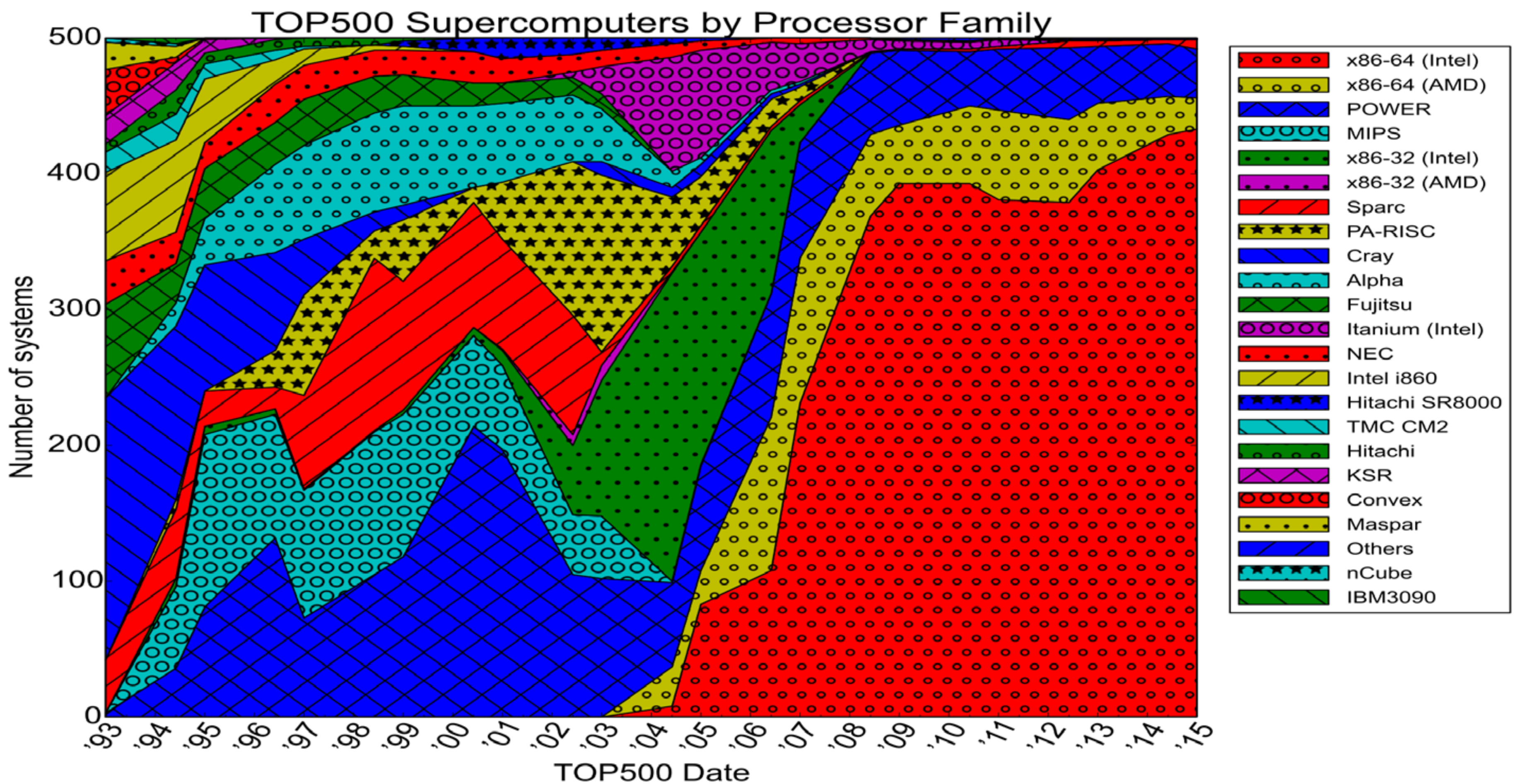
TOP500 List (2016 June)

	Country	System	Vendor	Power (kW)	#cores	Accelerator	Rmax	Rpeak (PFLOPS)
1	China	TaihuLight	NRCPC	15,371	10M		93.0	125.4
2	China	Tianhe-2	NUDT	17,808	3M	Xeon Phi	33.9	54.9
3	US	Titan	Cray	8,209	560K	Tesla K20X	17.6	27.1
4	US	Sequoia	IBM	7,890	1.5M		17.2	20.1
5	Japan	K	Fujitsu	12,660	705K		10.5	11.3
6	US	Mira	IBM	3,954	786K		8.6	10.0
7	US	Trinity	Cray		301K		8.1	11.1
8	Swiss	Piz Daint	Cray	2,325	116K	Tesla K20X	6.2	7.8

- Accelerator provides huge computing power
  - Titan’s Rmax without GPU was only 2K!!!

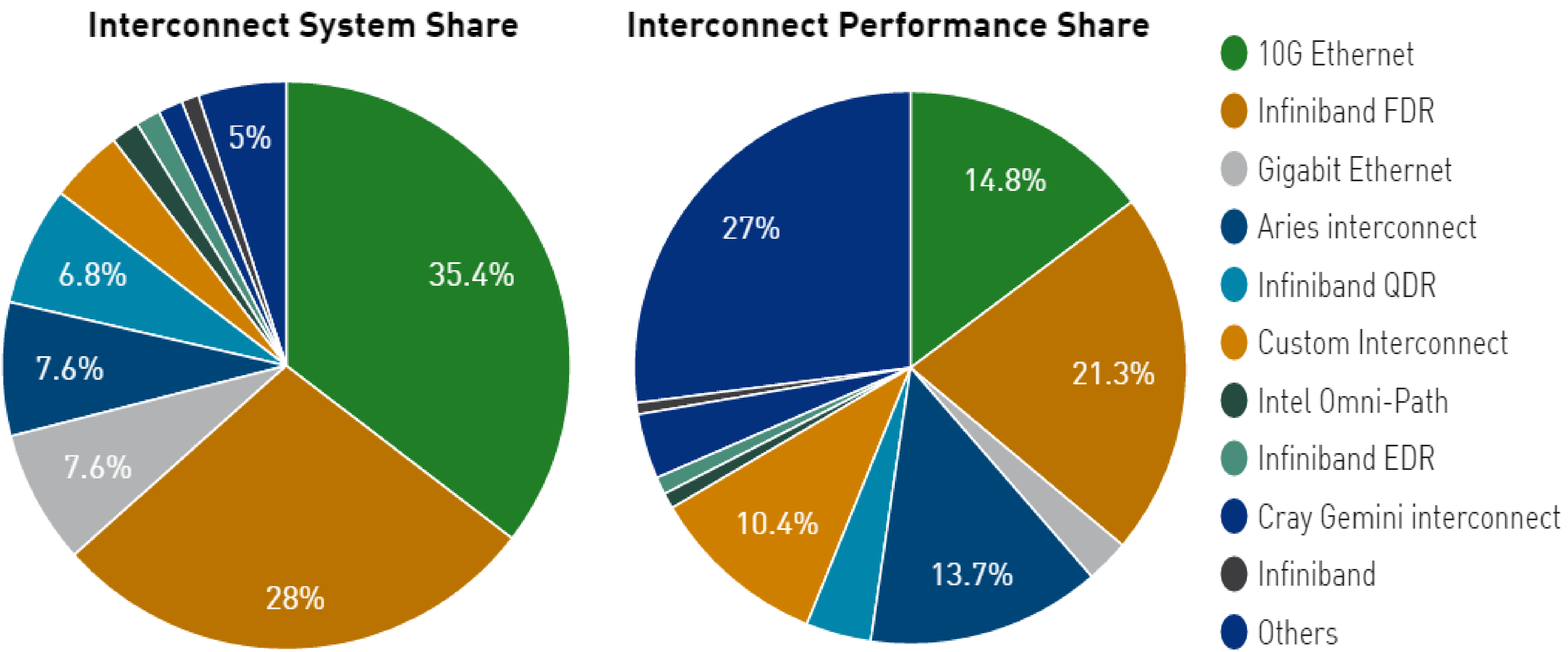
TOP500 Trend: CPU

- Intel CPU counts for more than 80%



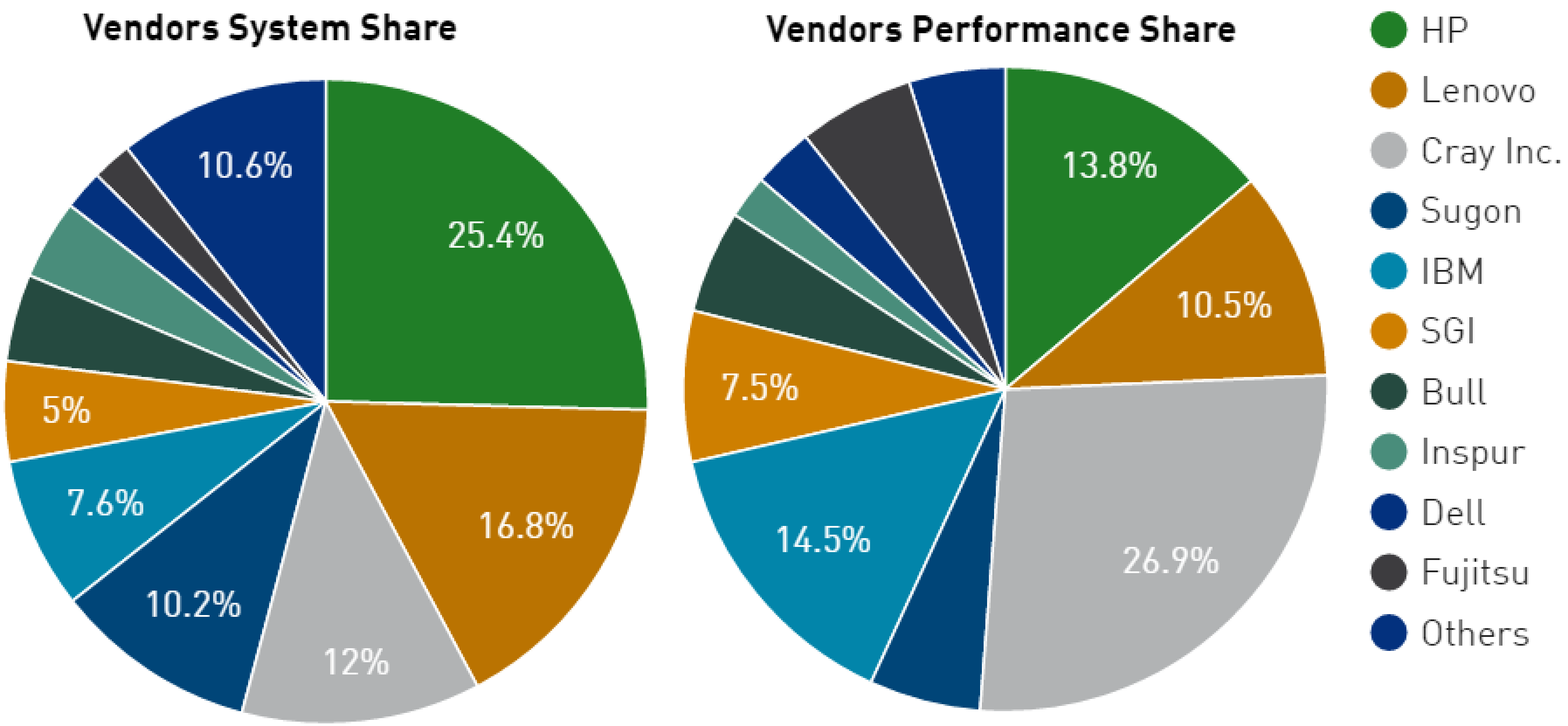
TOP500 Trend: Interconnect

- InfiniBand has much larger share in performance



TOP500 Trend: Vendor

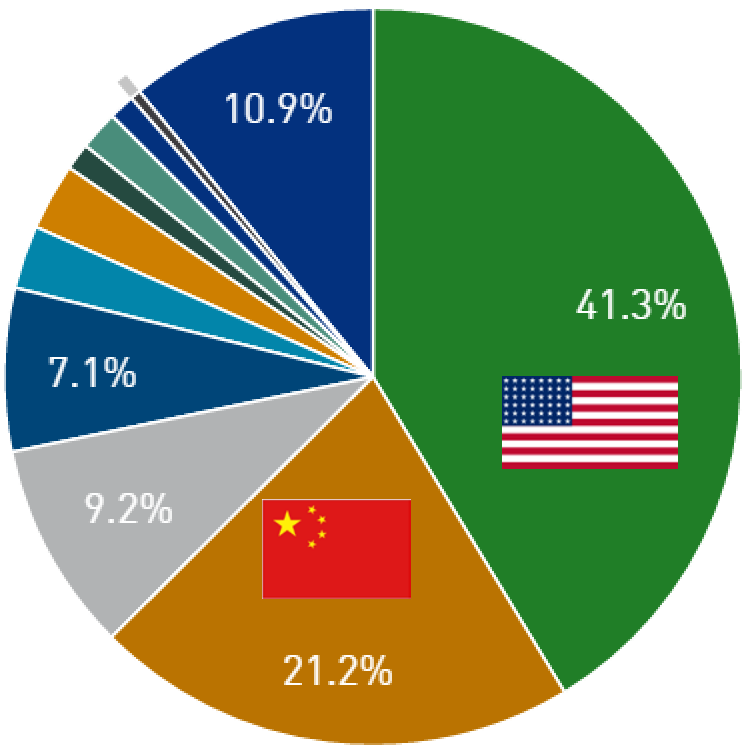
- CRAY and IBM still have larger share for performance



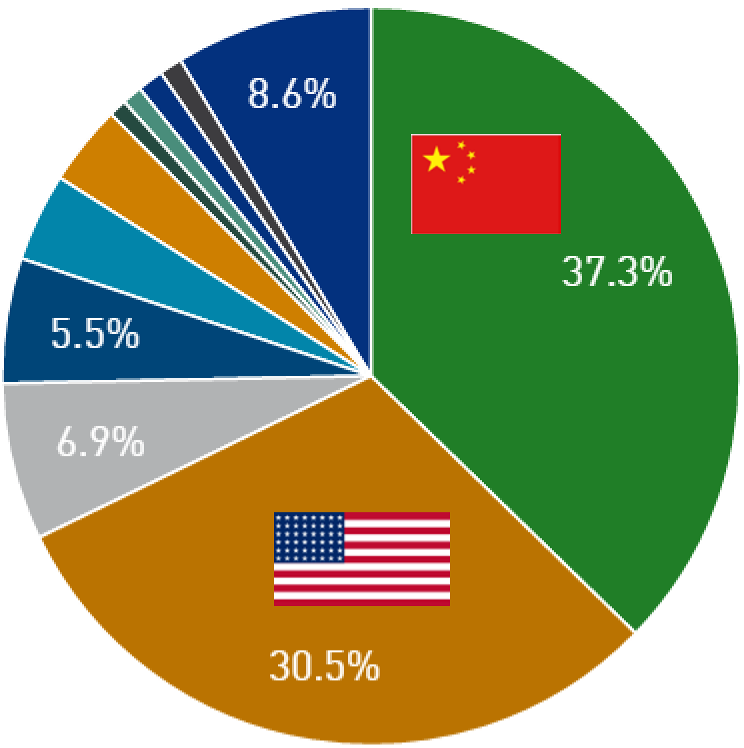
TOP500 Trend: Country

- China has a huge jump because of the new supercomputer

2015 Nov

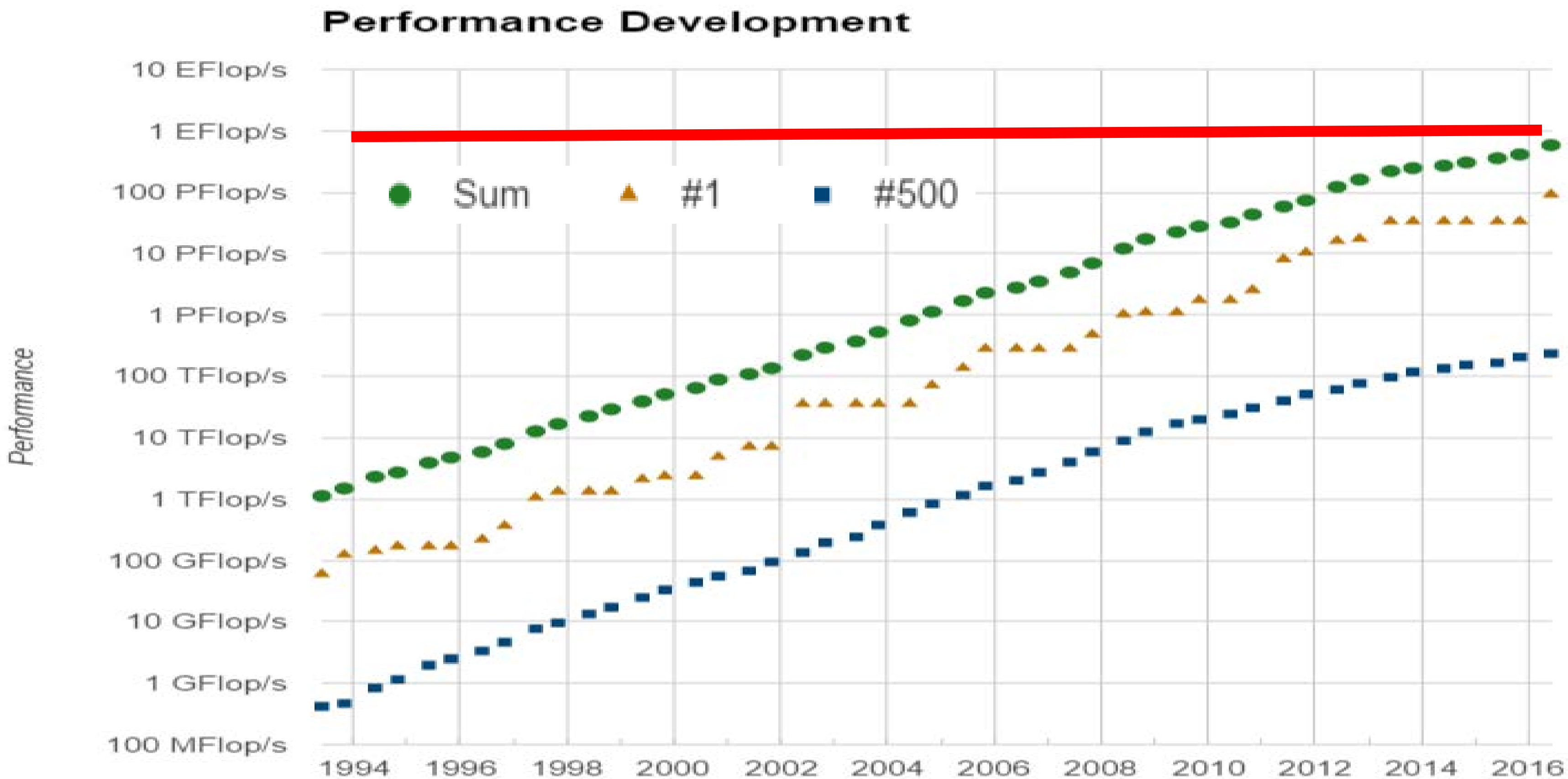


2016 June



TOP500 Trend: Computing power

- Goal is to reach Exascale computing 1EFlop (10^18) /s by 2020



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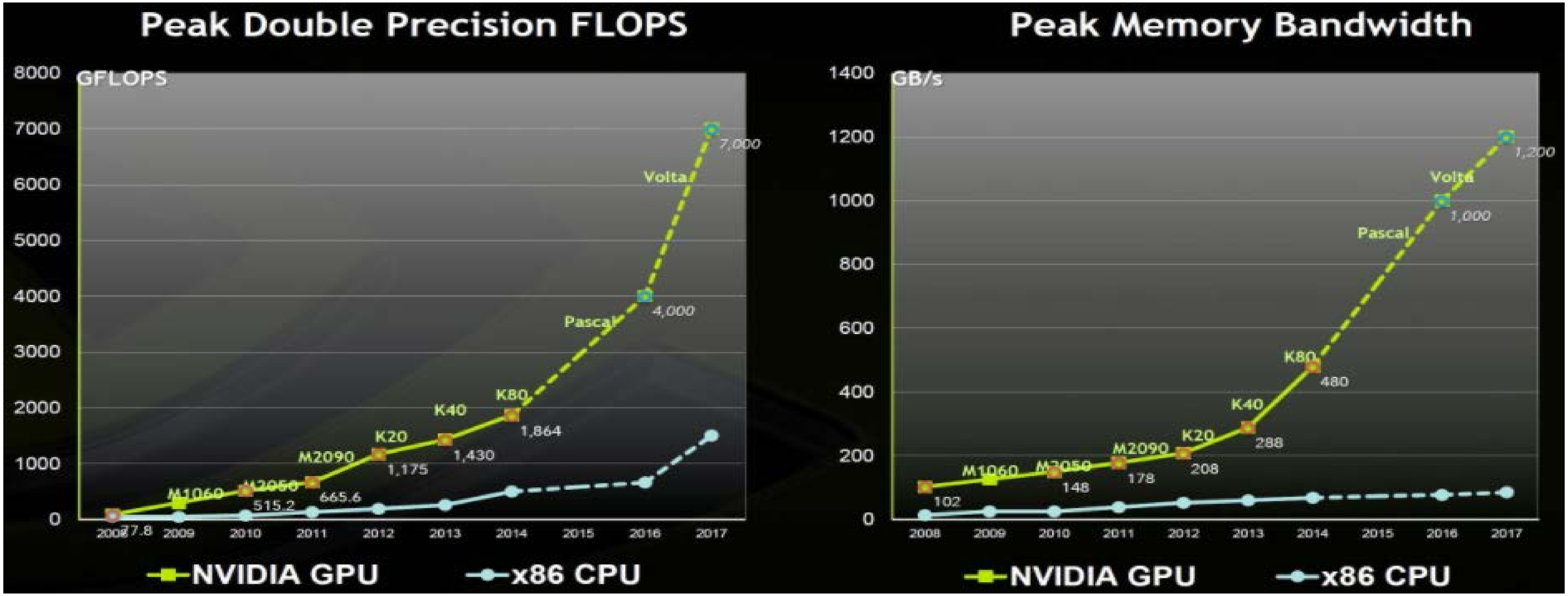
Limitation of CPU
General Purpose Processor

- A general purpose CPU (central processing unit) can do anything, but its design is against the goal of achieving the best performance for a specific application.



[source: nvidia]

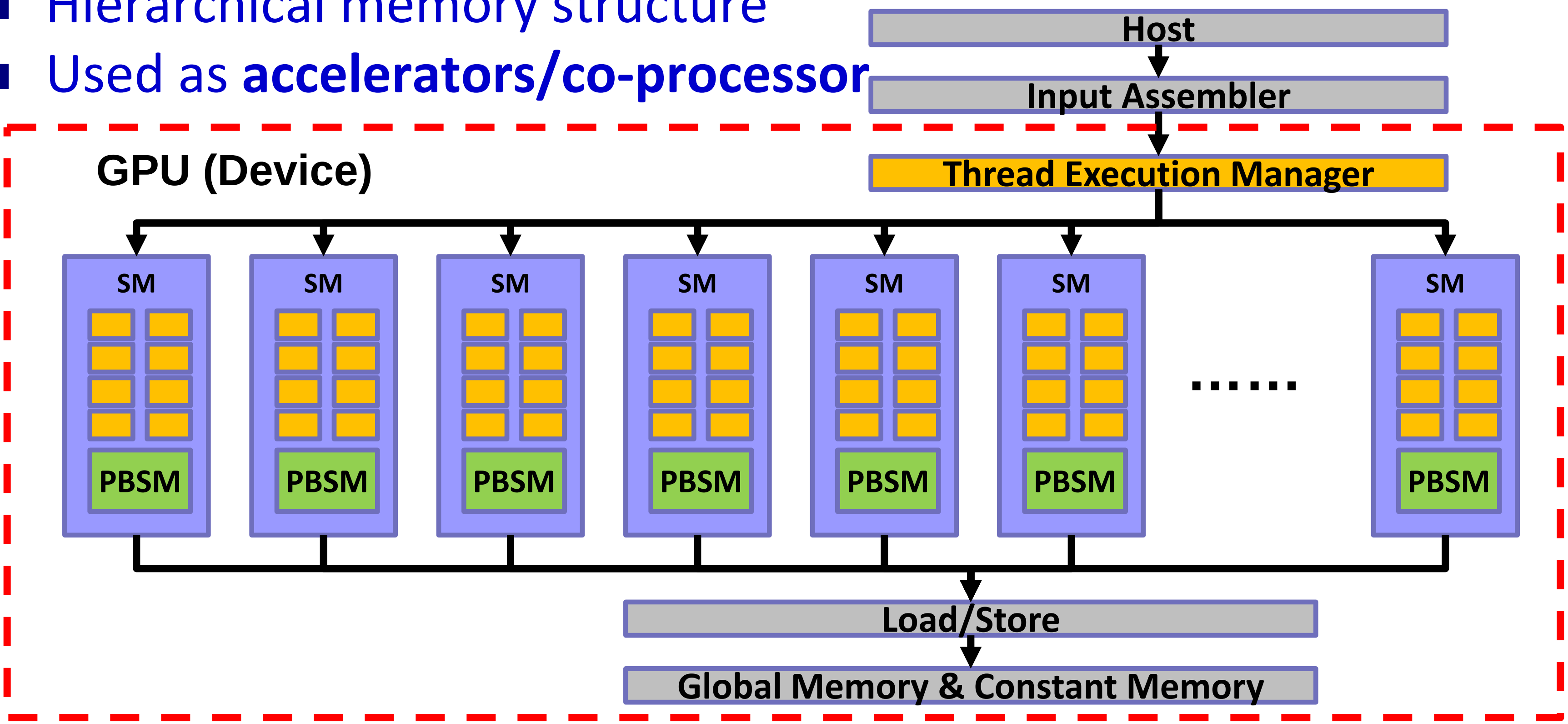
Comparison Numbers

	Intel Xeon E5-2697 v3 CPU (Haswell)	NVIDIA Tesla K80 GPU (Kepler)	Intel Xeon Phi 7120P (Knight's Corner)
Cores	2x14	2x13(SMX)	**61**
Logical Cores	2x28	2x2,496	244
Frequency	2.60GHz	562MHz	1.238GHz
GFLOPS(double)	2x583	2x1,455	1,208
Max memory	768GB	2x12GB	16GB
Max Mem BW	2x68GB/s	2x240GB/s **(Internal)**	352GB/s **(Internal)**
Price	2,700 USD	5,000 USD	4,000 USD

Source: https://www.xcelerit.com/computing-benchmarks/libor/haswell_k80_phi/

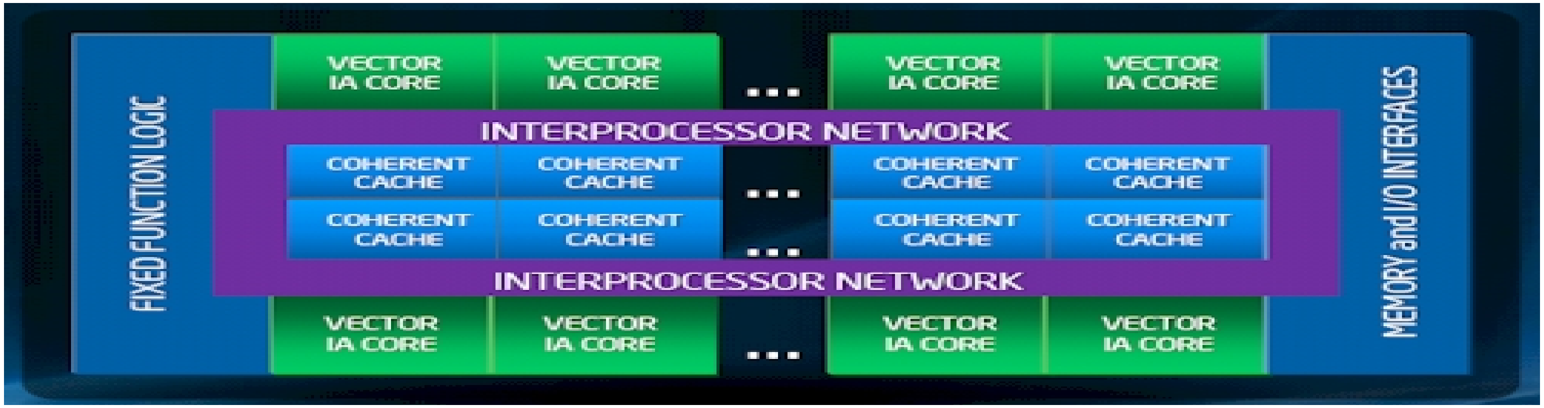
NVidia General Purpose GPU

- Extend GPU as a form of stream processor (or a **vector processor**) for general purpose computing
- Suited for **embarrassingly parallel** tasks and **vectorized operations**
- Hierarchical memory structure
- Used as **accelerators/co-processor**



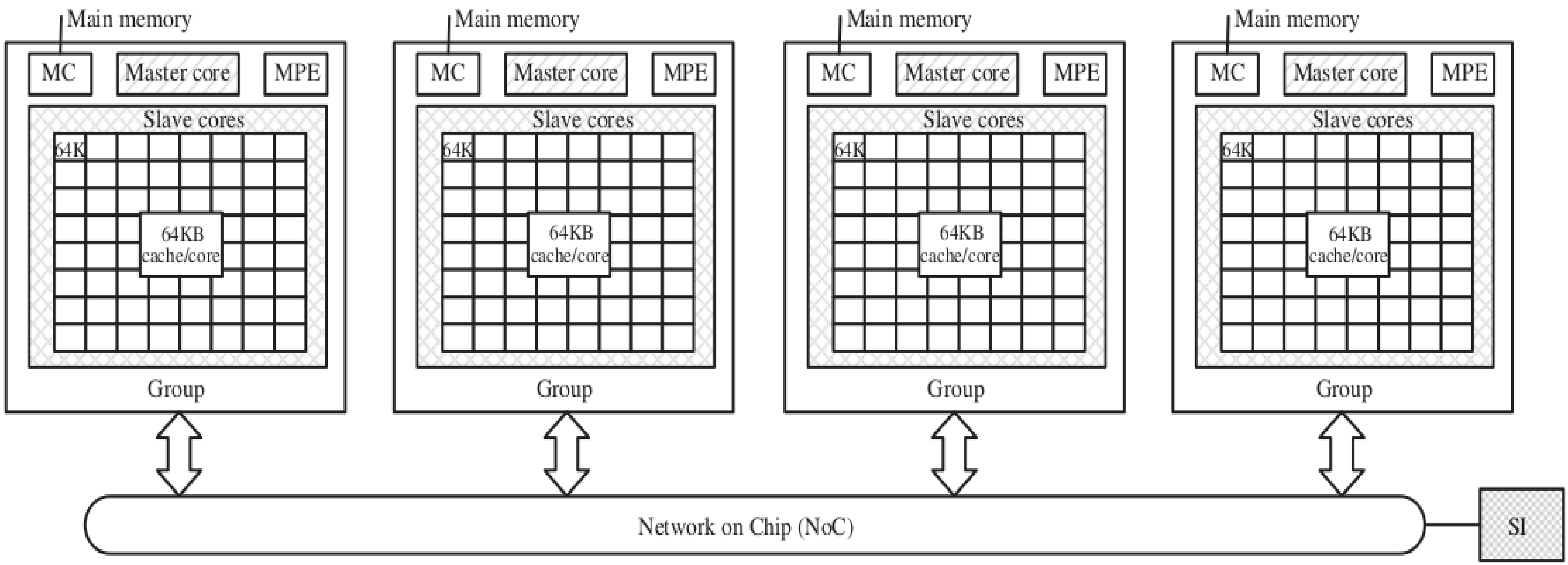
Intel Xeon Phi

- A brand name given to a series of manycore processors follows the Intel's MIC (Many Integrated Core) architecture
  - Typically it has **50-70 processors** on the die connected by a bidirectional Ring network
- More like a separate system
  - It runs **Intel assembly code** just like the main CPU in your computer
  - It has an **embedded linux**
  - Second generation chips (*Knights Landing*) could be used as a **standalone CPU**



Sunway TaihuLight SW26010

- Each node contains four clusters of 64 CPEs (SIMD)
- Each cluster is accompanied by a MPE (general purpose)



Google Tensor Processing Unit (TPU)

- Specifically for deep learning (tensorflow framework)
- 30–80X higher performance-per-watt than contemporary CPUs and GPUs
  - Only for **reduced precision computation** (e.g. 8-bit precision)
  - Matrix Multiplier Unit: use a to achieve hundreds of thousands of **matric operation** in a single clock cycle
  - Systolic array: The ALUs perform **only multiplications and additions in fixed patterns**
- Reference
  - https://cloud.google.com/blog/big-data/2017/05/an-in-depth-look-at-googles-first-tensor-processing-unit-tpu

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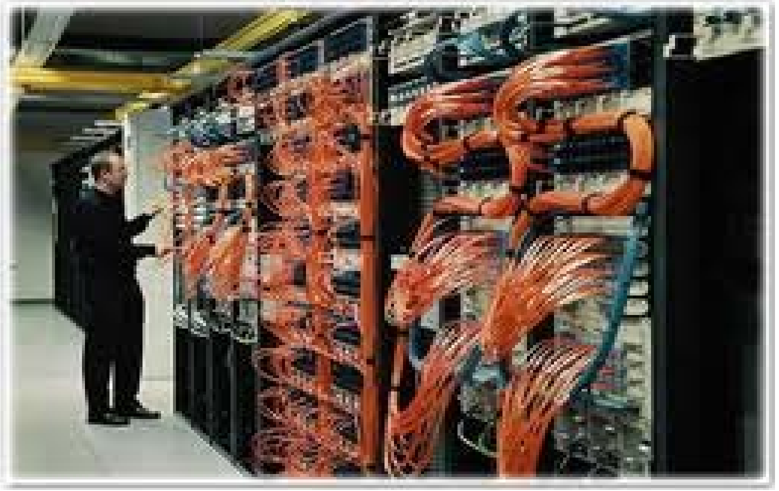
Communication

- Communication has the most impact to the performance of parallel programs (Even more critical to computing or memory).
  - Network is generally much slower than CPU
  - Communication is common to parallel programs
  - Synchronization is expensive and could grow exponentially to the number of servers



Interconnection Networks

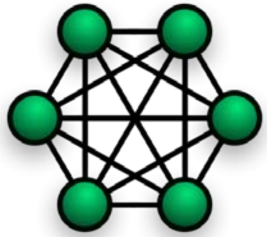
- Network design considerations
  - Scalability, Performance, Resilience and Cost

Application

- Communication pattern & protocol

Interconnection Network Topology

- Network diameter
- Re-routing path for fault tolerance
- # fan-in & fan-out degree per node



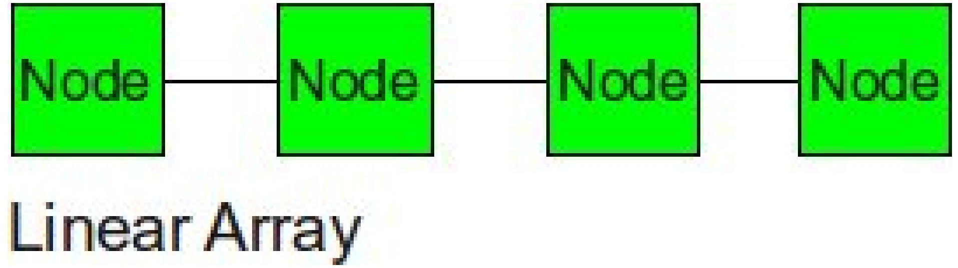
Network Devices (Cable, Switch, Adapter, etc.)

- Bandwidth: #bits transferred per second
- Latency: time to pack, unpack, and send a message
- Scalability: # of ports on the adapter and switch

Network Topology

	Diameter (latency)	Bisection (resilience)	#Links (cost)	Degree (scalability)
Linear array	P-1	1	P-1	2

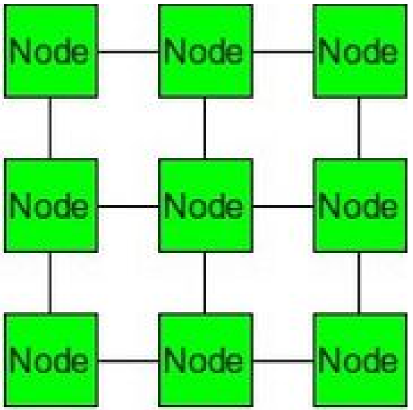
- Cheapest solution, but not reliable and long latency



Network Topology

	Diameter (latency)	Bisection (resilience)	#Links (cost)	Degree (scalability)
Linear array	P-1	1	P-1	2
Ring	p/2	2	P	2
Tree	$2\log_2 p$	1	2(p-1)	3
2-D Mesh	$2(\sqrt{p}-1)$	$\sqrt{p}$	$2\sqrt{p}(\sqrt{p}-1)$	4

- Particularly suitable for some of the applications such as the ocean application and matrix calculation
- Can be extended to 3-D mesh



2-D Mesh

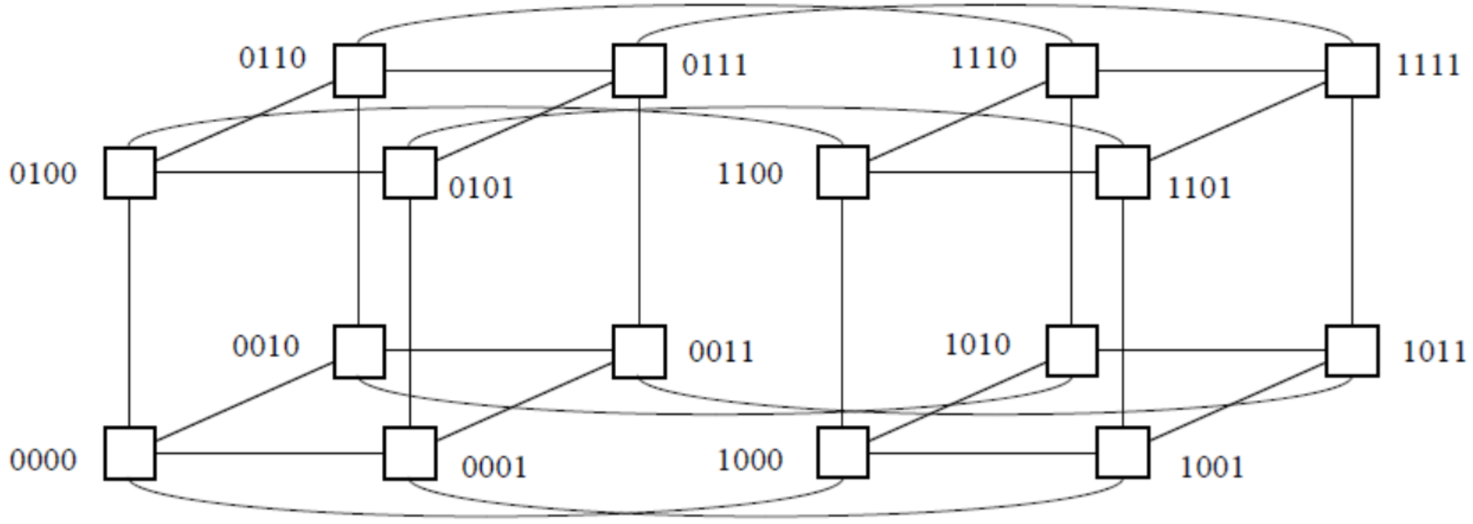
Network Topology

	Diameter (latency)	Bisection (resilience)	#Links (cost)	Degree (scalability)
Linear array	P-1	1	P-1	2
Ring	p/2	2	P	2
Tree	$2\log_2 p$	1	2(p-1)	3
2-D Mesh	$2(\sqrt{p}-1)$	$\sqrt{p}$	$2\sqrt{p}(\sqrt{p}-1)$	4
2-D Torus	$\sqrt{p}$-1	$2\sqrt{p}$	2p	4
Hypercube	$\log_2 p$	p/2	p/2 x $\log_2 p$	$\log_2 p$

- Smaller diameter, more bisection, but also higher cost and degree than Mesh and Torus
- More suitable for smaller scale systems

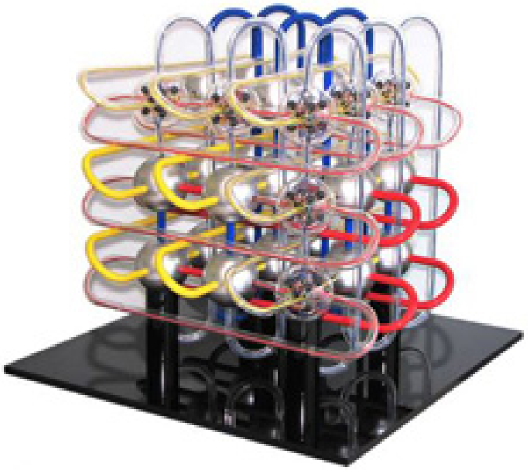
Network Topology

- 4-D hypercube
  - Each node is numbered with a bitstring that is $\log_2(p)$ bits long.
  - One bit can be flipped per hop so the diameter is $\log_2(p)$.



6-Dimensional Mesh/Torus on K-Computer

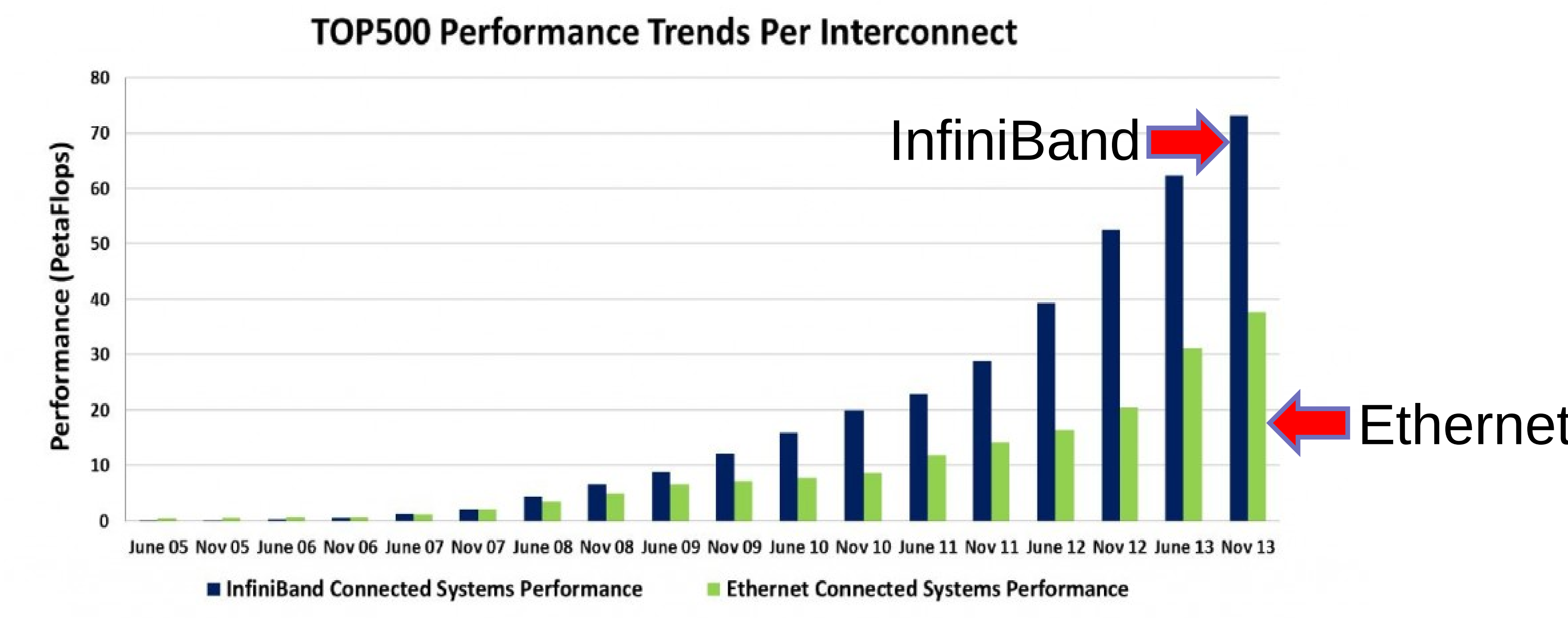
- K-computer (Kei means “京”)
  - Designed by FUJITSU, Japan
  - World’s #5 fastest supercomputer
  - 80,000 compute nodes; 640,000 cores
  - Network connection: Tofu
- Introduction video clip:
  - http://www.fujitsu.com/global/about/businesspolicy/tech/k/whatis/network/



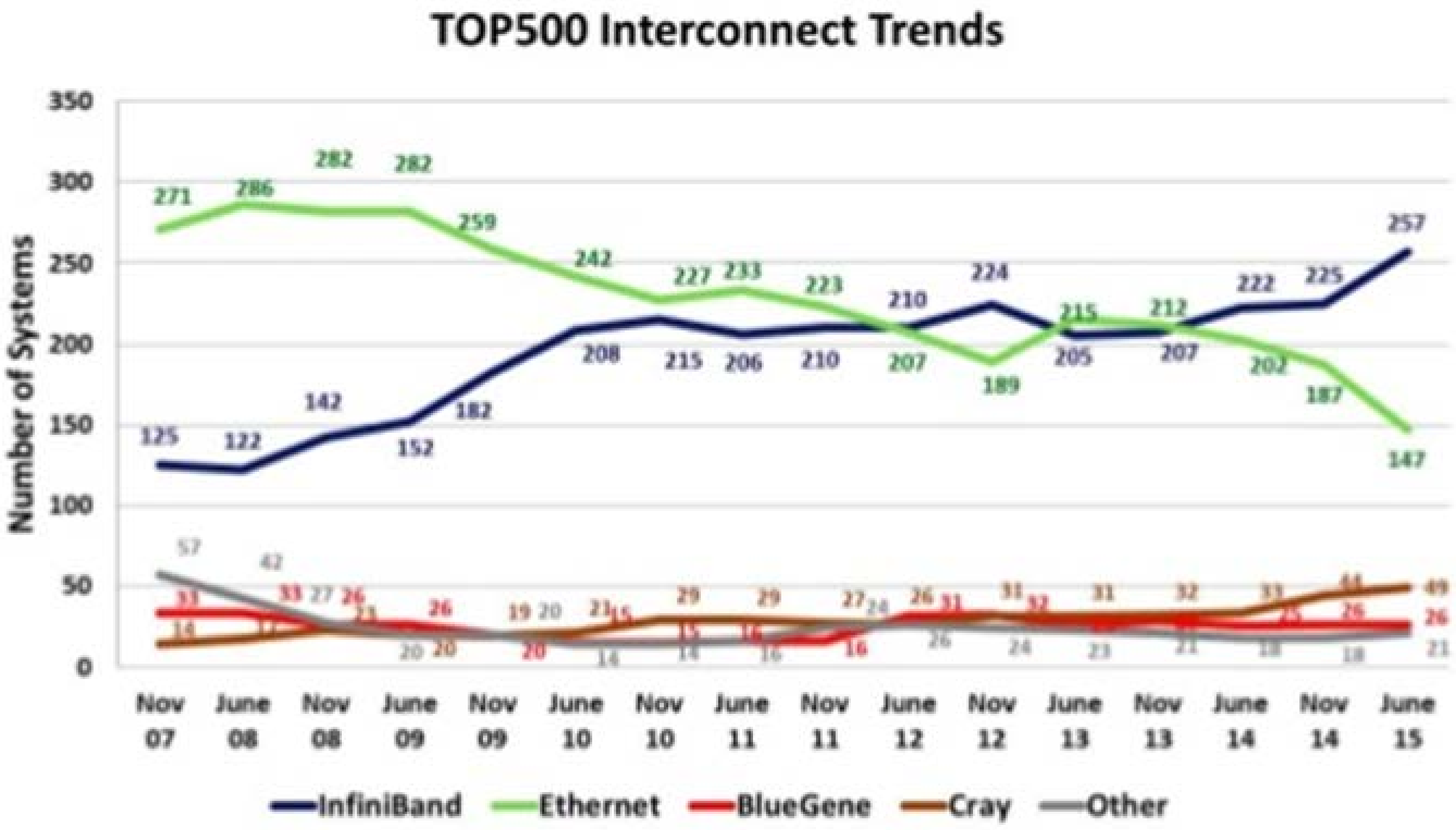
"6-dimensional mesh/torus" topology (model)

Network Device: InfiniBand

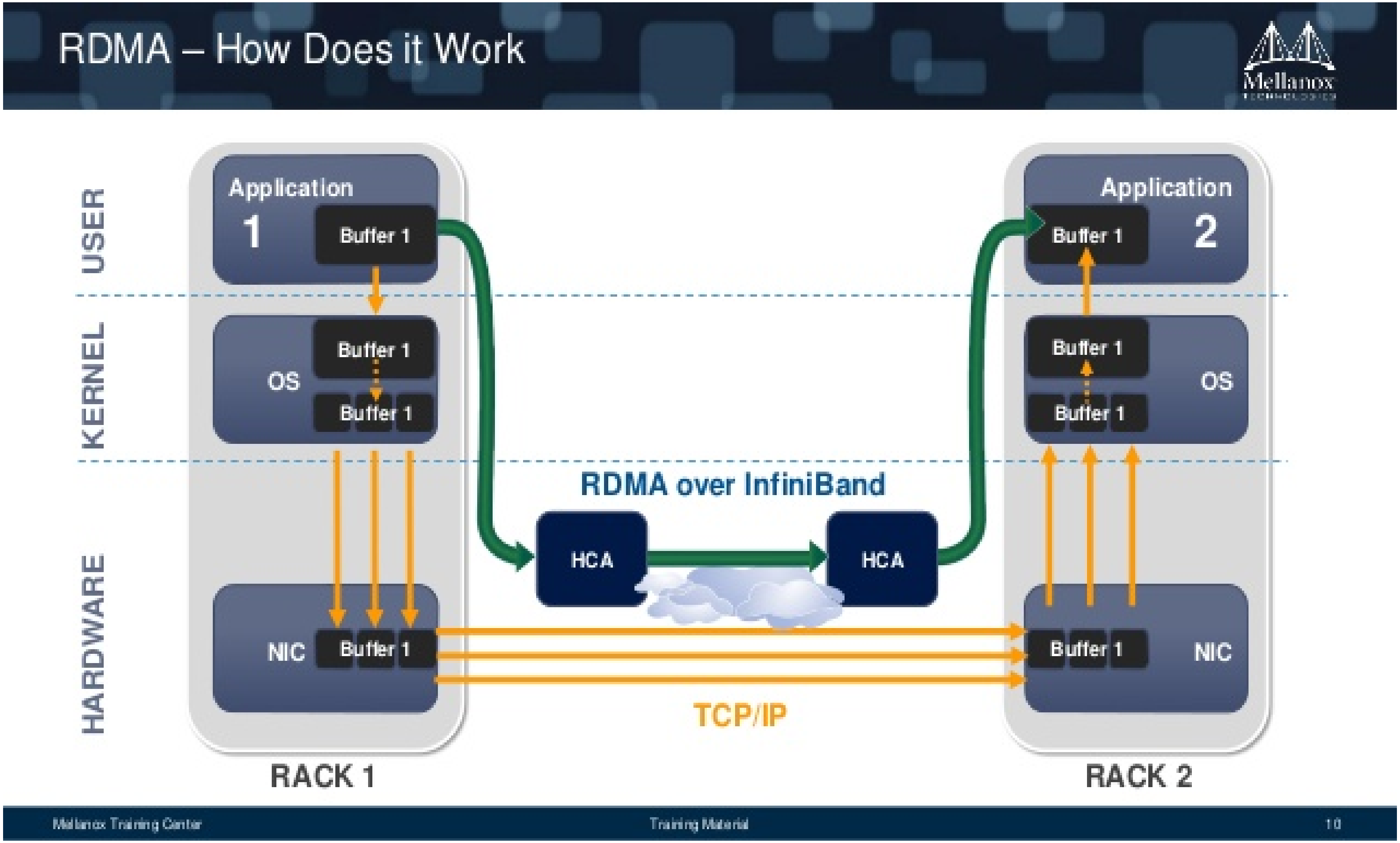
- A computer network communications link used in high-performance computing featuring very high throughput
- It is the most commonly used interconnect in supercomputers
- Manufactured by **Mellanox**



InfiniBand: Usage in TOP500



InfiniBand: RDMA



Source: Mellanox

InfiniBand vs. Gigabit Ethernet

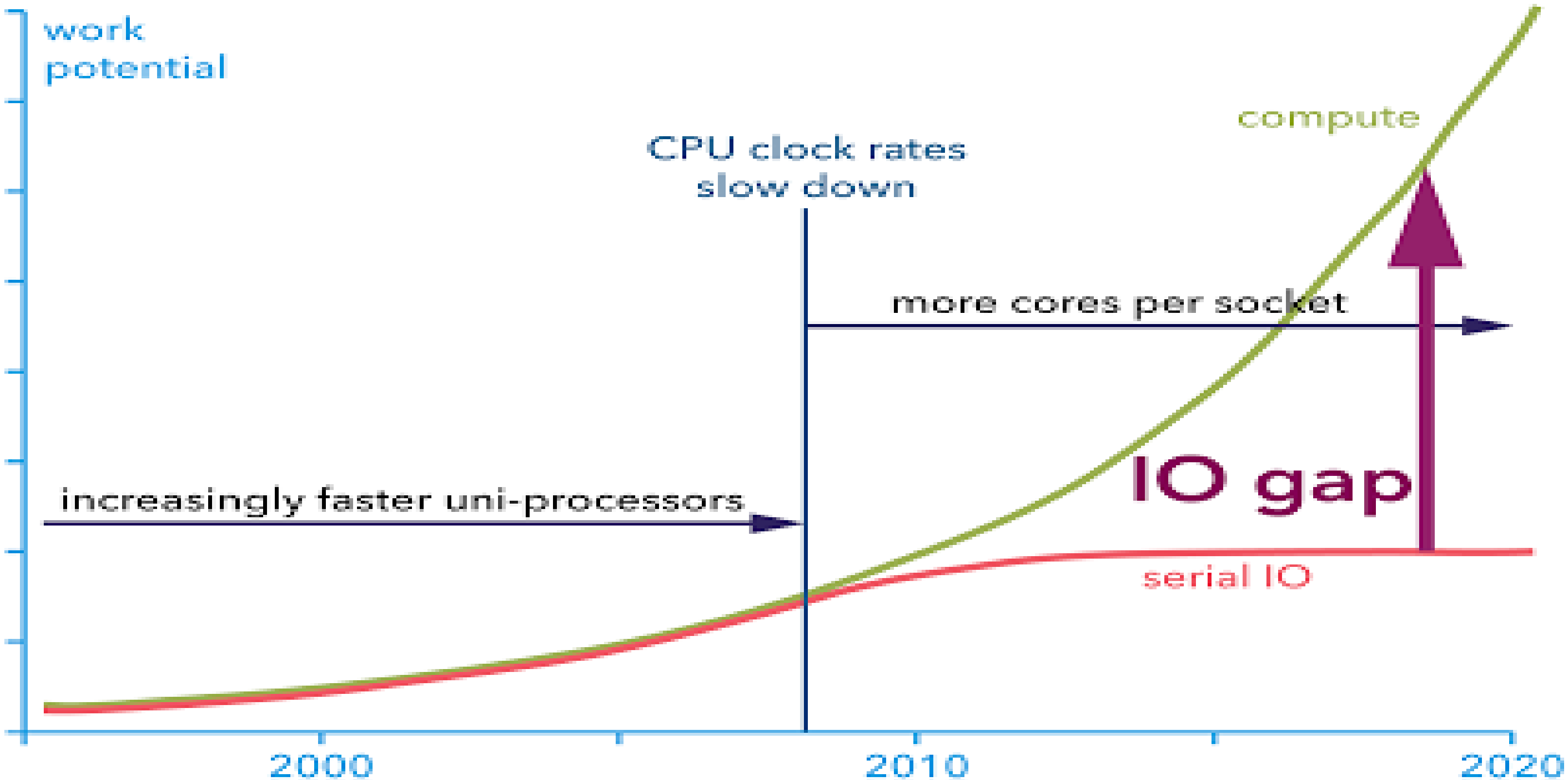
	InfiniBand	Ethernet
Protocol	Guaranteed credit based flow control	Best effort delivery
	End-to-End congestion management	TCP/IP protocol. Designed for L3/L4 switching
	Hardware based retransmission	Software based retransmission
RDMA	YES	NO (only now starting)
Latency	Low	High
Throughput	High	Low
Max cable length	4km	upto 70km
Price	36port switch: 25k USD QDR adapter: 500USD	36port switch: 1.5k USD Network card: 50 USD

Outline

- Parallel Computing Introduction
- Classifications of Parallel Computers & Programming Models
- Supercomputer & Latest technologies
  - Supercomputer
  - Processor technology
  - Interconnect & Network technology
  - I/O & Storage technology
- Parallel Program Analysis

How About I/O?

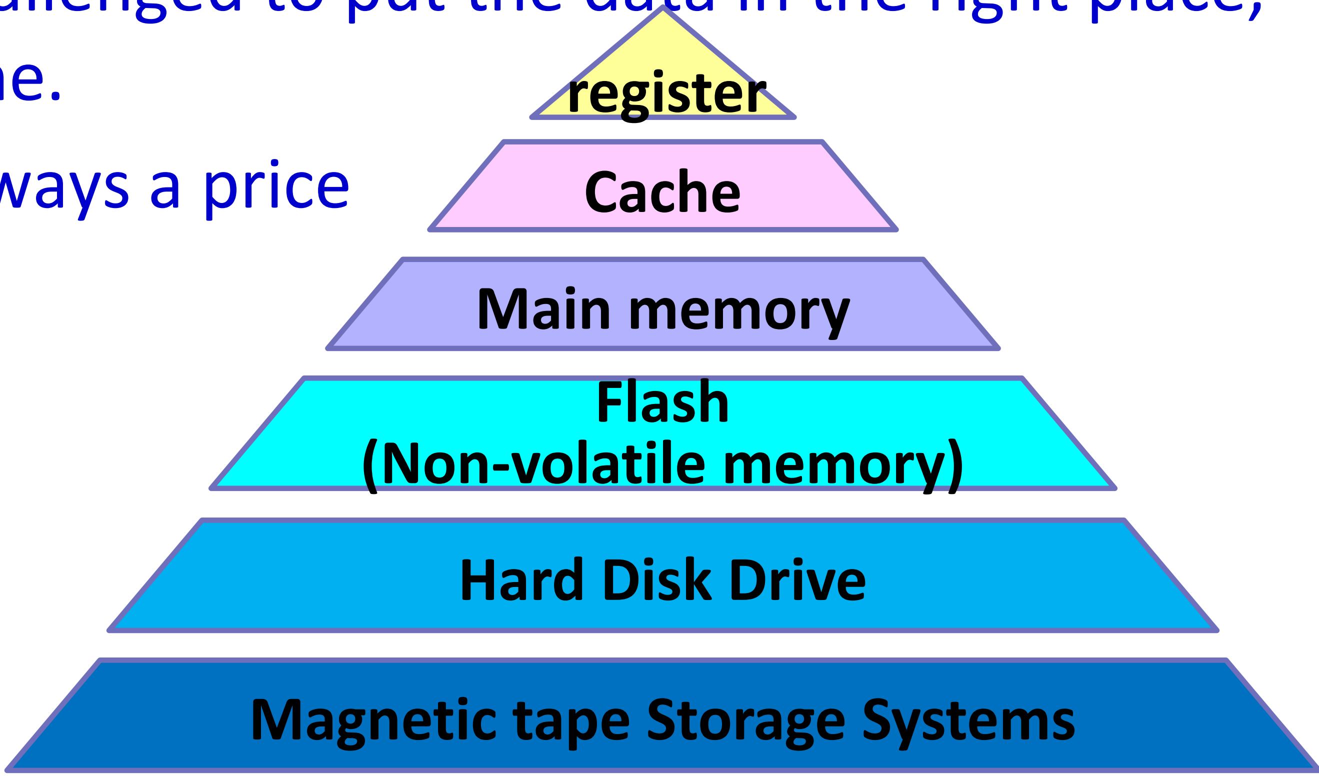
- Not so great…



Source: http://www.mostlycolor.ch/2015_10_01_archive.html

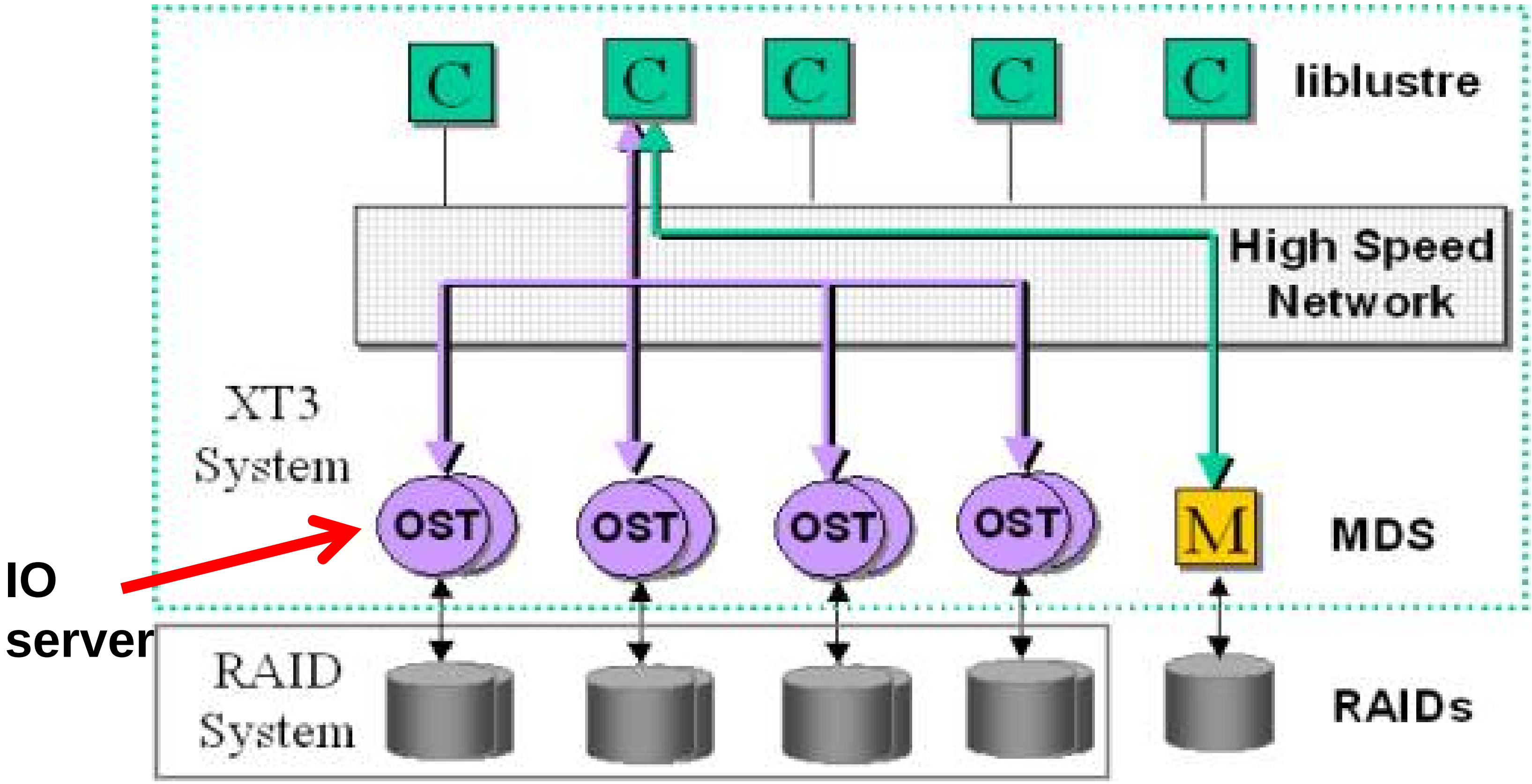
Opportunity in I/O

- Memory hierarchy
  - New storage technology is coming: Flash
  - It is still challenged to put the data in the right place, at right time.
  - There is always a price to pay



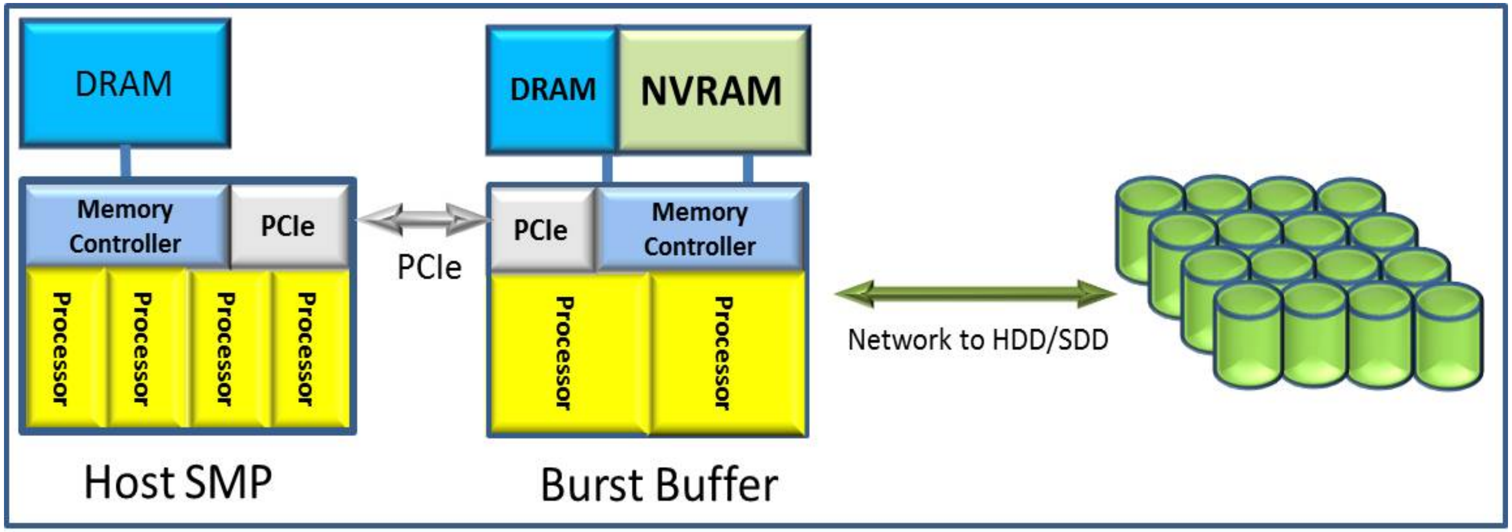
Opportunity in I/O

- Parallel file and IO systems
  - Lustre file system, MPI-IO



Opportunity in I/O

- Burst buffering
  - Add non-volatile RAM at the IO server nodes as a buffer to smooth the burst traffic pattern for improving the IO performance of storage systems, and reduce the IO latency



Summary

- People has been and will always be able to find a way to keep the growth of computing
  - Technology: CPU scaling, distributed computing, new processor architecture
  - Optimization: algorithm, data management, compiler
  - System design: network topology, file system
- It is more than just computing
  - Networks and IO become greater concerns
- Does the performance report from supercomputers really meets the needs of applications?
  - People start re-thinking what should be the right objective and benchmark for designing the next generation of supercomputers.

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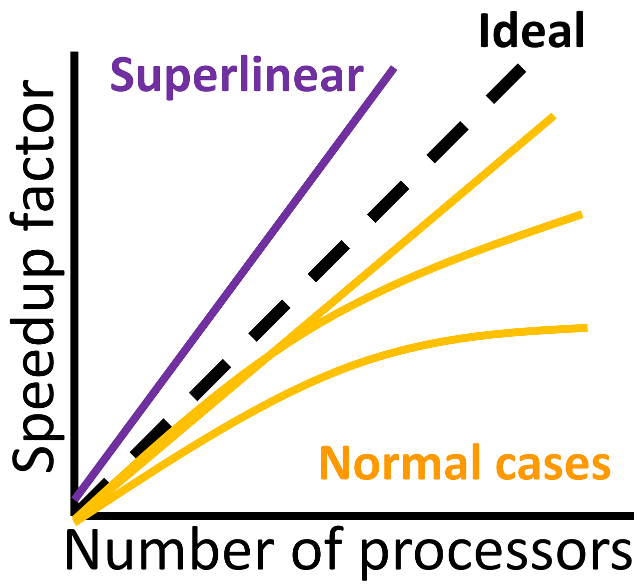
  - Strong scalability vs. Weak scalability
  - Time complexity & Cost optimality

Speedup Factor

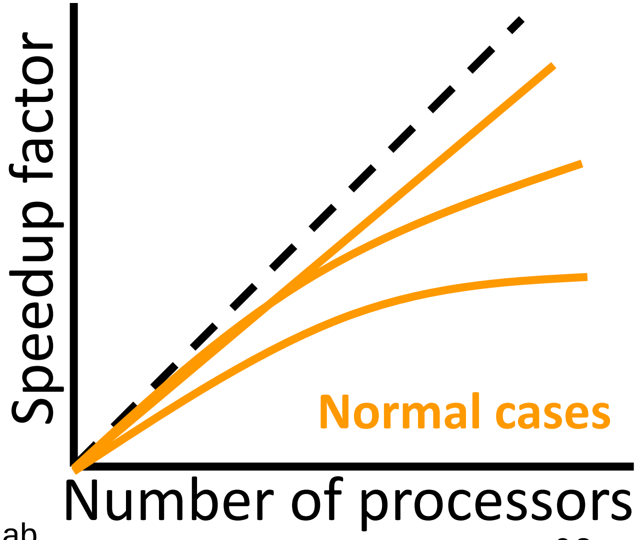
- Program **speedup factor**: $S(p) = \frac{T_s}{T_p}$
  - T_s: execution time using the BEST sequential algorithm
  - T_p: execution time using $\boldsymbol{p}$ processor
- Linear speedup: $S(p) = p$
  - Ideal maximum speedup in theory
- Superlinear speedup: $S(p) > p$
  - Occasionally happen in practice
  - Extra HW resource (e.g. memory)
  - SW or HW optimization (e.g. caching)



- **System efficiency**: $E(p) = \frac{T_s}{T_p \times p} = \frac{S(p)}{p} \times 100\%$

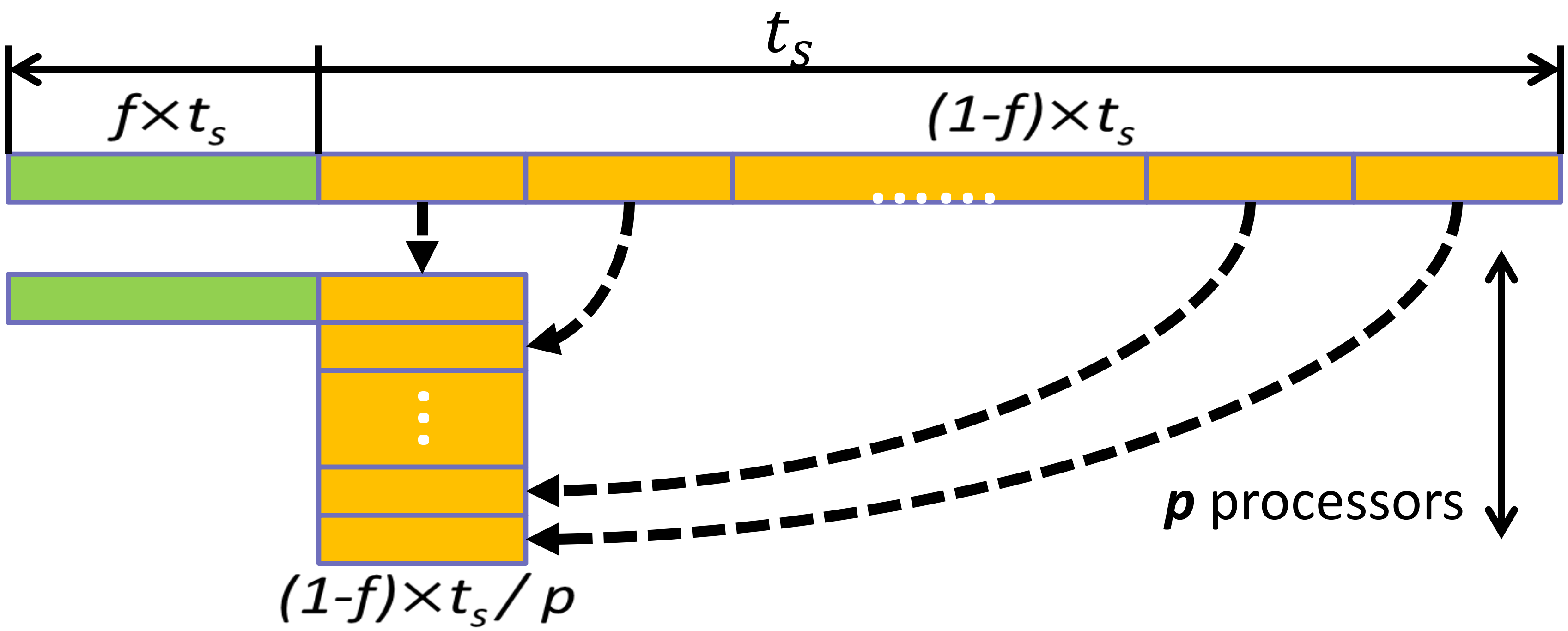
Maximum Speedup

- Difficult to reach ideal max. speedup: $S(p)=p$
  - Not every part of a computation can be parallelized (results in processor idle)
  - Need extra computations in the parallel version (i.e. due to synchronization cost)
  - Communication time between processes (normally the major factor)



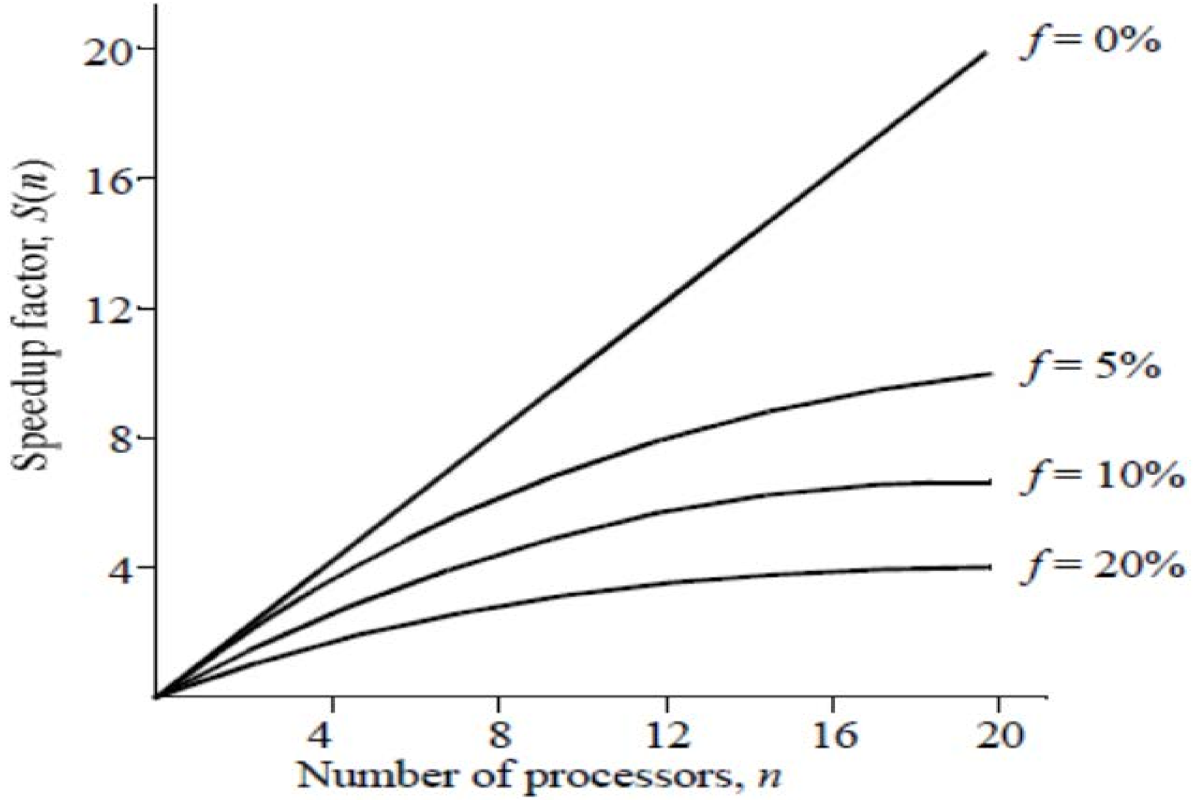
Maximum Speedup

- Let f be the fraction of computations that can **NOT** be parallelized
  - $S(p) = \frac{t_s}{f t_s + (1-f) t_s / p} = \frac{p}{1+(p-1)f}$



Maximum Speedup

- Even with infinite number of processors
  - $S(p)_{p \to \infty} \frac{p}{1+(p-1)f} = \frac{1}{f}$



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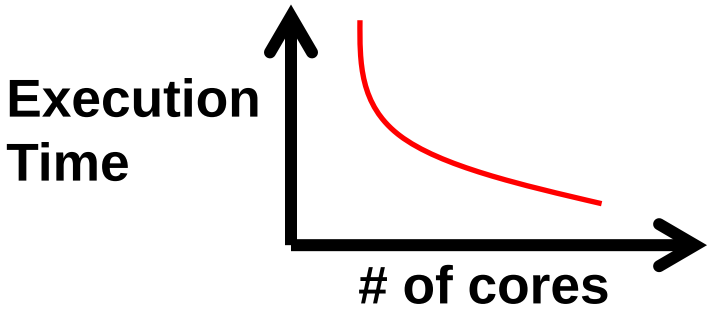
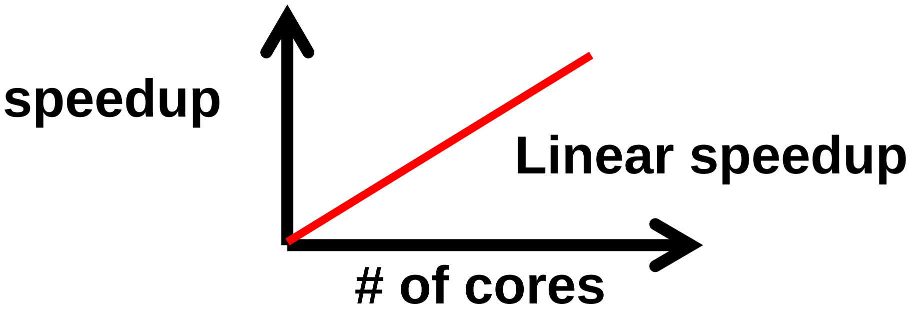
Strong Scaling

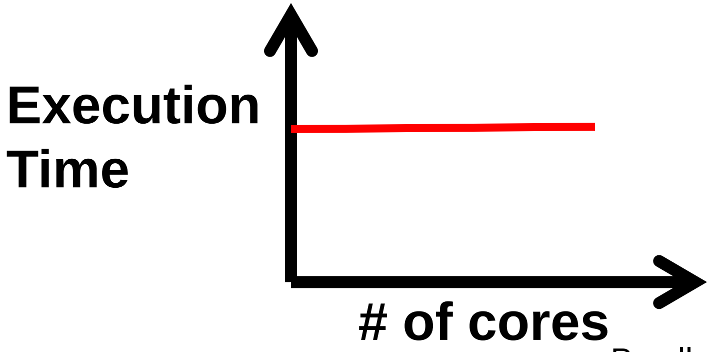
- The problem size stays fixed but the number of processing elements are increased.
- It is used to find a "sweet spot" that allows the computation to complete in a reasonable amount of time, yet does not waste too many cycles due to parallel overhead.
- **Linear scaling** is achieve if the **speedup is equal to the number of processing elements**.

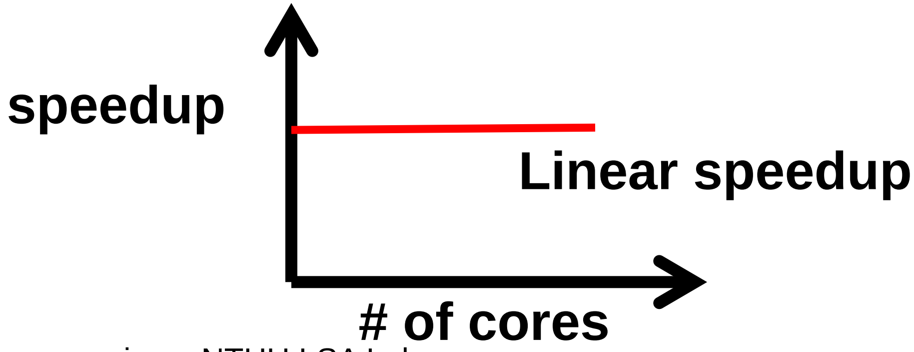




Weak Scaling

- The problem size (workload) assigned to **each processing element** stays fixed and additional processing elements are used to solve a **larger total problem**
- It is a justification for programs that take a lot of memory or other system resources (e.g., a problem wouldn't fit in RAM on a single node)
- **Linear scaling is** achieved if the run time stays constant while the workload is increased





Strong Scaling vs. Weak Scaling

- Strong scaling
  - Linear scaling is harder to achieve, because of the communication overhead may increase proportional to the scale
- Weak scaling
  - Linear scaling is easier to achieve because programs typically employ nearest-neighbor communication patterns where the communication overhead is relatively constant regardless of the number of processes used

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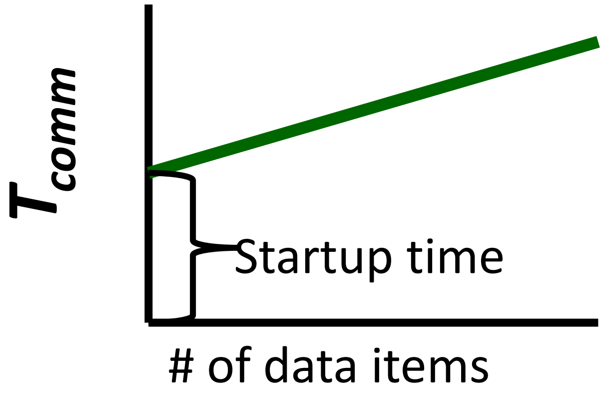
Time Complexity Analysis

- $T_p = T_{comp} + T_{comm}$
  - T_p: Total execution time of a parallel algorithm
  - T_{comp}: Computation part
  - T_{comm}: Communication part
- $T_{comm} = q\ (T_{startup} + n\ T_{data})$
  - $T_{startup}$: Message latency (assumed constant)
  - T_{data}: Transmission time to send one data item
  - n: Number of data items in a message
  - q: Number of message

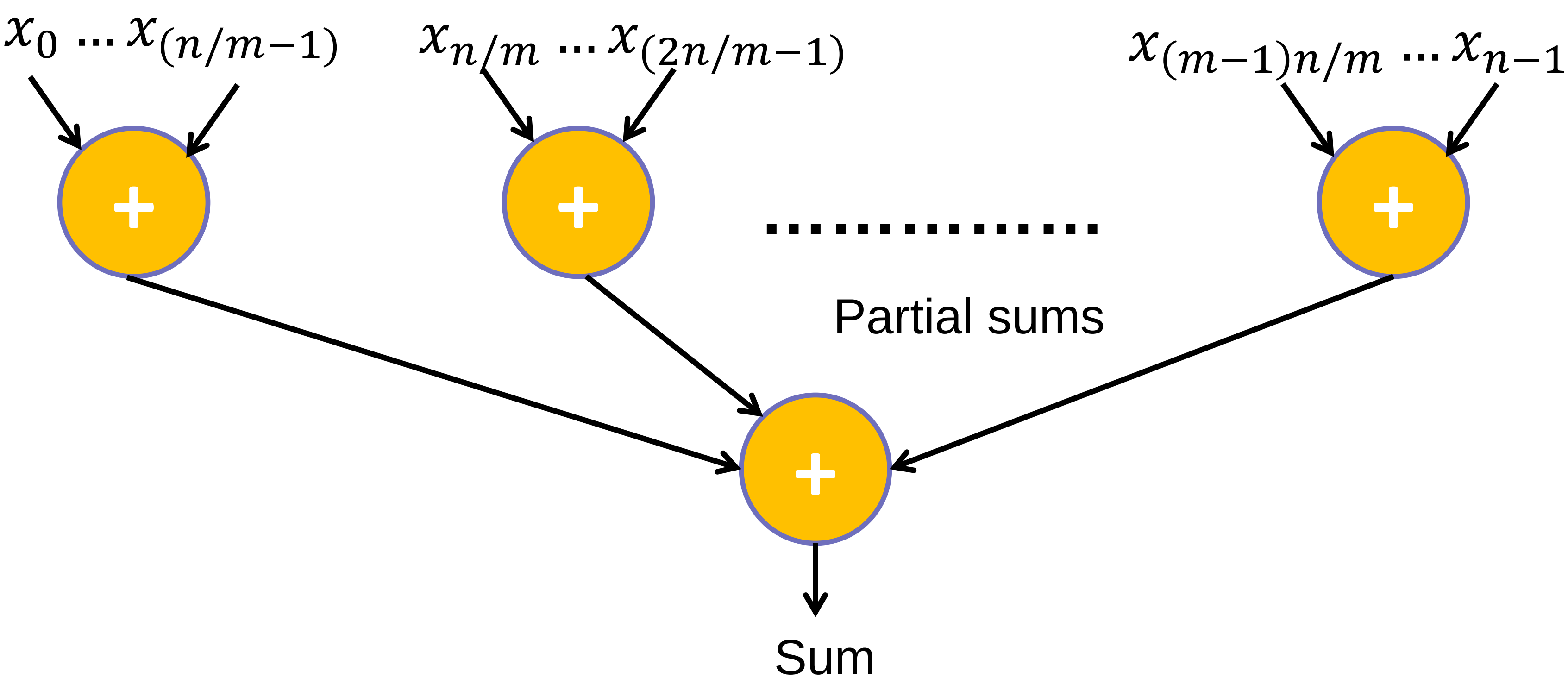


Time Complexity Example 1

- Algorithm phase:
  1. Computer 1 sends *n*/2 numbers to computer 2
  2. Both computers add *n*/2 numbers simultaneously
  3. Computer 2 sends its partial result back to computer 1
  4. Computer 1 adds the partial sums to produce the final result
- Complexity analysis:
  - Computation (for step 2 & 4):
    - $T_{comp} = n/2 + 1 = O(n)$
  - Communication (for step 1 & 3):
    - $T_{comm} = (T_{startup} + n/2 \times T_{data}) + (T_{startup} + T_{data})$
      $= 2T_{startup} + (n/2 + 1)\ T_{data} = O(n)$
  - Overall complexity: O(n)

Time Complexity Example 2

- Adding *n* numbers using ***m*** processes
  - Evenly partition numbers to processes



Time Complexity Example

- Sequential: $O(n)$
- Parallel:
  - Phase1: Send numbers to slaves

$$t_{comm1} = m(t_{startup} + (n/m)t_{data})$$

  - Phase2: Compute partial sum

$$t_{comp1} = n/m - 1$$

  - Phase3: Send results to master

$$t_{comm2} = m(t_{startup} + t_{data})$$

  - Phase4: Compute final accumulation

$$t_{comp2} = m - 1$$

  - Overall:

$$t_p = 2mt_{startup} + (n + m)t_{data} + m + \frac{n}{m} - 2 = O(m + n/m)$$

Tradeoff between **computation** & **communication**

Cost-Optimal Algorithm

- Definition:
  - Cost to solve a problem is proportional to the execution time on a single processor system
  - $O(T_p) \times N = O(T_s)$
- Example:
  - Sequential algo: O(N log N)
  - Parallel algo1: uses N processor with O(log N)
  - Parallel algo2: uses N^2 processor with O(1)

Reference

- Textbook: Parallel Computing Chap1
- TOP500: https://www.top500.org/
- Blaise Barney, Lawrence Livermore National Laboratory, Introduction to Parallel Computing, https://computing.llnl.gov/tutorials/parallel_comp/
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