# Introduction to Parallel Computing

National Tsing Hua University
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2019, Summer Semester



#### Outline

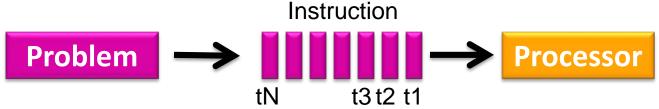
- Parallel Computing Introduction
  - What is parallel computing
  - Why need parallel computing
- Classifications of Parallel Computers & Programming Models
- Supercomputer & Latest technologies
- Parallel Program Analysis

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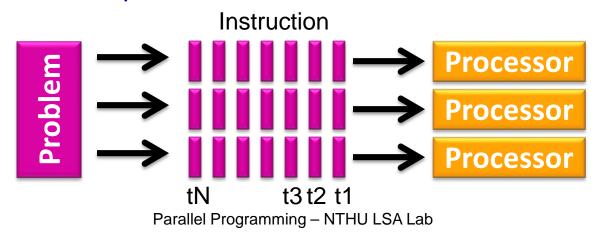
#### What is Parallel Computing?

"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
    Parallel Programming NTHU LSA Lab

#### 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 Finish in 1 hour!!!







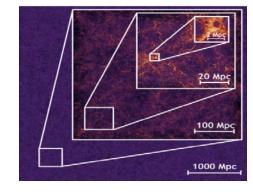


	DUAL XEON CPU server	DGX-1 GPU server ( 8 GPUs)		
FLOPS	3TF	170TF		
Node Mem BW	76GB/s	768GB/s		
Alexnet Train Time	150 Hr	2Hr		
Train in 2Hr	>250Nodes	1Node		

### 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)

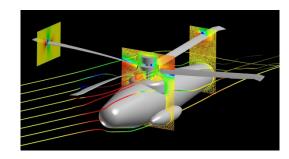




1 trillion particles, 4.225 Gpc box-size simulation, and 6 kpc force resolution.

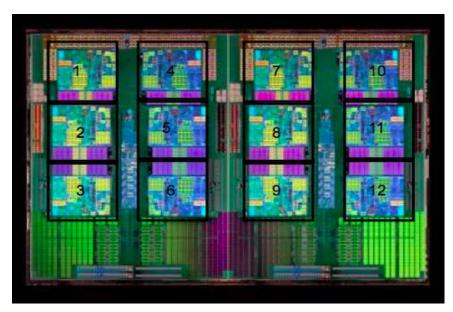




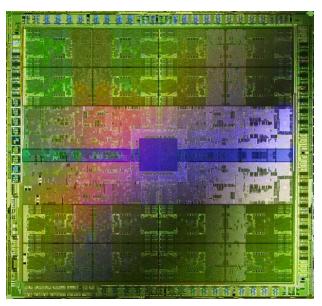


## Why need Parallel Computing

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



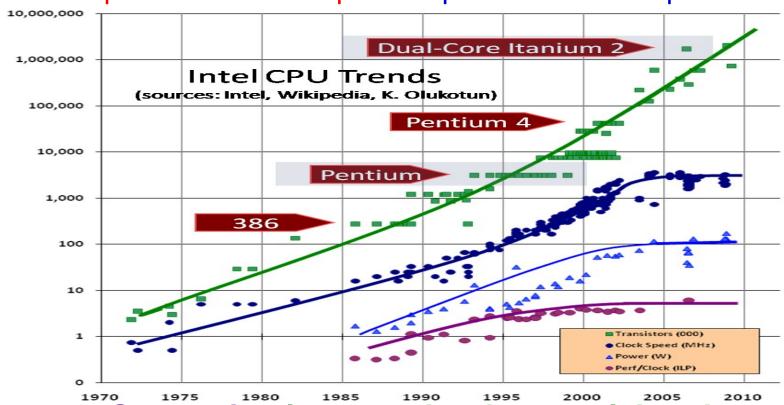
12 Cores IBM Blade Multi-core CPU



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 <u>trend</u> and <u>essential tools</u> in today's world!"

Parallel Programming – NTHU LSA Lab

## 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 ...

# Heterogeneous Systems Era

Enabled by:
Abundant data
parallelism
Power efficient GPUs

Constraint by:
Programming
models
Comm. overhead

Shader → CUDA → OpenCL ...

# Distributed System Era

Enabled by: Networking Constraint by:
Synchronization
Comm. overhead

MPI → MapReduce ...



#### Outline

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

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#### Parallel Computer Classification

#### **■ Flynn's classic taxonomy**

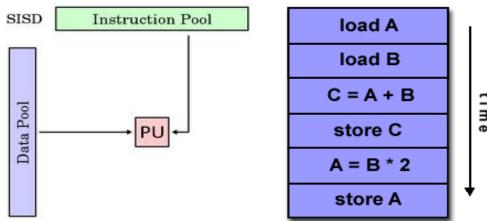
- > Since **1966** (50 years ago ...)
- ➤ From the process unit prospective: Classify computer architecture based two independent dimensions: Instruction & Data

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

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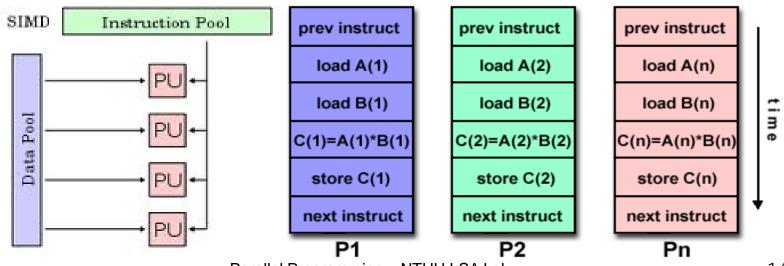
#### Flynn's classic taxonomy: SISD

- 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



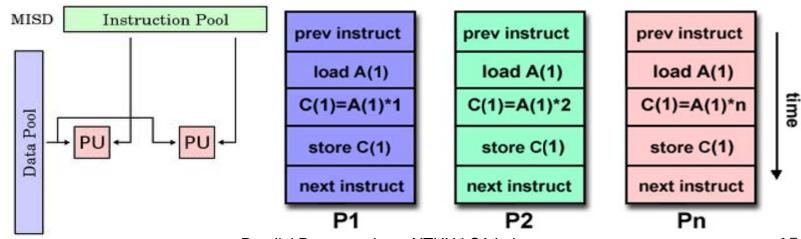
## Flynn's classic taxonomy: SIMD

- 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)



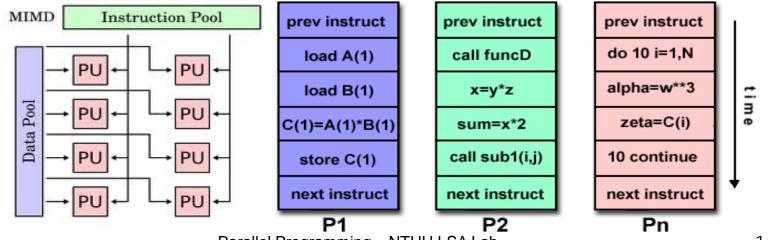
## Flynn's classic taxonomy: MISD

- 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

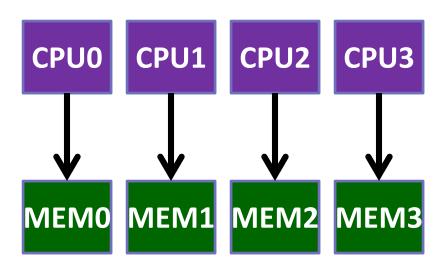




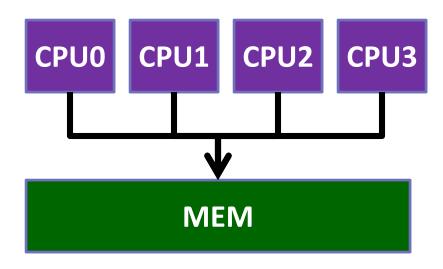
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  - > Programming model classification
- Supercomputer & Latest technologies
- Parallel Program Analysis

# Shared Memory vs. Distributed Memory Computer Architecture



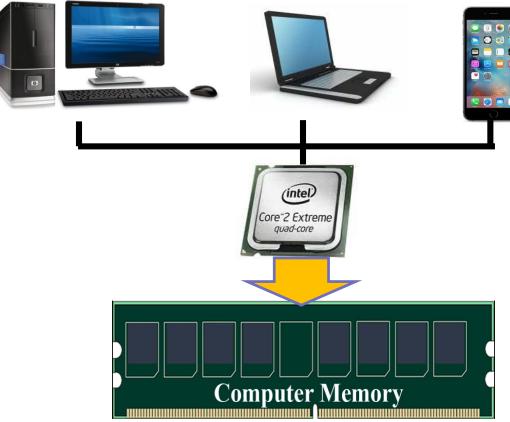
**Distributed memory** 



**Shared memory** 

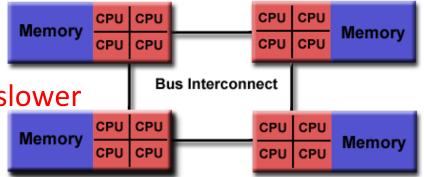
# Shared Memory Multiprocessor Computer System

Single computer with multiple internal multicore 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



Memory

CPU

CPU

#### 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

CPU

**CPU** 

Memory

Memory

Network fabric: Ethernet, InfiniBand Memory

Memory

**CPU** 

**CPU** 



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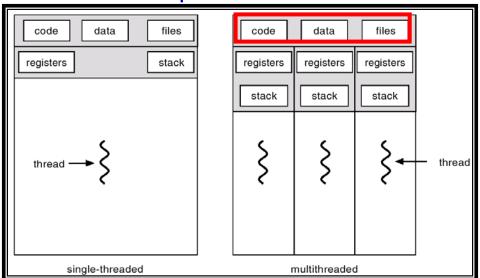
#### Parallel Programming Model

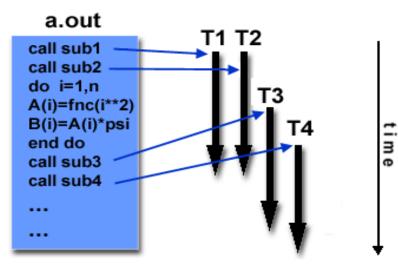
- Parallel programming models exist as an abstraction above hardware & memory architectures
- In general programming models are designed to match the computer architecture
  - Shared memory prog. model for shared memory machine
  - > Message passing prog. model for distributed memory machine
- But programming 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**

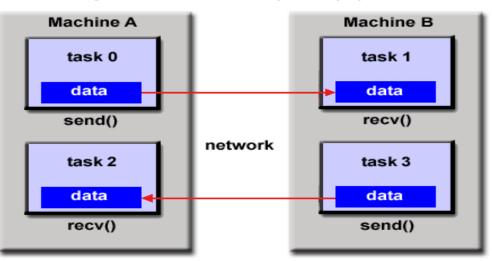
- Implementation
  - > A library of subroutines called from parallel source code
    - E.g.: POSIX Thread (Pthread)
  - A set of compiler directives imbedded in either serial or parallel source code
    - ♦ E.g.: OpenMP

```
#include <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

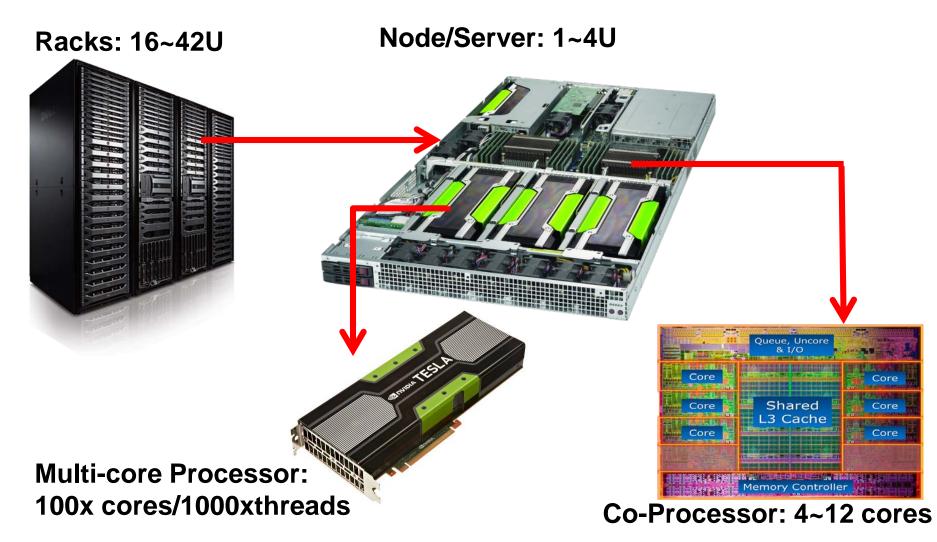
- The designs and popularity of **programming model** and **parallel systems** are highly influenced by each other
- openMP, MPI, Pthreads, CUDA are just some of the parallel languages for users to do parallel programming
- In reality, knowing what is parallel computing is more IMPORTANT than knowing 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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- Supercomputer & Latest technologies
  - Supercomputer
  - Processor technology
  - Interconnect & Network technology
  - ► I/O & Storage technology
- Parallel Program Analysis

## Today's Typical Parallel Computers





#### Supercomputers

- Definition: A computer with a high-level computational capacity compared to a general-purpose computer
- Its performance is measured in floatingpoint 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

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

- > 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 (2019 June)

	Country	System	Vendor	Power (kW)	#cores	Accelerator	Rmax	Rpeak (PFLOPS)
1	US	Summit	IBM	10,096	2.4M	Volta V100	148.6	200.8
2	US	Sierra	IBM	7,438	1.5M	Volta V100	94.6	125.7
3	China	TaihuLight	NRCPC	15,371	10M		93.0	125.4
4	China	Tianhe-2	NUDT	17,808	3M	Xeon Phi	33.9	54.9
5	US	Frontera	Cray		448K	Tesla P100	23.5	38.7
6	Swiss	Piz Daint	Cray	2,384	387K	Tesla P100	21.2	27.1

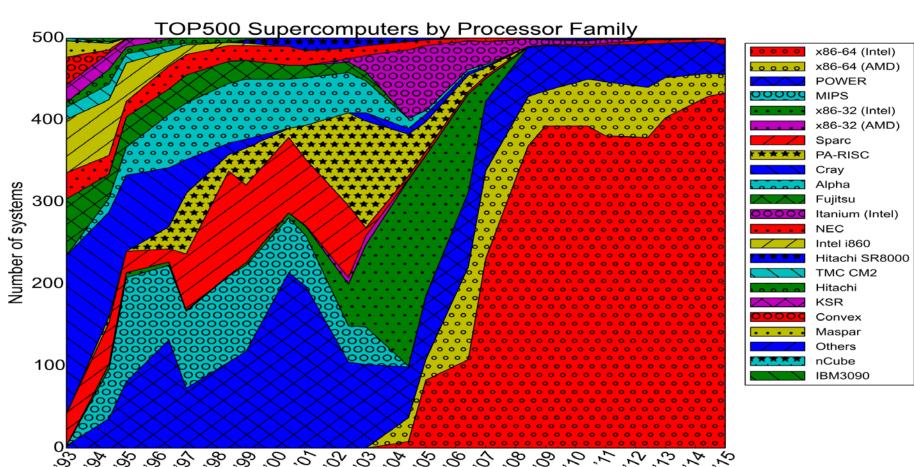
#### 2016 June

8	Swiss	Piz Daint	Cray	2,325	116K	Tesla K20X	6.2	7.8

#### Accelerator provides huge computing power

#### TOP500 Trend: CPU

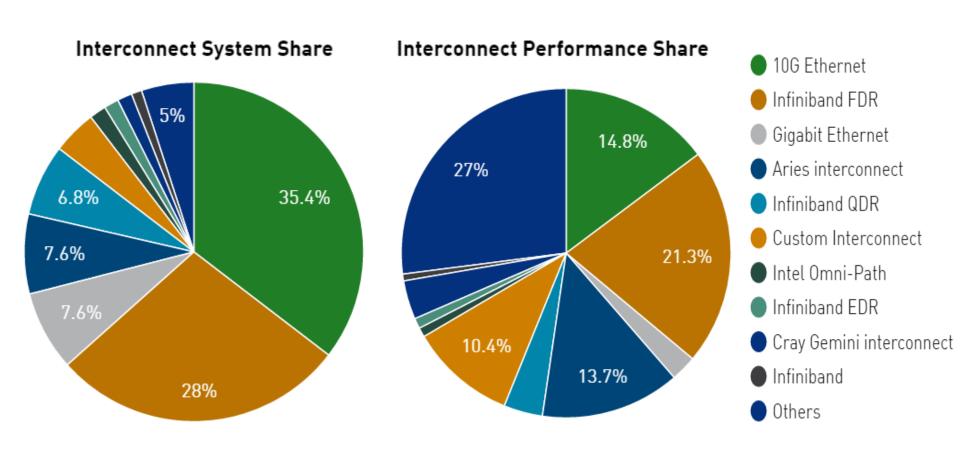
#### ■ Intel CPU counts for more than 80%





#### TOP500 Trend: Interconnect

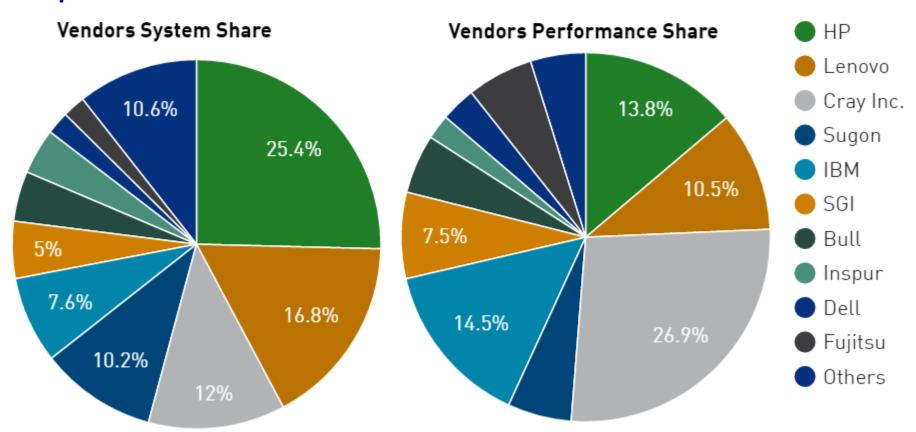
InfiniBand has much larger share in performance





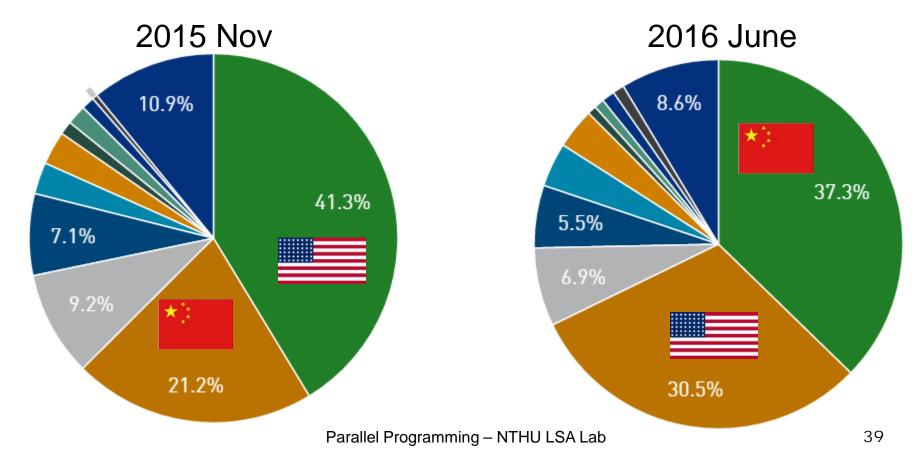
#### TOP500 Trend: Vendor

CRAY and IBM still have larger share for performance



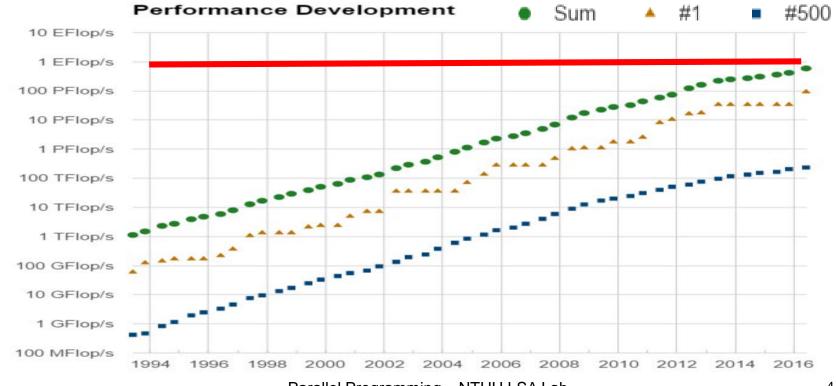
### TOP500 Trend: Country

China has a huge jump because of the new supercomputer



### TOP500 Trend: Computing power

- Goal is to reach Exascale computing 1EFlop (10^18) /s by 2020
  - It is estimated to be the order of processing power of the human brain at neural level
  - The target power of the Human Brain Project



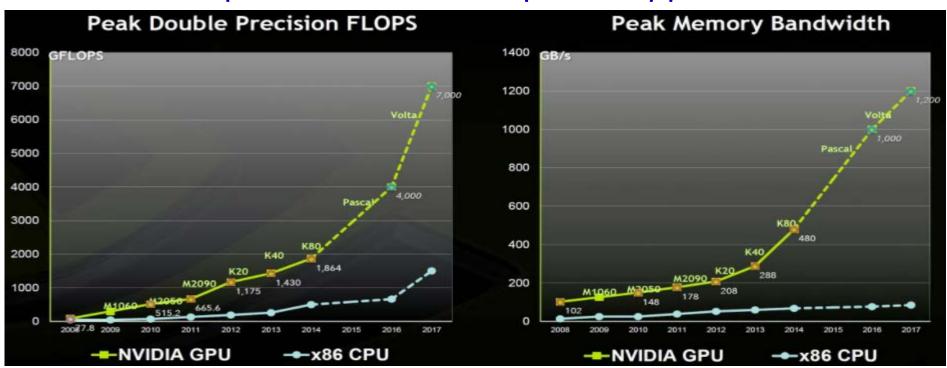


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### Limitation of CPU General Purpose Processor

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.



# **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)	<b>61</b>
Logical Cores	2x28	2x2,496	cores数多,需要减小 frequency(散热等), CPU靠的是frequency而 GPU靠的是core
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/

internal 指gpu访问内部 一的速度非常快(外部则非 堂慢)

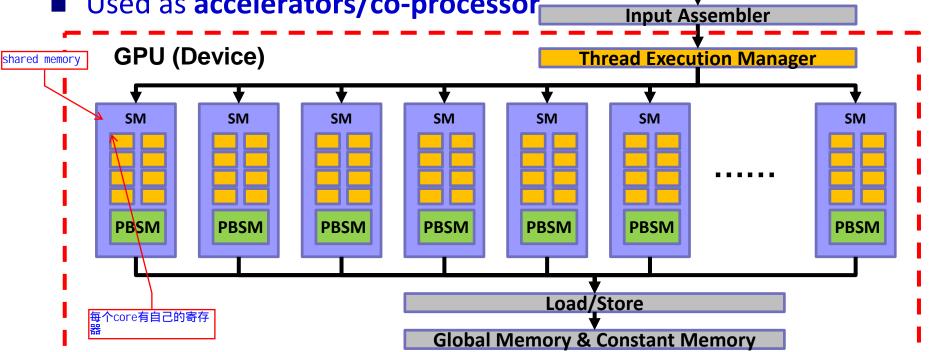
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### NVidia General Purpose GPU

- Extend GPU as a form of stream processor (or a vector processor) for general purpose computing
- Suited for embarrassingly parallel tasks and vectorized operations

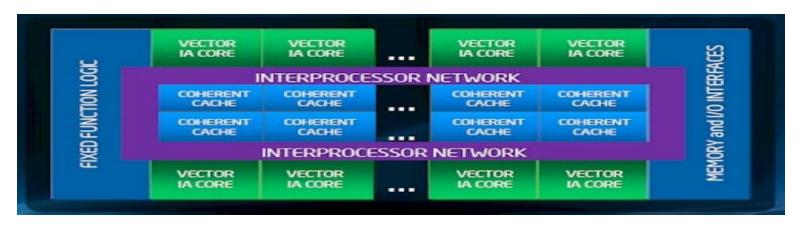
Host

- Hierarchical memory structure
- Used as accelerators/co-processor



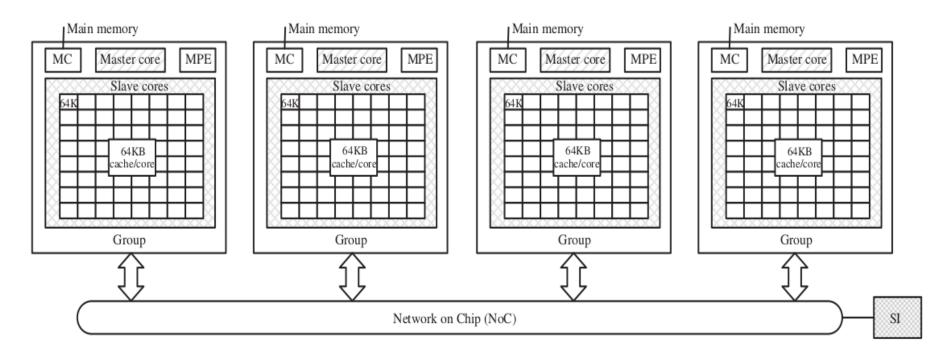
#### Intel Xeon Phi

- 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





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

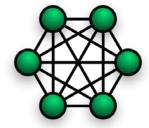
#### **Application**

Communication pattern & protocol



#### **Interconnection Network Topology**

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

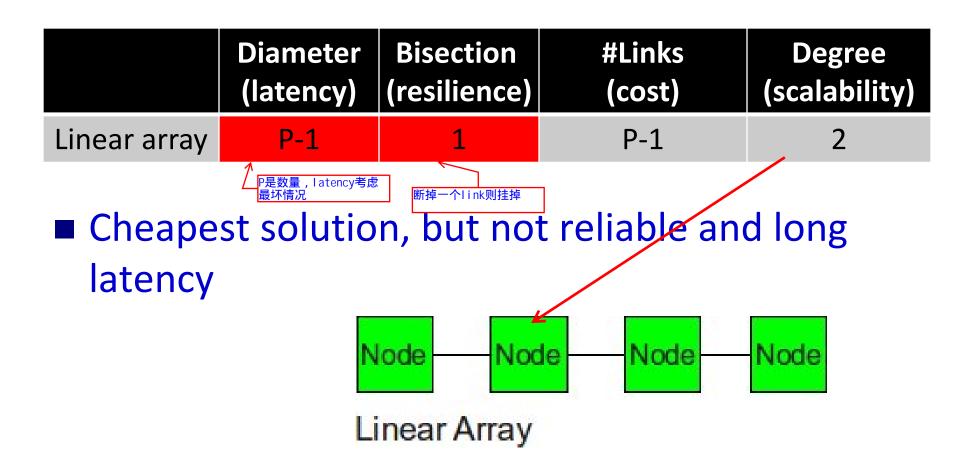


#### Network Devices (Cable, Switch, Adapter, etc.)

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





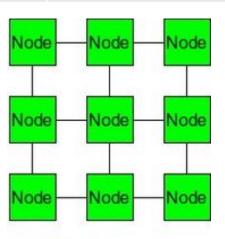


# **Network Topology**

这个越大越reliable

		Diameter (latency)	Bisection (resilience)	#Links (cost)	Degree (scalability)
	Linear array	P-1	1	P-1	2
	Ring	p/2	2	Р	2
bi nary	Tree	$2\log_2 p$	1	2(p-1)	3
z. nar y	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	Р	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	$p/2 \times \log_2 p$	$\log_2 p$

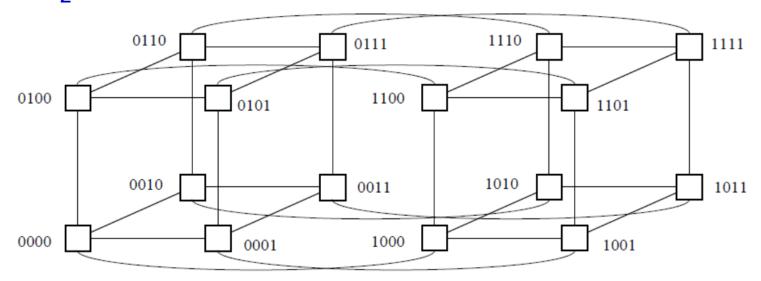
- Smaller diameter, more bisection, but also higher cost and degree than Mesh and Torus
- More suitable for smaller scale systems



#### Network Topology

#### ■ 4-D hypercube

- ➤ Each node is numbered with a bitstring that is log<sub>2</sub>(p) bits long.
- $\triangleright$  One bit can be flipped per hop so the diameter is  $log_2(p)$ .



### 6-Dimensional Mesh/Torus on K-Computer

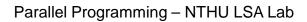
- K-computer (Kei means "京")
  - Designed by FUJITSU, Japan
  - World's #5 fastest supercomputer
  - ➤ 80,000 compute nodes; 640,000 cores
  - Network connection: Tofu
- Introduction video clip:

http://www.fujitsu.com/global/about/businesspolicy/tech/

k/whatis/network/



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

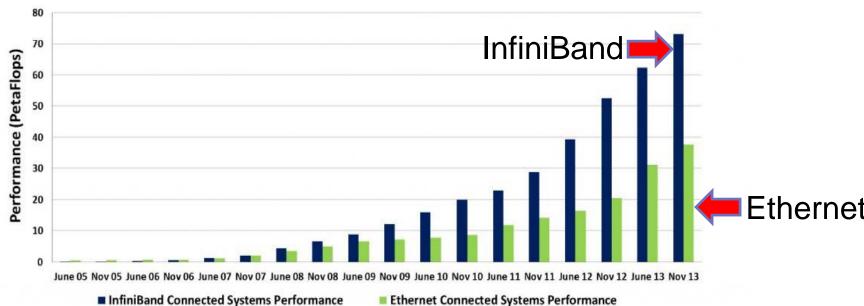


### Network Device: InfiniBand



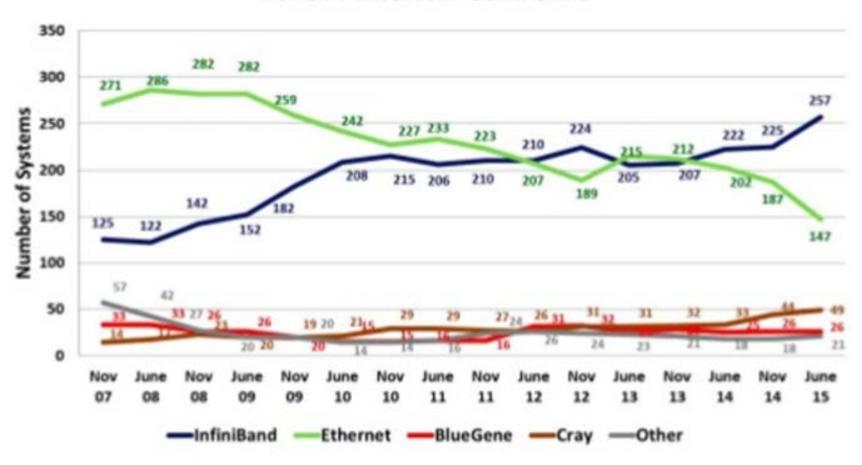
- A computer network communications link used in highperformance computing featuring very high throughput
- It is the most commonly used interconnect in supercomputers
- Manufactured by Mellanox





### InfiniBand: Usage in TOP500

#### TOP500 Interconnect Trends

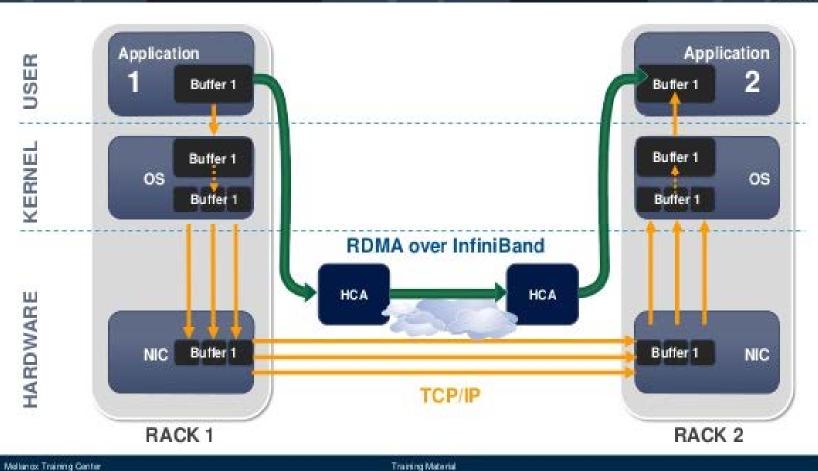






#### RDMA - How Does it Work





Source: Mellanox

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# InfiniBand vs. Gigabit Ethernet

	InfiniBand	Ethernet	
	Guaranteed credit based flow control	Best effort delivery	
Protocol	End-to-End congestion TCP/IP protocol. Design L3/L4 switching		
	Hardware based	Software based	
	retransmission	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	

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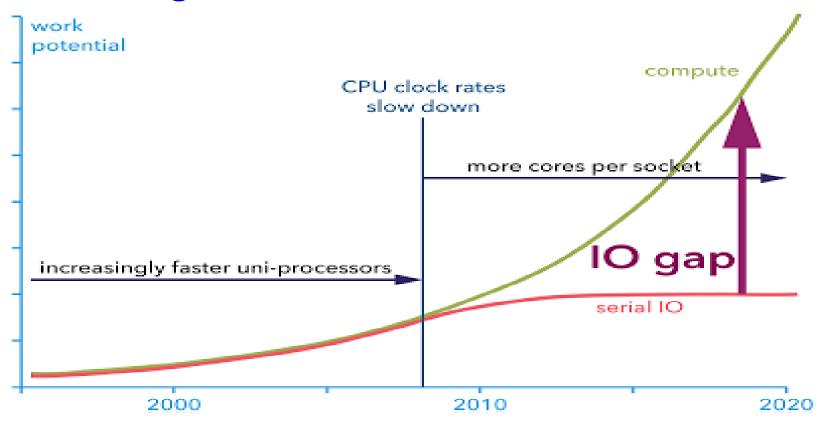
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#### How About I/O?

■ 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.

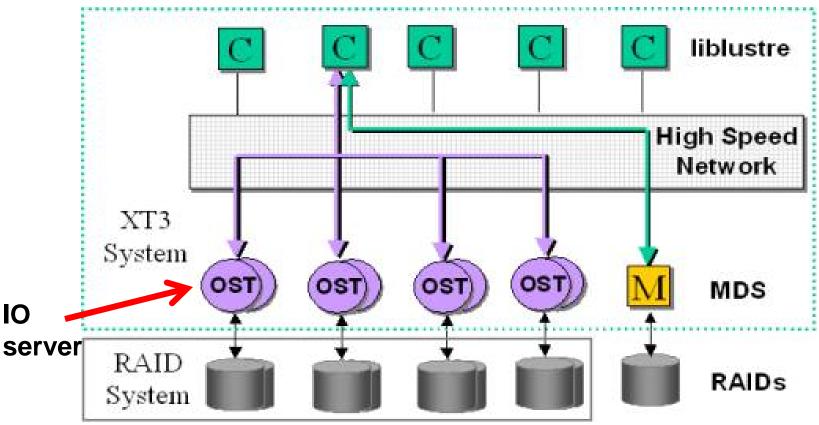
    register

**Hard Disk Drive** 

**Magnetic tape Storage Systems** 

### Opportunity in I/O

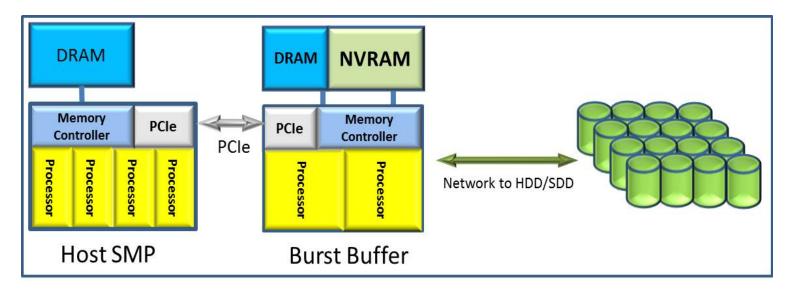
- Parallel file and IO systems
  - ➤ Lustre file system, MPI-IO





### 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. Parallel Programming NTHU LSA Lab



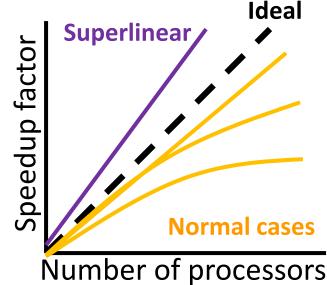
#### Outline

- Parallel Computing Introduction
- Classifications of Parallel Computers & Programming Models
- Supercomputer & Latest technologies
- Parallel Program Analysis
  - Speedup & Efficiency
  - Strong scalability vs. Weak scalability
  - Time complexity & Cost optimality



#### Speedup Factor

- Program speedup factor:  $S(p) = \frac{I_S}{T_p}$ 
  - $\succ T_s$ : execution time using the BEST sequential algorithm
  - $\succ T_p$ : execution time using **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)

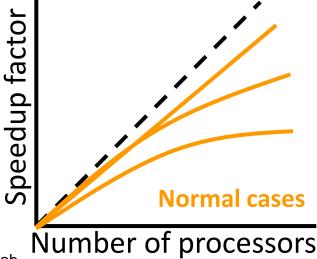


System efficiency: 
$$E(p) = \frac{T_S}{T_p \times p} = \frac{S(p)}{p} \times 100\%$$



#### Maximum Speedup

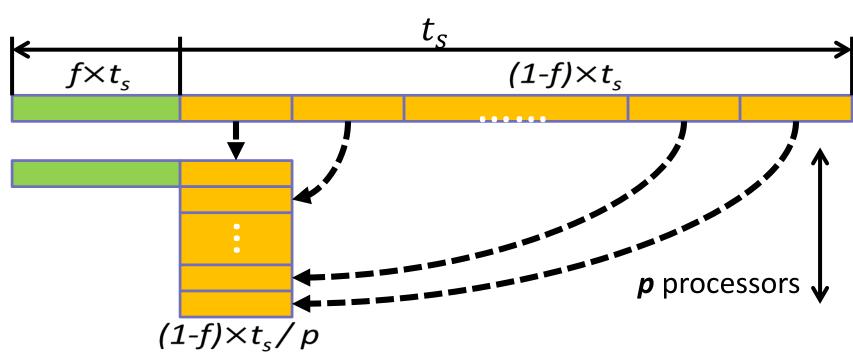
- Difficult to reach ideal max. speedup: S(p)=p
  - Not every part of a computation can be parallelized (results in processor idle)
  - Need extra computations in the parallel version (i.e. due to synchronization cost)
  - ➤ Communication time between processes (normally the major factor)



# Maximum Speedup

Let f be the fraction of computations that can NOT be parallelized

$$> S(p) = \frac{t_S}{ft_S + (1-f)t_S/p} = \frac{p}{1+(p-1)f}$$



# м

#### Maximum Speedup

■ Even with infinite number of processors

$$S(p)_{p\to\infty} \frac{p}{1+(p-1)f} = \frac{1}{f}$$

$$20^{-1}$$

$$f = 0\%$$

$$f = 10\%$$

$$f = 10\%$$

$$f = 20\%$$
Number of processors,  $n$ 
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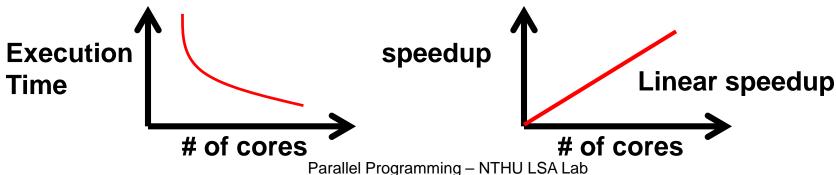


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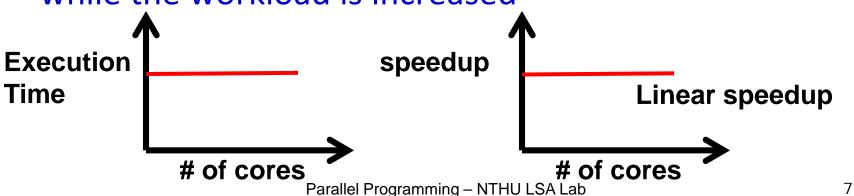


- The problem size stays fixed but the number of processing elements are increased.
- It is used to find a "sweet spot" that allows the computation to complete in a reasonable amount of time, yet does not waste too many cycles due to parallel overhead.
- Linear scaling is achieve if the speedup is equal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





- 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**

- $T_p = T_{comp} + T_{comm}$ 
  - $\succ T_p$ : Total execution time of a parallel algorithm

 $\mathcal{T}_{comm}$ 

- $\succ T_{comp}$ : Computation part
- > T<sub>comm</sub>: Communication part
- $T_{comm} = q (T_{startup} + n T_{data})$

- Startup time
  # of data items
- $\succ T_{startup}$ : Message latency (assumed constant)
- $\succ T_{data}$ : 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):

$$T_{comm} = (T_{startup} + n/2 \times T_{data}) + (T_{startup} + T_{data})$$

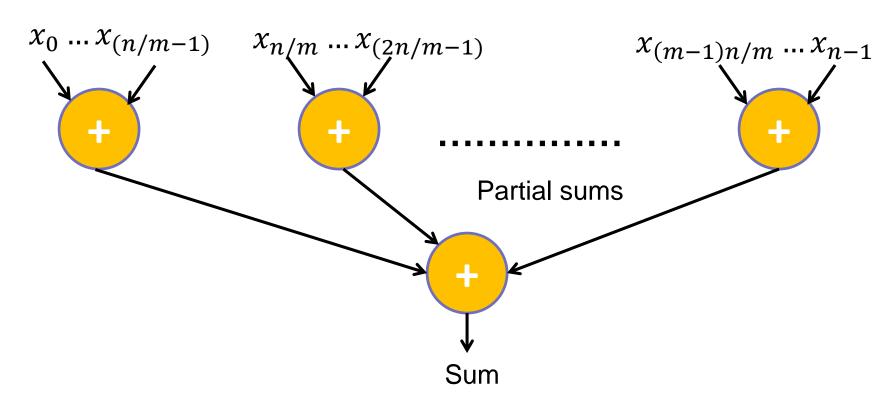
$$= 2T_{startup} + (n/2 + 1) \quad T_{data} = O(n)$$

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:

$$t_p = 2mt_{startup} + (n+m)t_{data} + m + \frac{n}{m} - 2 = O(m+n)$$
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Tradeoff between computation & communication



### **Cost-Optimal Algorithm**

#### ■ Definition:

- Cost to solve a problem is proportional to the execution time on a single processor system
- $\triangleright O(T_p) \times N = O(T_s)$

#### ■ Example:

- Sequential algo: O(N log N)
- ➤ Parallel algo1: uses N processor with O(log N)
- ➤ Parallel algo2: uses N² processor with O(1)



#### Reference

- Textbook: Parallel Computing Chap1
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