



**21st Summer  
School of  
PARALLEL  
COMPUTING**

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# Introduction to High Performance Computing

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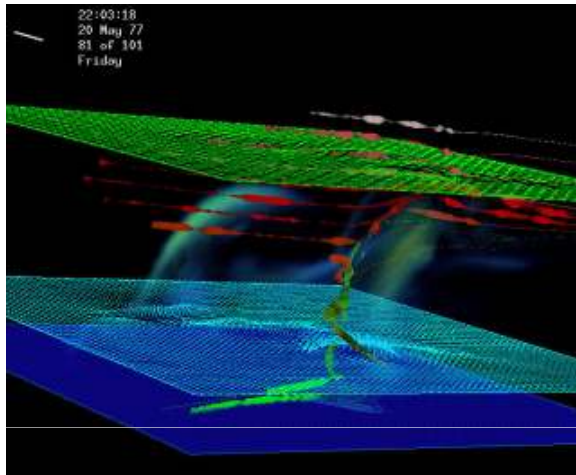


## Outline

Computational Sciences  
High Performance Computing  
von Neumann Model  
Pipelining  
Memory  
Flynn Taxonomy  
Vector Architectures  
Parallel Architectures  
Accelerators



# Computational Sciences

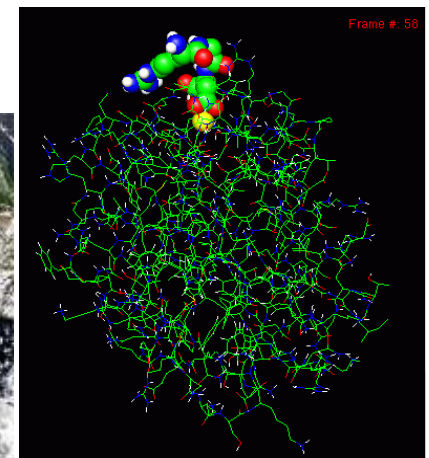


Identify the scientific disciplines that use mathematical models and computing systems to analyze and solve scientific problems.

Computational methods allow us to study complex phenomena, giving a powerful impetus to scientific research.

The use of computers to study physical systems allows to manage phenomena

- **very large**  
*(meteo-climatology, cosmology, data mining, oil reservoir)*
- **very small**  
*(drug design, silicon chip design, structural biology)*
- **very complex**  
*(fundamental physics, fluid dynamics, turbulence)*
- **too dangerous or expensive**  
*(fault simulation, **nuclear tests**, crash analysis)*





# Computational Sciences / 1

Computational science (with theory and experimentation), is the “third pillar” of scientific inquiry, enabling researchers to build and test models of complex phenomena



## The Nobel Prize in Chemistry 1998

"for his development of the density-functional theory"



**Walter Kohn**

"for his development of computational methods in quantum chemistry"



**John A. Pople**

## Owen Willans Richardson, Years '20

Nobel Prize in Physics 1928

*for his work on the thermionic phenomenon and especially for the discovery of the law named after him"*



## John Von Neumann, Years '40



## Kenneth. Wilson, Years '80

Nobel Prize in Physics 1982

*"for his theory for critical phenomena in connection with phase transitions"*





## Size of computational applications

### Computational Dimension:

number of operations needed to solve the problem,  
in general is a function of the size of the involved  
data structures ( $n$ ,  $n^2$ ,  $n^3$ ,  $n \log n$ , etc.)

### flop - Floating point operations

indicates an arithmetic floating point operation.

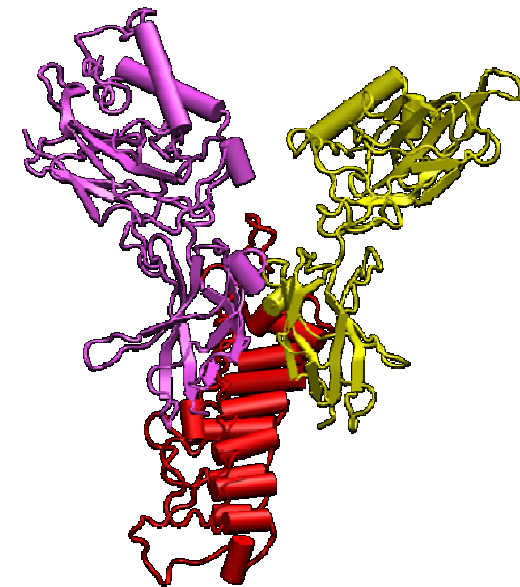
### flop/s - Floating points operations per second

is a unit to measure the speed of a computer.

computational problems today:  $10^{15} - 10^{22}$  flop

One year has about  $3 \times 10^7$  seconds!

Most powerful computers today have reach a sustained  
performance in the order of Tflop/s ( $10^{12}$  flop/s).





# Example: Weather Prediction

Forecasts on a global scale (a little too accurate)

## - 3D Grid to represent the Earth

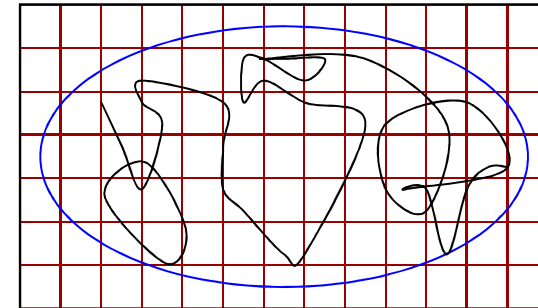
- Earth's circumference:  $\cong 40000$  km
- radius:  $\cong 6370$  km
- Earth's surface:  $\cong 4\pi r^2 \cong 5 \cdot 10^8$  km<sup>2</sup>

## - 6 variables:

- temperature
- pressure
- umidity
- wind speed in the 3 Cartesian directions

## - cells of 1 km on each side

- 100 slices to see how the variables evolve on the different levels of the atmosphere
- a 30 seconds time step is required for the simulation with such resolution
- Each cell requires about 1000 operations per time step (Navier-Stokes turbulence and various phenomena)



On a **global scale** is currently a precision quite impossible.  
unimaginable!  
On a **local scale** normally the cells are 10-15 km on each side

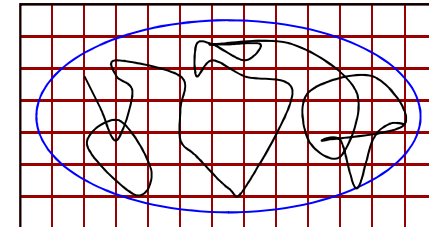


# Example: Weather Prediction / 1

**Grid:  $5 \cdot 10^8 \cdot 100 = 5 \cdot 10^{10}$  cells**

- each cell is represented with 8 Byte
- Memory space:

$$(6 \text{ var}) \cdot (8 \text{ Byte}) \cdot (5 \cdot 10^{10} \text{ cells}) \cong 2 \cdot 10^{12} \text{ Byte} = 2\text{TB}$$



A 24 hours forecast needs:

- $24 \cdot 60 \cdot 2 \cong 3 \cdot 10^3$  time-step
- $(5 \cdot 10^{10} \text{ cells}) \cdot (10^3 \text{ oper.}) \cdot (3 \cdot 10^3 \text{ time-steps}) = 1.5 \cdot 10^{17} \text{ operations !}$

A computer with a power of 1Tflop/s will take  $1.5 \cdot 10^5 \text{ sec.}$

- 24 hours forecast will need 2days to run

..... but we shall obtain a very accurate forecast

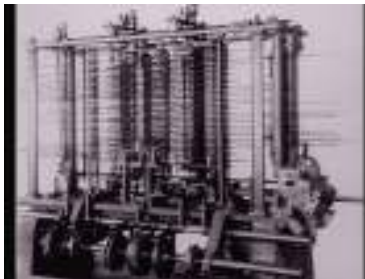




# Supercomputer

supercomputer are defined as the more powerful computers available in a given period of time.

**Powerful** is meant in terms of execution speed, memory capacity and accuracy of the machine.



**Supercomputer:** "*new statistical machines with the mental power of 100 skilled mathematicians in solving even highly complex algebraic problems*".

**New York World,** march 1920

to describe the machines invented by Mendenhall and Warren, used at Columbia University's Statistical Bureau.





# More powerful computers

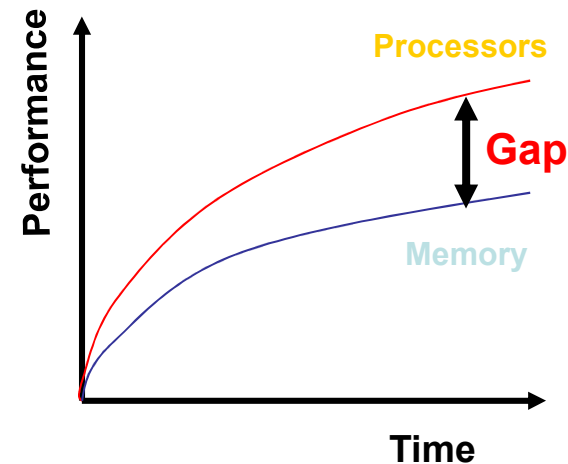
Increase the speed of microprocessors:

Physical limitations to size and speed of a single chip:

- speed of light,
- size of atoms,
- dissipation of heat

Solution:

- increase the degree of parallelism
- use many CPUs cooperatively on the same problem



*“Serial computing is dead, and the parallel computing revolution has begun: Are you part of the solution, or part of the problem?”*

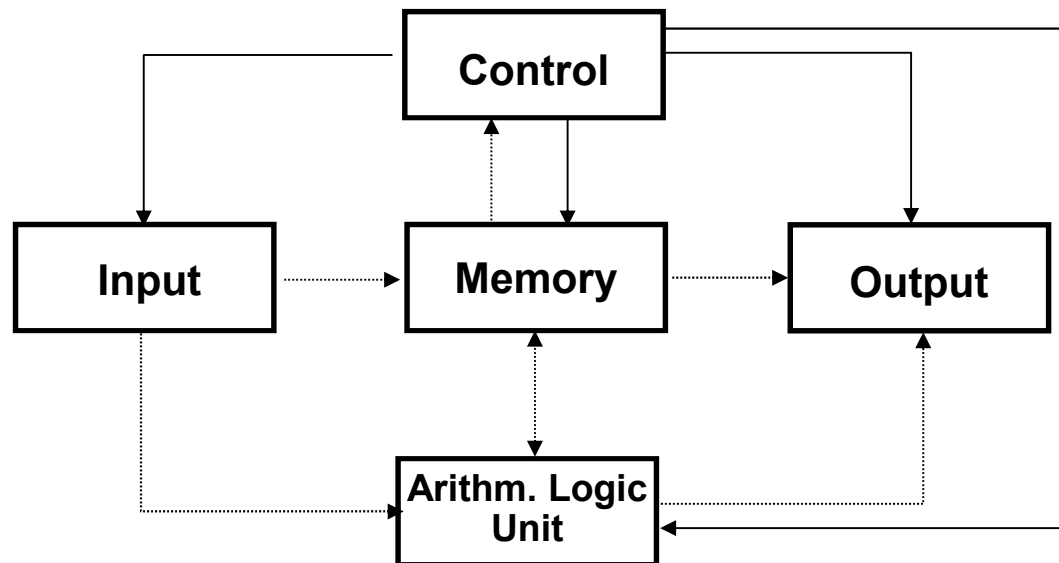
Dave Patterson,

UC Berkeley, Usenix conference June 2008



# von Neumann Model

## Conventional Computer



*Von Neumann Model of Computer Architecture*



..... **Data**  
——— **Control**

### Instructions are processed sequentially

- 1 A single instruction is loaded from memory (**fetch**) and decoded
- 2 Compute the addresses of operands
- 3 Fetch the operands from memory;
- 4 Execute the instruction ;
- 5 Write the result in memory (**store**).



## Speed of Processors: Clock Cycle and Frequency

The **clock cycle**  $\tau$  is defined as the time between two adjacent pulses of oscillator that sets the time of the processor.

The number of these pulses per second is known as **clock speed** or **clock frequency**, generally measured in GHz (gigahertz, or billions of pulses per second).

The clock cycle controls the synchronization of operations in a computer: All the operations inside the processor last a multiple of  $\tau$ .

Processor	$\tau$ (ns)	freq (MHz)
CDC 6600	100	10
Cyber 76	27.5	36,3
IBM ES 9000	9	111
Cray Y-MP C90	4.1	244
Intel i860	20	50
PC Pentium	< 0.5	> 2 GHz
Power PC	1.17	850
IBM Power 5	0.52	1.9 GHz
IBM Power 6	0.21	4.7 GHz

### Increasing the clock frequency:

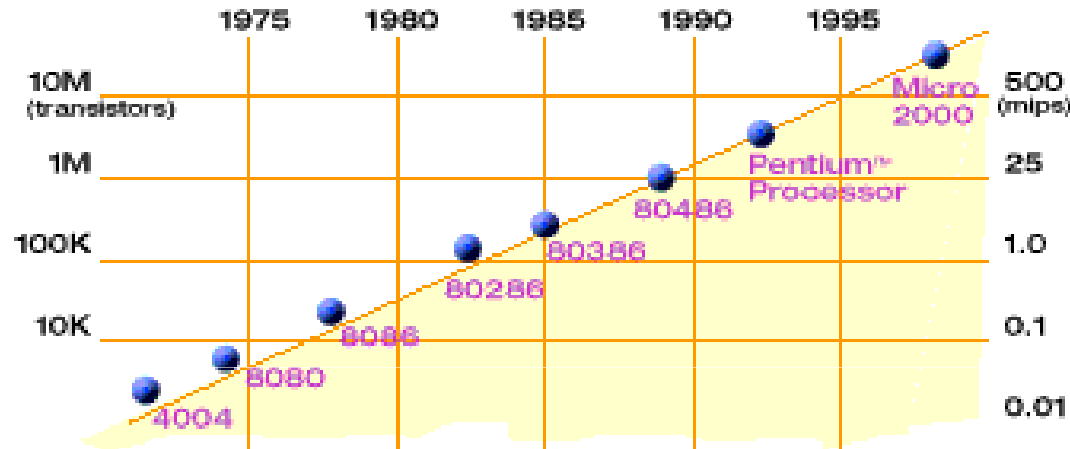
The **speed of light** sets an upper limit to the speed with which electronic components can operate .

Propagation velocity of a signal in a vacuum: **300.000 Km/s = 30 cm/ns**

**Heat dissipation** problems inside the processor.



# Moore's Law



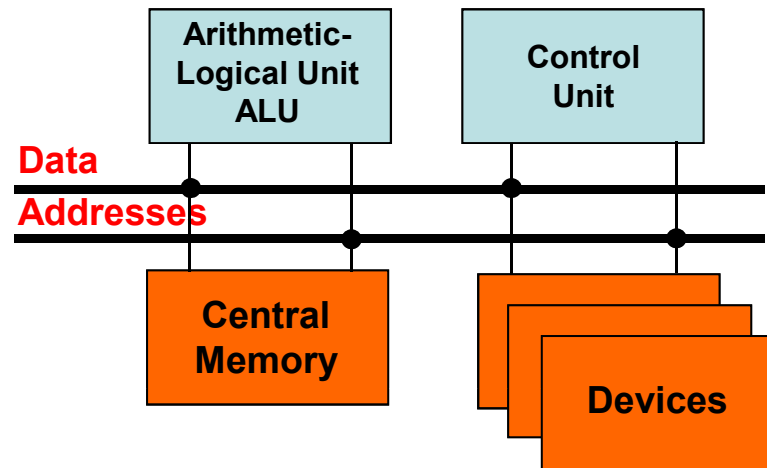
Empirical law which states that the complexity of devices (number of transistors per square inch in microprocessors) doubles every 18 months..

**Gordon Moore**, INTEL co-founder, 1965

It is estimated that Moore's Law still applies in the near future but applied to the number of cores per processor



## Other factors that affect Performance



In addition to processor power, other factors affect the performance of computers:

- Size of memory
- Bandwidth between processor and memory
- Bandwidth toward the I/O system
- Size and bandwidth of the cache
- Latency between processor, memory, and I/O system



# Memory hierarchies

**Time to run code = clock cycles running code + clock cycles waiting for memory**

**Memory access time:** the *time* require by the processor to *access* data or to write data from / to *memory*

The hierarchy exists because

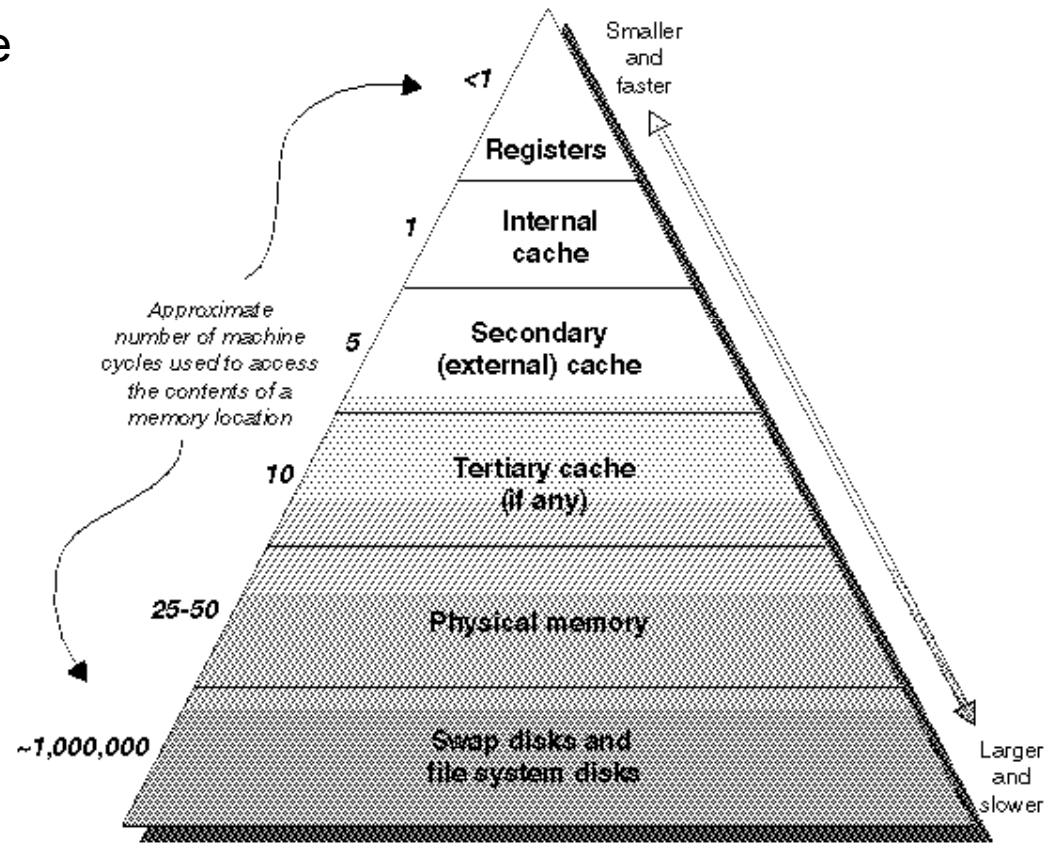
- fast memory is expensive and so is small
- slow memory is cheap and can be big

## Latency

- how long do I have to wait for the data?
- (cannot do anything while waiting)

## Throughput

- how many Data / second?
- not important when you're waiting



ZK-1083U-AI

**Total time = latency + (amount of data / throughput)**





## Cache Memory

Memory unit with a small size used as a buffer for data to be exchanged between the main memory and the processor.

- Reduces the time spent by the processor waiting for data from the main memory.
- Cache efficiency depends on the locality of the data references:

### Principle of locality

**Temporal locality** refers to the reuse of specific data within relatively small time durations.

**Spatial locality** refers to the use of data elements within relatively close storage locations.

A special case of spatial locality, occurs when data elements are arranged and accessed linearly (sequentially), e.g., traversing the elements in a one-dimensional array.

**Cache** can contain Data, Instructions or both





## Cache Memory / 1

The code performance improve when the instructions that compose a heavy computational kernel (eg. a loop) fit into the cache

The same applies to the data, but in this case the work of optimization involves also the programmer and not just the system software.

### **DEC Alpha 21164 (500 MHz):**

#### ***Memory access time***

Registers	2 ns
L1 On-chip	4 ns
L2 On-Chip	5 ns
L3 Off-Chip	30 ns
Memory	220 ns

### **IBM SP Power 6 (4.7 GHz):**

#### ***Memory access time (in clock cycles)***

Registers	
L1: 2 x 64KB	< 5
L2: 2 x 4MB	22 cc
L3: 32 MB	160 cc
Memory 128 GB	400 cc

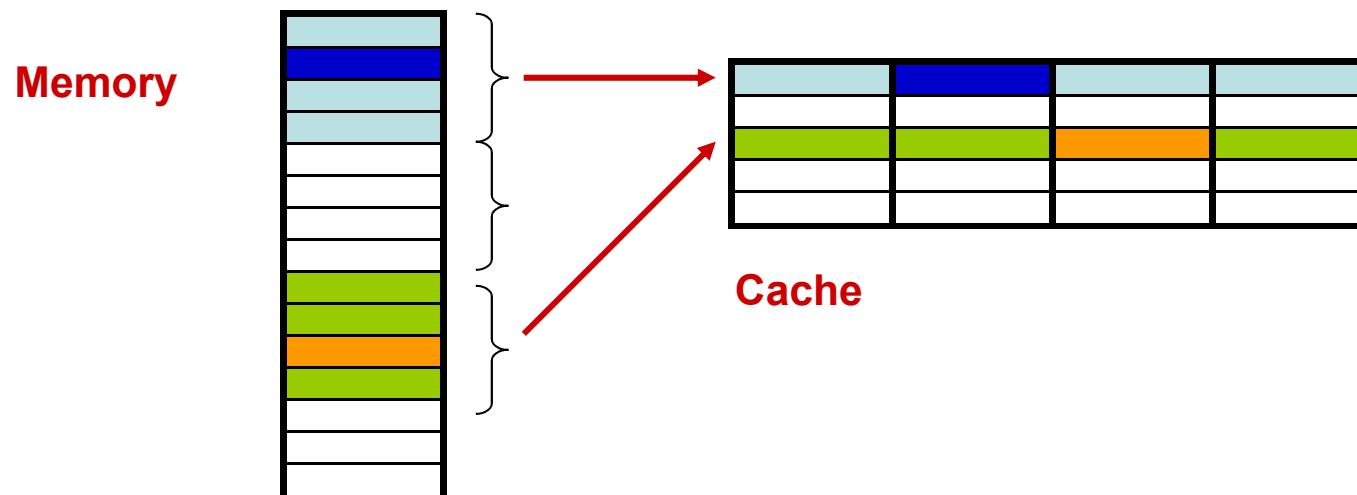


## Cache organisation

The cache is divided into slots of the same size (**lines**)

Each line contains  $k$  consecutive memory locations (ie 4 words).

When a data is required from memory, (if not already in the cache) the system loads from memory, the entire cache line that contains the data, overwriting the previous contents of the line.



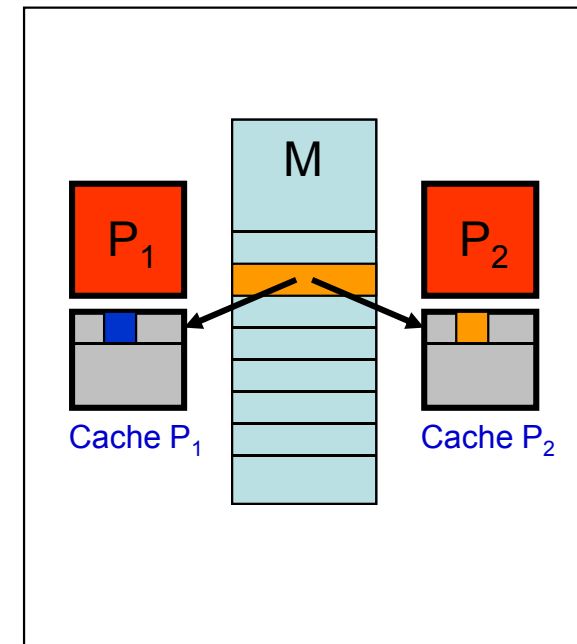


## Cache organisation / 1

When the CPU writes out a value the data must be updated in main memory

- **Cache write-back**: data written in the cache will stay there until the cache line is not required to store other data. When the cache line must be replaced, the data is written in memory.
- **Cache write-through**: data are written in cache and immediately to main memory.

In multi-processors systems, **cache coherency** must be managed: we need to access updated data in main memory





# Mapping

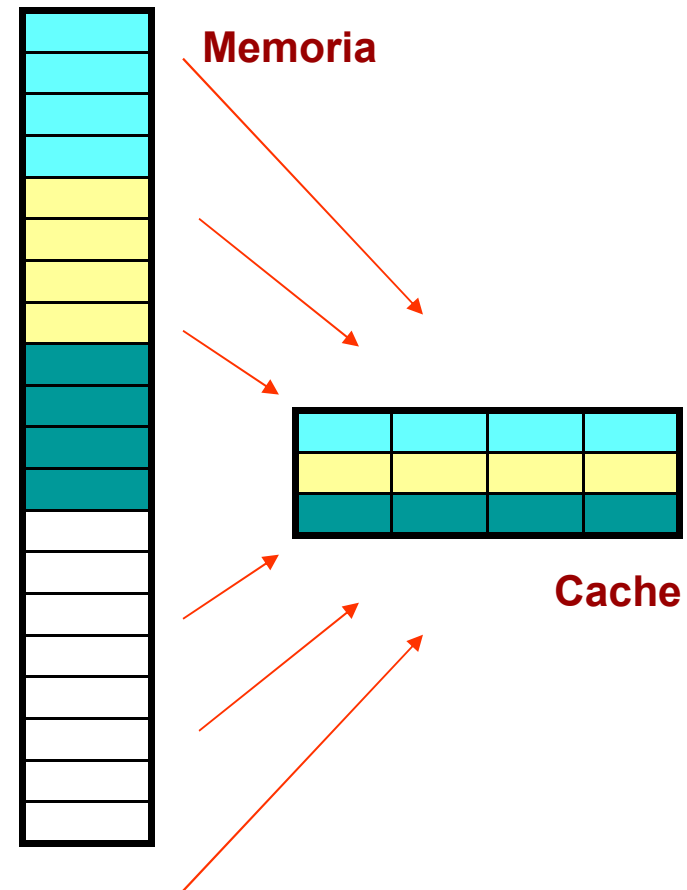
Time by time the cache can contain only a sub-set of the data in memory.

A set of memory locations must be associated to a cache line (**mapping**).

Based on the mapping cache can be organized in one of the following ways:

- *Direct mapped*
- *Fully associative*
- *Set associative*

The way in which memory locations are mapped in the cache lines can affect the performance of the programs: **two memory locations heavily used can be mapped or not on the same line.**



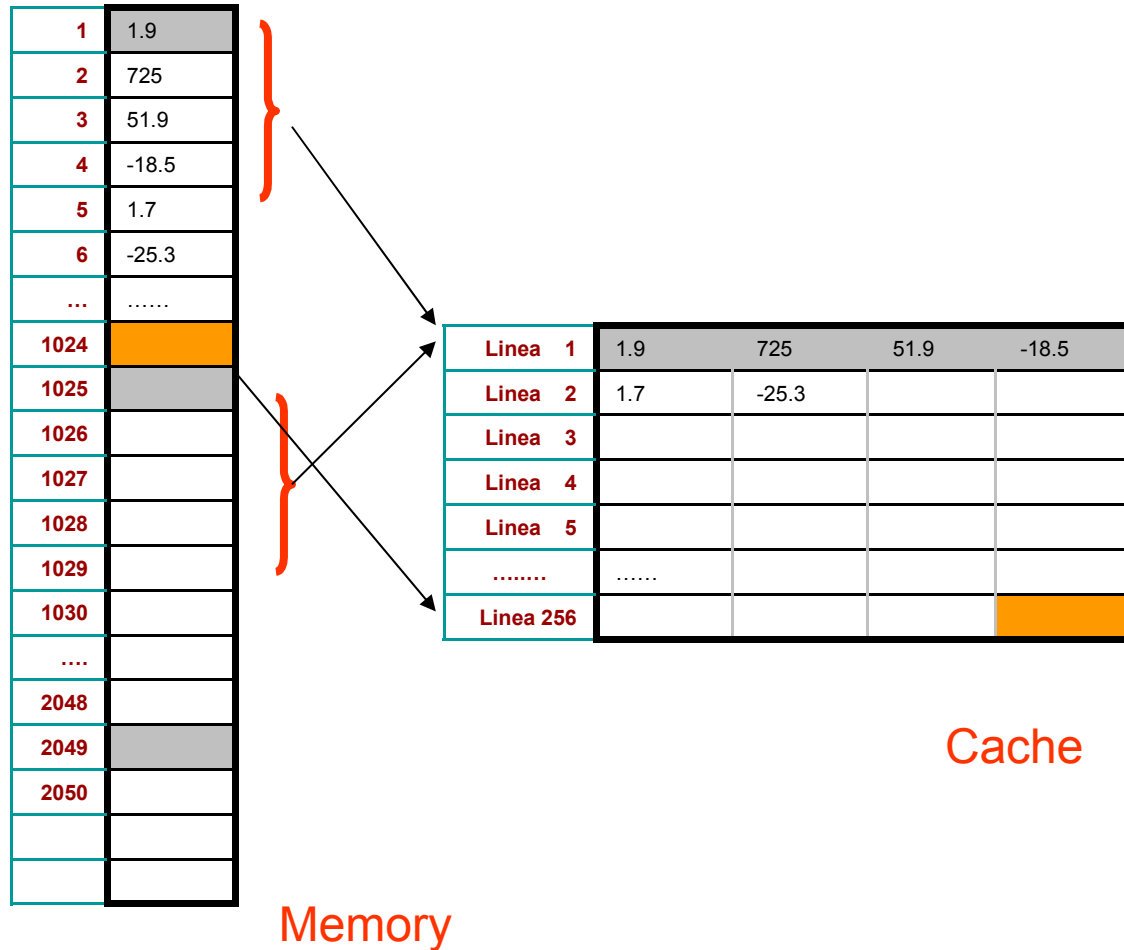


## Cache Direct Mapping

With this scheme the first memory location (word 1) is mapped in line 1, as well as the location  $d+1$ ,  $2d+1$ ,  $3d+1$  etc. where

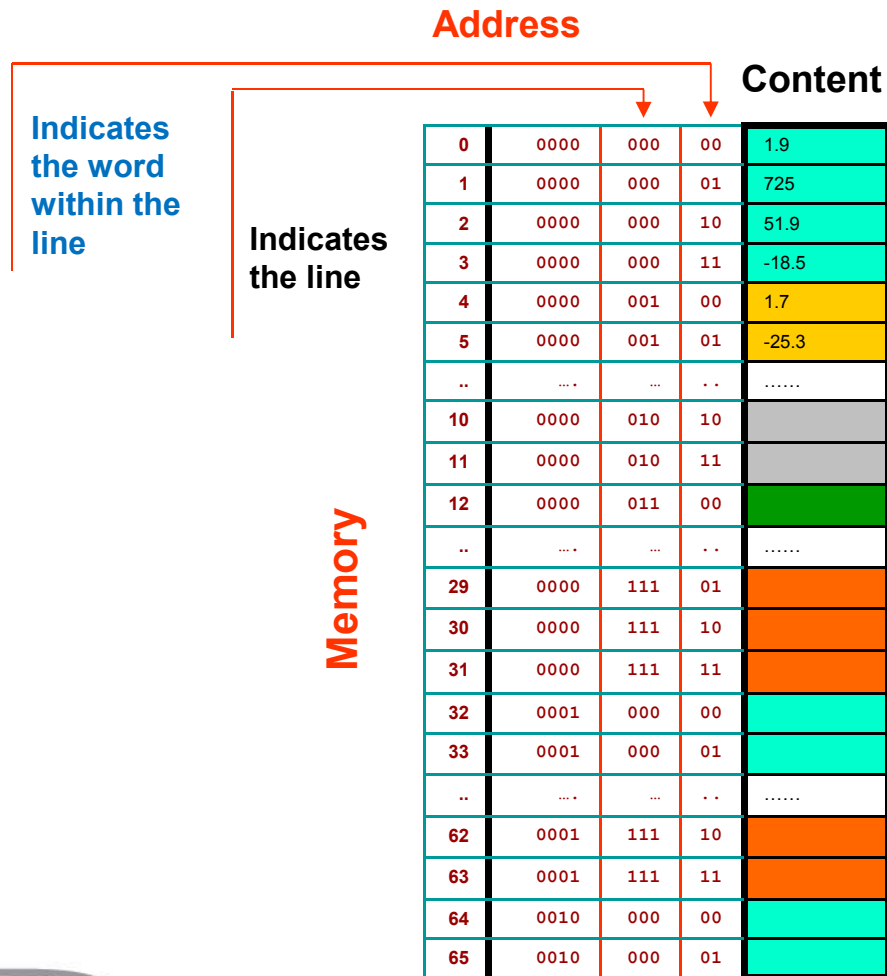
$$d = N^{\circ}_{\text{lines}} * N^{\circ}_{\text{words per line}}$$

If different memory references in turn point to the same cache line (eg, word 1, word 1025, word 2049), each reference causes a **cache miss** and the line just inserted must be replaced.  
A lot of extra work (**overhead**) is generated.  
This phenomenon is called **thrashing**.





# Cache Direct Mapping / 1



<b>Linea 0</b>	1.9	725	51.9	-18.5
<b>Linea 1</b>	1.7	-25.3		
<b>Linea 2</b>				
<b>Linea 3</b>				
<b>Linea 4</b>				
<b>Linea 5</b>				
<b>Linea 6</b>				
<b>Linea 7</b>				

**Cache**  
 8 lines  
 4 word per line





## Cache Fully Associative

With this scheme, each memory location can be mapped to any cache line, regardless of the memory location.

The name comes from the type of memory used to build this type of cache (**associative memory**).

When the CPU needs a given data, this is required in all the cache lines simultaneously. If a line contains the data, this is sent to CPU, otherwise a cache miss occurs.

In general, the least recently used line will be overwritten with the new data. (**LRU policy**)

Fully associative caches are costly but provide a higher usage when compared to the direct mapped cache





## Cache Set Associative

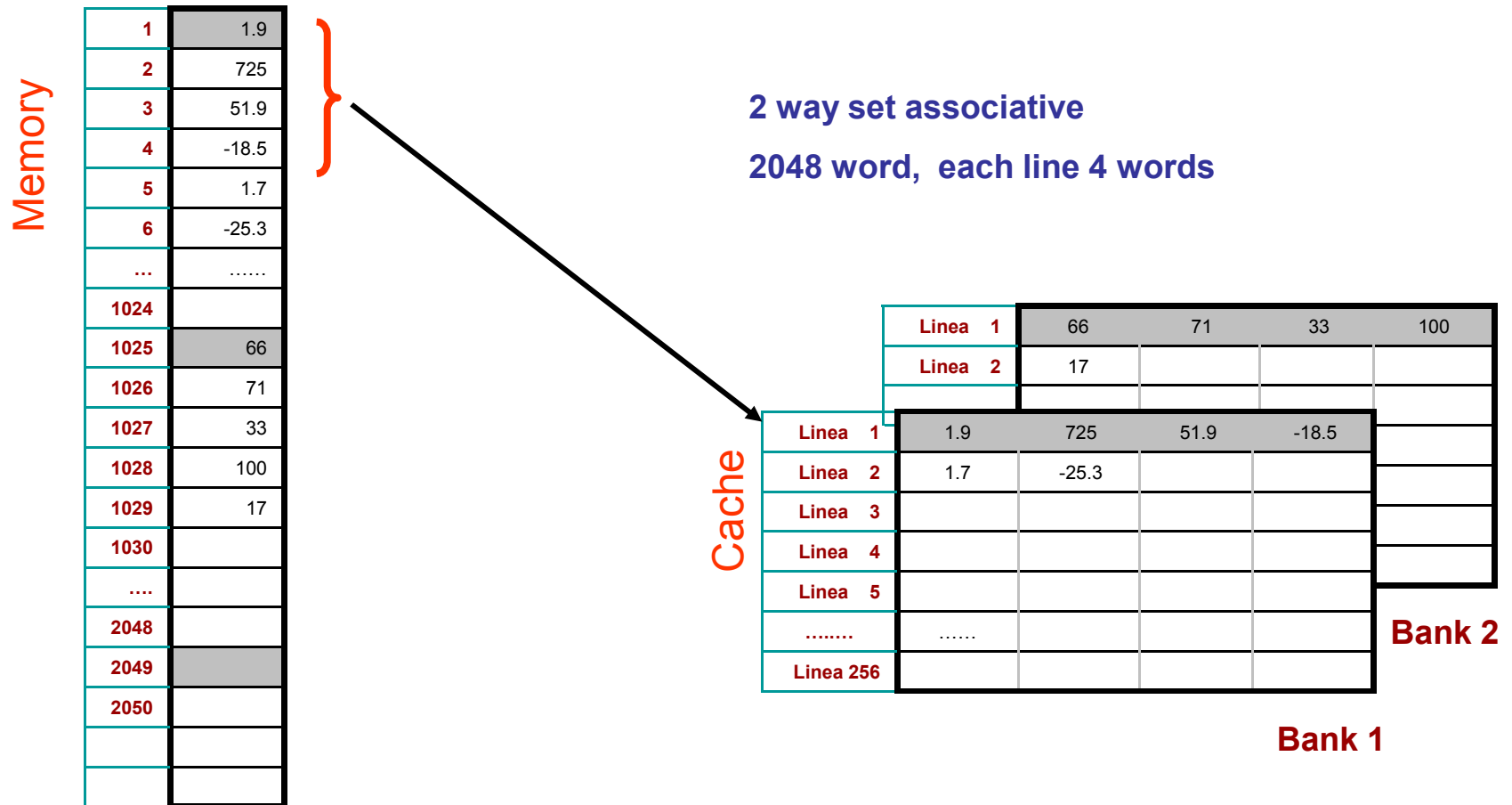
Practically it is a direct mapped cache replicated in multiple copies (**banks**)  
i.e. 2 or 4 separate banks of cache (*two-way, four-way set associative*).

With this scheme, if a memory location is mapped in line  $k$ , a further reference to a memory location always mapped to the same line, will be allocated in line  $K$  of a different bank.

**Set Associative** cache is less susceptible to **cache thrashing** compared to a direct mapped cache with the same size.



# Cache Set Associative





## Multiple Functional Units

Arithmetic logic unit (**ALU**) executes the operations.

ALU is designed as a set of **independent functional units**, each in charge of executing a different arithmetic or logical operation,

- Add
- Multiply
- Divide
- Integer Add
- Integer Multiply
- Branch ....

The functional units can operate in parallel. This aspect represents the **first level of parallelism**. It is a parallelism **internal to the single CPU**.

The **compiler** analyses the different instructions and determine which operations can be done in parallel, without changing **the semantics of the program**.



## Pipelining

Is a technique where more instructions, belonging to a stream of sequential execution, overlap their execution

This technique improves the performance of the processor

The concept of pipelining is similar to that of **assembly line** in a factory where in a flow line (**pipe**) of assembly stations the elements are assembled in a continuous flow.

All the assembly stations must operate at the **same processing speed**, otherwise the station slower becomes the **bottleneck** of the entire pipe.

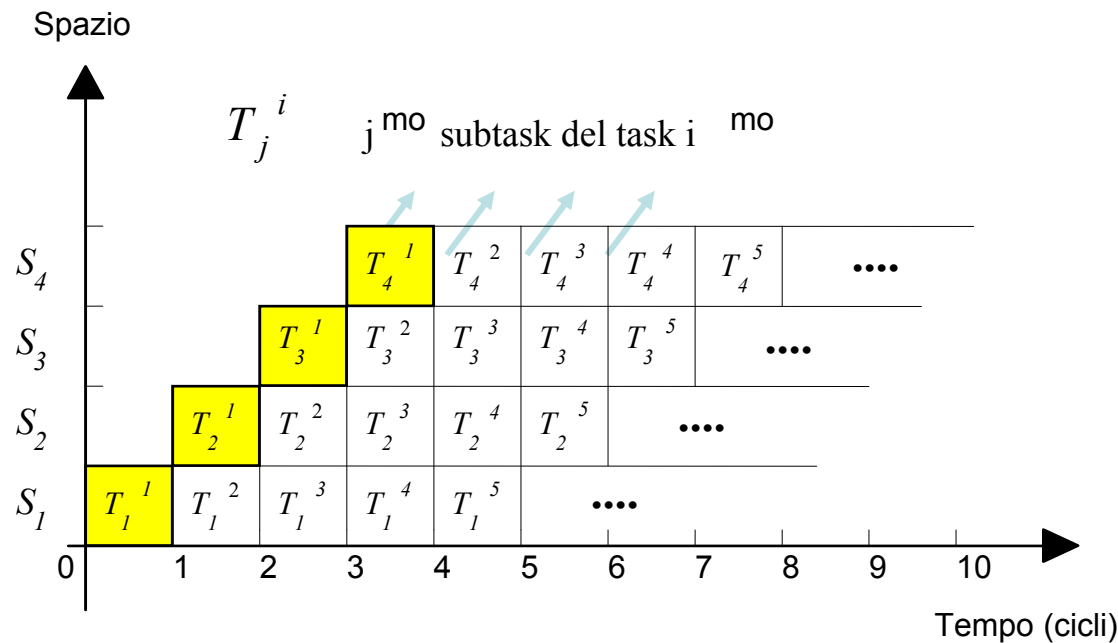




# Pipelining / 1

A task T is decomposed into a set of sub-tasks  $\{T_1, T_2, \dots, T_k\}$  linked by a **dependency relationship**: Task  $T_j$  can not start until all previous sub-tasks  $\{T_i, \forall i < j\}$  are completed

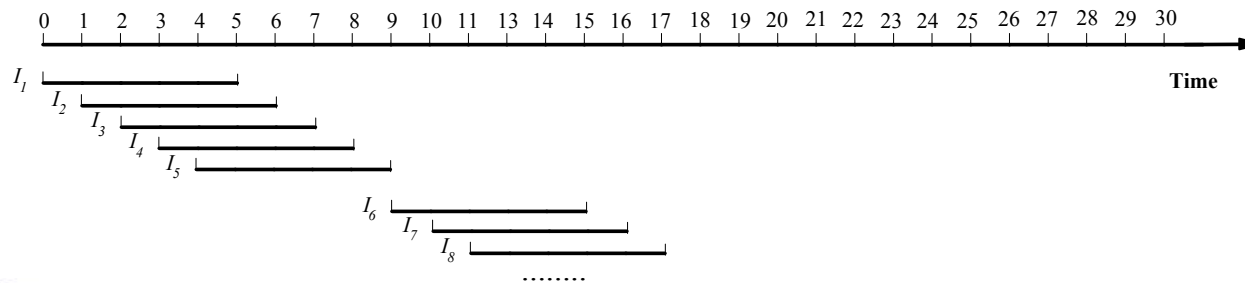
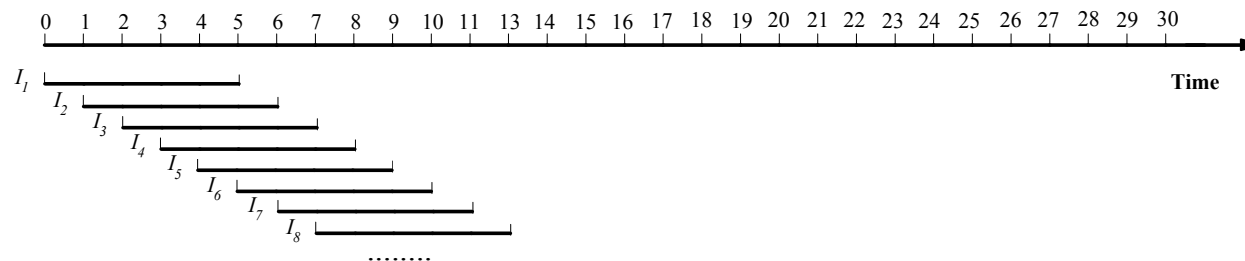
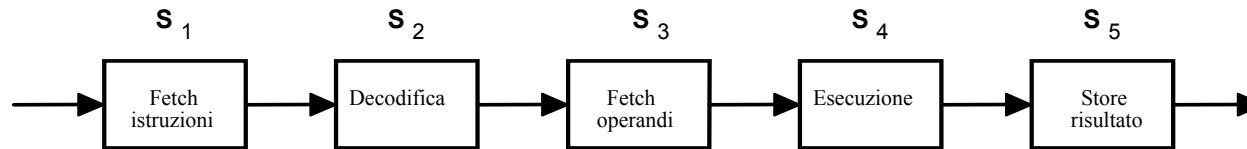
## Overlapping operations in a four stages pipe



**Space-time diagram**



# Pipeline di Istruzioni





## Vector Computers

Vector computer architectures adopt a set of **vector instructions**, in conjunction with the scalar instruction set. The vector instructions operate on a set of **vector registers** each of which is able to contain more than one data element.

- **Cray vector systems** of the 80s and 90s
- **Cray C90**: 8 vector registers each with 128 elements at 64-bits
- Also the **current microprocessors** have a set of vector registers and a set of vector instructions

The vector instructions implement a particular operation to be performed on a given set of operands called **vector**.

Functional units when executing vector instructions exploit pipelining to perform the same operation on all data operands stored on vector registers.

Data transfer to and from the memory is done through **load** and **store** operations operating on vector registers.





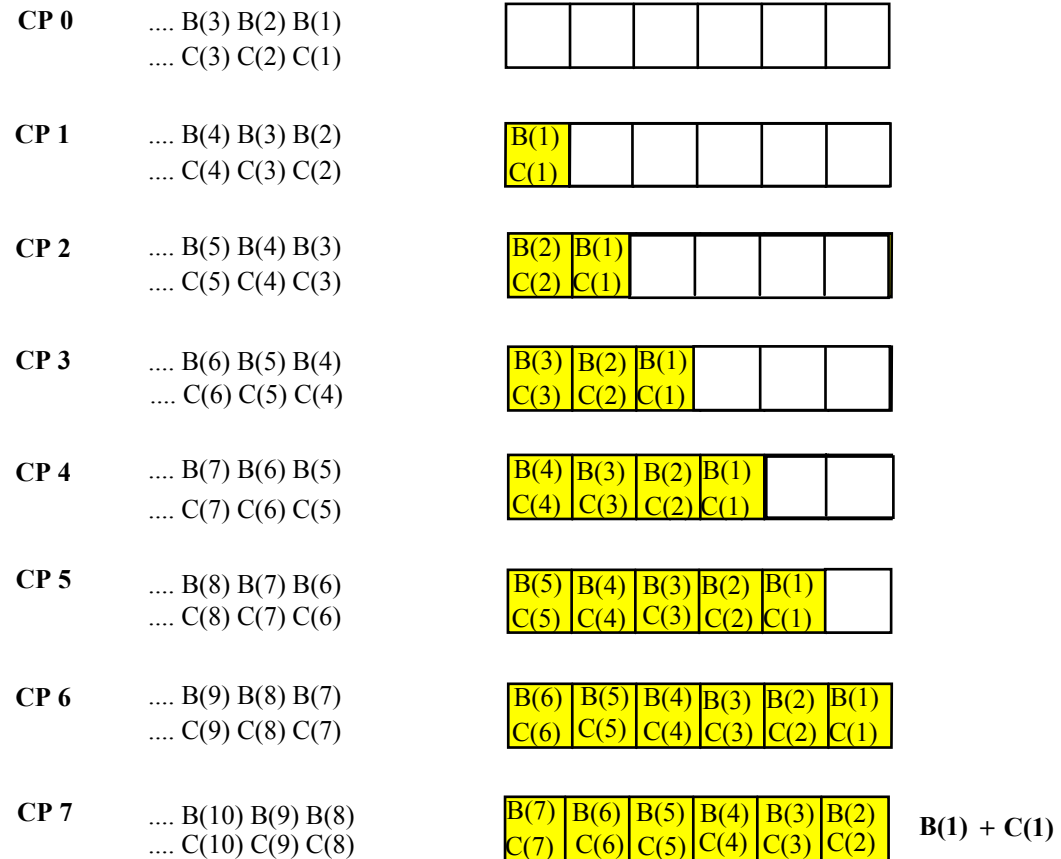


# Example

```
do i = 1, N
  A(i) = B(i)+C(i)
end do
```

$$V0 \leftarrow V1 + V2$$

Functional Unit Add Floating Point





# Flynn Taxonomy

**M. J. Flynn**

*Very high speed computing systems*, proceedings of the IEEE (1966).

*Some computer organizations and their effectiveness*, IEEE Transaction on Computers.(1972).

*"The multiplicity is taken as the maximum possible number of simultaneous operations (instructions) or operands (data) being in the same phase of execution at the most constrained component of the organization"*

- A computer architecture is categorized by the multiplicity of hardware used to manipulate **streams of instructions** (sequence of instructions executed by the computer) and **streams of data** (sequence of data used to execute a stream of instructions).

**SI** Single Instruction stream

**SD** Single Data stream

**MI** Multiple Instruction stream

**MD** Multiple Data stream

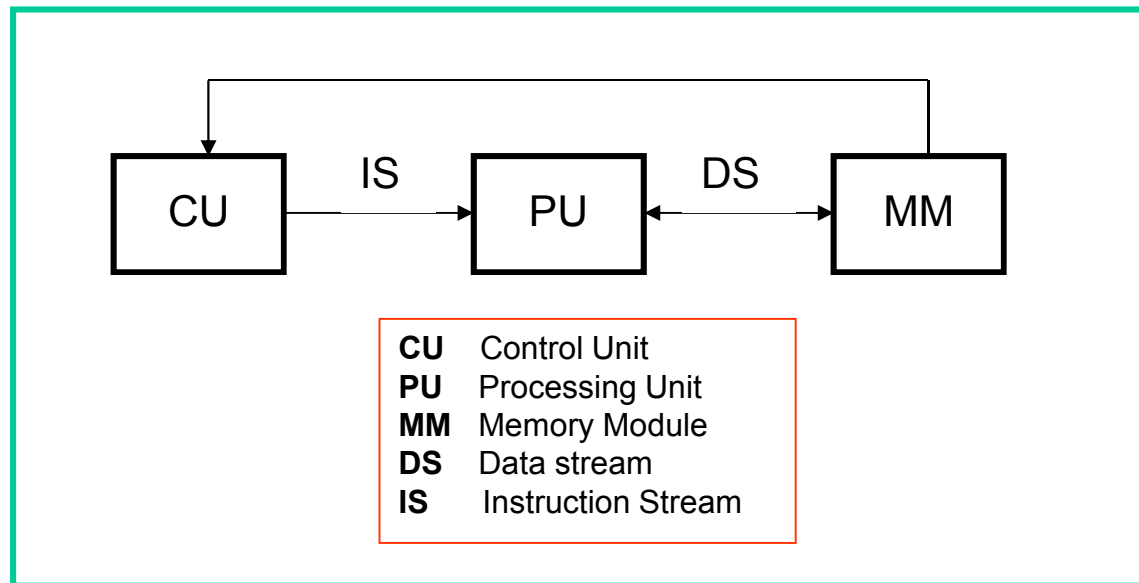
4 possible combinations : **SISD, SIMD, MISD, MIMD**



## SISD Systems

### Sequential systems

- Classical von Neumann architecture.
- Scalar mono-processor systems (single core).
- The execution of the instructions can be pipelined (Cyber 76).
- Each arithmetic instruction starts an arithmetic operation.





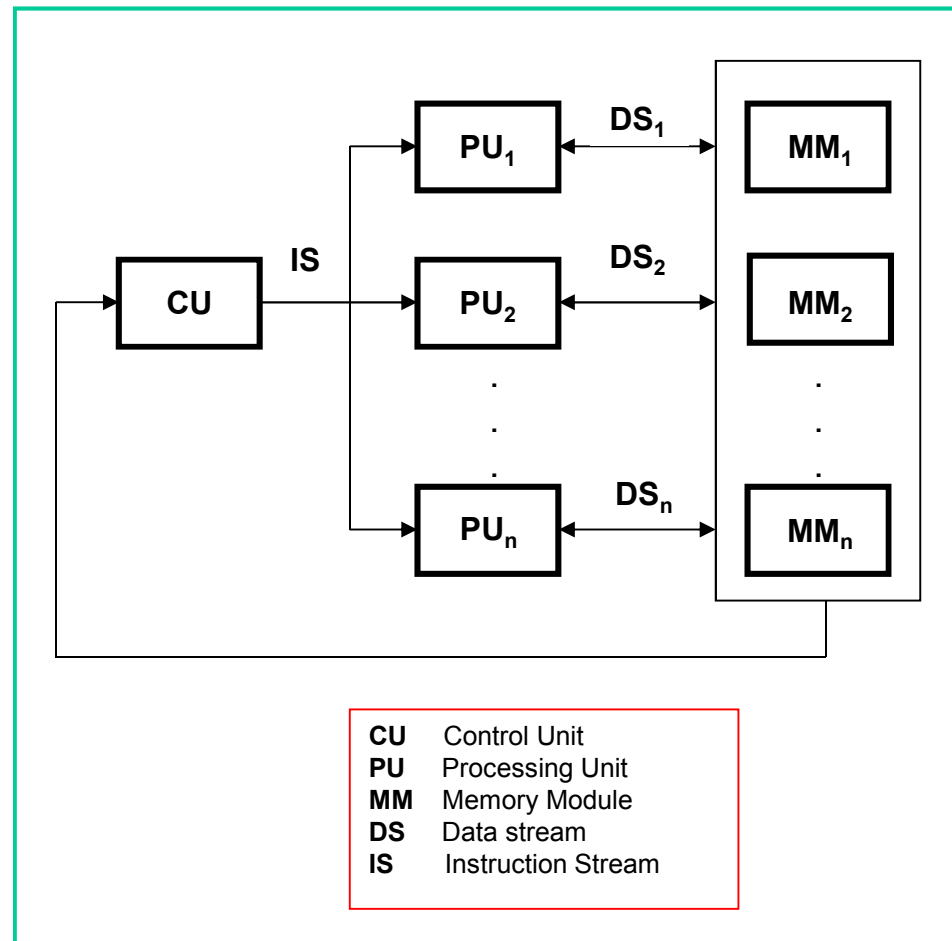
# SIMD Systems

## Synchronous parallelism

SIMD systems presents a single control unit

A single instruction operates simultaneously on multiple data.

Array processor and vector systems fall in this class





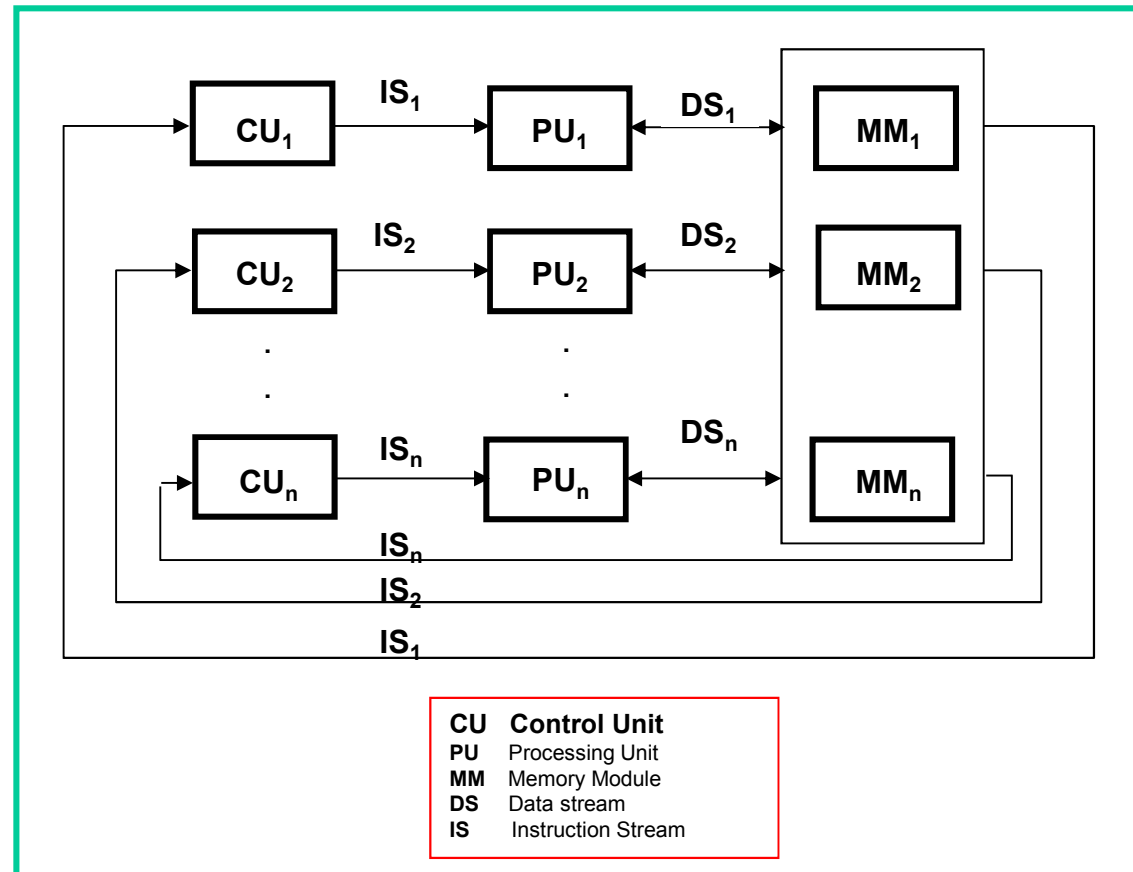
# MIMD Systems

## Asynchronous parallelism

Multiple processors execute different instructions operating on different data.

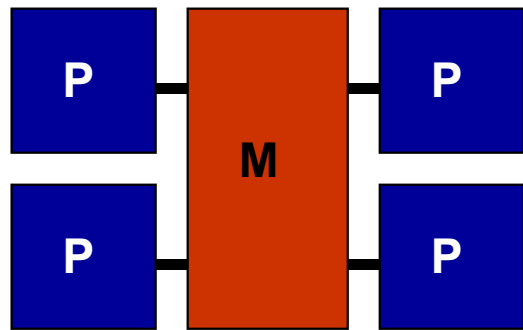
Represents the multiprocessor version of the SIMD class.

Wide class ranging from multi-core systems to large MPP systems.

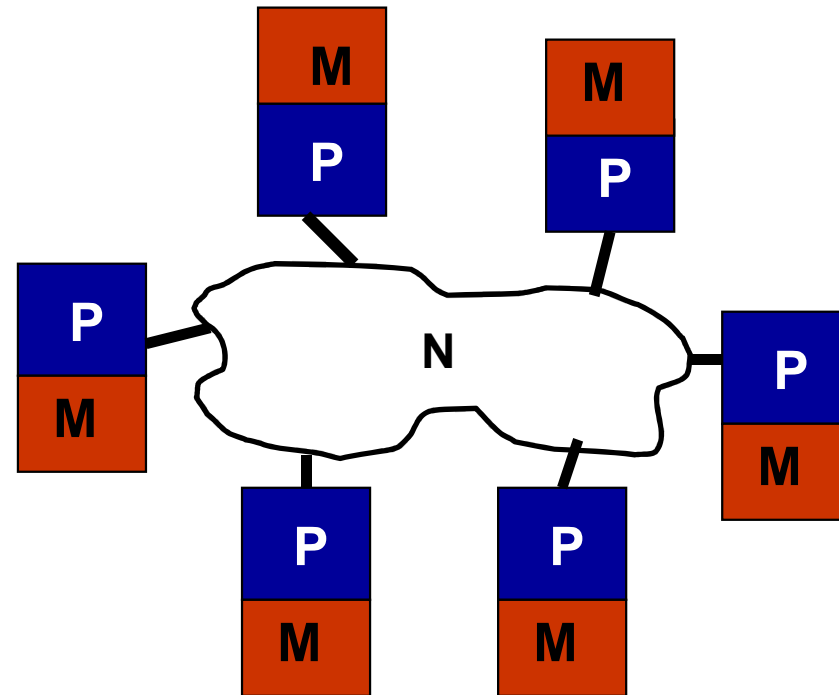




# Classification based on the Memory



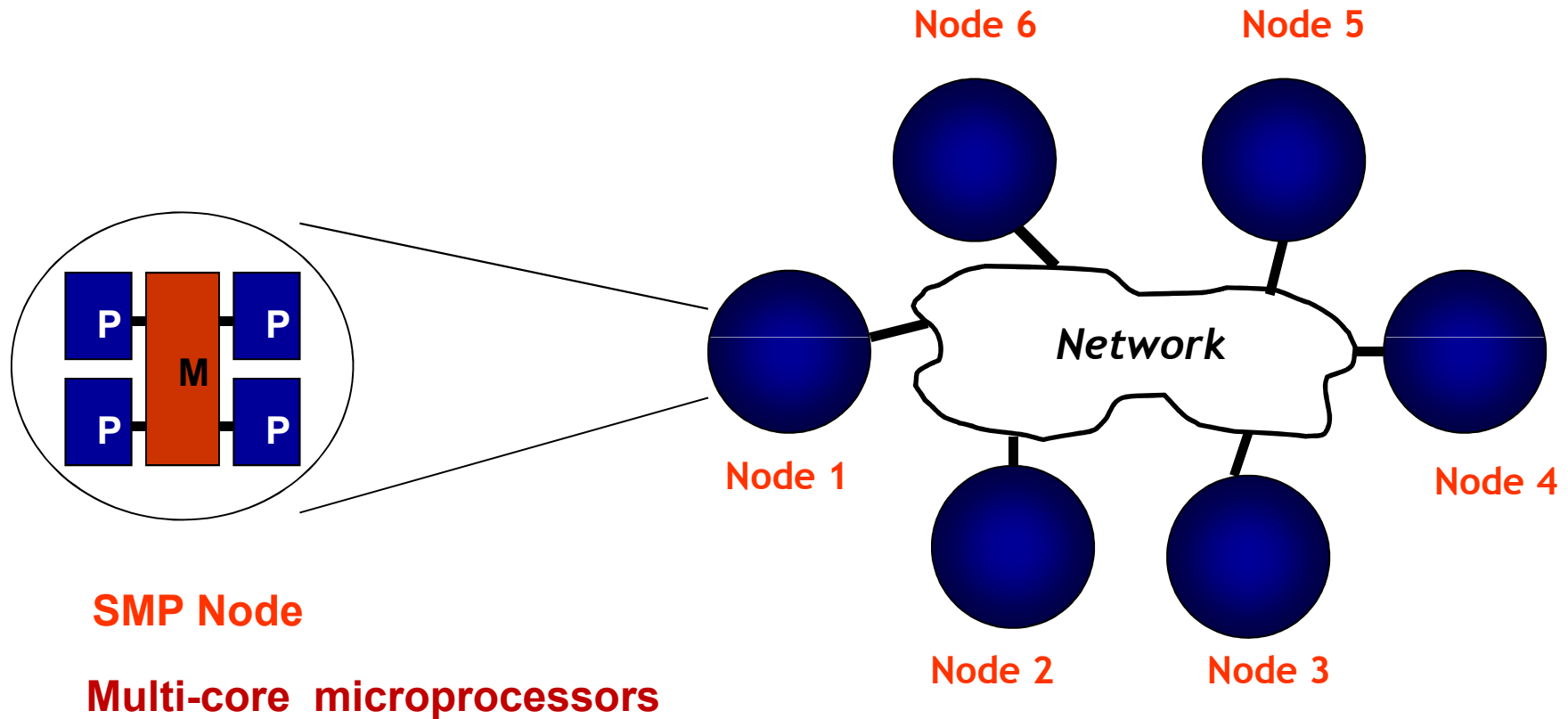
Shared Memory System



Distributed Memory System



# The concept of Node





## Shared memory systems

All the processors (cores) share the main memory.

The memory can be addressed globally by all the processors of the system

*Uniform Memory Access (UMA) model*  $\Leftrightarrow$  **SMP: Symmetric Multi Processors**

The memory access is **uniform**: the processors present the same access time to reference any of the memory locations.

Processor-Memory interconnection via **common bus**, **crossbar switch**, or **multistage networks**.

Each processor can provide local caches,

Shared memory systems can not support a high number of processors





## Distributed memory systems

The memory is physically distributed among the processors (**local memory**).

Each processor can access directly only to his own local memory

- **NO-Remote Memory Access (NORMA) model**

Communication among different processors occurs via a specific communication protocol (**message passing**).

The messages are routed on the interconnection network

In general distributed memory systems can scale-up from a small number of processors  $O(10^2)$  to huge numbers of processors  $O(10^6)$  but the power of the single cores is not too high, to reduce global costs and power consumption but power is not too high, called processing nodes.

The performance of the system are influenced by:

- **Power of the node**
- **Topology of the interconnection network**



## NUMA systems

### *Non Uniform Memory Access (NUMA) model*

Memory is **physically distributed among all the processors** (each processor has its own local memory) but the collection of the different local memories forms a global address space accessible by all the processors

Hw support to ensure that each processor can access directly the memory of all the processors

The **time** each processor needs to access the memory **is not uniform**:

- Access time is faster if the processor accesses its own local memory;
- when accessing the memory of the remote processors **delay** occurs, due to the interconnection network crossing.



## Interconnection network

It is the set of links (**cables**) that define how the different processors of a parallel computer are connected between themselves and with the memory unit.

The time required to transfer the data depends on the type of interconnection.

The transfer time is called the **communication time**.

### Features of an interconnection network:

- **Bandwidth**: identifies the amount of data that can be sent per unit time on the network. **Bandwidth must be maximized.**
- **Latency**: identifies the time required to route a message between two processors. Latency is defined also as the time needed to transfer a message of length zero. **Bandwidth must be minimized.**

Other points to consider:

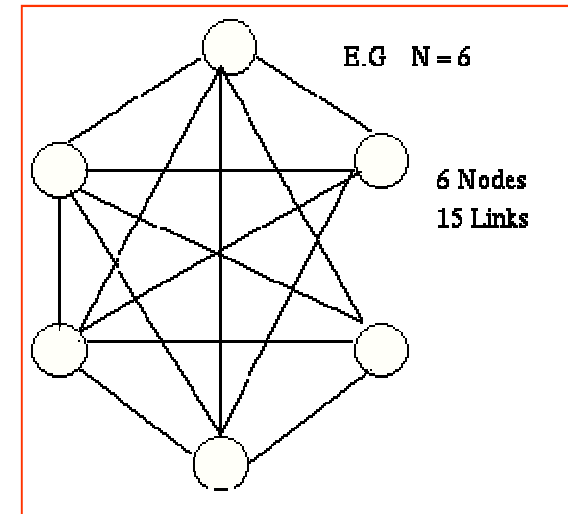
- **Cost**
- **Scalability**
- **Reliability**
- **Diameter**
- **Degree**



## Connectivity

### Complete Interconnection (ideal)

- each node can communicate **directly** with all other nodes (in parallel)
- with  $n$  nodes the bandwidth is proportional to  $n^2$ .
- the cost increases proportionally to  $n^2$ .



### Indirect Interconnection (practical)

- Only a few nodes are connected directly. A direct or indirect path allows to reach all nodes.
- the worst case is represented by a single communication channel, shared by all the nodes (eg. a cluster of workstations connected by a LAN).
- Need for intermediate solutions that **balance cost** and **performance** (mesh, tree, shuffle-exchange, omega, hypercube, ...).



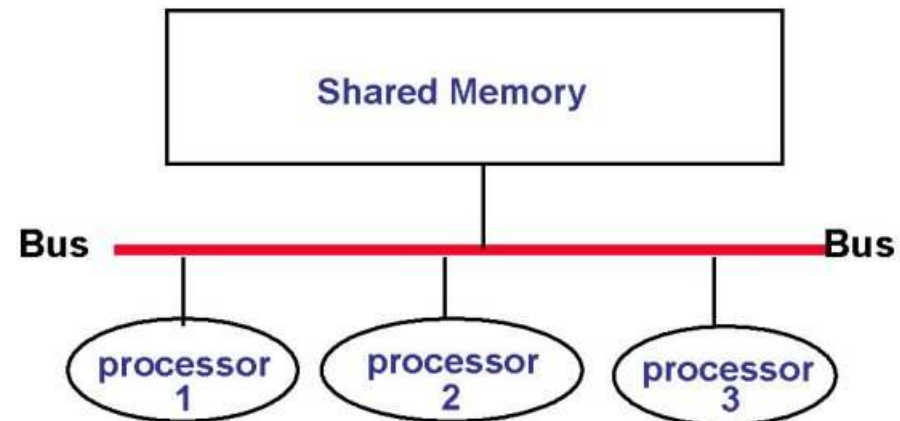
## Bus Network

The bus topology is constituted by a coaxial cable (bus) to which are connected all devices

The benefits of a network based on bus are the **simplicity to Implement** and the very **low cost**.

The negative aspects are the limited data transmission rate and consequently the non scalability in terms of performance.

Bus Network Diagram





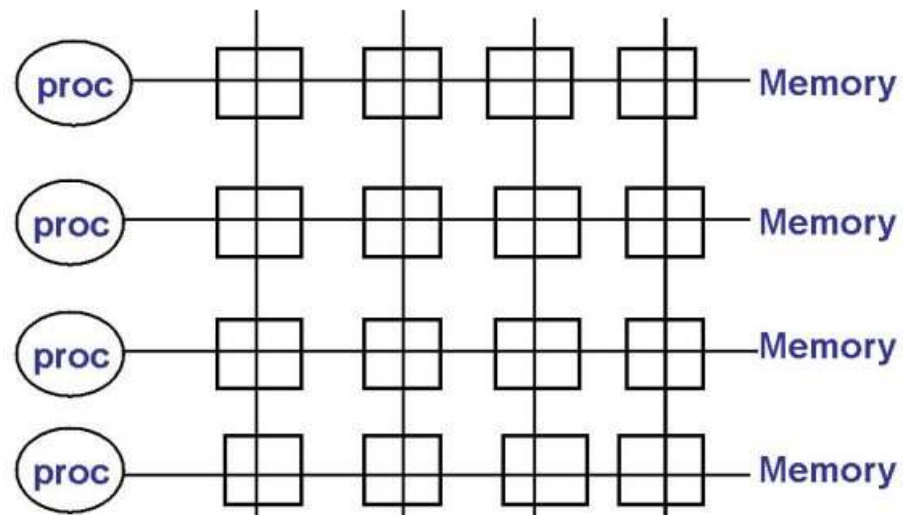
## Cross-bar Switch Network

A cross-bar switch is a network that operates according to a switching mechanism to connect devices to other devices (processors, memory).

Mechanism similar to that adopted by the telephone systems.  
Scales better than the bus but has higher costs

- The processors communicate via the switch boxes to access the memory modules.
- Multiple paths exist for communication between a processor and a certain memory module.
- The switch determines the optimal path to be taken.

**Cross-bar Switch Network Diagram**





## Mesh topology

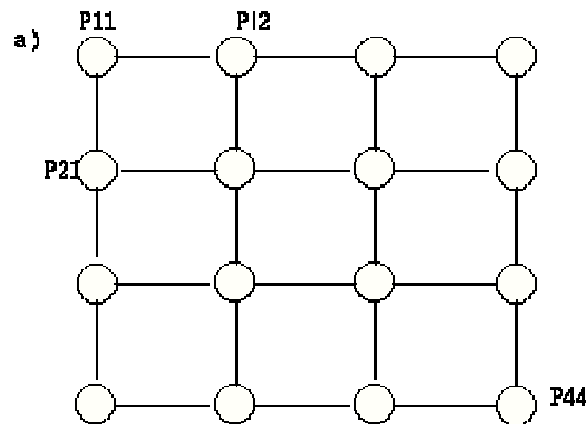
In a mesh network, the nodes are arranged as a **k**-dimensional lattice with width **w**, for a total of **w<sup>k</sup>** nodes

- **k=1** (a linear array)
- **k=2** (2D array) es. ICL DAP, Intel Paragon,

Direct communication is allowed only between neighboring nodes.

The internal nodes communicate directly with other **2k** nodes.

### EXAMPLE



2D mesh of width 4 with  
no wraparound connections  
on edge or corner nodes

corner nodes have degree 2  
edge nodes have degree 3

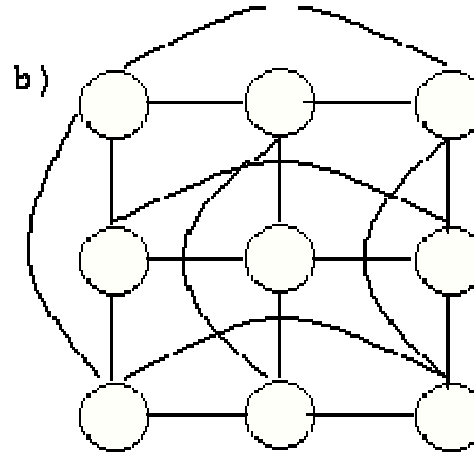


# Toroidal Topology

Some variations of the mesh model have **wrap-around type** connections between the nodes to the edges of the mesh (**torus topology**).

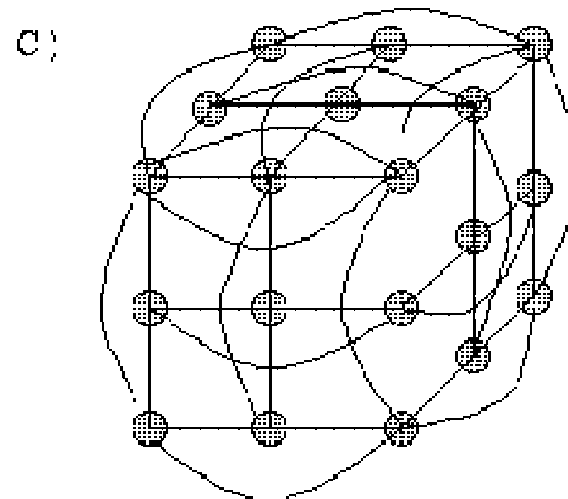
The **Cray T3E** adopts a 3D torus topology

**IBM BG/Q** has adopted a 5D torus topology



2D mesh of width 3 with wraparound connections between nodes on same row or column

Edge and corner nodes have degree 4



$k = 3 \quad w = 3$

i.e.  $3^3 = 27$  nodes

with wraparound connections

all nodes have degree 6 ( $2k$ )





## Hypercube Topology

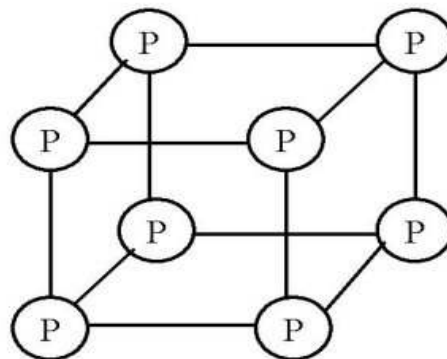
A hypercube topology (**cube-connected**) is formed by  $n = 2^k$  nodes connected according to the vertexes of a cube with  $k$  dimensions.

Each node is directly connected to  $k$  other nodes.

The **degree** of a hypercube topology is  $\log n$  and also the **diameter** is  $\log n$ .

Examples of computers with this type of network are **CM2**, **Ncube-2**, **Intel iPSC860**, **SGI Origin**.

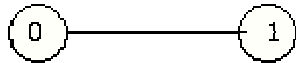
Hypercube Network Diagram



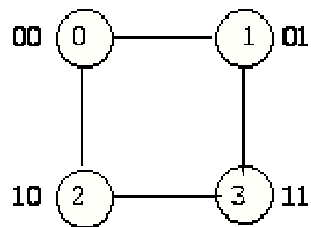


# Hypercube Topology / 1

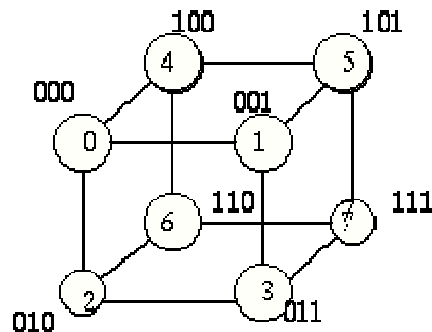
E.g. 1D hypercube ( 2 nodes)



E.g. 2D hypercube ( 4 nodes)



E.g. 3D hypercube ( 8 nodes)

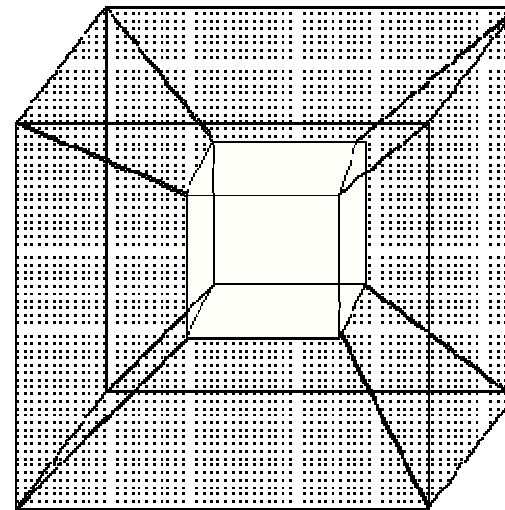


**Recursive definition:**  $H(i) = H(H(i-1), H(i-1))$

Each node is connected to **k** other nodes  
**k** represents the distance between the two most distant points  
**(diameter)**.

A cube connected network is a network butterfly whose columns are collapsed into single nodes.

4D Hypercube or Binary 4-Cube





## Tree Topology

The processors are located in the terminal nodes (**leaves**) of a **binary tree**

The **degree** of a network with tree topology with  $N$  nodes is  $\log_2 N$  and the **diameter** is  $2 \log_2(N) - 2$

### Fat tree

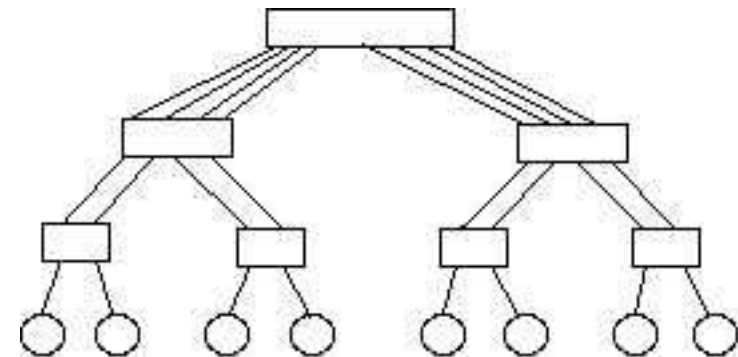
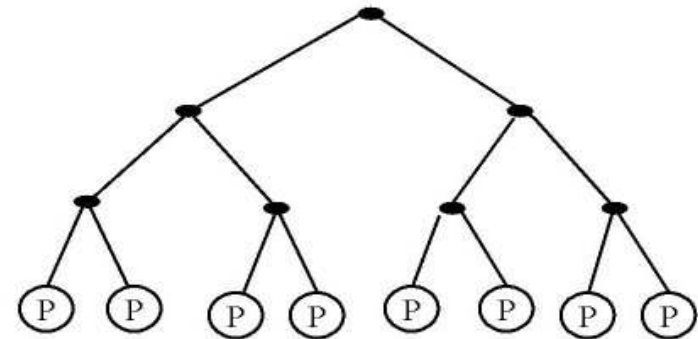
tree topology where the bandwidth of the network increases with the level of the network.

CM-5, Network Myrinet e QSNet

### Pyramid

A pyramidal network of amplitude  $p$  is a complete  $p$ -ary tree with levels, where the nodes of each level are connected in a bi-dimensional mesh.

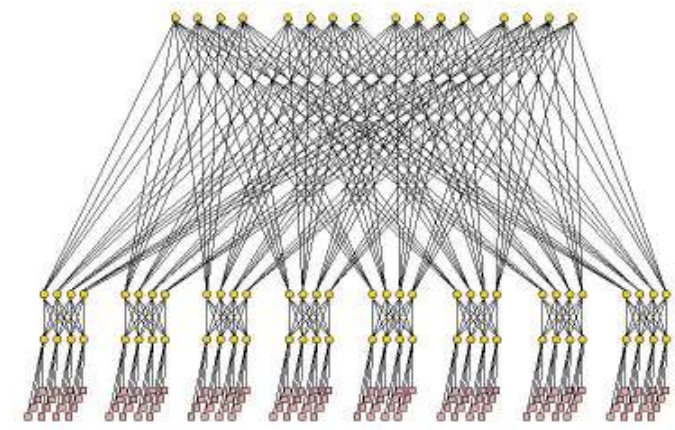
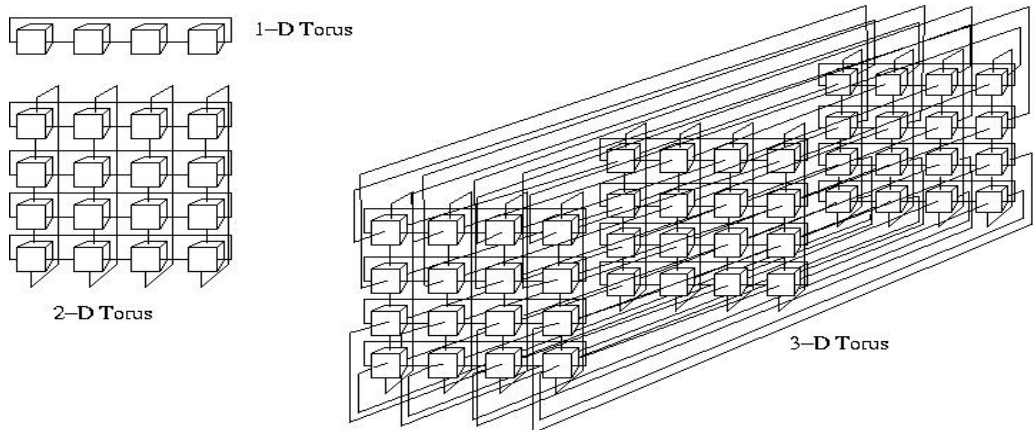
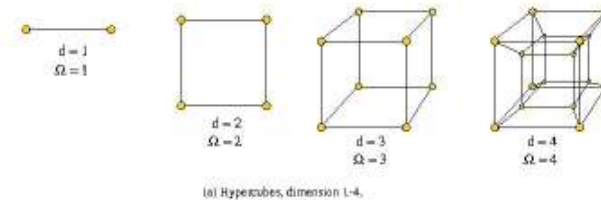
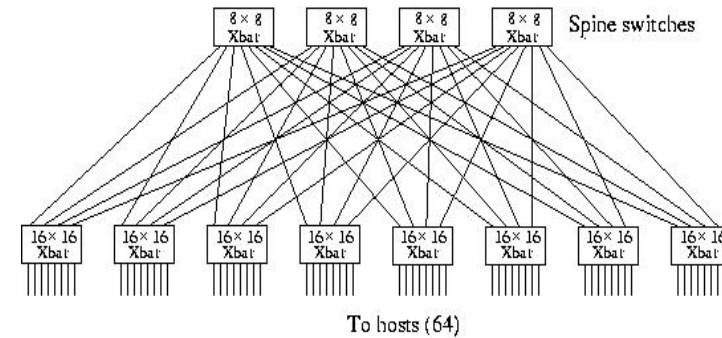
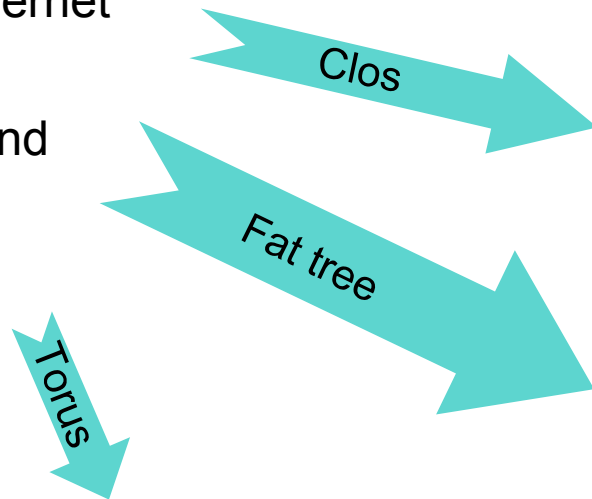
Tree Network Diagram





# Commodity Interconnects

- Gig Ethernet
- Myrinet
- Infiniband
- QsNet
- SCI



(b) A 128-way fat tree.





# HPC Architectures

Performance comes from:

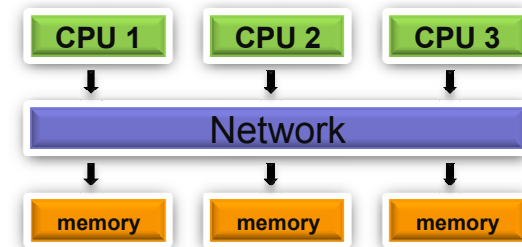
- Device Technology
- Computer Architecture

Characteristics of HPC system:

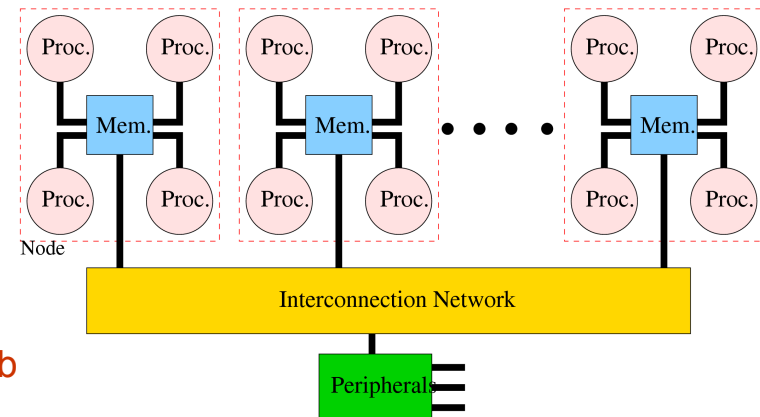
- Multi-processor/multi-core nodes  
(not necessarily SMP nodes anymore!)
- Node architecture may differ, even with similar components
- Network interconnecting nodes
- Parallelism
  - Number of operations per cycle per processor
    - Instruction level parallelism (ILP)
    - Vector processing
  - Number of processors per node
  - Number of nodes in a system
- Hybrids, combining
  - standard processors with accelerators.

The macro-architecture of HPC systems is presently remarkably uniform: but this aspect will change soon

Shared Memory Systems



Distributed Memory





## HPC architectures /1

There are several factors that have an impact on the system architectures in the present:

- 1 Power consumption has become a primary headache.
- 2 Processor speed is never enough.
- 3 Network complexity/latency is a main hindrance.
- 4 There is still the memory wall.

Interestingly, solutions for point 1 and 2 can often be combined.

Since a few years computational accelerators of various kinds are offered that may address speed and power consumption.

Fitting accelerators into a general purpose system:

This is a general problem that is met by at least AMD and Intel.

Goal: Let accelerator communicate directly with the system's memory and General Purpose Computational Cores.





## HPC Architectures: Parameters affecting Performance

Peak floating point performance

Main memory capacity

Bi-section bandwidth

I/O bandwidth

Secondary storage capacity

Organization

- Class of system
- # nodes
- # processors per node
- Accelerators
- Network topology

Control strategy

- MIMD
- Vector, PVP
- SIMD
- SPMD



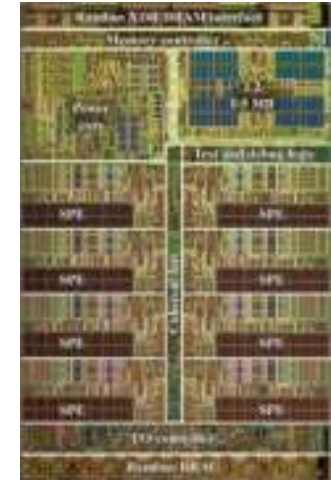
# Heterogeneous Multicore Architecture

## Combines different types of processors

- Each optimized for a different operational modality
  - Performance >  $Nx$  better than other  $N$  processor types
- Synthesis favors superior performance
  - For complex computation exhibiting distinct modalities

## Conventional co-processors

- Graphical processing units (GPU)
- MIC
- Network controllers (NIC)
- Efforts underway to apply existing special purpose components to general applications



## Purpose-designed accelerators

- Integrated to significantly speedup some critical aspect of one or more important classes of computation
- IBM Cell architecture

ClearSpeed SIMD attached array processor

## Drawback of all accelerators: **No standard (yet).**

- Software Development Kits far from uniform (but improving rapidly, OpenFPGA initiative, OpenCL ...).

Programming is hard work.

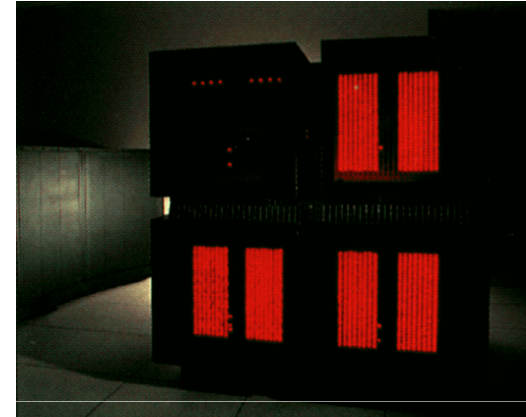






## HPC systems evolution

- Vector Processors
  - Cray-1
- SIMD, Array Processors
  - Goodyear MPP, MasPar 1 & 2, TMC CM-2
- Parallel Vector Processors (PVP)
  - Cray XMP, YMP, C90 NEC Earth Simulator, SX-6
- Massively Parallel Processors (MPP)
  - Cray T3D, T3E, TMC CM-5, Blue Gene/L
- Commodity Clusters
  - Beowulf-class PC/Linux clusters
  - Constellations
- Distributed Shared Memory (DSM)
  - SGI Origin
  - HP Superdome
- Hybrid HPC Systems
  - Roadrunner
  - Chinese Tianhe-1A system
  - GPGPU systems





# HPC systems evolution in CINECA

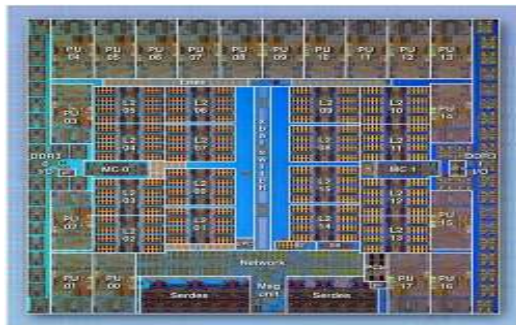
- 1969: CDC 6600      1<sup>st</sup> system for scientific computing
- 1975: CDC 7600      1<sup>st</sup> supercomputer
- 1985: Cray X-MP / 4 8      1<sup>st</sup> vector supercomputer
- 1989: Cray Y-MP / 4 64
- 1993: Cray C-90 / 2 128
- 1994: Cray T3D 64      1<sup>st</sup> parallel supercomputer
- 1995: Cray T3D 128
- 1998: Cray T3E 256      1<sup>st</sup> MPP supercomputer
- 2002: IBM SP4 512      1 Teraflops
- 2005: IBM SP5 512
- 2006: IBM BCX      10 Teraflops
- 2009: IBM SP6      100 Teraflops
- 2012: IBM BG/Q      2 Petaflops





## BG/Q in CINECA

- 10 BGQ Frame
- 10240 nodes
- 1 PowerA2 processor per node
- 16 core per processor
- 163840 cores
- 1GByte / core
- 2PByte of scratch space
- 2PFlop/s peak performance
- 1MWatt liquid cooled



- 16 core chip @ 1.6 GHz
- a crossbar switch links the cores and L2 cache memory together.
- 5D torus interconnect

The Power A2 core has a **64-bit instruction set** (unlike the prior 32-bit PowerPC chips used in BG/L and BG/P

The A2 core have **four threads** and has **in-order dispatch**, execution, and completion instead of out-of-order execution common in many RISC processor designs.

The A2 core has **16KB of L1** data cache and another **16KB of L1** instruction cache.

Each core also includes a **quad-pumped double-precision floating point unit:**

Each FPU on each core has four pipelines, which can be used to execute scalar floating point instructions, four-wide SIMD instructions, or two-wide complex arithmetic SIMD instructions.



# LINPACK Benchmark



The TOP500 project was started in 1993 to provide a reliable basis for tracking and detecting trends in high-performance computing. Twice a year, a list of the sites operating the 500 most powerful computer systems is assembled and released. The best performance on the **Linpack** benchmark is used as performance measure for ranking the computer systems. The list contains a variety of information including the system specifications and its major application areas.

<http://www.top500.org/>

The LINPACK Benchmark was introduced by Jack Dongarra. The LINPACK Benchmark is to solve a dense system of linear equations. For the TOP500, is used that version of the benchmark that allows the user to scale the size of the problem and to optimize the software in order to achieve the best performance for a given machine.

*This performance does not reflect the overall performance of a given system, as no single number ever can. It does, however, reflect the performance of a dedicated system for solving a dense system of linear equations. Since the problem is very regular, the performance achieved is quite high, and the performance numbers give a good correction of peak performance.*

By measuring the actual performance for different problem sizes  $n$ , a user can get not only the maximal achieved performance  $R_{max}$  for the problem size  $N_{max}$  but also the problem size  $N_{1/2}$  where half of the performance  $R_{max}$  is achieved. These numbers together with the theoretical peak performance  $R_{peak}$  are the numbers given in the TOP500. In an attempt to obtain uniformity across all computers in performance reporting, the algorithm used in solving the system of equations in the benchmark procedure must conform to the **standard operation count for LU factorization with partial pivoting**. In particular, the operation count for the algorithm must be  $\frac{2}{3}n^3 + O(n^2)$  floating point operations. This excludes the use of a fast matrix multiply algorithm like "Strassen's Method". This is done to provide a comparable set of performance numbers across all computers.



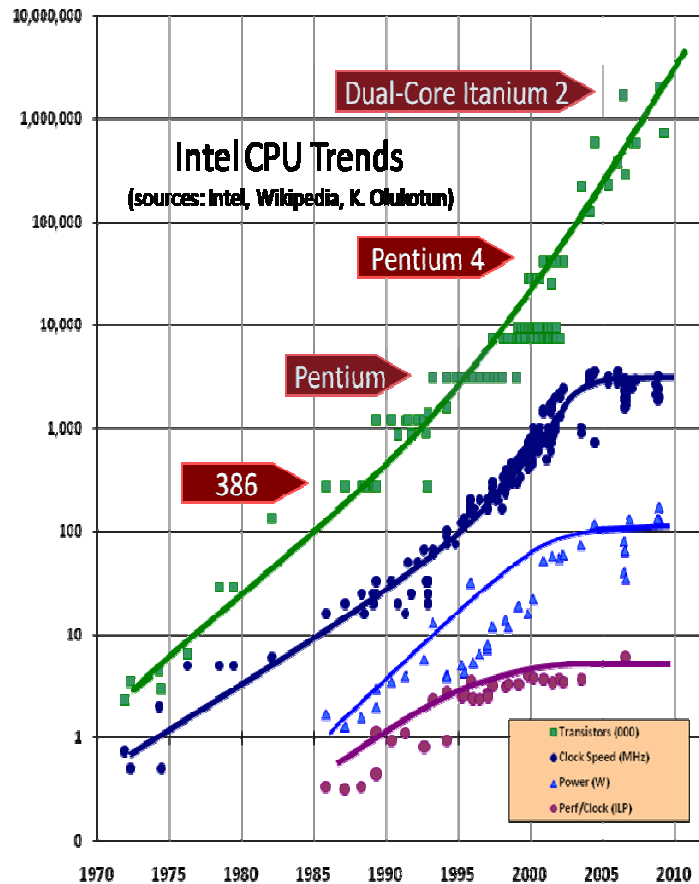
## Top 500: some facts

- 1976** Cray 1 installed at Los Alamos: peak performance 160 MegaFlop/s ( $10^6$  flop/s)
- 1993** (1° Edition Top 500) N. 1 59.7 GFlop/s ( $10^{12}$  flop/s)
- 1997** Teraflop/s barrier ( $10^{12}$  flop/s)
- 2008** Petaflop/s ( $10^{15}$  flop/s): [Roadrunner](#) (LANL) Rmax 1026 Gflop/s, Rpeak 1375 Gflop/s hybrid system: 6562 processors dual-core AMD Opteron accelerated with 12240 IBM Cell processors (98 TByte di RAM)
- 2011** 11.2 Petaflop/s : K computer (SPARC64 VIIIfx 2.0GHz, Tofu interconnect) RIKEN Japan
  - 62% of the systems on the top500 use processors with six or more cores
  - 39 systems use GPUs as accelerators (35 NVIDIA , 2 Cell , 2 ATI Radeon)





# HPC Evolution



## Moore's law is holding, in the number of transistors

- Transistors on an ASIC still doubling every 18 months at constant cost
- 15 years of *exponential* clock rate growth has ended

## Moore's Law reinterpreted

- Performance improvements are now coming from the increase in the number of cores on a processor (ASIC)
- #cores per chip doubles every 18 months *instead of clock*
- 64-512 threads per node will become visible soon
- Million-way parallelism

## Heterogeneity: Accelerators

- GPGPU
- MIC



From Herb Sutter <hsutter@microsoft.com>



## Real HPC Crisis is with Software

A supercomputer application and software are usually much more long-lived than a hardware

- Hardware life typically four-five years at most.
- Fortran and C are still the main programming models

Programming is stuck

- Arguably hasn't changed so much since the 70's

Software is a major cost component of modern technologies.

- The tradition in HPC system procurement is to assume that the software is free.

It's time for a change

- Complexity is rising dramatically
- Challenges for the applications on Petaflop systems
- Improvement of existing codes will become complex and partly impossible
- The use of  $O(100K)$  cores implies dramatic optimization effort
- New paradigm as the support of a hundred threads in one node implies new parallelization strategies
- Implementation of new parallel programming methods in existing large applications has not always a promising perspective

There is the need for new community codes  
multidisciplinary applications



# PRACE



Partnership for Advanced Computing in Europe

<http://www.prace-project.eu/>

PRACE is part of the ESFRI roadmap and has the aim of creating a European Research Infrastructure providing world class systems and services and coordinating their use throughout Europe.

It covers both hardware at the multi petaflop/s level and also very demanding software (parallel applications) to exploit these systems.



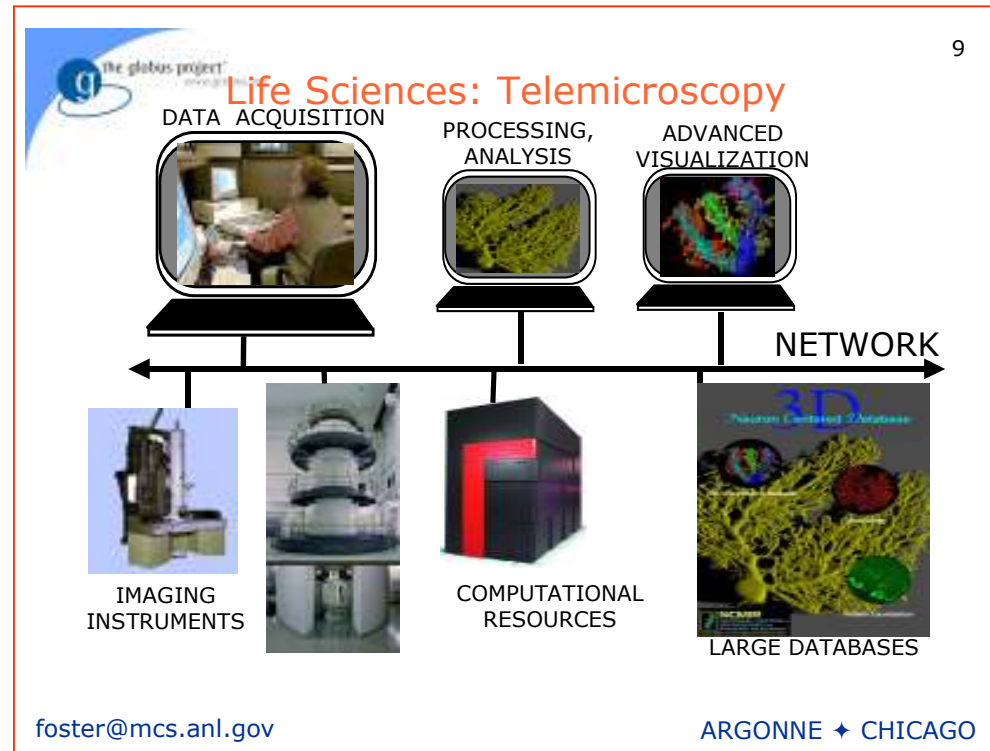




# HPC and Grid Computing

## Grid computing

Networked infrastructure for advanced research that can seamlessly connect distributed teams to the high-end computing systems, instruments, advanced simulation and visualization software, and sensor networks they need to work collaboratively on data- and computation-intensive problems.



HPC and Grid are non-orthogonal but complementar



## Bit and Byte on Information Society

### Gigabyte [ 1,000,000,000 bytes OR $10^9$ bytes ]

- 500 megabytes: A CD-ROM
- 100 megabytes: 1 meter of shelved books
- 10 megabytes: A minute of high-fidelity sound
- 5 megabytes: The complete works of Shakespeare
- 2 megabytes: A high-resolution photograph
- 1 megabyte: A small novel OR a 3.5-inch floppy disk

### Megabyte [ 1,000,000 bytes OR $10^6$ bytes ]

- 200 kilobytes: A box of punched cards
- 100 kilobytes: A low-resolution photograph
- 50 kilobytes: A compressed document image page
- 10 kilobytes: An encyclopaedia page
- 2 kilobytes: A typewritten page
- 1 kilobyte: A very short story

### Kilobyte [ 1,000 bytes OR $10^3$ bytes ]

- 100 bytes: A telegram or a punched card
- 10 bytes: A single word
- 1 byte: A single character

Byte [ 8 bits ]

Bit [ A binary digit - either 0 or 1 ]



## Bits and Bytes on Information Society/1

### **Zettabyte [ 1,000,000,000,000,000,000 bytes OR $10^{21}$ bytes ]**

5 exabytes: All words ever spoken by human beings

2 exabytes: Total volume of information generated worldwide annually

### **Exabyte [ 1,000,000,000,000,000,000 bytes OR $10^{18}$ bytes ]**

200 petabytes: All printed material

8 petabytes: All information available on the Web

2 petabytes: All U.S. academic research libraries

1 petabyte: 3 years of Earth Observing System (EOS) data (2001)

### **Petabyte [ 1,000,000,000,000,000 bytes OR $10^{15}$ bytes]**

400 terabytes: National Climatic Data Center (NOAA) database

50 terabytes: The contents of a large mass storage system

10 terabytes: The printed collection of the U.S. Library of Congress

2 terabytes: An academic research library

1 terabyte: 50,000 trees made into paper and printed OR daily rate of EOS data (1998)

### **Terabyte [ 1,000,000,000,000 bytes OR $10^{12}$ bytes ]**

500 gigabytes: The biggest FTP site

100 gigabytes: A floor of academic journals

50 gigabytes: A floor of books

2 gigabytes: 1 movie on a Digital Video Disk (DVD)

1 gigabyte: A pickup truck filled with paper