

Lecture 1

Introduction to HPC architecture

What is High Performance Computing ?

High *Productivity* Computing

HPC is computing on *supercomputer* or a computer with contemporary processing capacity- with high calculation speed and memory.

HPC can happen on:

- A workstation, desktop, laptop, *smartphone* !
- A supercomputer
- A Linux/MacOS/Windows/... cluster
- A cloud
- Cyberinfrastructure = any combination of the above

Why do we need Computers in Science ?

- Numerical solution to complex problems
- Performing “numerical” experiments that are otherwise impossible to perform in a lab
- Verifying the correctness of theories and models

High *Performance* Computing

Why performance is so important ?



1988: PC: 0.25 million FLOPs

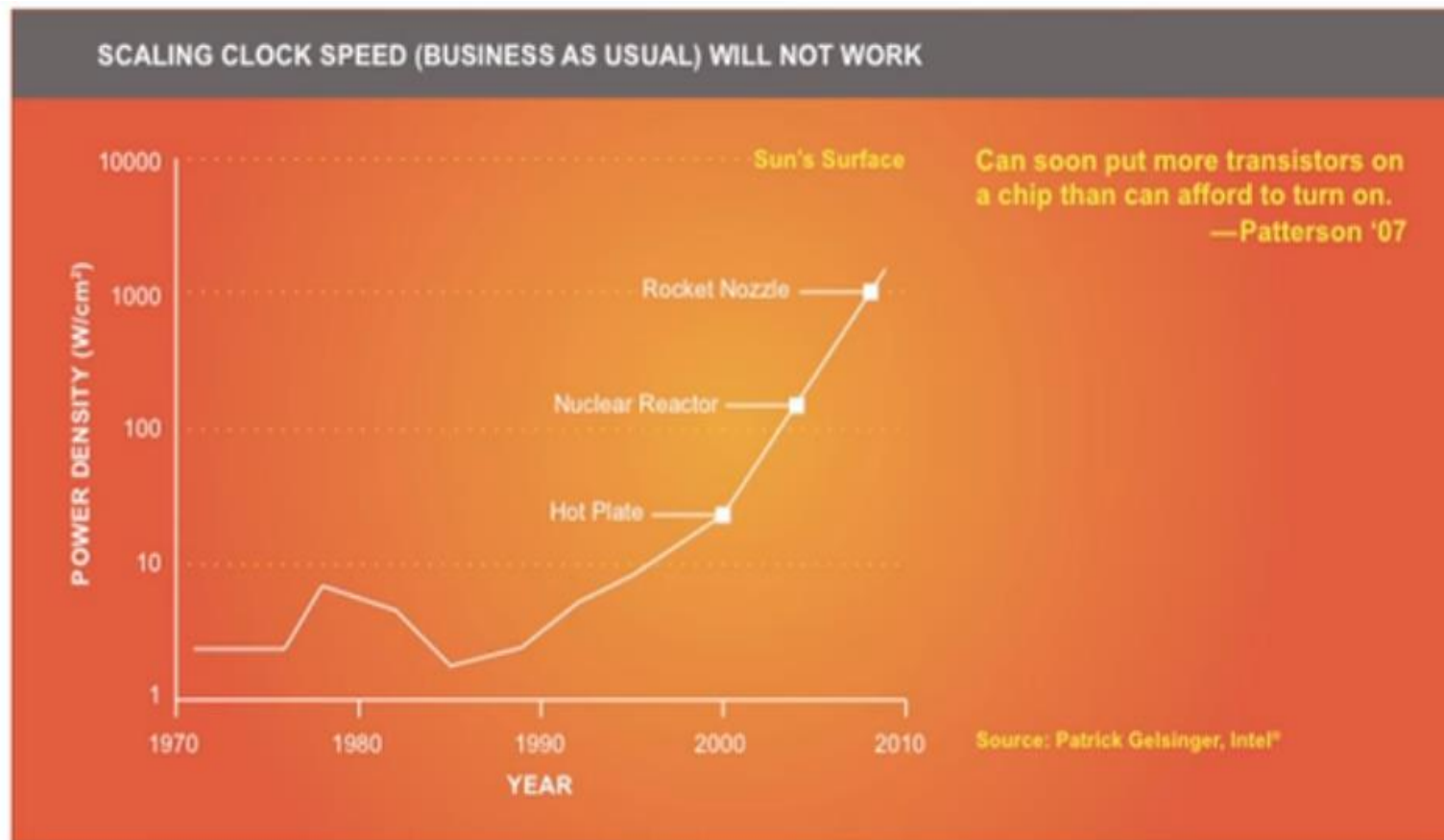
400 PCs = 100 million FLOPs ?

Why HPC ?

- Scientific applications / simulations require greater computing power.
- Single core processors cannot be made more efficient:
 - Faster clock speeds cannot be obtained due to cost and power/heat limitations.
 - Huge memory on a processor cannot be put → expensive

Solution: parallel computing

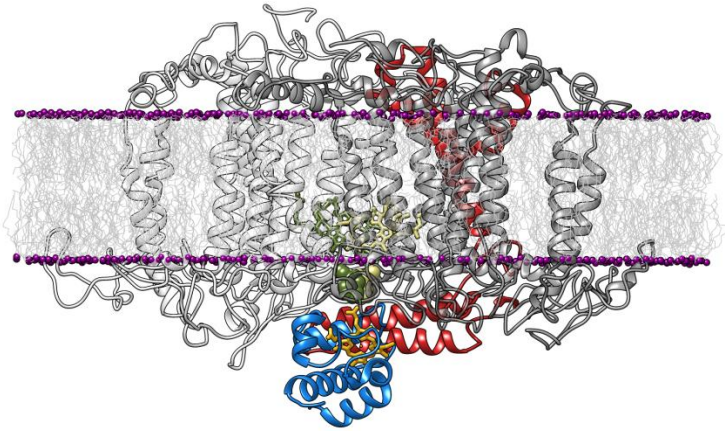
Can putting more transistors on processor chip enhance performance ?



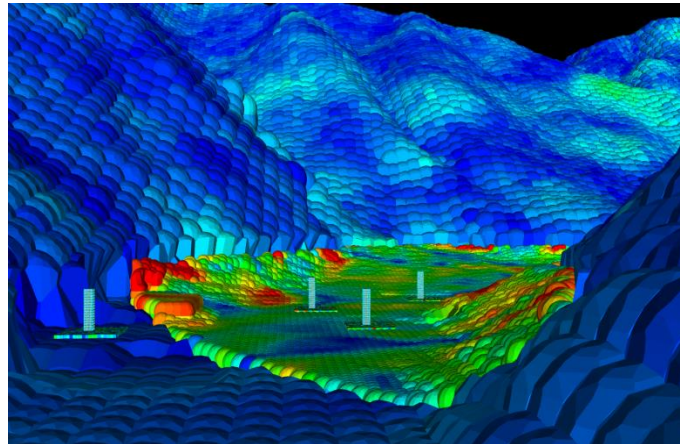
TEDxUIUC - William Gropp - Petascale Computing in Scientific Research (Blue Waters)

Where is HPC needed ?

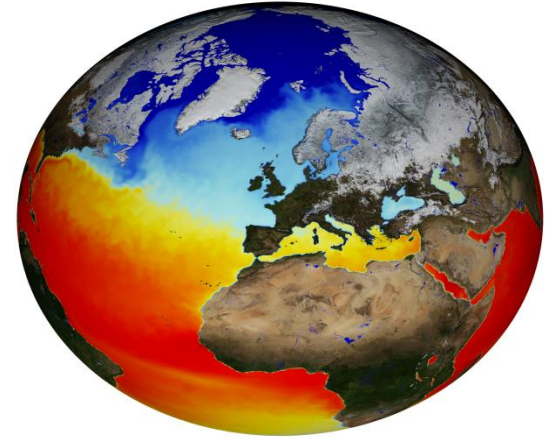
Applications: Scientific research and industrial innovation



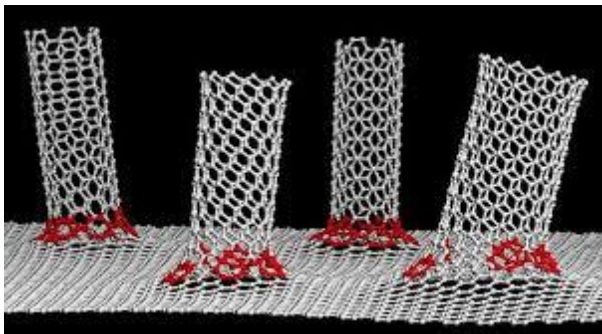
Biology



Earth sciences

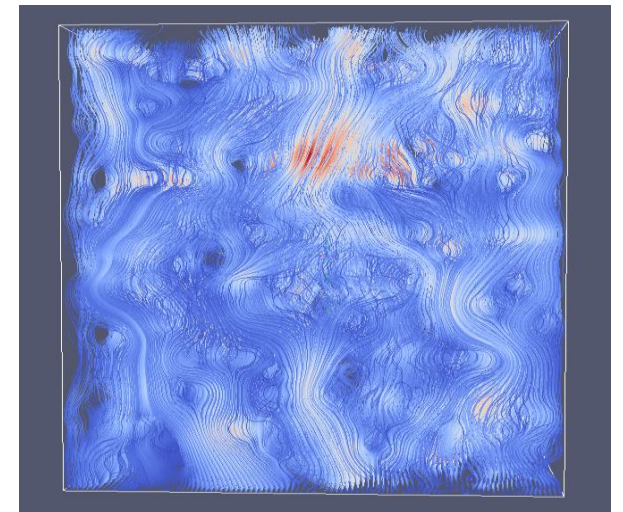


Climate modeling



Material science

Mesoscopic
hydrodynamics



Top500 List of Supercomputers

Rank	Site	System	Cores	Rmax (TFlop/s)	Rpeak (TFlop/s)	Power (kW)
1	DOE/SC/Oak Ridge National Laboratory (/site/48553) United States	Summit - IBM Power System AC922, IBM POWER9 22C 3.07GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband (/system/179397) IBM	2,414,592	148,600.0	200,794.9	10,096
2	DOE/NNSA/LLNL (/site/49763) United States	Sierra - IBM Power System S922LC, IBM POWER9 22C 3.1GHz, NVIDIA Volta GV100, Dual-rail Mellanox EDR Infiniband (/system/179398) IBM / NVIDIA / Mellanox	1,572,480	94,640.0	125,712.0	7,438
3	National Supercomputing Center in Wuxi (/site/50623) China	Sunway TaihuLight - Sunway MPP, Sunway SW26010 260C 1.45GHz, Sunway (/system/178764) NRCP	10,649,600	93,014.6	125,435.9	15,371
4	National Super Computer Center in Guangzhou (/site/50365) China	Tianhe-2A - TH-IVB-FEP Cluster, Intel Xeon E5-2692v2 12C 2.2GHz, TH Express-2, Matrix-2000 (/system/177999) NUDT	4,981,760	61,444.5	100,678.7	18,482
5	Texas Advanced Computing Center/Univ. of Texas (/site/48958) United States	Frontera - Dell C6420, Xeon Platinum 8280 28C 2.7GHz, Mellanox InfiniBand HDR (/system/179607) Dell EMC	448,448	23,516.4	38,745.9	
6	Swiss National Supercomputing Centre (CSCS) (/site/50422) Switzerland	Piz Daint - Cray XC50, Xeon E5-2690v3 12C 2.6GHz, Aries interconnect , NVIDIA Tesla P100 (/system/177824) Cray Inc.	387,872	21,230.0	27,154.3	2,384
7	DOE/NNSA/LANL/SNL (/site/50334) United States	Trinity - Cray XC40, Xeon E5-2698v3 16C 2.3GHz, Intel Xeon Phi 7250 68C 1.4GHz, Aries interconnect (/system/178610) Cray Inc.	979,072	20,158.7	41,461.2	7,578
8	National Institute of Advanced Industrial Science and Technology (AIST) (/site/50762) Japan	AI Bridging Cloud Infrastructure (ABCI) - PRIMERGY CX2570 M4, Xeon Gold 6148 20C 2.4GHz, NVIDIA Tesla V100 SXM2, Infiniband EDR (/system/179393)	391,680	19,880.0	32,576.6	1,649

Some of the fastest HPC facilities around the world



“Summit” supercomputer: Oak Ridge National Laboratory, USA
200 PetaFLOPs



“Sierra” supercomputer: Lawrence Livermore National Laboratory, USA
125 PetaFLOPs



Sunway TaihuLight, China
93 PetaFLOPs

Source: Top500 List

Supercomputing in India

Top500 List:

53	Indian Institute of Tropical Meteorology (/site/50296) India	Pratyush - Cray XC40, Xeon E5-2695v4 18C 2.1GHz, Aries interconnect (/system/179416) Cray Inc.	119,232	3,763.9	4,006.2	1,353
86	National Centre for Medium Range Weather Forecasting (/site/50235) India	Mihir - Cray XC40, Xeon E5-2695v4 18C 2.1GHz, Aries interconnect (/system/179418) Cray Inc.	83,592	2,570.4	2,808.7	955

<https://www.top500.org/list/2019/06/>

Supercomputing in India (National Supercomputing Mission)



Param Shakti
IIT Kharagpur 1.3 PetaFLOPs



Param Shivay
IIT BHU 833 TeraFLOPs



Param Brahma
IISER Pune 797 TeraFLOPs

Other Supercomputing Facilities in India



“Pratyush” 4 PetaFLOPs
Indian Institute of Tropical Meteorology



“Mihir” 2.5 PetaFLOPs
*National Centre for Medium Range
Weather Forecasting*

Some definitions...

1. **Desktop computer** or Personal computer
 2. **Workstation**: a desktop computer, networked and more powerful than a personal computer
 3. **Servers**: a computer on a network that manages network resources.
 4. **Cluster**: collection of desktop computers or servers connected by local area network to act as single large computer.
 5. Floating point operations per second: computing performance
- FLOPs** = no. of cores * cycles per sec * FLOP per cycle

Your desktop computer

Intel Core i7 4790 (Haswell) processor

4 cores at 4.0 GHz

Floating point operations per second

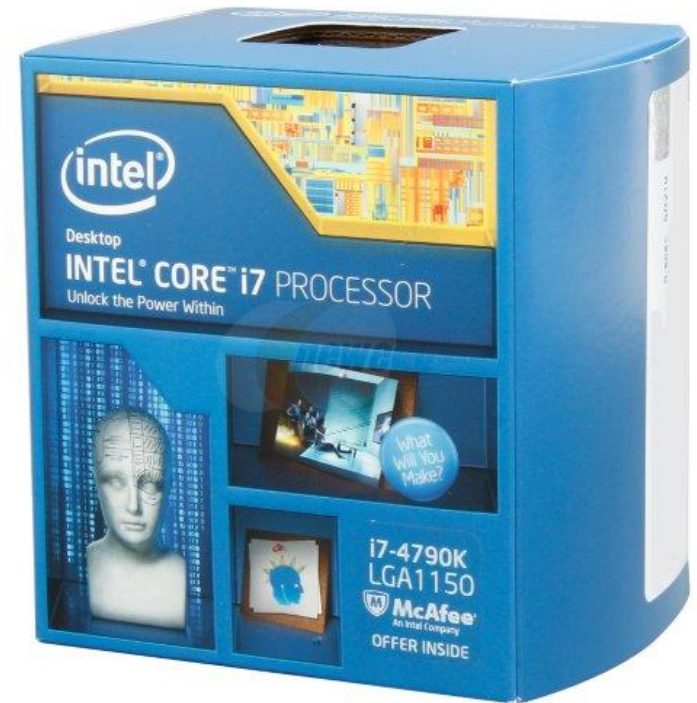
$\text{FLOPs} = \text{no. of cores} * \text{cycles per sec} * \text{FLOP per cycle}$

8 double precision floating point operations per second (FLOP/s)

Desktop PC ~ 128 GFLOPs

HPC cluster at IIT Kharagpur: 1.3 PFLOPs

Exascale computing



High *Performance* Computing

Why performance is so important ?

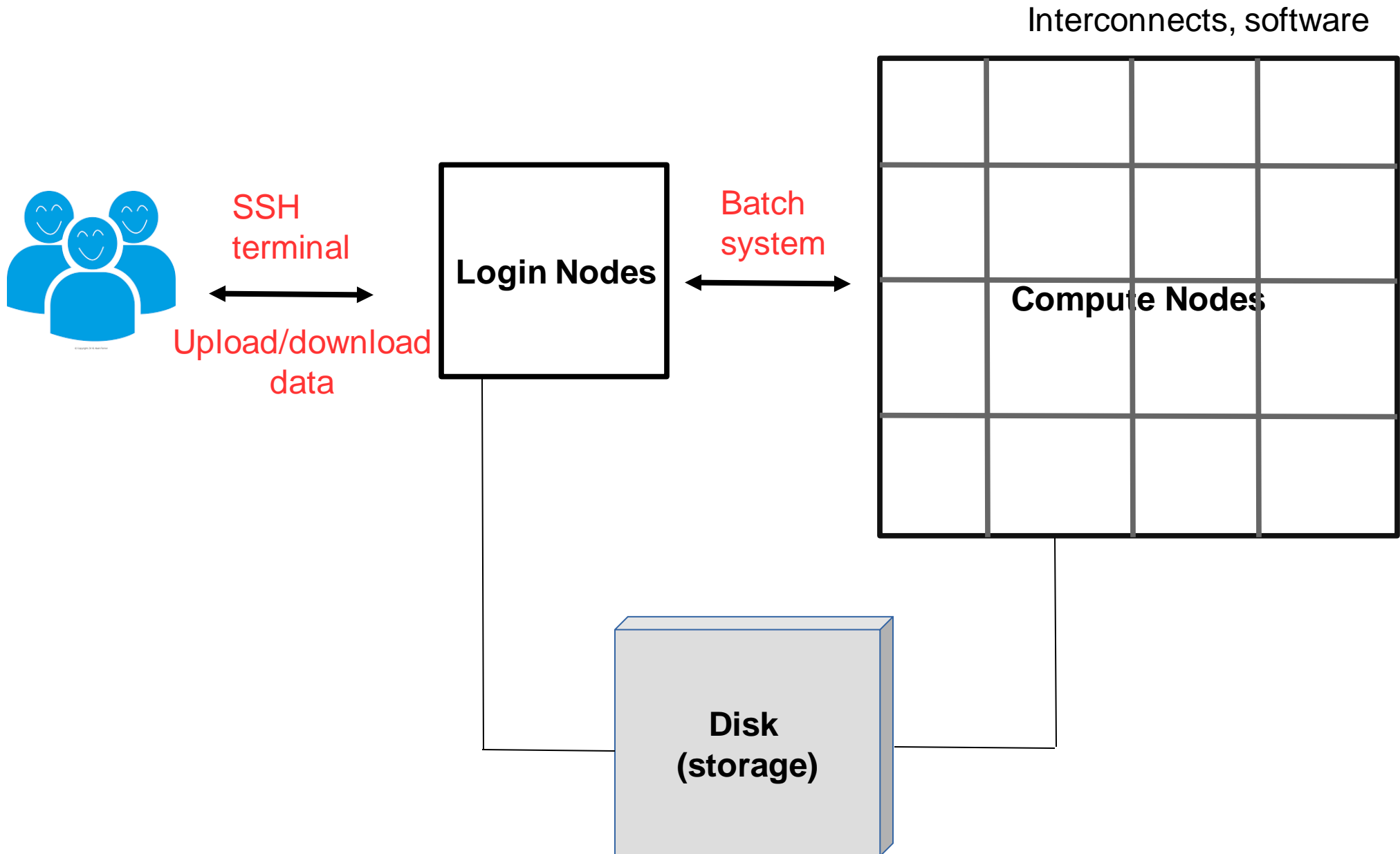


1988: PC: 0.25 million FLOPs

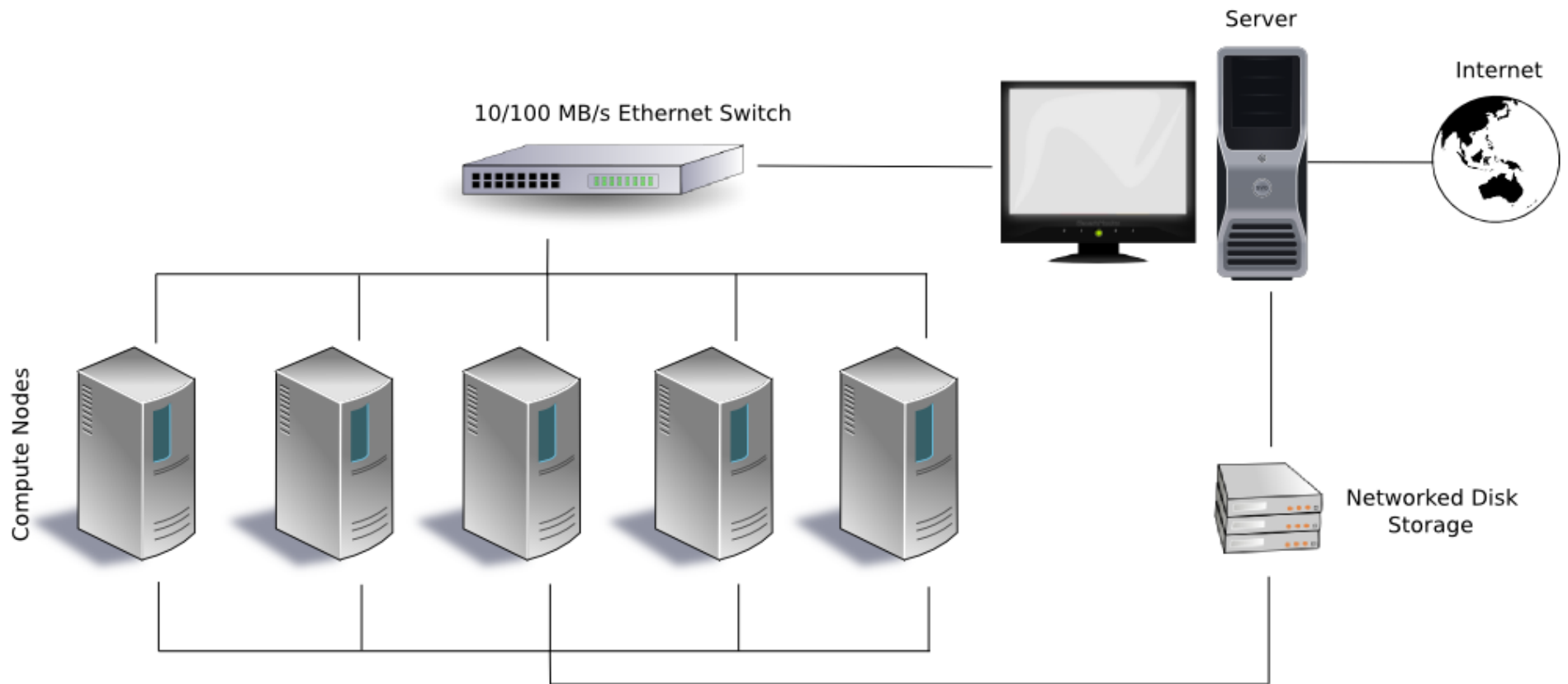
400 PCs = 100 million FLOPs ?

HPC Layout

Basic HPC Layout



A typical HPC cluster...



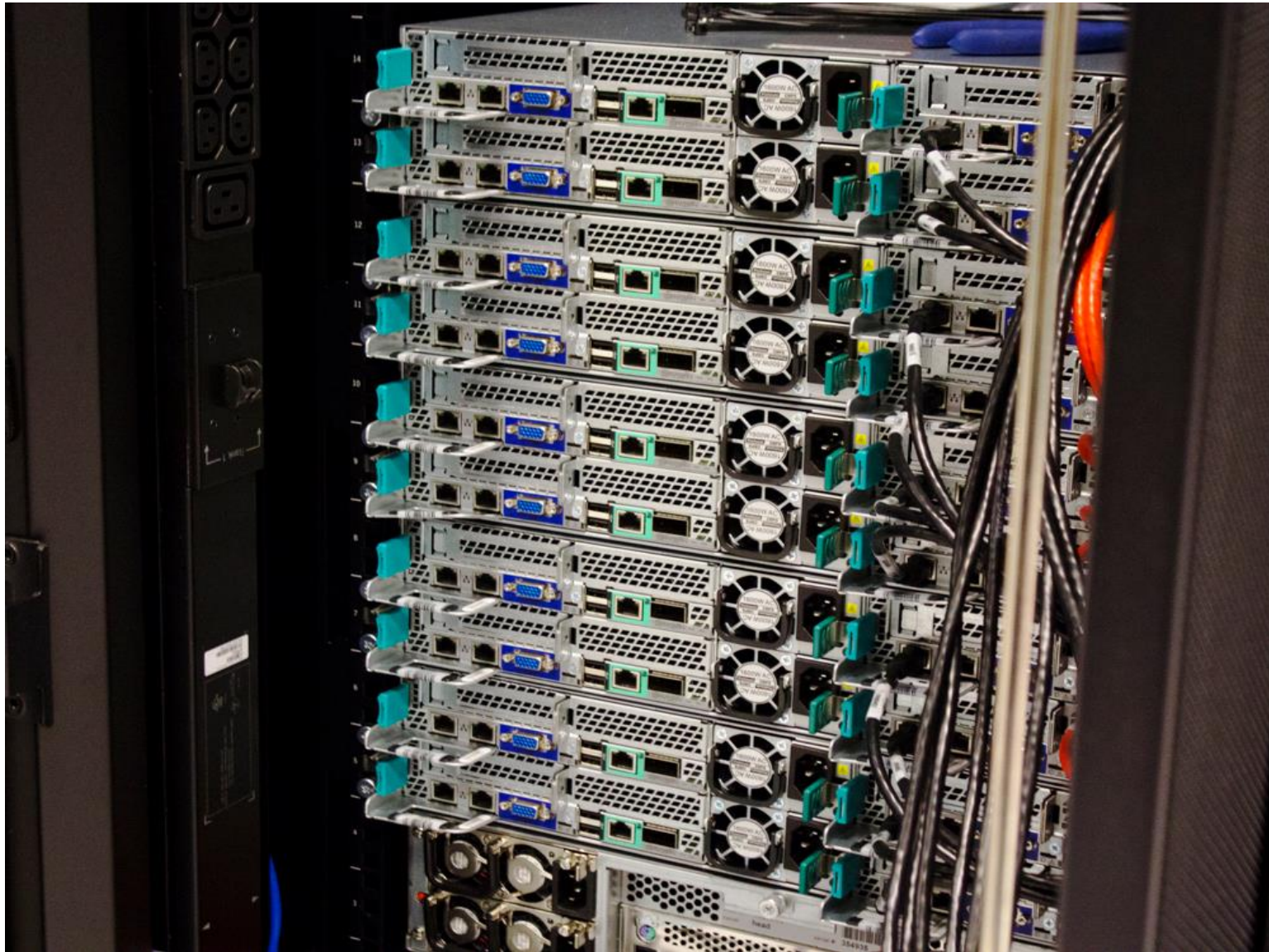
A cluster in 2002



The Ugly part...

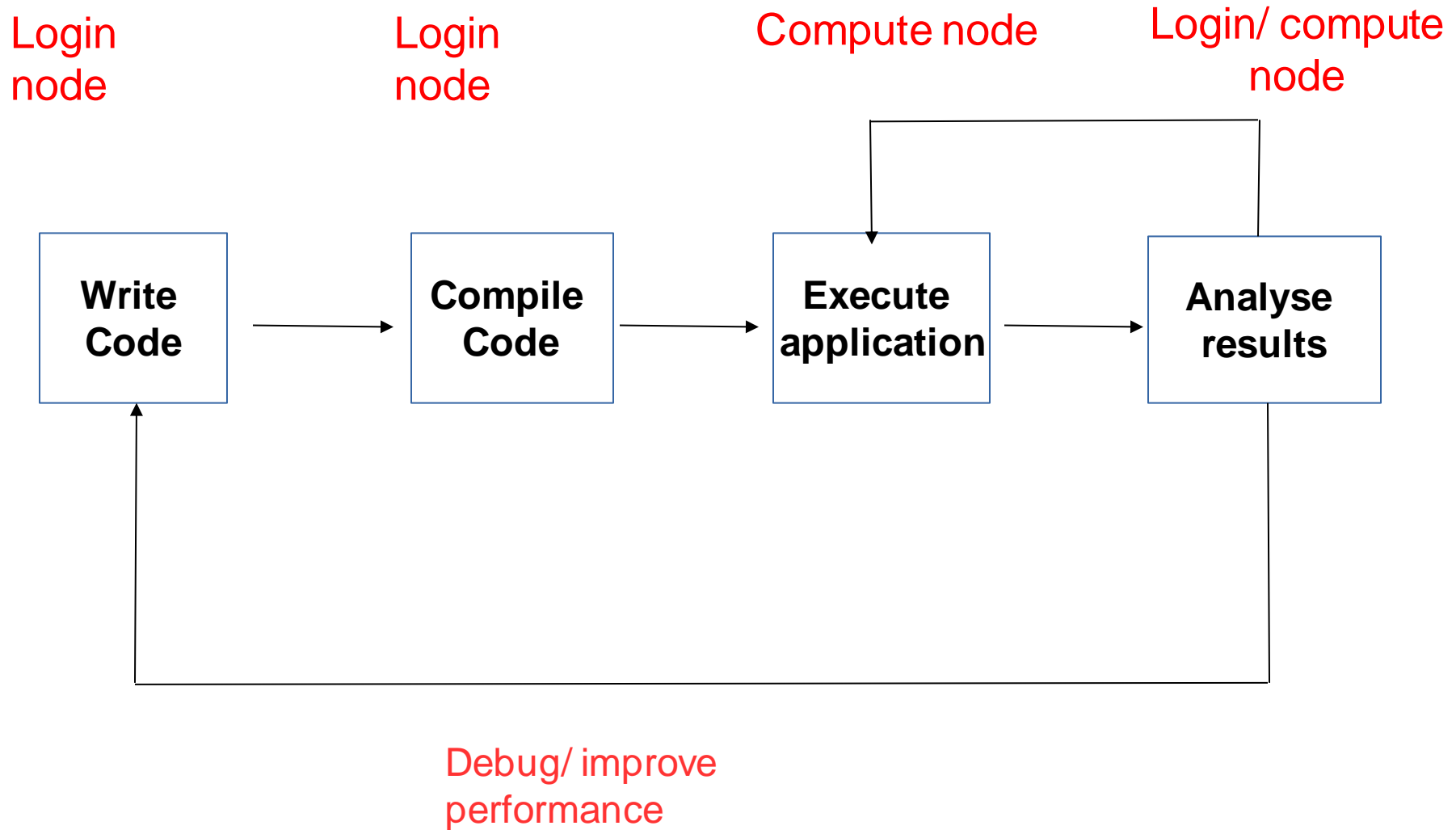


HPC cluster these days...

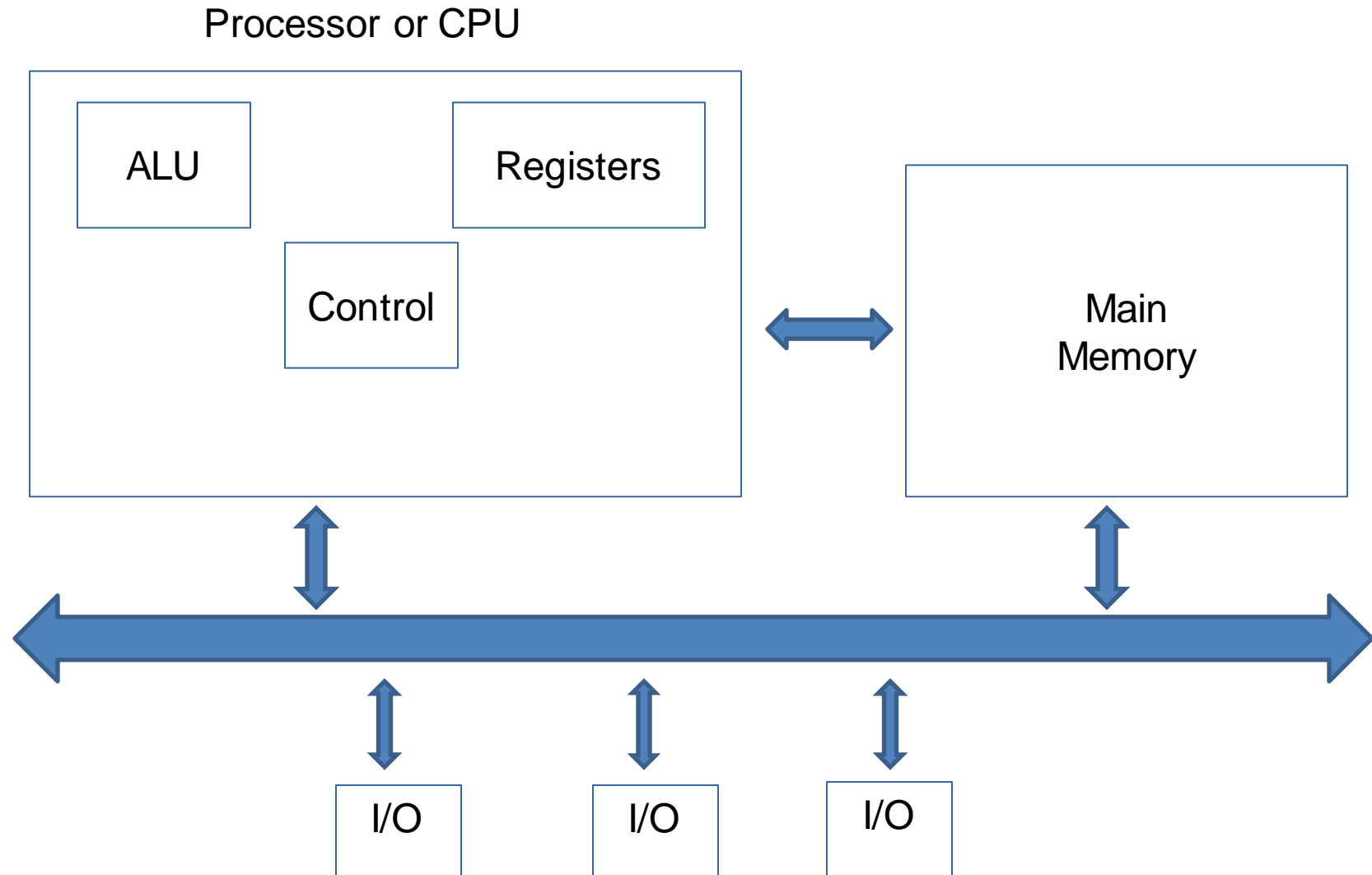




How we use the HPC ?

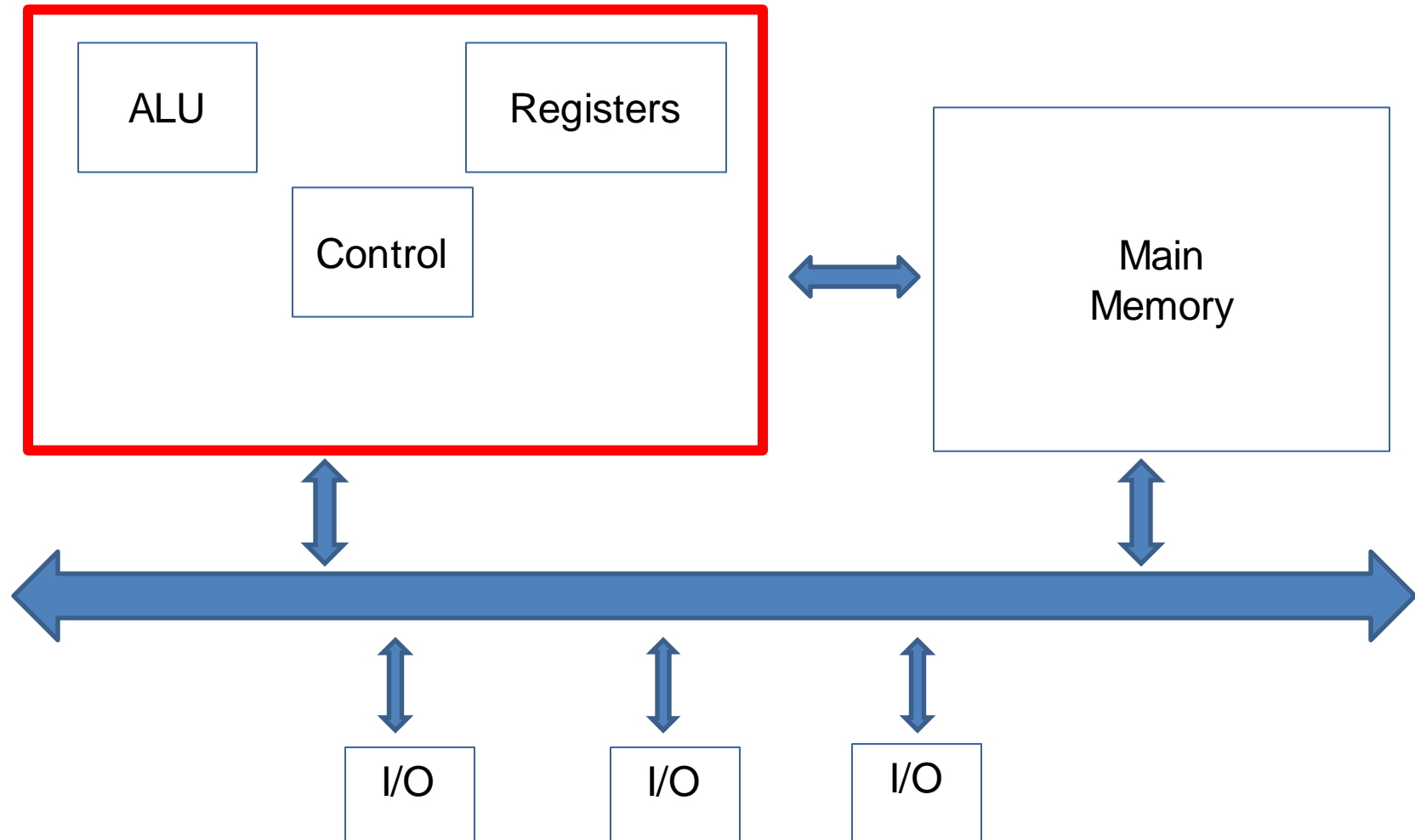


Basic Computer Architecture

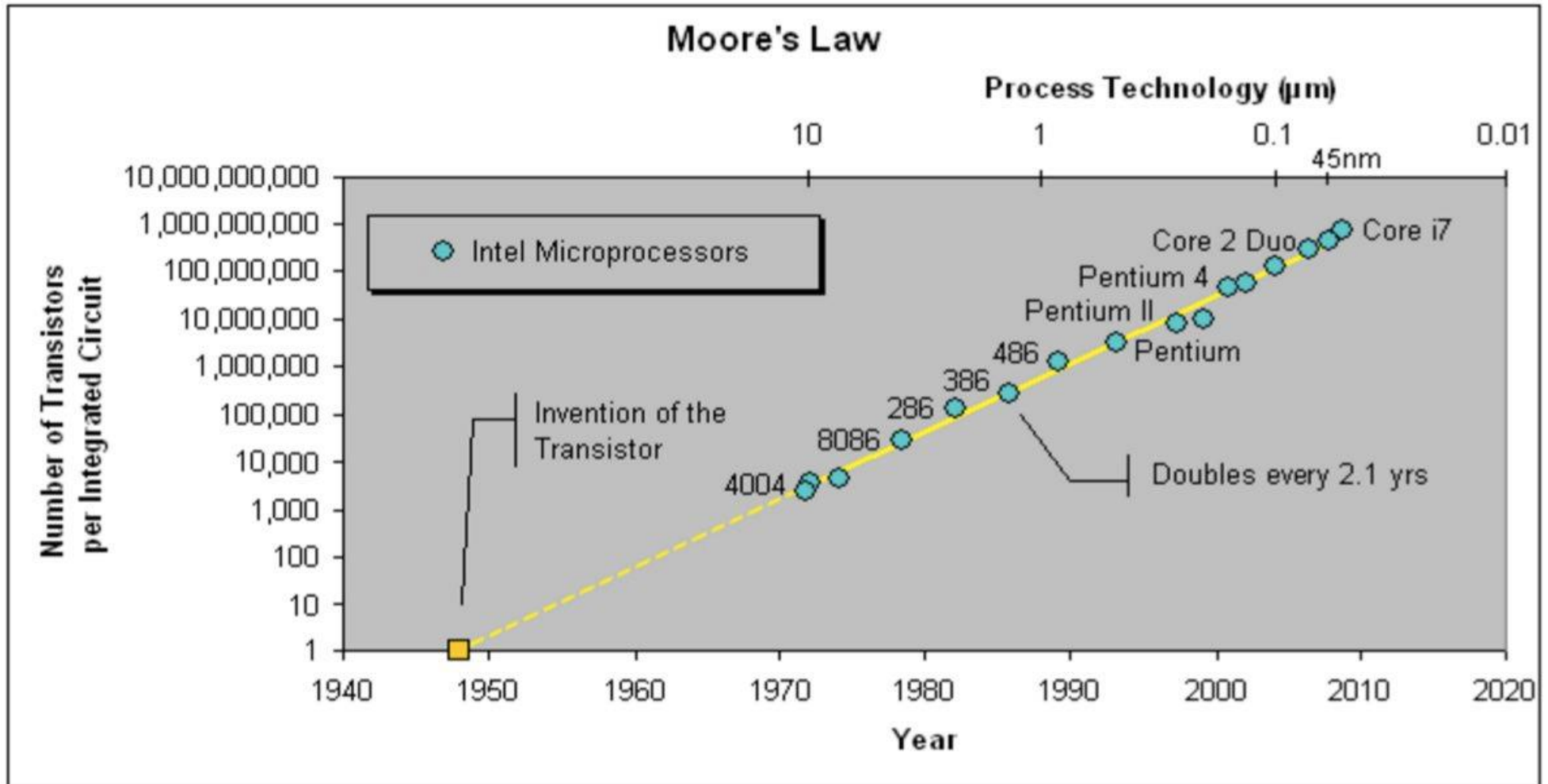


Basic Computer Architecture (*von Neumann architecture*)

Processor or CPU



Moore's law



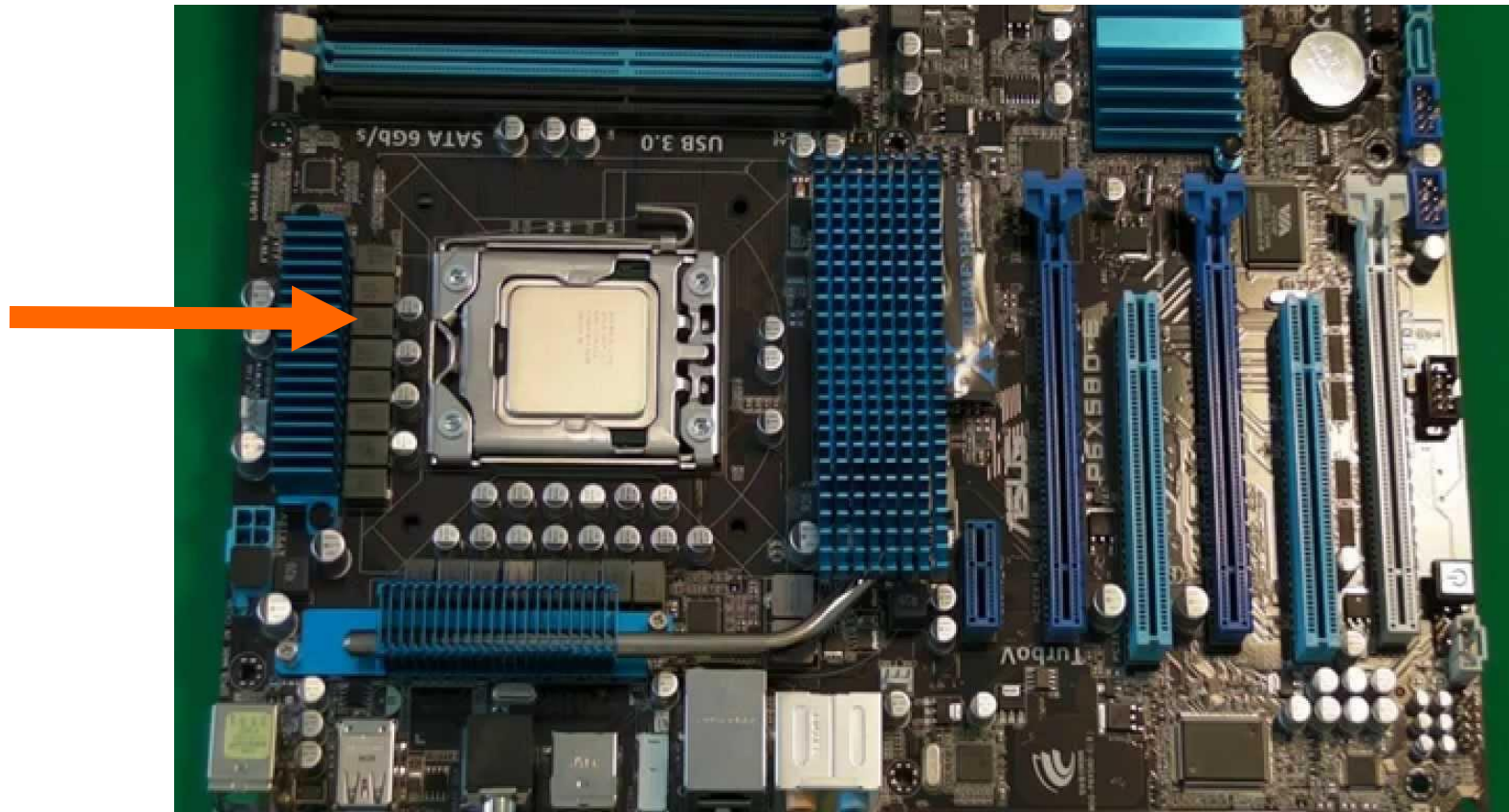
Gordon Moore (Intel cofounder) "Cramming more components onto integrated circuits" 1995, Electronics Magazine

Number of transistors in a dense integrated circuit (IC) doubles about every two years.

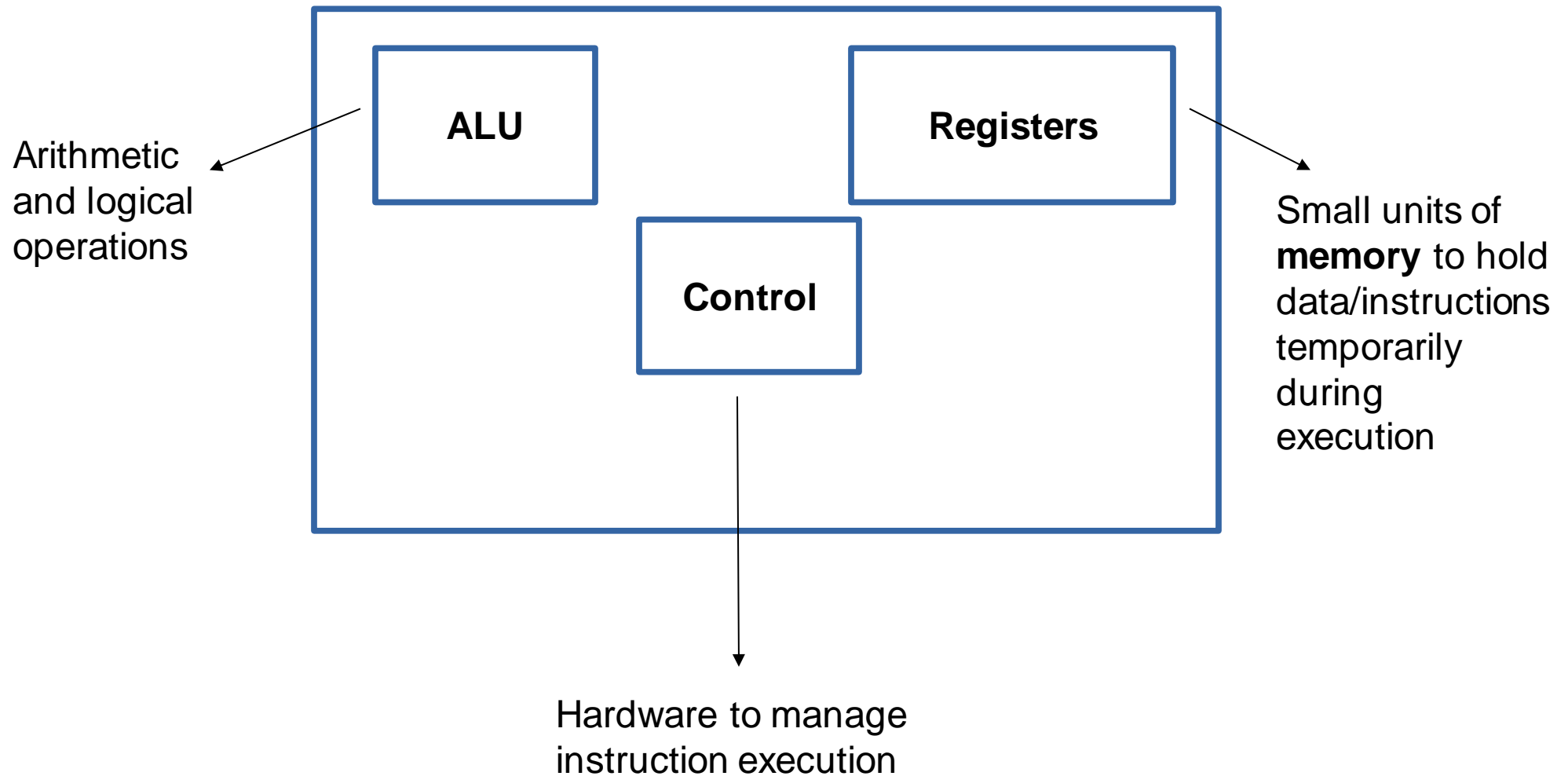
Processor building technology

Year	Technology used in computers	Relative performance/unit cost
1951	Vacuum tube	1
1965	Transistor	35
1975	Integrated circuit	900
1995	Very large-scale integrated circuit	2,400,000
2013	Ultra large-scale integrated circuit	250,000,000,000

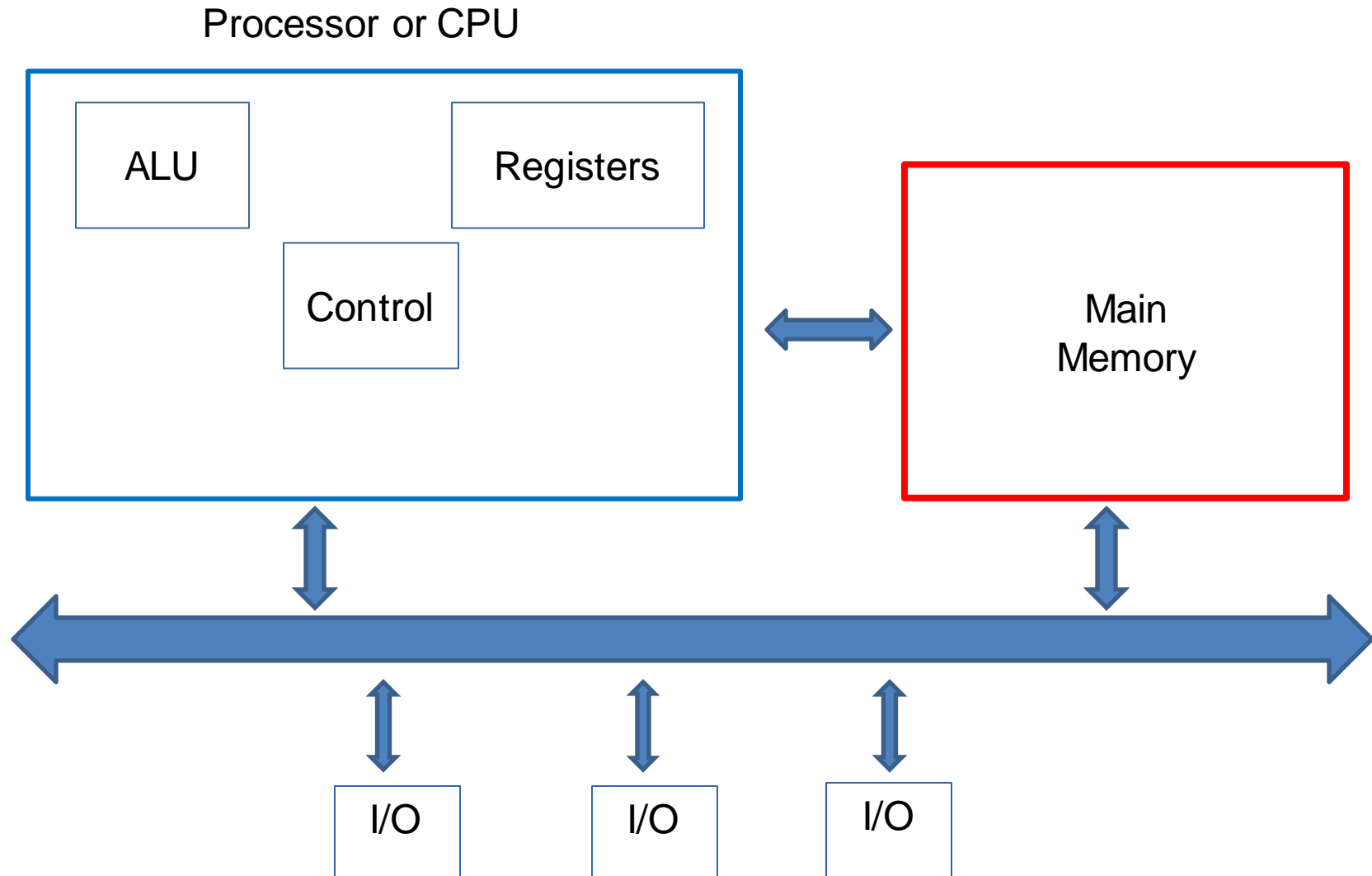
Processor chip



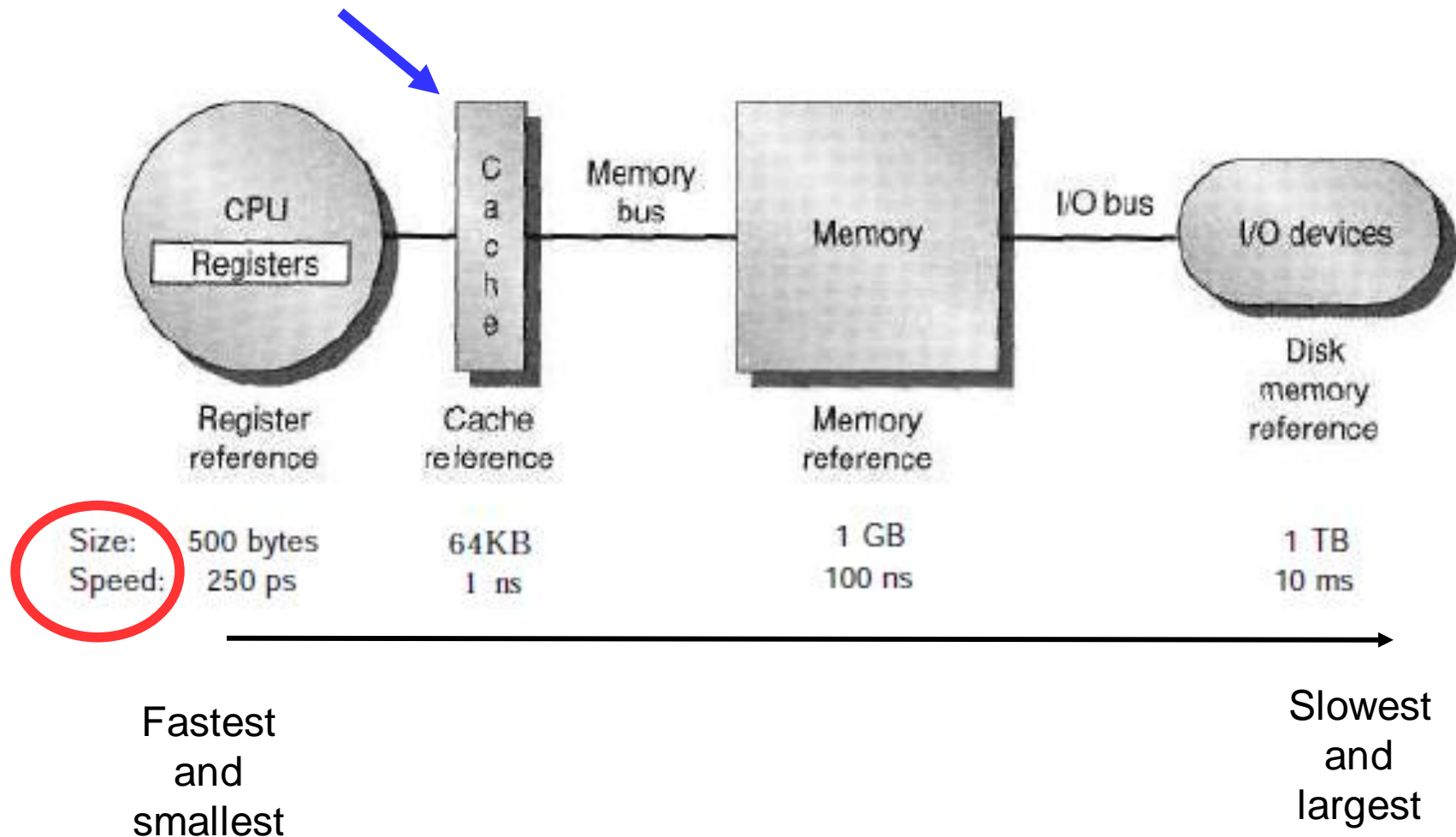
Processor architecture



Basic Computer Architecture

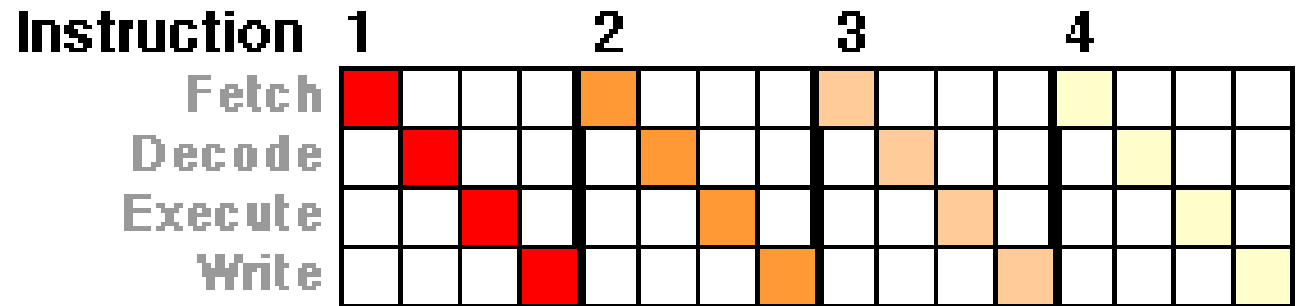


Memory Hierarchy

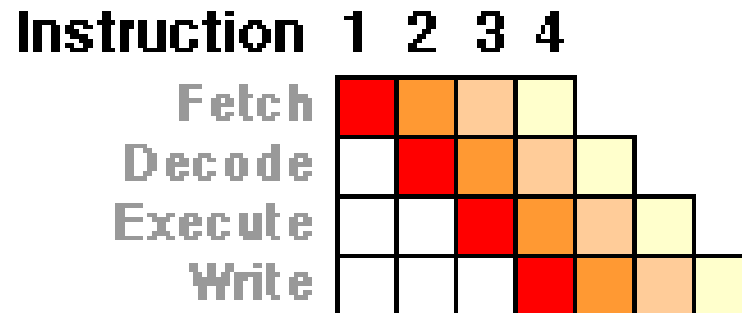


Machine Cycle /Instruction Set

1. Fetch
2. Decode
3. Execute
4. Write/Store



Non-Pipelined



Pipelined

Cycles/Time →

Registers

(Small units of memory inside Processor)

Special Purpose registers: (hold program state)

1. Program Counter (PC)
2. Instruction Register (IR)
3. Processor Status Register

Registers

(Small units of memory inside Processor)

General Purpose Registers (GPRs): (store a data or a memory location address)

- Available to use for any *program or user*
- Large speed disparity between *processor* and the *main memory* where instructions and data are stored
- A typical processor has 32 GPRs.

Processor is 100 times faster than the type of memory

Cache

- Like a temporary storage
- Provides ability to access data at high speed
- **Principle of locality**: Most programs do not access all code or data uniformly.
- **Temporal locality**: least recently used objects are least likely to be referenced in future.
- **Spatial locality**: neighbours of recently referenced locations are likely to be referenced in the near future.

Main Memory: RAM (Random Access Memory)

Able to handle arbitrary ordered requests without favouring any particular request

- SRAM (Static Random Access Memory)
- DRAM (Dynamic Random Access Memory)

Speed and capacity can vary

Video on how processors are made

<https://www.youtube.com/watch?v=qm67wbB5Gml>