INTENSIVE COMPUTATION

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2021-2022

Lecture 1

COURSE INFORMATION

Course topics

Updated course program

- Changes to the order of the topics
- New topics
- Some topics in more detail and less in detail others

In particular, **this year course** will:

- start from the part dedicated to computer architectures
- place greater emphasis on interconnection topologies for HPC and PD systems and the related communication problems
- introduce Quantum Computing, with particular regard to quantum arithmetic circuits

Course topics

Part 1 – Architectures

- Overview on the Von Neumann architecture
- Motivation to parallel architectures and their classifications
- SIMD class: vector architecture and GPUs
- MIMD class: interconnection networks and related problems for HPC systems
- Circuits for arithmetic operations and circuit evaluation
- Number representations for Fast Arithmetic
- Quantum Computing and quantum arithmetic circuits
- Performance metrics and measurements for computer architectures evaluation

Course topics

Part 2 – Methods and applications

- Sparse matrices: compact storage methods
- Errors
- Methods for solving linear systems
- Eigenvalues and eigenvectors: methods and applications.
- Molecular Dynamics: Hooke's Law Model, Lennard-Jones Model, Hard Sphere Model

Disclaimer – it is possible that some of these latter topics will be only touched on or completely skipped

Time and venue

- **G0 room: Wednesday** 11:00-13:00 & **Friday** 10:00-13:00

- Lectures will be given mainly by using slides (or by using the blackboard/tablet)

- To get information on the lessons in streaming, access the course material and receive notices, you must **register on Classroom** for the **imcilwm** course using your Sapienza email address

- Course page is:
  http://twiki.di.uniroma1.it/twiki/view/CI/WebHome

Exam

- **Written exam**
  - Two partial exams or a final exam - *Midterm + end-of-term and final exams consist in a written test with exercises*
- **Oral part**
  - **Oral exam** ***or*** **Project** (one course topic) ***or*** **Presentation** of one-two papers (on one course topic)
  - *NOTICE that project and papers for presentation* ***must be approved by the teacher***
- **Homeworks** will be assigned during the course and will contribute to the final grade

There is not a book - I will give you slides and references on the topics of the course

INTRODUCTION

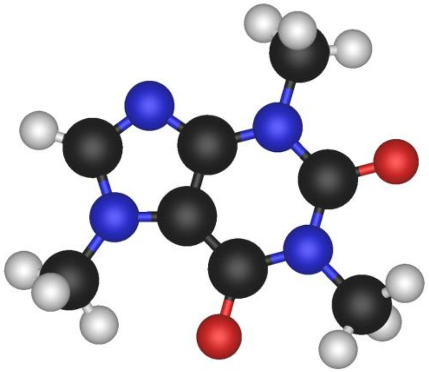
Introduction

- Traditional **methods in science** and **engineering** are:
  - To develop *theories* and *projects*
  - To execute *experiments* and
  - To build *systems*

- The realization of these tasks can be :
  - Too ***difficult*** → wind tunnel
  - Too ***expensive*** → crash testing
  - Too ***slow*** → the evolution of a galaxy
  - Too ***dangerous*** → drugs, toxic gas diffusion

Chlorine release, 2010 Jack Rabbit I Program

Introduction

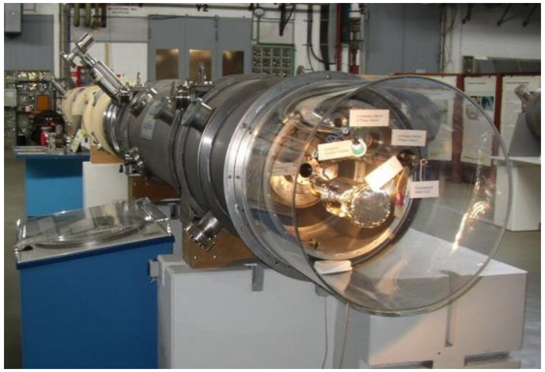


- **Computers** represent the fundamental tool for the simulation and can be seen both as a **microscope** and as a **telescope** with respect to space and to the time

- **Examples**
  - Model molecules in details
  - Travel to the origin of the universe and study its evolution
  - Provide weather forecasts or climate changes

Introduction

Instruments as particle accelerator, telescopes, scanner, etc., produce big quantity of data



Data are elaborated by a computer and are:

- Reduced and transformed
- Represented and visualized

Objectives of **data elaboration** are:

- To understand the meaning of the produced data
- To develop new theories
- To verify different kind of phenomena

COMPUTATIONAL SCIENCE

Computational Science

- Computational science is concerned with:
  - Mathematical models
  - Quantitative analysis techniques
  - **Computer** elaboration
  - Analysis and solution of scientific problems

$$\frac{\mathrm{dLs}}{\mathrm{dt}} = N * K_1 - (d_1 + r) * Ls + \delta_1$$

$$\frac{\mathrm{dLux}}{\mathrm{dt}} = \left(\frac{K_2}{1 + A * Ls1^2}\right) * N - (d_2 + r) * Lux + \delta_2$$

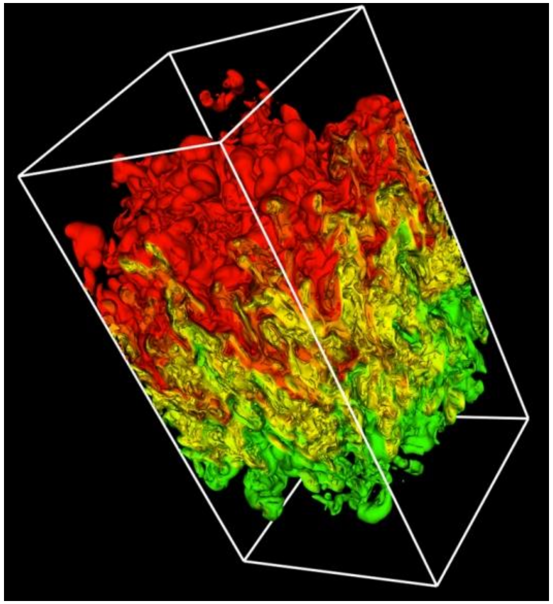
$$Z = Z_1 + Z_2$$

$$Z_1 = K_3 * Lux$$

$$Z_2 = \iint_{0,0}^{2\pi,D} e^{-K_4 s} * Z_{i,j} ds$$

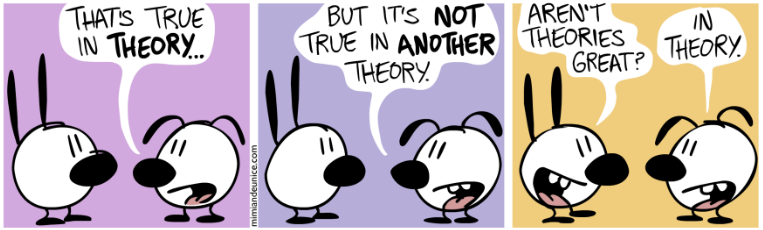
$$\frac{\mathrm{dLs1}}{\mathrm{dt}} = Ls * \left(1 - \frac{Ls}{K5}\right) * Z * \left(1 - \frac{Z}{K6}\right) \qquad (1)$$

- Computational science involves:
  - The application of **computer** simulation
  - Different forms of computation (numerical analysis, theoretical computer science, etc.)
  - Problems in various scientific disciplines



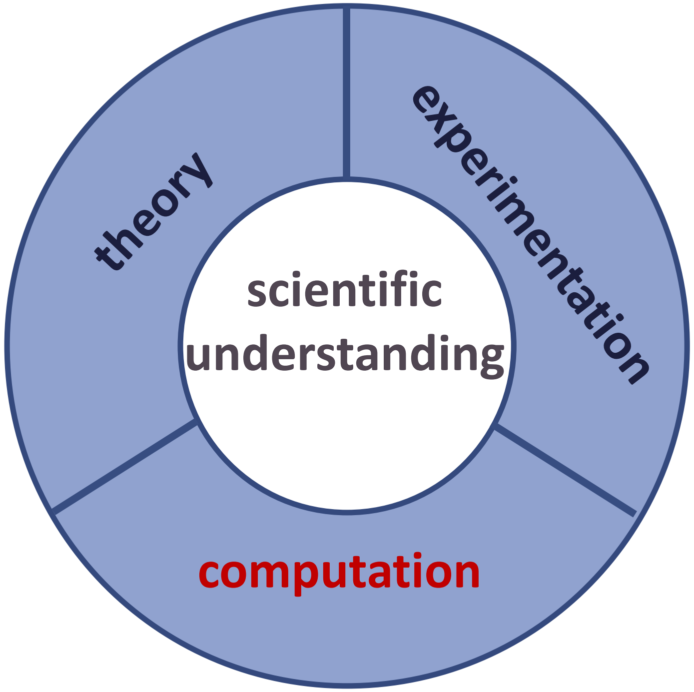
Computational Science

- The **scientific computing approach** is to gain understanding, mainly through the analysis of mathematical models implemented on **computers**



Computational science:

- Is different from **theory** and **laboratory experiments**, traditional forms of science and engineering
- Is now considered a **third mode of science**, besides theory and experimentation/observation



Computational Science

- Scientists and engineers develop **computer** programs and application software, that model systems being studied

- These programs are run with various sets of input parameters

- In most cases, these models require **massive amounts of calculations** (usually floating-point numbers) that are executed on **supercomputers** or **distributed computing systems**

FUNDAMENTALS OF QUANTITATIVE DESIGN AND ANALYSIS

Computer Architecture: A Quantitative Approach

J. L. Hennessy, D. A. Patterson - Morgan Kaufmann, 2012

Computer architectures evolution

- The dramatic growth rate in computer performance in the 20th century has been **fourfold**
- **First impact**
  - Significant enhancement of the capability available to computer users
  - In fact, for many applications, the highest-performance microprocessors of today outperform the supercomputer of less than 20 years ago
- **Second impact**
  - New classes of computers
  - In the 1980s: personal computers and workstations thanks to microprocessor
  - Last two decades: smart cell phones and tablet computers, used as primary computing platforms instead of PCs exploiting the Internet to access warehouses containing tens of thousands of servers, as they were a single gigantic computer

Computer architectures evolution

- **Third impact**
  - Improvement of semiconductor manufacturing – predicted by Moore’s law - led to the dominance of microprocessor-based computers
  - Minicomputers, traditionally made from gate arrays, were replaced by servers made using microprocessors
  - Even mainframe computers and high-performance supercomputers are all collections of microprocessors
  - The hardware innovations led to a **renaissance in computer design**, which emphasized both architectural innovation and efficient use of technology improvements
  - By 2003, high-performance microprocessors were 7.5 times faster than what would have been obtained by relying solely on technology, including improved circuit design
  - That is, 52% per year versus 35% per year

Computer architectures evolution

- **Fourth impact**
  - The hardware renaissance had impact on software development
  - In place of performance-oriented languages like C and C++, much more programming today is done in managed programming languages like Java and C#
  - Scripting languages like Python and Ruby, which are even more productive, gained in popularity
  - To maintain productivity, interpreters with just-in-time compilers and trace-based compiling are replacing the traditional compiler and linker of the past
  - Software deployment is changing as well, with Software as a Service (SaaS) used over the Internet replacing software running on a local computer
  - The nature of applications is also changing: speech, sound, images, and video are becoming increasingly important, along with predictable response time that is so critical to the user experience

Computer architectures evolution

- At a certain point, the hardware renaissance seemed to be over
- In 2004 Intel canceled its high-performance uniprocessor projects and joined others in declaring that the road to higher performance would be via ***multiple processors per chip*** *rather than via faster uniprocessors*
- There has been a historic shift from relying solely on the instruction-level parallelism (ILP) to data-level parallelism (DLP) and thread-level parallelism (TLP)
- Now also the warehouse-scale computers and the request-level parallelism (RLP) need to be considered

GENERATION OF COMPUTERS AND CLASSES

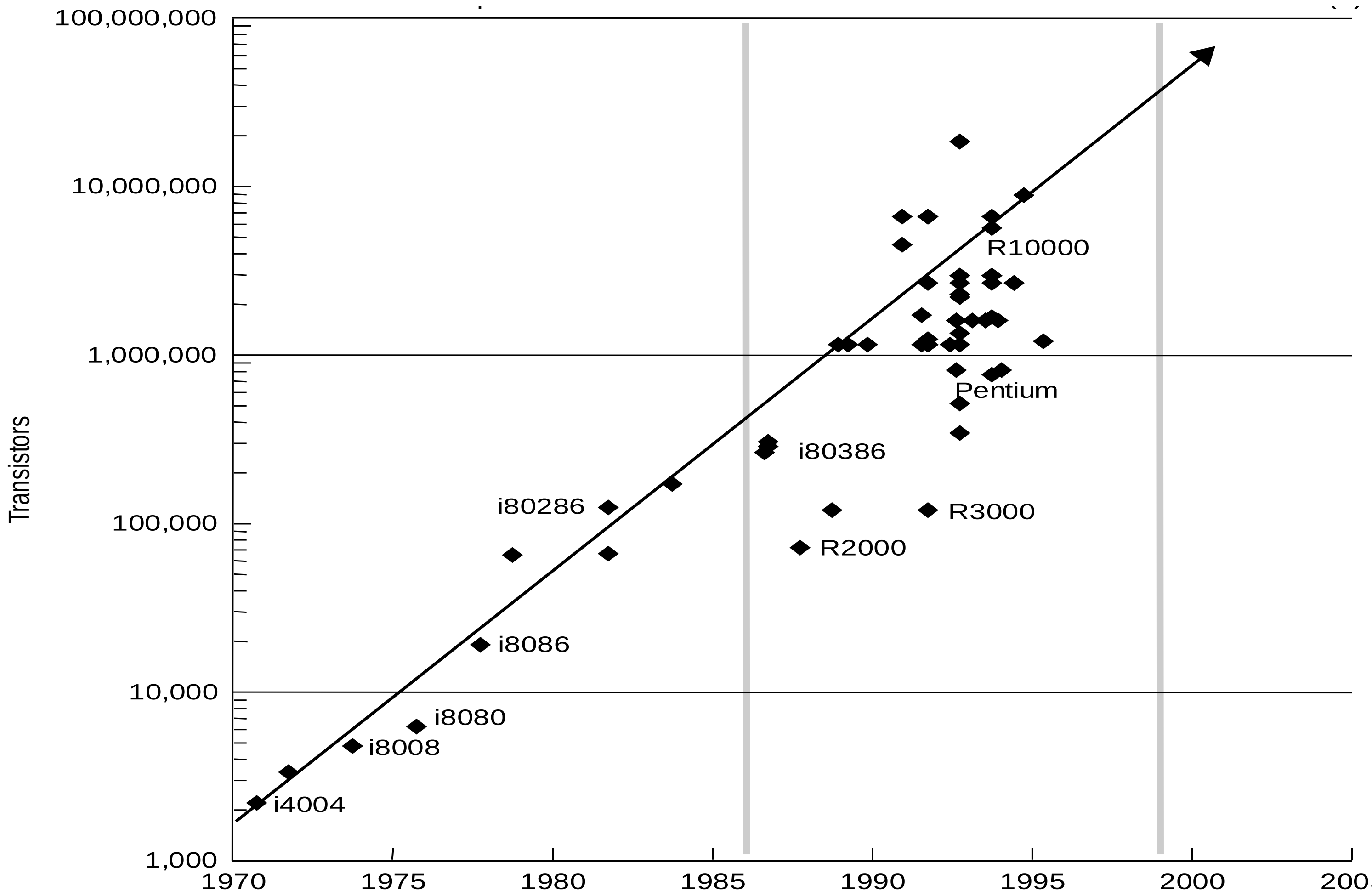
Generations of Computers

- The history of computer architecture is traditionally divided into **four generations** (basic logic technology):

  - **1 - Vacuum tube** - 1946-1957
  - **2 - Transistor** - 1958-1964
  - **3 - Integrated circuits**
    Small scale integration - 1965 on
    Up to 100 devices on a chip
    Medium scale integration - to 1971
    100-3,000 devices on a chip
    Large scale integration - 1971-1977
    3,000 - 10^5 devices on a chip
  - **4 - VLSI**
    Very large scale integration - 1978-1991
    10^5 - 10^8 devices on a chip
    Ultra large scale integration - 1991-
    Over 10^8 devices on a chip

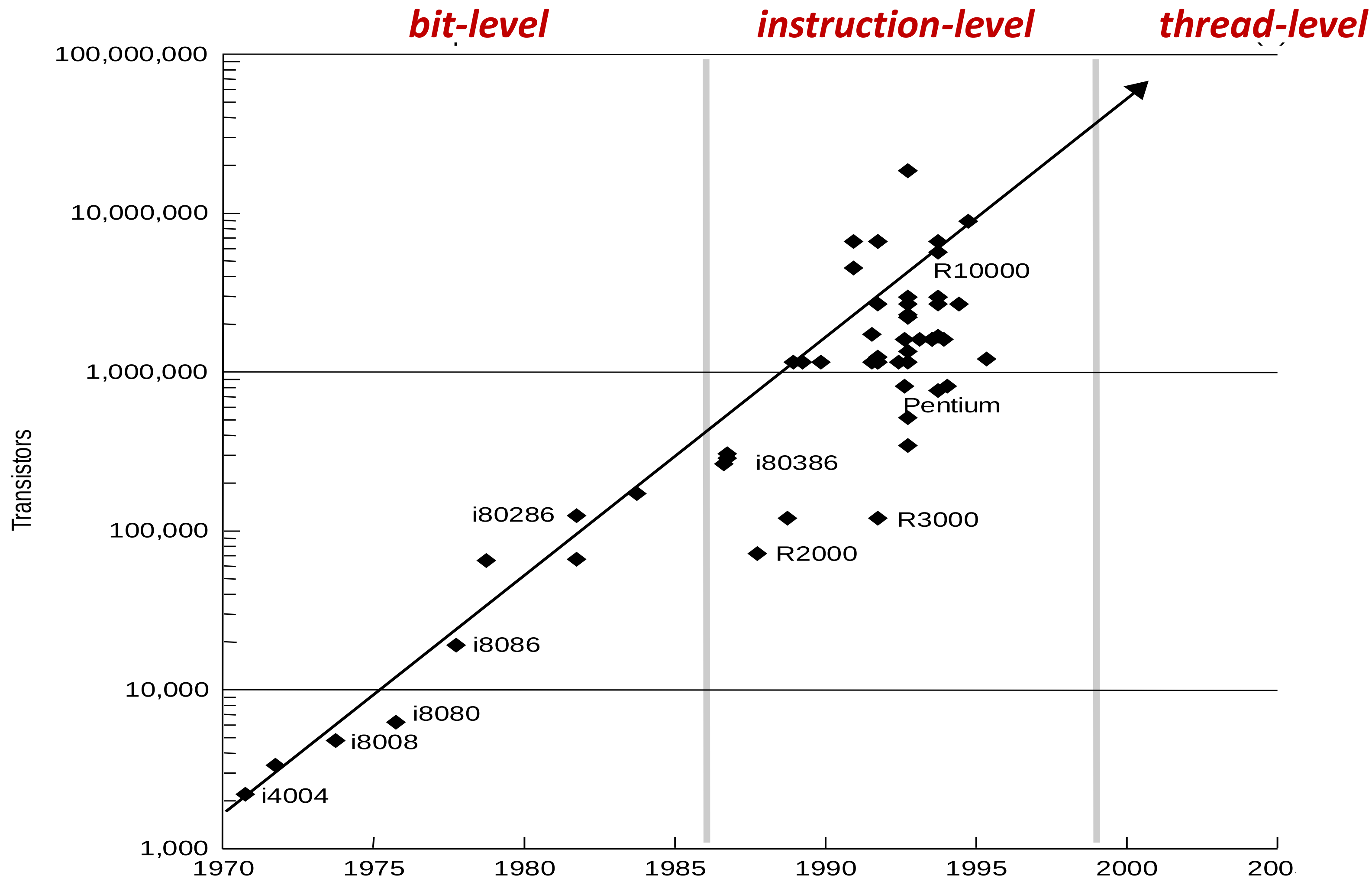
Architectural Trends

- The most interesting period is the fourth - VLSI generation - with its tremendous architectural advance



Architectural Trends

The strongest delineation in VLSI generation is the **kind of parallelism** exploited



Classes of Computers

- The changes we have described above have influenced the computer markets in this new century also because our vision of computing and computer applications has changed considerably

- Since the creation of the personal computer, there have been no changes as evident as they are today in the appearance of computers and in the way they are used

- These changes in computer use have led to five different computing markets, each characterized by different applications, requirements, and computing technologies

Classes of Computers

- **Personal mobile device** (PMD) is the term applied to a collection of wireless devices with multimedia user interfaces such as cell phones, tablet computers, and so on

- Cost is a prime concern determining the consumer price
- Energy efficiency is driven by both battery power and heat dissipation
- The memory can be a substantial portion of the system cost, and it is important to optimize memory size
- The importance of memory size translates to an emphasis on code size, since data size is dictated by the application

Classes of Computers

- **Desktop computing** spans from low-end netbooks, sold at low price, to high-end, heavily configured workstations that are more expensive
- Since 2008, more than half of the desktop computers made each year have been battery operated laptop computers
- The desktop market tends to be driven to optimize *price-performance*:
  - **performance** is measured primarily in terms of compute performance and graphics performance
  - **price** is what matters most to customers in this market, and hence to computer designers
- As a result, the newest, highest-performance and cost-reduced microprocessors often appear first in desktop systems

Classes of Computers

- Since the 1980s, the role of **servers** has grown to provide larger-scale and more reliable file and computing services, replacing the traditional mainframe
- First key feature is availability, since most servers must operate seven days a week, 24 hours a day and a failure can be catastrophic – consider, e.g., the servers running ATM machines for banks or airline reservation systems
- A second key feature is scalability, since server systems often grow in response to an increasing demand for the services they support or an increase in functional requirements
- Finally, servers are designed for efficient throughput, and the overall performance of the server is what is crucial

Classes of Computers

- The growth of Software as a Service (SaaS) for many applications has led to the growth of a class of computers called **clusters**
- Clusters are collections of desktop computers or servers connected by local area networks to act as a single larger computer
- The largest of the clusters are called **warehouse-scale computers** (WSCs), and tens of thousands of servers can act as one
  - Price-performance, power and availability are critical to WSCs
  - WSCs emphasize interactive applications, large-scale storage, dependability, and high Internet bandwidth
- **Supercomputers** or **HPC systems** are related to WSCs in that they are equally expensive
  - Supercomputers emphasize floating-point performance and run communication-intensive batch programs that can run for weeks

Classes of Computers

- **Embedded computers** are found in everyday machines: microwaves, washing machines, most printers, most networking switches, and all cars contain simple embedded microprocessors
- The ability to run third-party software is the dividing line between non-embedded and embedded computers, so as PMD is a different category with respect to embedded computers
- Although the range of computing power in the embedded computing market is very large, price is a key factor in the design of embedded computers
- Performance requirements do exist, of course, but the primary goal is often meeting the performance need at a minimum price, rather than achieving higher performance at a higher price

Classes of Parallelism and Parallel Architectures

- **Parallelism** at multiple levels is now the driving force of computer design across all classes of computers, with energy and cost being the primary constraints

- There are basically two kinds of parallelism in applications:

1. Data-Level Parallelism (DLP) arises because there are many data items that can be operated on at the same time

2. Task-Level Parallelism (TLP) arises because tasks of work are created that can operate independently and largely in parallel

Classes of Parallelism and Parallel Architectures

Computer hardware in turn can exploit these two kinds of application parallelism in four major ways:

1. **Instruction-Level Parallelism** exploits data-level parallelism at modest levels with compiler help using ideas like pipelining and at medium levels using ideas like speculative execution

2. **Vector Architectures and Graphic Processor Units (GPUs)** exploit data-level parallelism by applying a single instruction to a collection of data in parallel

Classes of Parallelism and Parallel Architectures

Computer hardware in turn can exploit these two kinds of application parallelism in four major ways:

3. **Thread-Level Parallelism** exploits either data-level parallelism or task-level parallelism in a tightly coupled hardware model (shared memory systems) that allows for interaction among parallel threads

4. **Request-Level Parallelism** exploits parallelism among largely decoupled tasks specified by the programmer or the operating system

Taxonomy of Computer Architectures

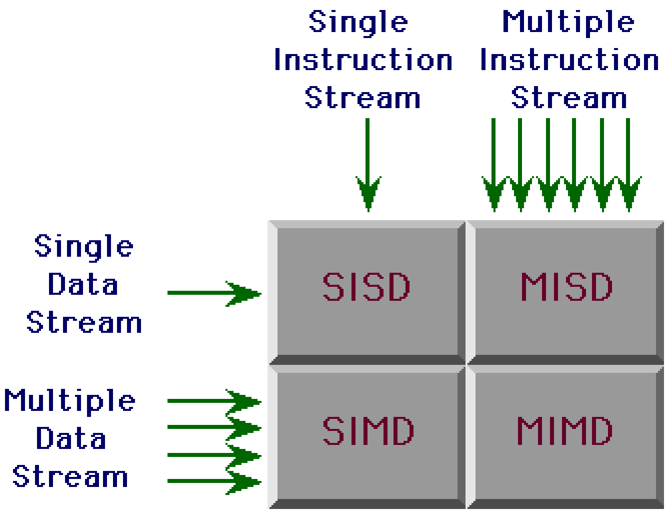
- These four ways for hardware to support the data-level parallelism and task-level parallelism go back to the 60s

- **Michael Flynn** studied the parallel computing efforts in that period, and introduced a **taxonomy** of computer architectures that is still the *most common way of categorizing* systems defining abbreviations we still use today

- He looked at the parallelism in the instruction and data streams called for by the instructions at the most constrained component of the multiprocessor, and placed all computers into one of four categories

Taxonomy of Computer Architectures

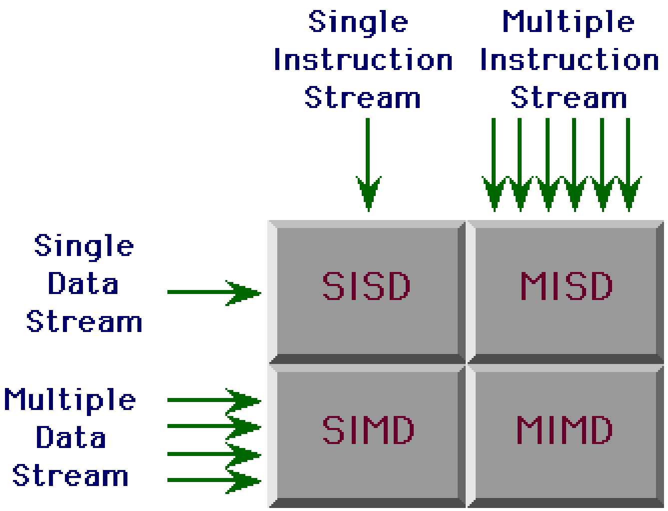
- In Flynn's classification, machines are classified based on how many **data** items they can process concurrently and how many different **instructions** they can execute at the same time
  - Single Instruction, Single Data - **SISD**
  - Single Instruction, Multiple Data - **SIMD**
  - Multiple Instruction, Single Data - **MISD**
  - Multiple Instruction, Multiple Data - **MIMD**



Taxonomy of Computer Architectures

Single Instruction stream, Single Data stream – SISD

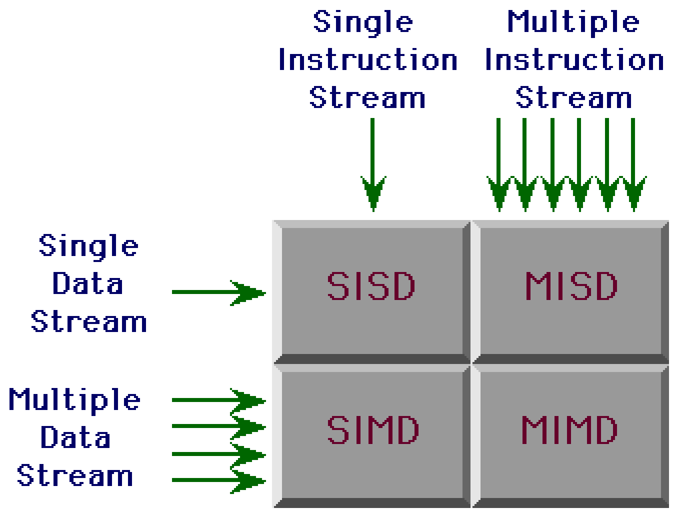
- This category is the uniprocessor
- The programmer thinks of it as the standard sequential computer, but it can exploit instruction-level parallelism
- SISD architectures use ILP techniques such as superscalar and speculative execution



Taxonomy of Computer Architectures

Single Instruction stream, Multiple Data stream - SIMD

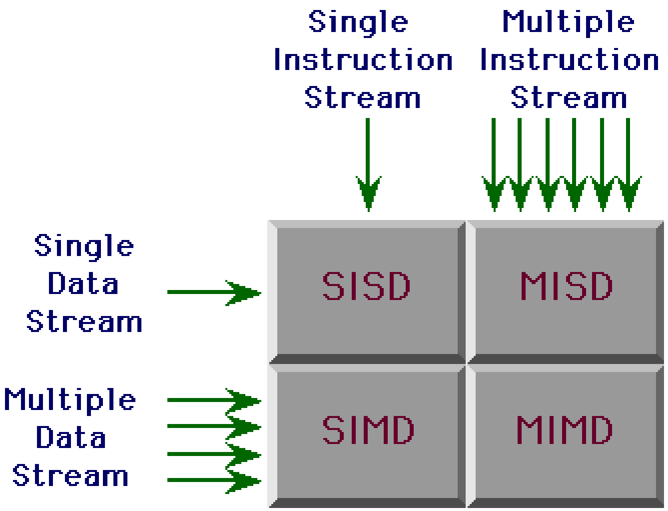
- The same instruction is executed by multiple processors using different data streams
- SIMD computers exploit data-level parallelism by applying the same operations to multiple items of data in parallel
- Each processor has its own data memory, but there is a single instruction memory and control processor, which fetches and dispatches instructions
- Examples are:
  - vector architectures
  - GPUs



Taxonomy of Computer Architectures

Multiple Instruction stream, Single Data stream – MISD

- **No** commercial multiprocessor of this type has been built to date
- But there can be possible future realizations/applications



Taxonomy of Computer Architectures

Multiple Instruction stream, Multiple Data stream – MIMD

- Each processor fetches its own instructions and operates on its own data, and it targets task-level parallelism
- MIMD computers can also exploit data-level parallelism, even if the overhead is likely to be higher than in a SIMD computer
- **Tightly coupled** MIMD architectures exploit thread-level parallelism since multiple cooperating threads operate in parallel
- **Loosely coupled** MIMD architectures - clusters and warehouse-scale computers - exploit request-level parallelism, where many independent tasks can proceed in parallel naturally with little need for communication or synchronization

High performance computers

- 1961 **IBM 7030 Stretch** → **10^6** Flops/sec (**megaFLOPS** *or* **MFLOPS**)
  - scalar processors
- 1984 **M-13** → **10^9** Flops/sec (**gigaFLOPS** *or* **GFLOPS**)
  - vector processors, shared memory
- 1997 **ASCI Red** → **10^{12}** Flops/sec (**teraFLOPS** *or* **TFLOPS**)
  - massive parallelism, distributed systems, message passing
- 2008 **IBM Roadrunner Red** → **10^{15}** Flops/sec (**petaFLOPS** *or* **PFLOPS**)
  - multicore processors, precision extension, fault tolerance
- 2012 **Fujitsu K** → **10,5 petaFLOPS**
- 2016 **Sunway TaihuLight** → **93 petaFLOPS**
- 2018 **Summit** → **200 petaFLOPS**

See https://www.top500.org/