INTENSIVE COMPUTATION

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2020-2021

Lecture 1

COURSE INFORMATION

Course topics

The course will cover **topics** that are in some sense related to **intensive computation**:

- Matlab (an introduction)
- Sparse matrices
- Eigenvectors and eigenvalues (graph connectivity, etc.)
- Errors
- Simulations
- Molecular Dynamics
- Computer architecture – Parallel architectures
- GPU (an introduction)
- Performance metrics and measurements

Time and venue

- **G0 room: Wednesday** 11:00-13:00 & **Friday** 10:00-13:00
- The course requires a quantity of hand-on work
- We will have **lectures** and **laboratory classes**

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

Course page is:

http://twiki.di.uniroma1.it/twiki/view/CI/WebHome

Exam

- **Homeworks** will be assigned during the course (usually due the next laboratory lesson)
- **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** (Matlab or GPU on 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***

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*

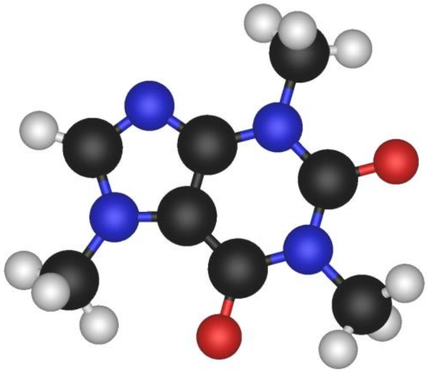
- The realization of these tasks can be :
  - Too ***difficult*** ------- wind tunnel
  - Too ***expensive*** ---- crash testing
  - Too ***slow*** ---------- the evolution of a galaxy
  - Too ***dangerous*** --- drugs, toxic gas diffusion

Chlorine release, 2010 Jack Rabbit I Program

Introduction

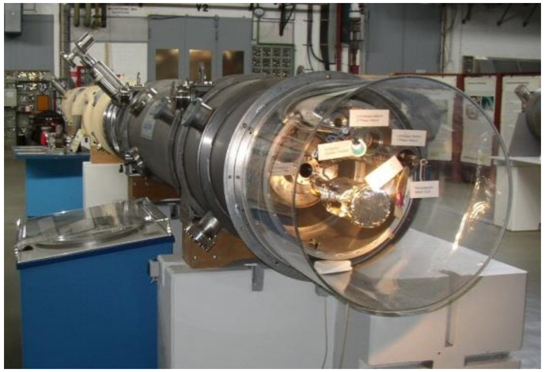
- **Computers** represent the fundamental tool for the simulation and can be seen both as a **microscope** and as a **telescope** with respect to space and to the time

- Examples:
  - To model molecules in details
  - To travel to the origin of the universe and study its evolution
  - To 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

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

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

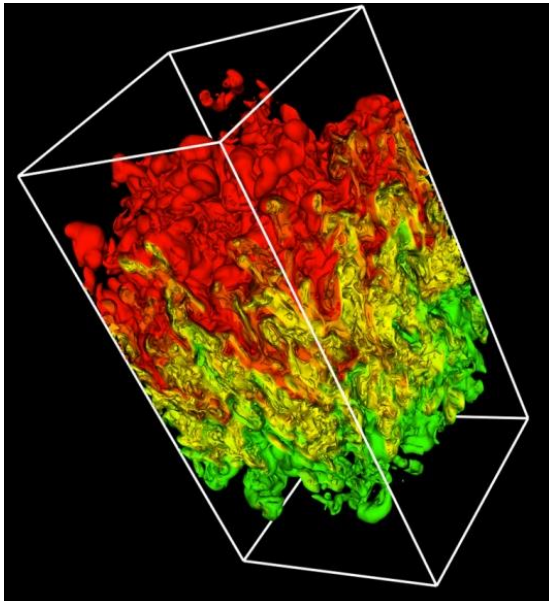
$$Z = Z_1 + Z_2$$

$$Z_1 = K_3 * Lux$$

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

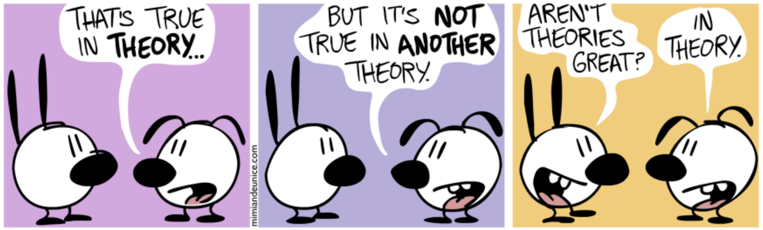
$$\frac{\mathrm{dLs1}}{\mathrm{dt}} = Ls * \left(1 - \frac{Ls}{K5}\right) * Z * \left(1 - \frac{Z}{K6}\right) \quad (1)$$

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



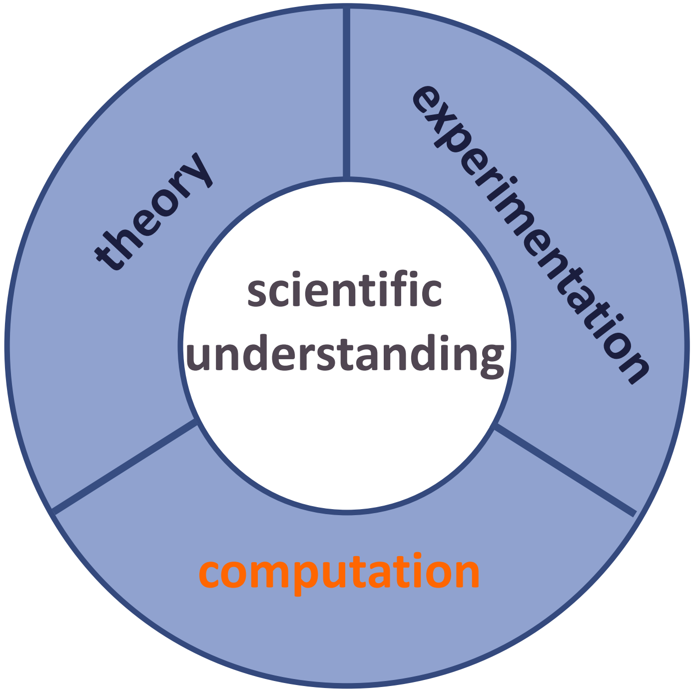
Computational Science

- 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

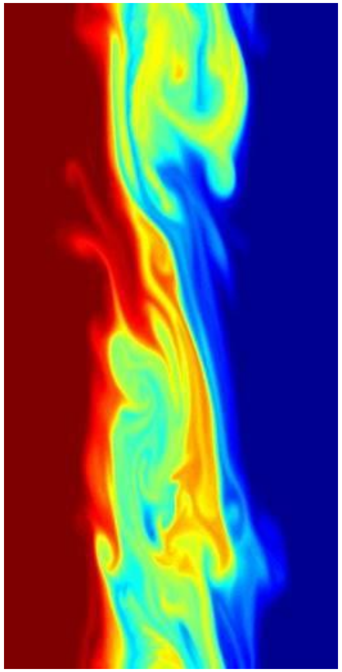
- In most cases, these models require **massive amounts of calculations** (usually floating-point numbers) that are executed on **supercomputers** or **distributed computing systems**

GRAND CHALLENGE PROBLEMS

Grand challenges

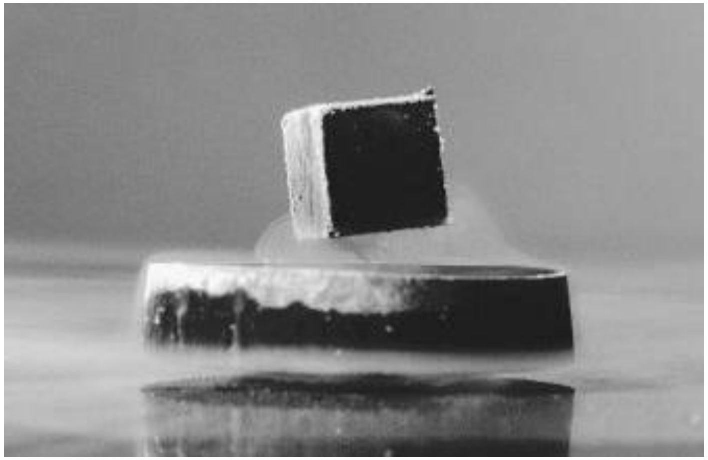
- **Grand Challenges** were USA policy terms set as goals in the late 1980s for funding high-performance computing and communications research
- *A grand challenge is a **fundamental problem** in science or engineering, with broad applications, whose solution would be enabled by the application of **high performance computing** resources that could become available in the near future*

Grand challenges

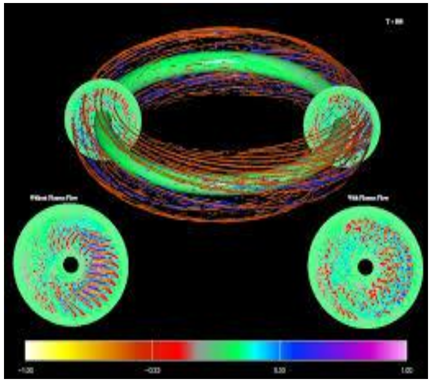


- **Computational fluid dynamics** for:
  - design of hypersonic aircraft, efficient automobile bodies, and extremely quiet submarines
  - weather forecasting for short and long term effects
  - efficient recovery of oil and other applications

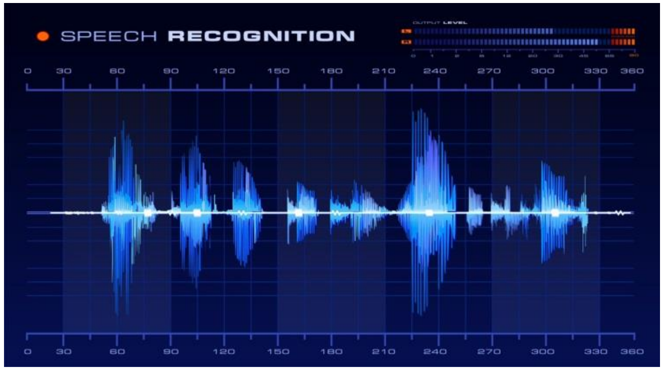
- Electronic structure calculations for the **design of new materials** such as:
  - chemical catalysts
  - immunological agents
  - superconductors



Grand challenges



- **Plasma dynamics** for fusion energy technology and for safe and efficient military technology
- Calculations to understand the fundamental **nature of matter**, including quantum chromodynamics and condensed matter theory

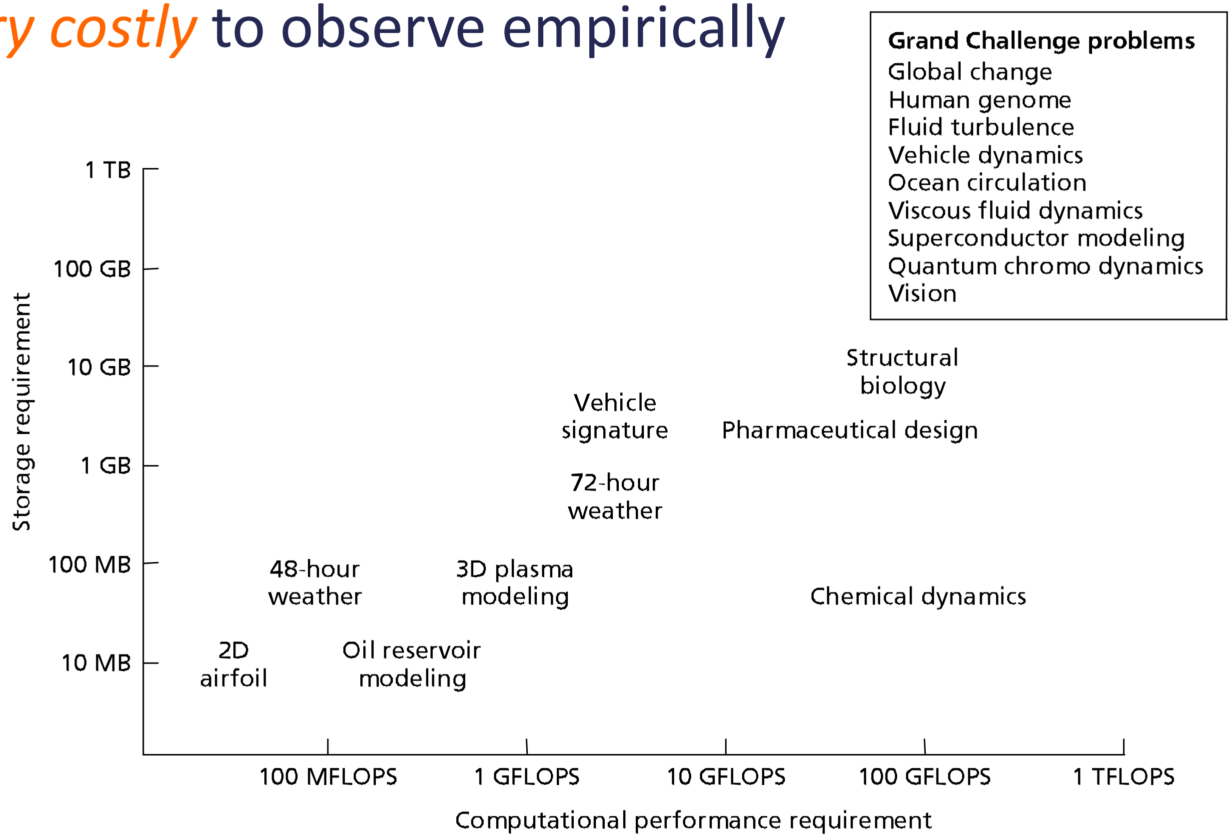


- Symbolic computations
  - speech recognition
  - computer vision
  - natural language understanding
  - automated reasoning
  - tools for design, manufacturing, and simulation of complex systems

Scientific Computing Demand

- The direct reliance on increasing levels of performance is most apparent in the field of computational science and engineering
- Computers are used to simulate physical phenomena that are *impossible* or *very costly* to observe empirically

Figure indicates the computational rate and storage capacity required to tackle a number of important science and engineering problems (1993)



21st Century Grand Challenges

- On April 2, 2013, President Obama called on companies, research universities, foundations, and philanthropists to join him in identifying and pursuing the Grand Challenges of the 21st century

- Grand Challenges are ambitious but achievable goals that harness **science**, **technology**, and **innovation** to solve important national or global problems and that have the potential to capture the public's imagination

AN EXAMPLE OF GRAND CHALLENGE PROBLEM

Greenhouse effect simulation

- As an example we describe an experiment done in the late ’90s for studying **global warming** a problem that is still studied and has been the subject of international attention
- This problem is studied by **computer simulations** to understand how changing concentrations of carbon dioxide in the atmosphere contribute to global warming through the greenhouse effect

- A study of this type requires **modeling the climate** over a long period of time

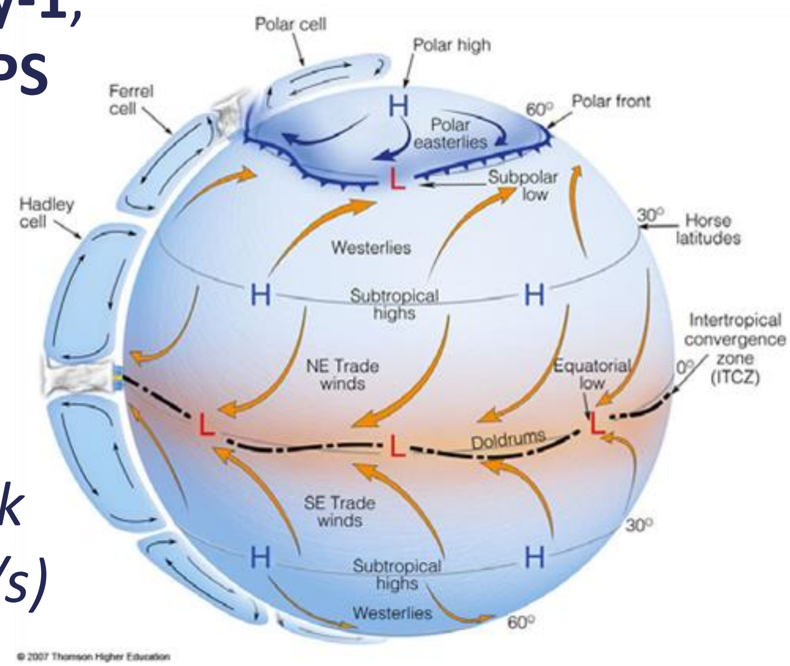
Greenhouse effect simulation

The climate model known as the **General Circulation Model**, GCM, was used by the National Center for Atmospheric Research

They studied the *warming which would be caused* by **doubling the concentration of carbon dioxide over a period of 20 years**

- The computations were done on a **Cray-1**, with a peak speed of about **200 MFLOPS** (200×10^6 flops/s):
  - 110 s per simulated day
  - 400 computational hours per two 19-year simulations

Today, a desktop processor (Intel i7) peak speed is about ***70 GFLOPS*** *(70×10^9 flops/s)*

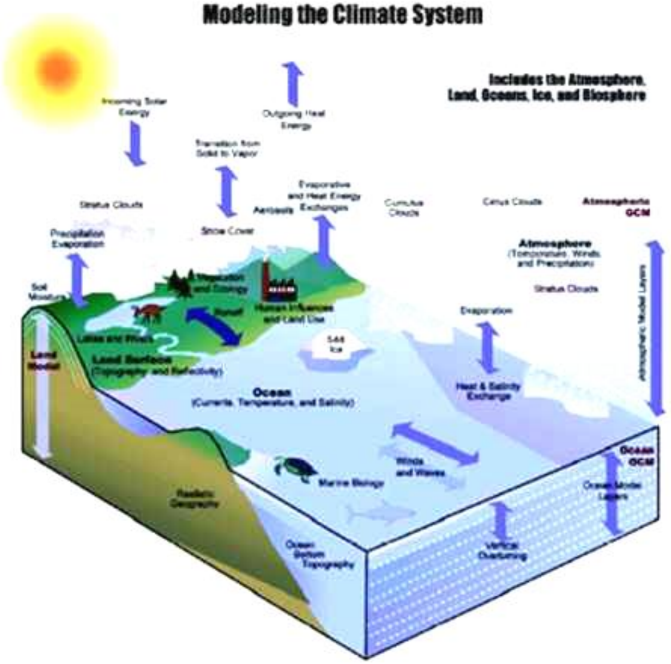


Greenhouse effect simulation

The effects that the GCM attempts to model are:

- The **atmosphere is a fluid** → the behaviour of fluids is described by **partial differential equations**

- Computer solution of these equations is obtained by means of the **finite difference algorithm** in which derivatives with respect to spatial coordinates and time are approximated by difference formulas

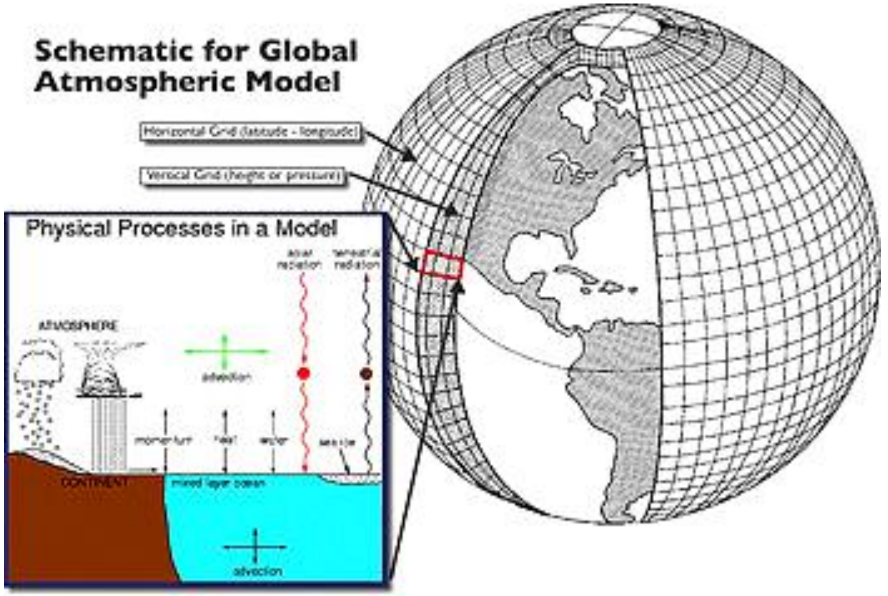


Greenhouse effect simulation

- A **3D mesh in space** is considered

The mesh used in the computations was composed by:

- about **2000 points** to cover the surface of the earth
- **9 layers** of different altitudes



- There are **8-9 variables at each mesh point** that must be updated (*temperature, CO_2 concentration, wind velocity, etc.*)

- Computer **performance** is very important!!

Greenhouse effect simulation

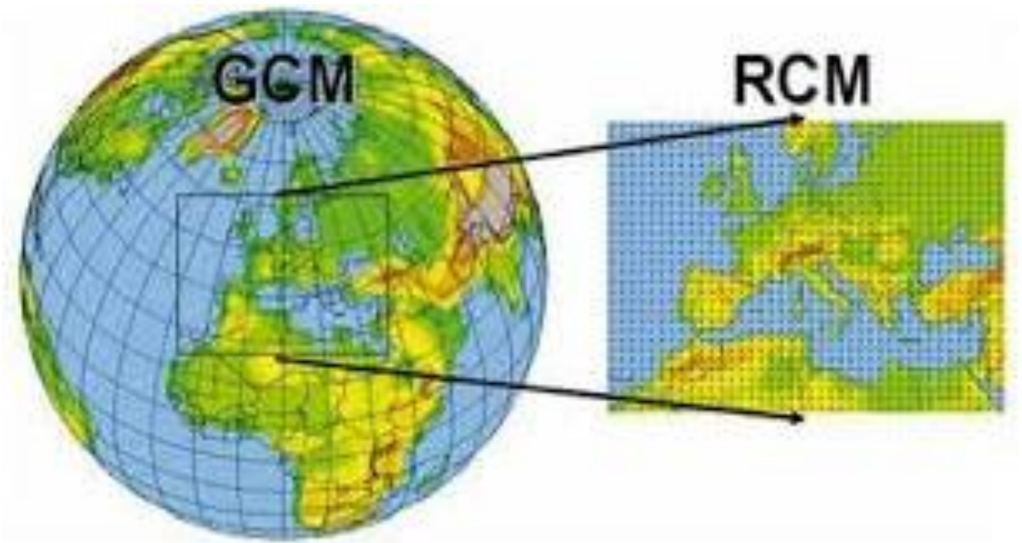
- Solution of the problem needs a ***set of initial conditions*** for which values are assigned to the variables at each mesh point and stepping forward in time updating these variables at the end of each step

- **Observation** The mesh is *extremely coarse*!!

- Infact the surface of the earth is 5,1 x 10^8 km^2 → one mesh point over an area 2,6 x 10^5 km^2, that is on a *land area like Spain-Portugal there are 2 mesh points*!

Greenhouse effect simulation

- We would like to have a **greater accuracy**, that is more mesh points
- If we **double** the density of points in each of the three directions:
  - We increase the number of mesh points of a factor of 8
  - The computation that took ***400 hours*** in this case would take over **3000 hours**, but we still have only ***few points*** on Spain-Portugal

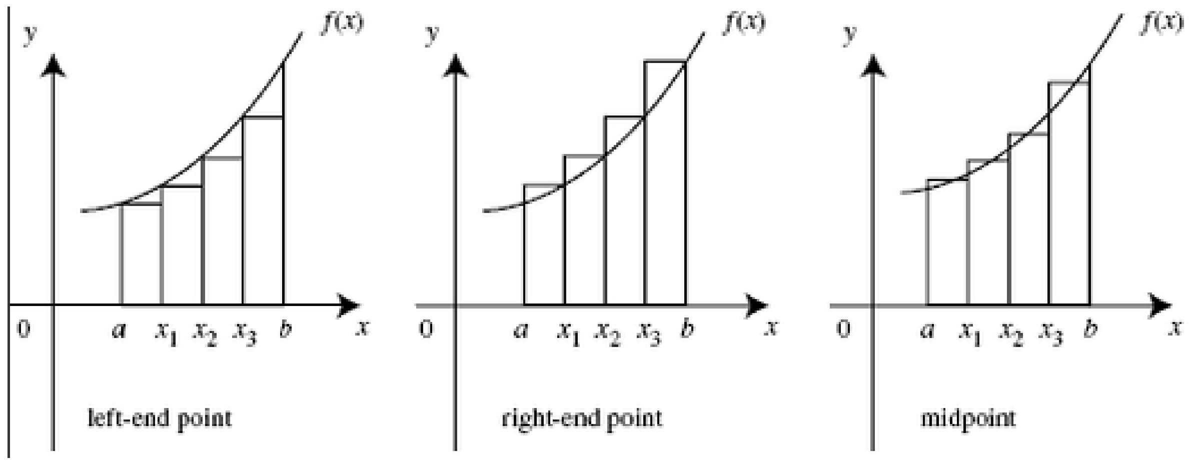


GENERAL STRATEGY

General Strategy

When we define a **solution for a computational problem**, the general strategy is:

- To substitute a ***difficult problem*** by an **easier problem** with the ***same solution or solution quite similar***



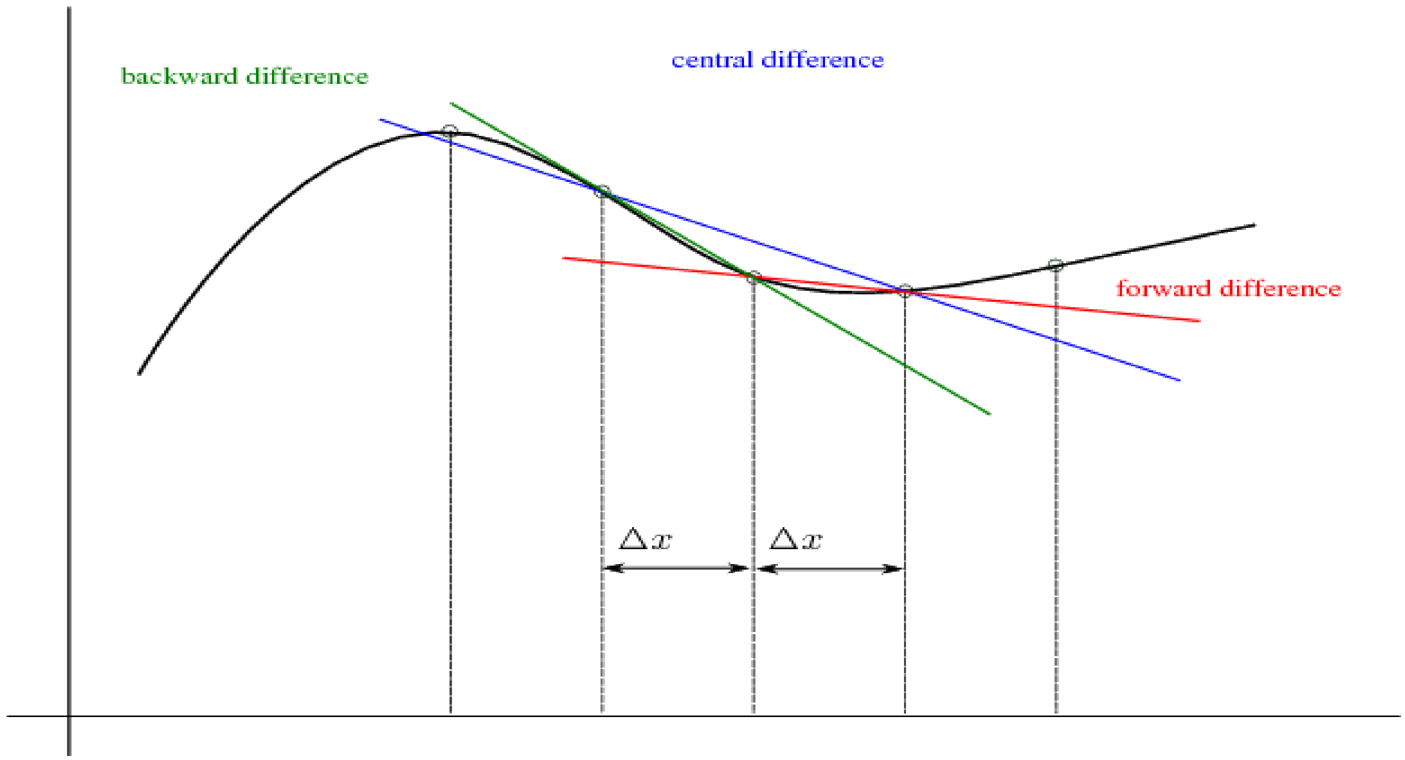
General Strategy

To this end we can:

- substitute ***infinite spaces*** with **spaces of finite dimension**
- substitute ***infinite processes*** with **finite processes**
  - for example we can substitute ***integrals*** or ***infinite series*** with **finite sums** or we can substitute ***derivatives*** with **finite differences**
- substitute ***differential equations*** with **algebraic equations**
- substitute ***non linear problems*** with **linear problems**
- substitute ***higher degree problems*** with **lower degree problems**
- substitute ***difficult functions*** with **simpler functions** (polynomials)
- substitute ***general matrices*** with **simpler matrices**

General Strategy

At each step it is needed to ***verify that the solution doesn't change*** or it changes within a threshold with respect to real solution



Example

To solve a **system of nonlinear differential equations** (dynamical systems) we can:

- Substitute the system of differential equations with a system of **algebraic equations**
- Substitute the nonlinear algebraic system with a **linear system**
- Substitute the matrix of the linear system with a **matrix with a simpler solution** to compute

$$\frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} = 0 \quad \text{is linear} .$$

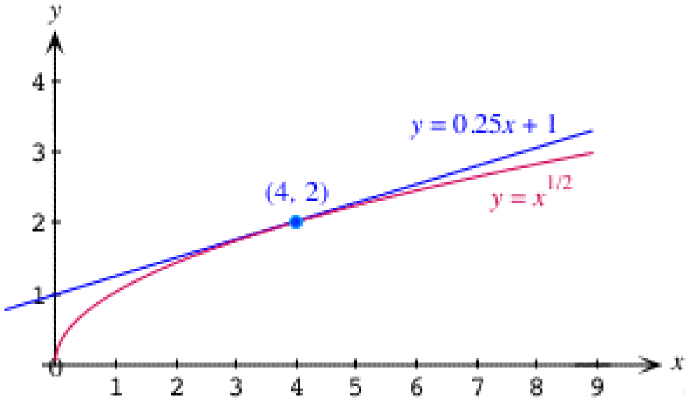
$$\frac{\partial u}{\partial x_1} + \left(\frac{\partial u}{\partial x_2}\right)^2 = 0 \quad \text{is nonlinear}$$

$$\frac{\partial u}{\partial x_1} + \frac{\partial u}{\partial x_2} + u^2 = 0 \quad \text{is nonlinear}$$

General Strategy

- To make the general strategy appliable, we need:
  - A problem or a class of problems **easier to solve**
  - A ***transformation*** from the given problem to the simplified problem that ***preserve the solution***

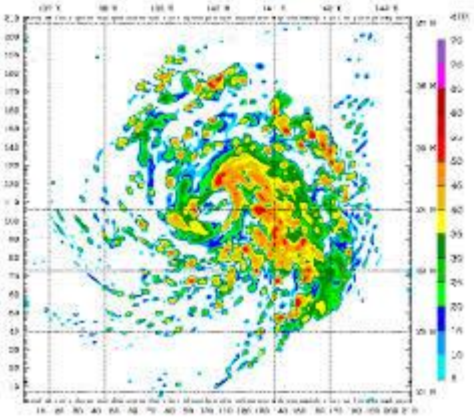
- If the **solution** of the new problem (the transformed problem) is an **approximation of the real solution**, then we have to estimate the **accuracy** and to compute the **convergence toward the real solution**
- The accuracy can be made as good as we want by using time consuming and memory consuming computations

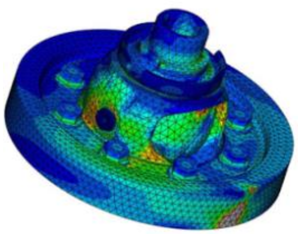


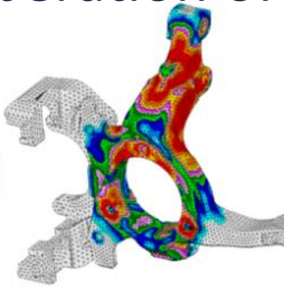
SIMULATION AND SOLUTIONS

Simulations

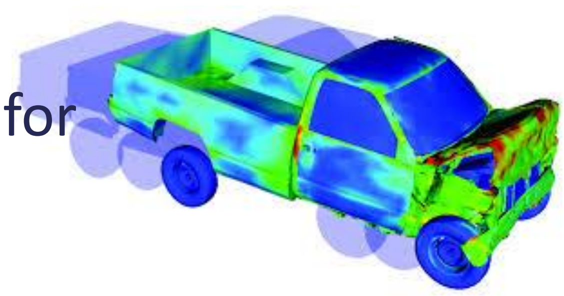
- Computer simulation has become an important part of modeling:
  - natural systems in physics, chemistry and biology
  - human systems in economics and social science
  - engineering to gain insight into the operation of systems







- Typical problems:
  - Handle big quantity of data
  - Consider scale with very small or huge values for distances and time (molecules, astronomy)



Simulations

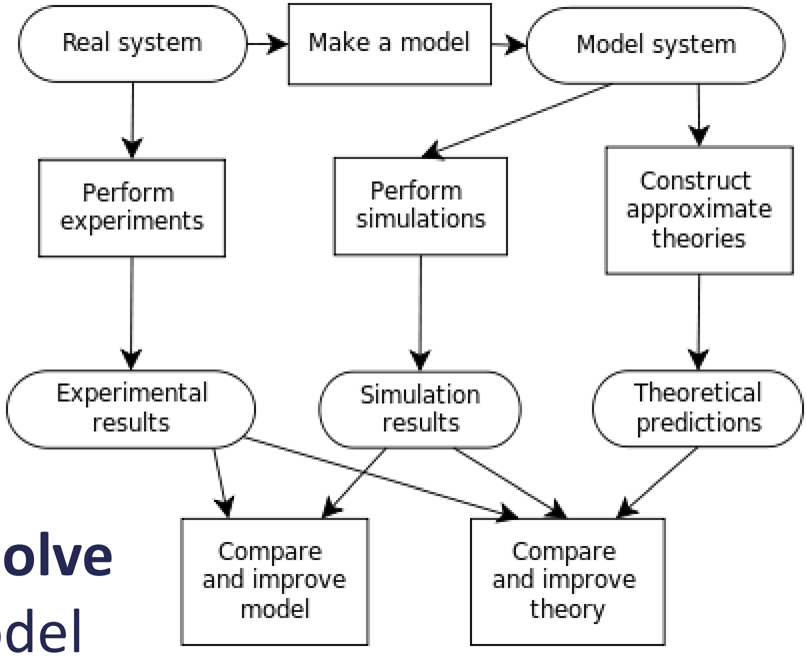
By using **computer simulations** it is possible:

- To test the behaviour of a model by varying the value of a set of **parameters**
- To consider different **options** in a way which is **faster**, **cheaper** and **safer** if compared with real or traditional tests (e.g. crash testing)

Solutions and simulations

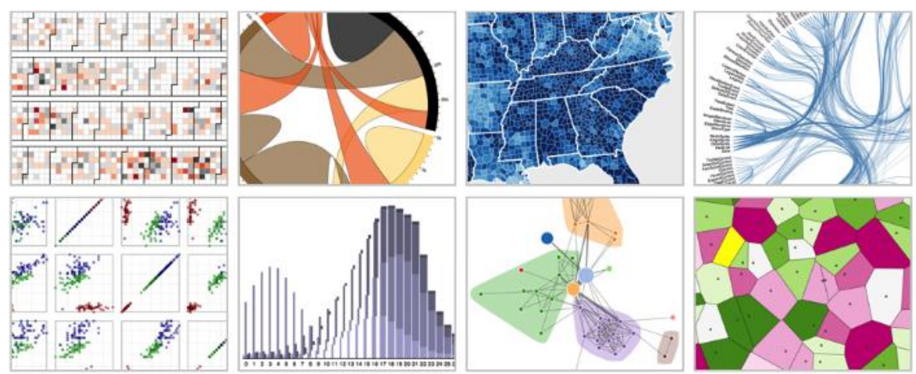
The solution of a problem by means of computational simulations requires a ***sequence of steps***:

- To develop a **mathematical model**, consisting of equations describing the **physical system or phenomenon of interest**
- To develop **algorithms** to numerically **solve the equations** of the mathematical model
- To implement the algorithms with a **suitable language** or in a **suitable software environment**
- …



Solutions and simulations

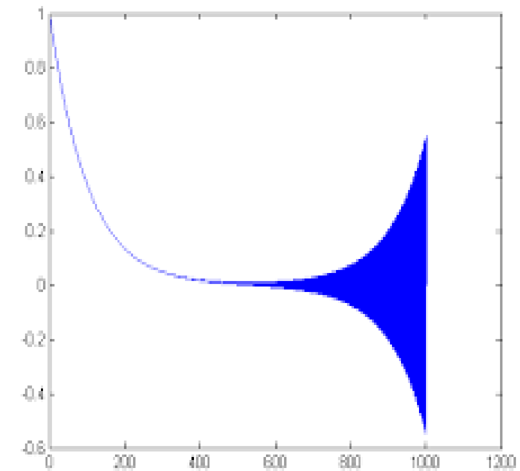
- To run programs on a **high performance computer** selected for the specific problem
- To represent computed data using a **graphical visualization** that makes them **understandable**
- To **validate** and to **interpretate** the obtained results



- In this process each step influences and is influenced by the other steps → it is common to repeate some of the steps

Solutions and simulations

- A problem is said **well-posed** (Hadamard 1923) if:
  - a **solution exists**,
  - the solution is **unique** and
  - it **continuously changes with the initial conditions**
- Continuum models must often be discretized in order to obtain a numerical solution
- While solutions may be continuous with respect to the initial conditions, they may suffer from **numerical instability** when solved with **finite precision** or with **errors in the data**

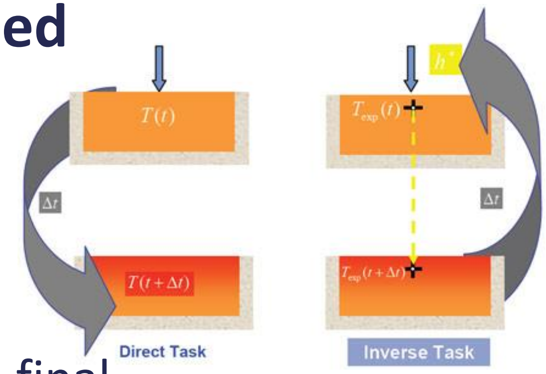


Solutions and simulations

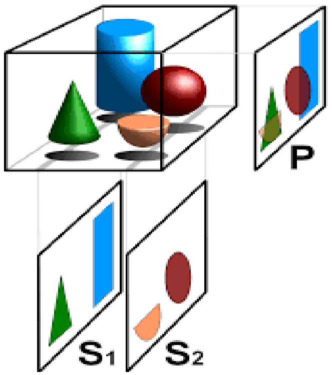
- If the problem is well-posed, then it stands a good chance of solution on a computer using a stable algorithm
- If it is not well-posed, it needs to be re-formulated for numerical treatment
- Typically, this involves including **additional assumptions**, such as smoothness of solution
- Even if a problem is well-posed, it may still be **ill-conditioned**, meaning that a ***small error in the initial data can result in much larger errors in the solution***

Solutions and simulations

- Problems that are not well-posed are said **ill-posed**



- **Inverse problems** are often ill-posed
  - ***Inverse heat equation***
    - Deduces a previous distribution of temperature from final data
    - It is not well-posed → the solution is highly sensitive to changes in the final data
  - ***Internal structure of a physical system*** from an external observation, as in tomography or in seismology
    - Often the derived problems are ill-posed because ***very different configurations*** can assume the ***same external appearance***



AN EXAMPLE IN THE PARALLEL CONTEXT

Example for parallel architectures

- Let us consider an example from the Grand Challenge program to understand the **interaction** between applications, architecture, and technology in the context of parallel machines

- A 1995 study examined the effectiveness of a wide range of parallel machines on a variety of applications

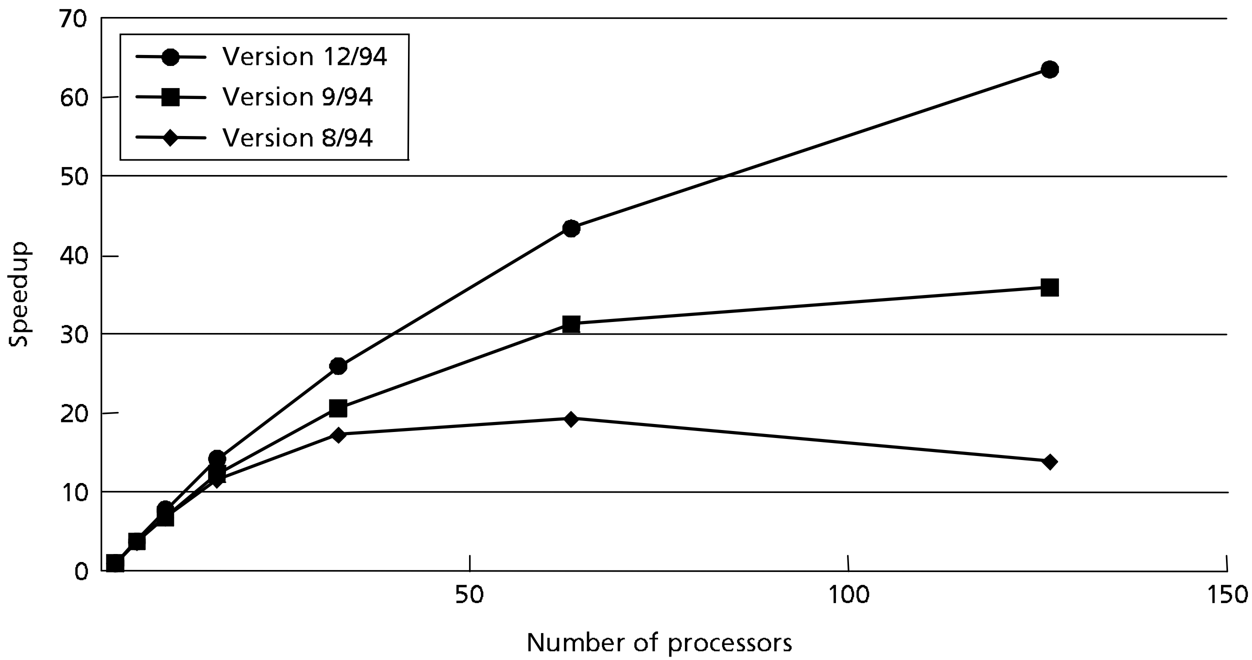
- **AMBER** (Assisted Model Building through Energy Refinement) - a *molecular dynamics package*
- AMBER is widely used to simulate the motion of large biological models such as proteins and DNA

Example for parallel architectures

- The code was developed on **Cray vector supercomputers**, which employ:
  - custom ECL-based processors
  - large expensive SRAM memories (instead of caches)
  - machine instructions that perform arithmetic or data movement on *vector* of data values

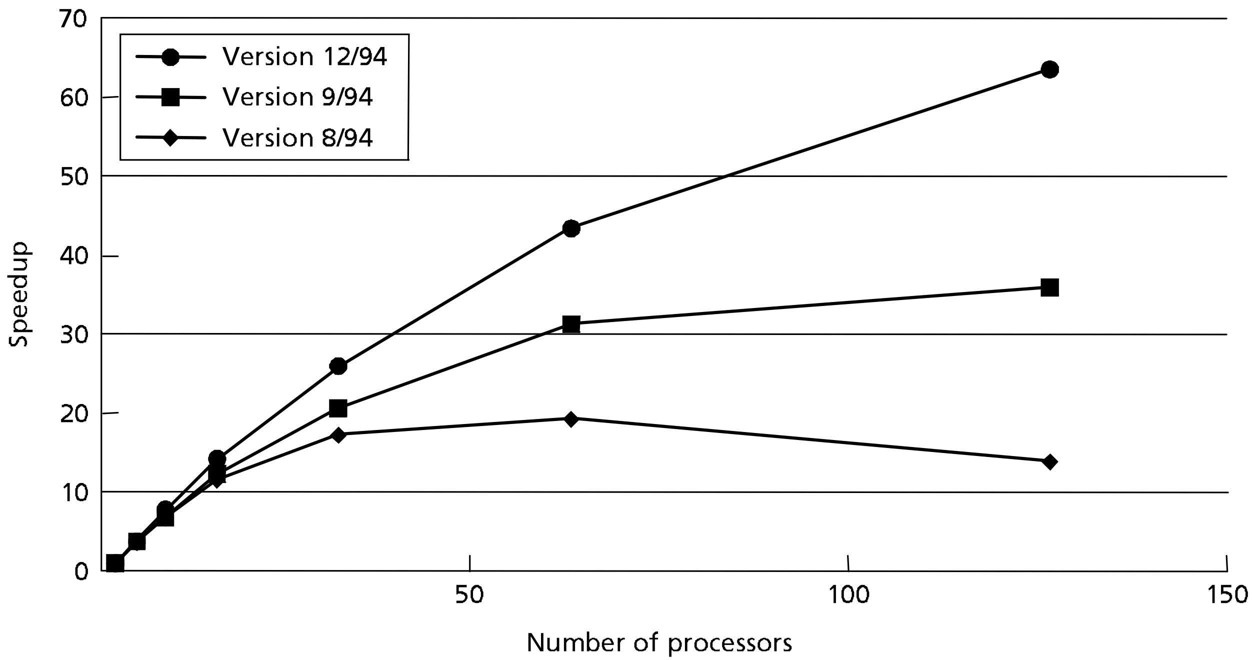
- The test involves the simulation of a protein solvated by water: 99 *amino acids*, 3,375 *water molecules* for a total of about 11,000 *atoms*

Example for parallel architectures



- Figure shows the speedup obtained on *three versions* of code on the Intel Paragon a 128-processor microprocessor-based machine
- **vers. 8/94 -** ***initial parallelization*** → good speedup for small configurations, but poor speedup on larger configurations

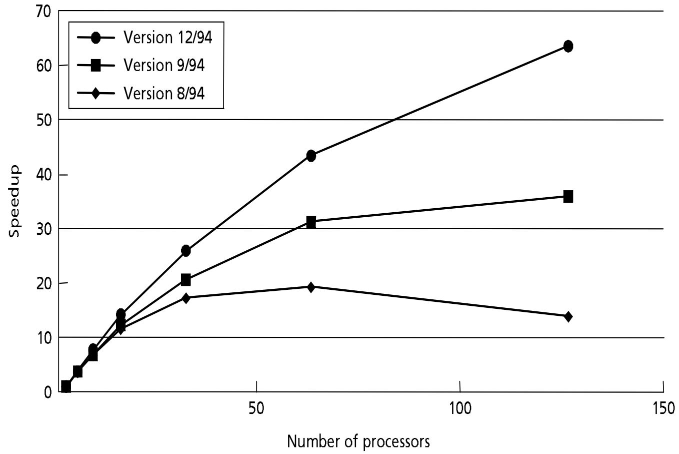
Example for parallel architectures



- **vers. 9/94 -** the ***balance of work*** done by each processor improved the scaling of the application significantly
- **vers. 12/94 -** ***optimization of the communication*** produced a highly scalable version

Example for parallel architectures

- This sort of *learning curve* is quite typical in the parallelization of important applications, as is the *interaction between application and architecture*
- The **application writer** studies the application to understand the demands it places on the available architectures and how to improve its performance on a given set of machines
- The **architect** studies these demands to understand how to make the machine more effective on a given set of applications
- The **end user** of the application enjoys the benefits of both efforts



GENERATION OF COMPUTERS AND TAXONOMY

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 - 100,000 devices on a chip
4. **VLSI**
   - Very large scale integration - 1978-1991

     100,000 - 100,000,000 devices on a chip
   - Ultra large scale integration - 1991-

     Over 100,000,000 devices on a chip

High performance computing

High Performance Computing (HPC):

- Generally refers to the practice of aggregating computing power to deliver higher performance with respect to a typical desktop computer or workstation
- It is used to solve large problems in science, engineering, or business

HPC tasks are characterized as needing ***large amounts of computing power***

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**

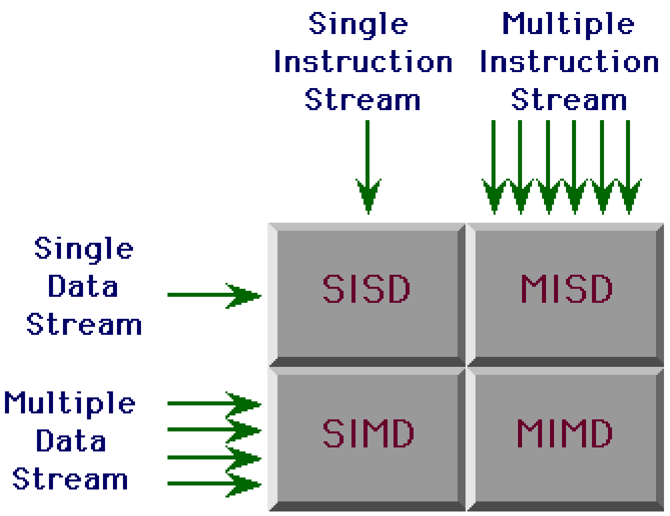
Taxonomy of Computer Architectures

- The idea of obtaining more performance by utilizing multiple resources is quite dated

- In 1966 Michael Flynn introduced a **taxonomy** of computer architectures that is still the *most common way of categorizing* systems with **parallel processing capability**

Taxonomy of Computer Architectures

- 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**

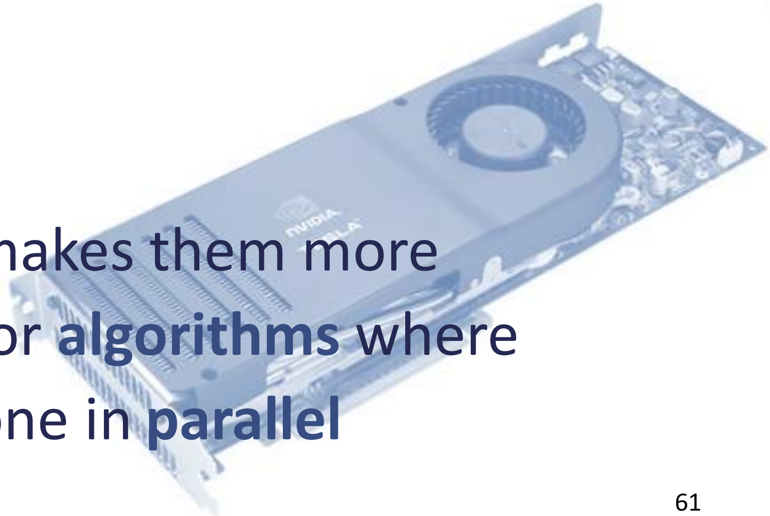


GPU and GPGPU

- **GPU, Graphics Processing Unit,** is a specialized electronic circuit designed to rapidly manipulate computer graphics and to render 3D images

- **GPGPU** (General Purpose computing on GPU) is the utilization of a GPU to perform computation in applications traditionally handled by CPU

- The highly parallel structure of GPUs makes them more effective than general-purpose CPUs for **algorithms** where processing of large blocks of data is done in **parallel**



GPU and GPGPU

Some of the areas where GPUs have been used for general purpose computing are:

- Weather forecasting
- Molecular dynamics
- Computational finance
- Protein alignment and genoma project

MATLAB

MATLAB (**Mat**rix **Lab**oratory) allows **matrix** manipulations, plotting of **functions and data**, implementation of **algorithms**, creation of user interfaces, and interfacing with programs written in other languages (including C, Java and Fortran)

MATLAB provides:

- mathematical functions for linear algebra, statistics, Fourier analysis, filtering, optimization, numerical integration, and solving ODE
- graphic functions for 2D and 3D data representation
- many specialized toolboxes