INTENSIVE COMPUTATION

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Course topics

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

- Matlab (an introduction)
- GPU (an introduction)
- Sparse matrices
- Eigenvectors and eigenvalues, graph connectivity
- Molecular Dynamics
- Global search
- IEEE floating point representation and arithmetic
- Errors
- Simulations

Time and venue

- **Aula Alfa:** **Tuesday** 14:00-15:30 and **Thursday** 12:00-13:30

- The course requires a quantity of hand-on work

- We will have **lectures** and **laboratory classes**

- **Laboratory** (**Colossus**??) according to the previous lecture

- Lectures will be given by using slides or by using the blackboard

Course page is:

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

Exam

- **Homeworks** will be assigned during the course (due the next laboratory lesson)
- Two mid-term exams or a final exam - written
  - Mid-term and final exams consist in a written test and exercises
- Oral exam or Project (Matlab or GPU on one course topics)

There is not a book

– I will give you slides and references on the topics of the course

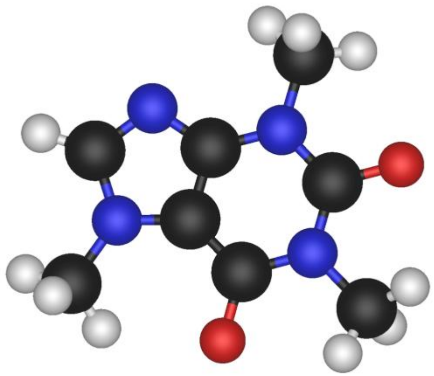
Introduction

- 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

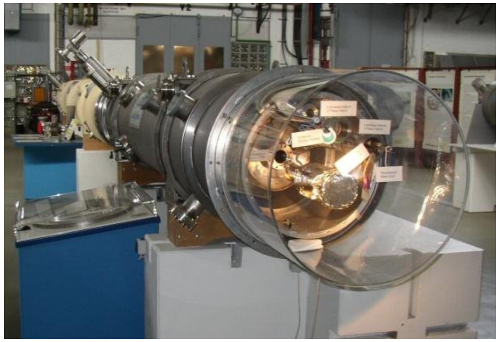
- **Computers** represent the fundamental tool for the simulation and can be seen both as a **microscope** and as a **telescope** with respect to space and to the time



- 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 is concerned with:
  - mathematical models
  - quantitative analysis techniques
  - using computers
  - to analyze and solve scientific problems

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

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

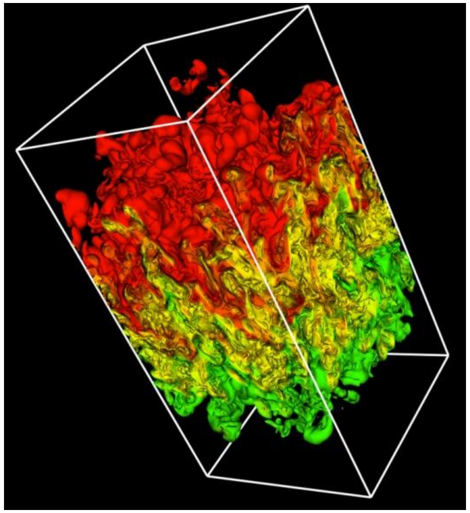
$$\mathrm{Z} = Z_1 + Z_2$$

$$Z_1 = K_3 * Lux$$

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

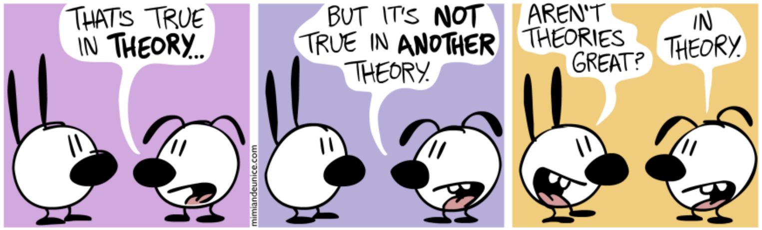
$$\frac{\mathrm{dLs1}}{\mathrm{dt}} = Ls * \left(1 - \frac{Ls}{K5}\right) * Z * \left(1 - \frac{Z}{K6}\right) \qquad (1)$$

- 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 experimentation/observation and theory

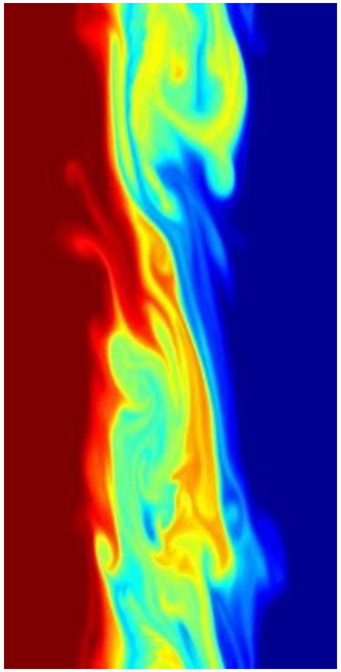
Computational Science

- 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**

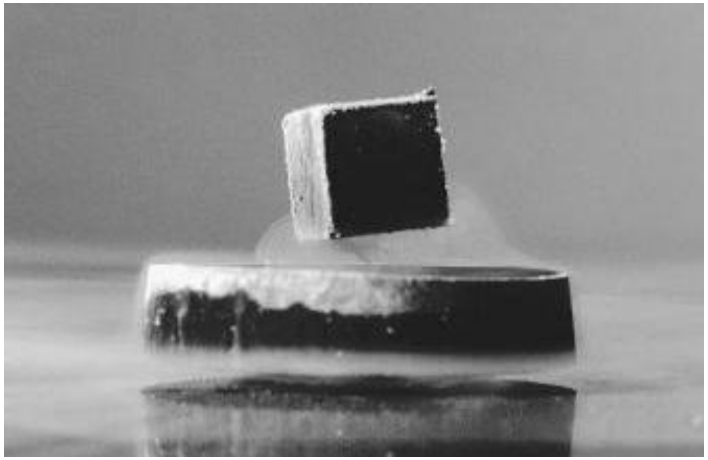
Grand challenges

- **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

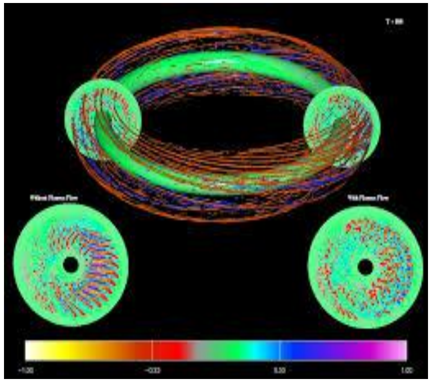


- **Computational fluid dynamics** for:
  - design of hypersonic aircraft, efficient automobile bodies, and extremely quiet submarines
  - weather forecasting for short and long term effects
  - efficient recovery of oil and other applications
- Electronic structure calculations for the **design of new materials** such as:
  - chemical catalysts
  - immunological agents
  - superconductors

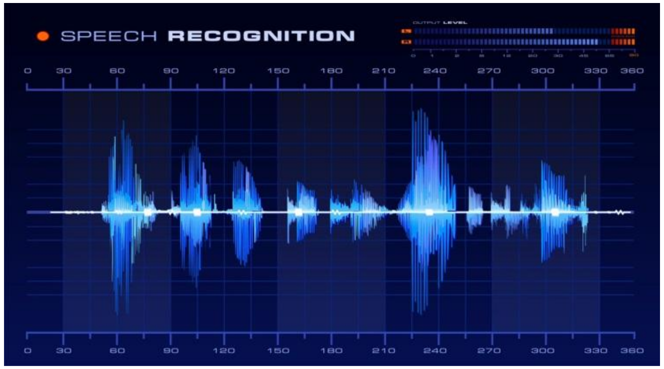


Grand challenges

- **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 including speech recognition



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

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

Greenhouse effect simulation

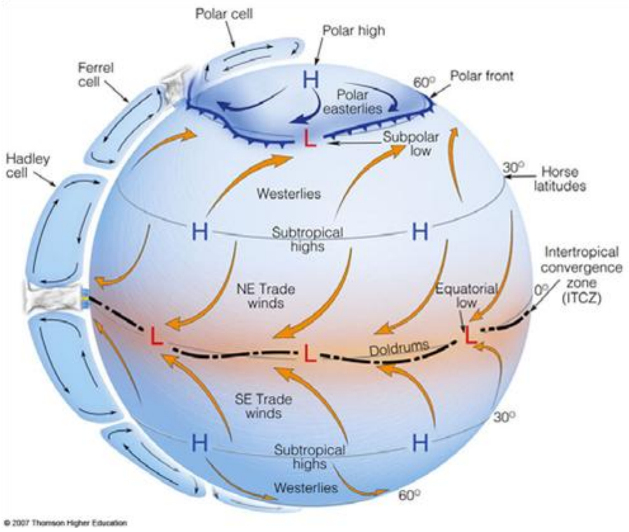
- As an example we describe an experiment done in the late ’90s for studying **global warming** a problem that is still studied and has been the subject of international attention
- This problem is studied by **computer simulations** to understand how changing concentrations of carbon dioxide in the 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 to study 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** ($2x10^2x10^6$ flops/s):
  - 110 s per simulated day
  - 400 computational hours per two 19-year simulations



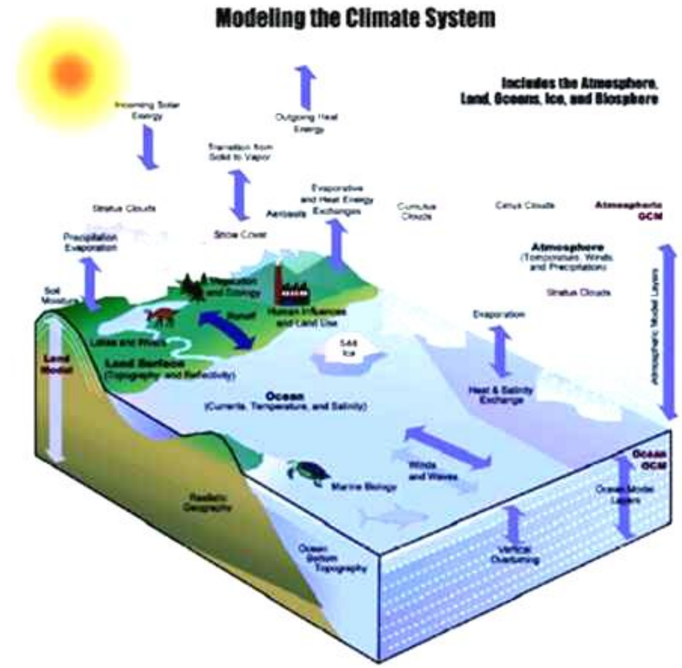
Today, a desktop processor (Intel i7) peak speed is about **70 GFLOPS** ($70x10^9$ flops/s)

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.

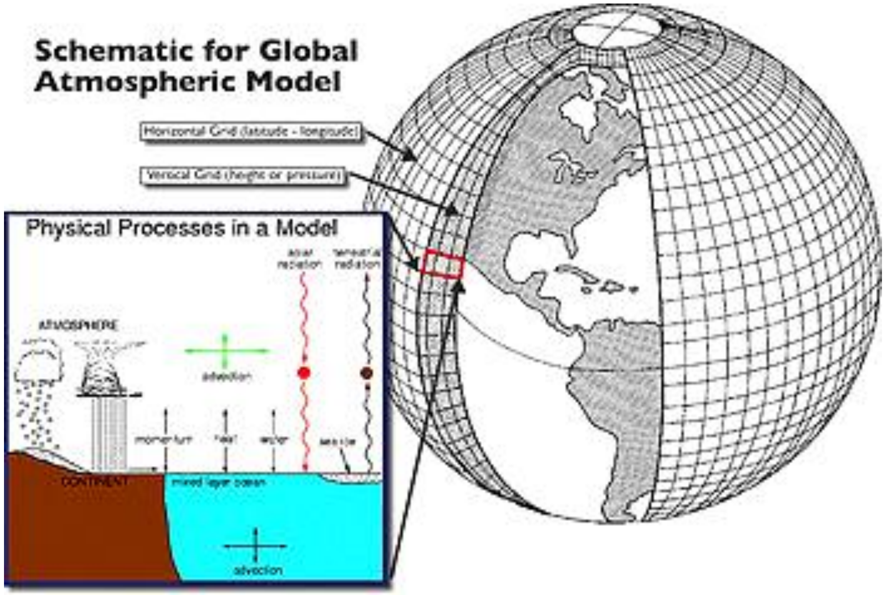


Greenhouse effect simulation

- 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 and 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

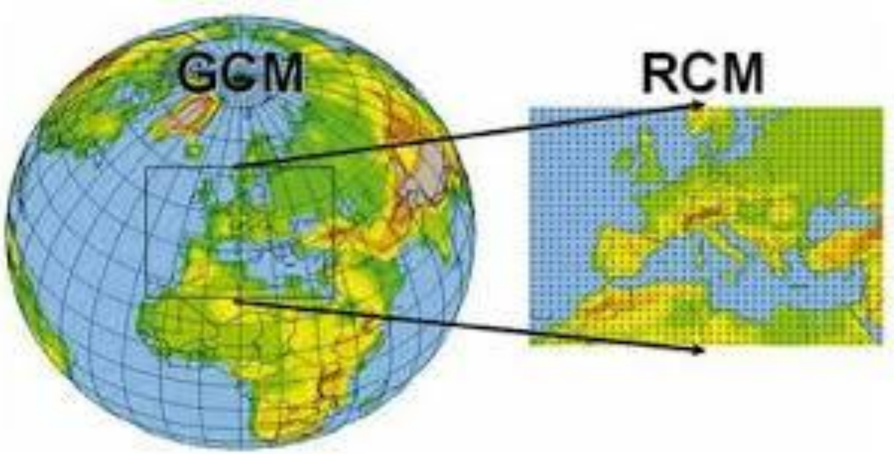
- **Observation** The mesh is extremely coarse!!

- 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

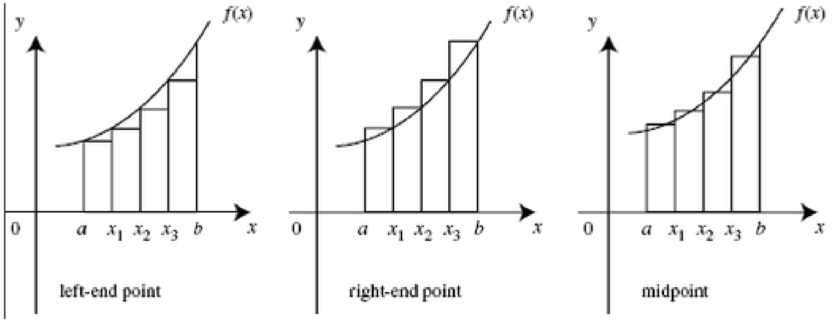
- If we **double** the density of points in each of the three directions:
  - we increase the number of mesh points of a factor of 8
  - the computation that took ***400 hours*** in this case would take over **3000 hours**, but we still have only **few points** on Spain-Portugal



General Strategy

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***



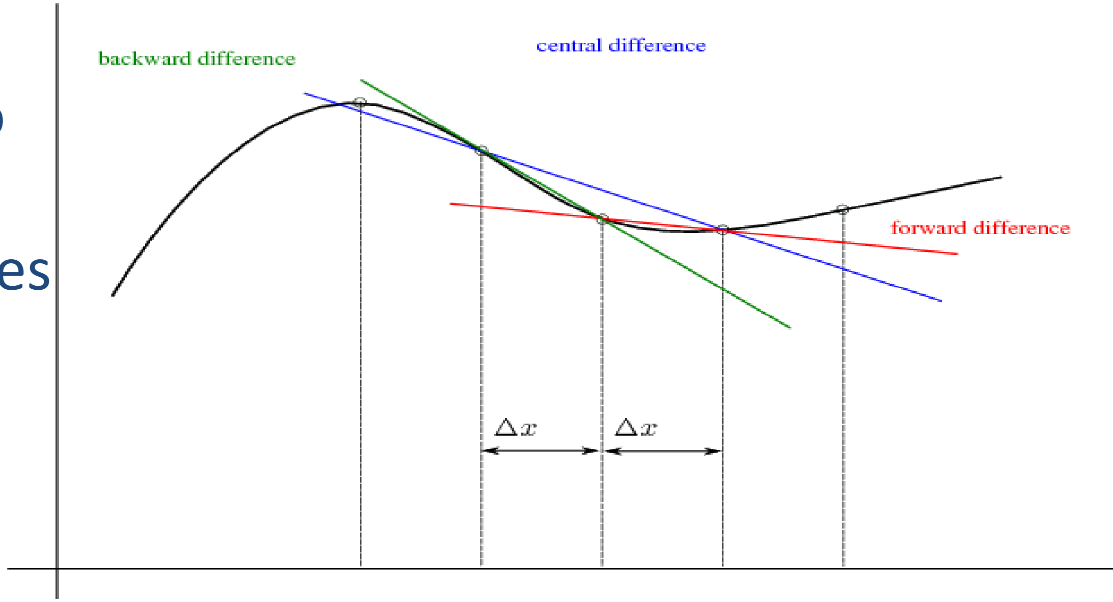
To this end we can:

- 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**

General Strategy

- 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**

- 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

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

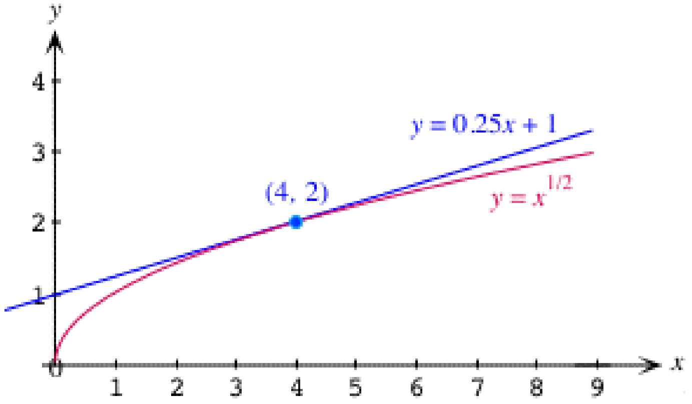
$$\frac{\partial u}{\partial x_1} + \left(\frac{\partial u}{\partial x_2}\right)^2 = 0 \quad \text{is nonlinear}$$

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

General Strategy

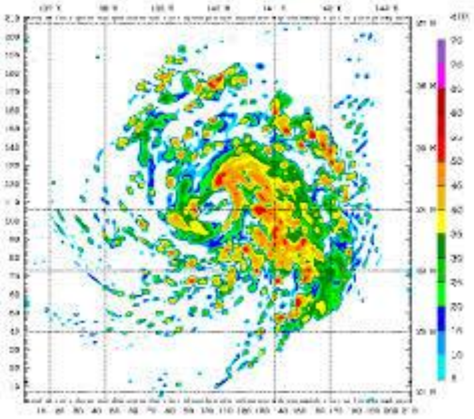
- To make the general strategy appliable, we need:
  - A problem or a class of problems **easier to solve**
  - A ***transformation*** from the given problem to the simplified problem that ***preserve the solution***

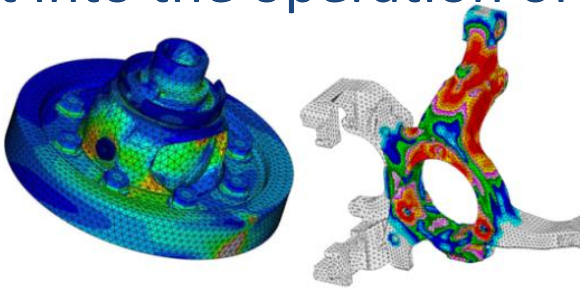
- If the **solution** of the new problem (the transformed problem) is an **approximation of the real solution**, then we have to estimate the **accuracy** and to compute the **convergence toward the real solution**
- The accuracy can be made as good as we want by using time consuming and memory consuming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



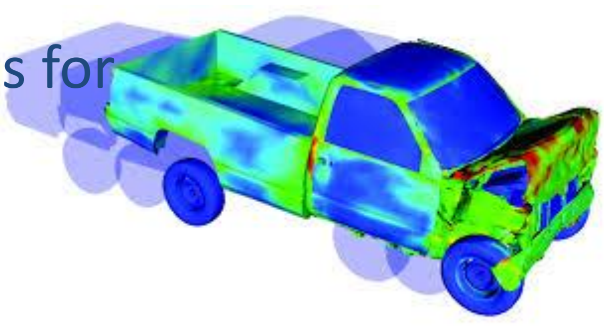
Simulations

- 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

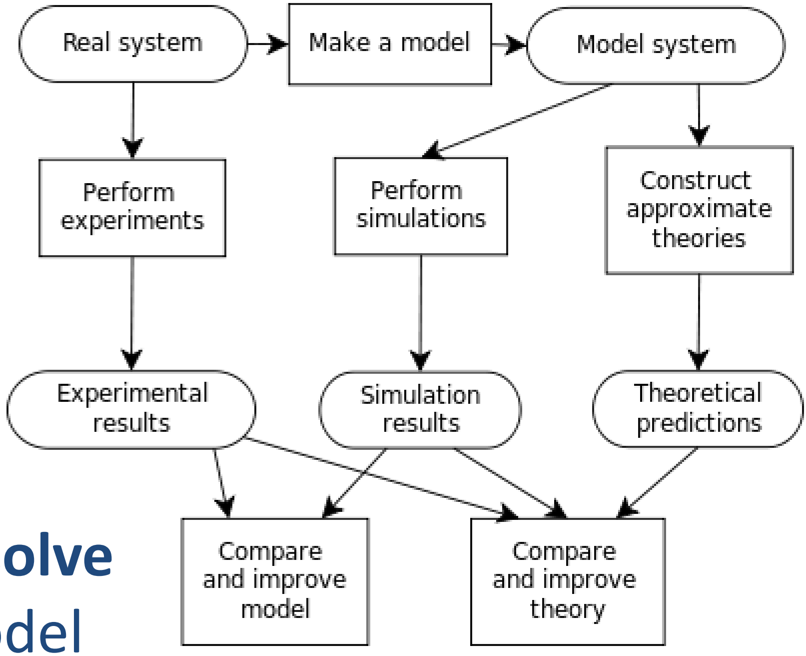
By using **computer simulations** it is possible:

- 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

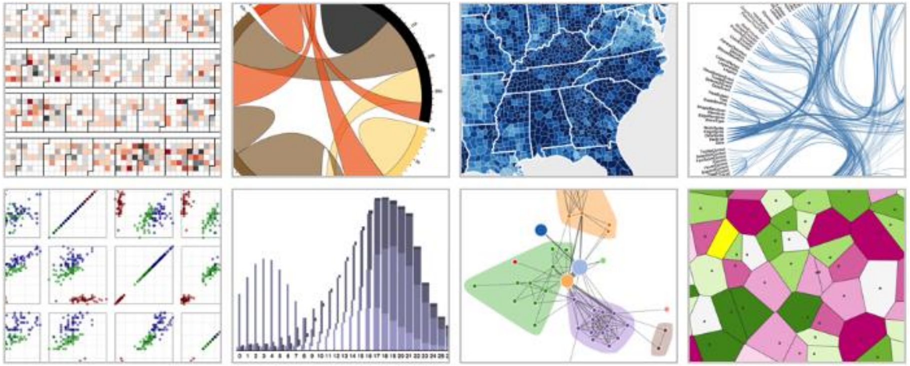
The solution of a problem by means of computational simulations requires a sequence of steps:

- 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, and to repeate some of the previous steps



- Note that in this process each step influences and is influenced by the other steps

Solutions and simulations

- A problem is said **well-posed** 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 termed **ill-posed**

- **Inverse problems** are often ill-posed
  - For example, the ***inverse heat equation***, deducing a previous distribution of temperature from final data, is not well-posed in that the solution is highly sensitive to changes in the final data
  - Another example is the study of ***internal structure of a physical system*** from an external observation, as in the case of tomography or in seismology. Often the derived problems are ill-posed because very different configurations can assume the same external appearance

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
- 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

- **25 years ago**
  - **1×10^6** Flops/sec (**Mflop/s**)
  - scalar processors

- **15 years ago**
  - **1×10^9** Flops/sec (**Gflop/s**)
  - vector processors, shared memory

- **A few years ago**
  - **1×10^{12}** Flops/sec (**Tflop/s**)
  - massive parallelism, distributed systems, message passing

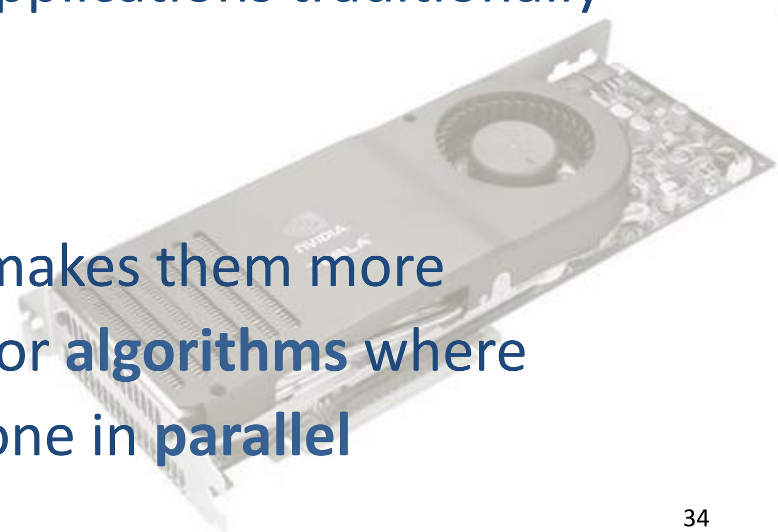
- **Today**
  - **1×10^{15}** Flops/sec (**Pflop/s**)
  - multicore processors, precision extension, fault tolerance

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