# "Modeling and Simulations": A Short Introduction to Numerical Simulations

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Course web page: https://elearn.uoc.gr/ Course: Τμήμα Μαθηματικών και Εφαρμοσμένων Μαθηματικών, *«ΜΕΜ-286 Μαθηματική Μοντελοποίηση και Αριθμητική Προσομοίωση»*

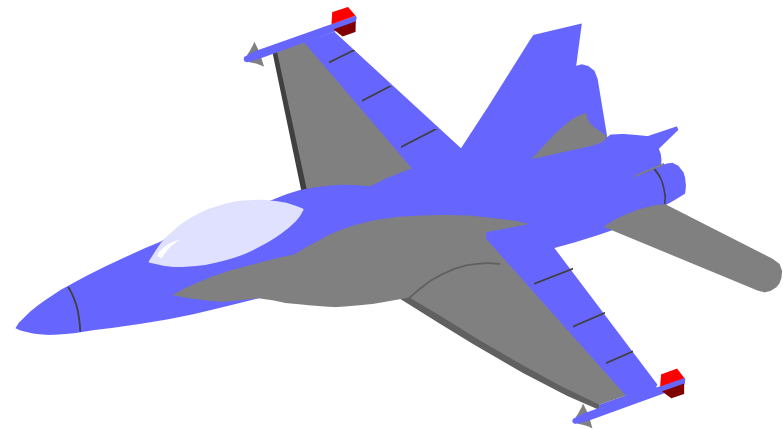**Any idea?**

❑ **Webster's Dictionary:**

*" to assume the mere appearance of ,
without the reality"*

# What are Simulations?

❑ **Definition:**

*"Simulation is the process of designing a model of a real system and conducting experiments with this model for the purpose of either understanding the behavior of the system and/or evaluating various strategies for the operation of the system."*

- *Introduction to Simulation Using SIMAN*
  *(2nd Edition)*

# Why do we need Simulations?

❑ **Simulation allow us:**

➢ Model *complex systems* in a detailed way

➢ Describe the *behavior* of systems

➢ Construct *theories or hypotheses* that account for the observed behavior

➢ Use the model to *predict future behavior*, that is, the effects that will be produced by changes in the system

➢ *Analyze* proposed systems


❑ *Simulation is one of the* *most widely used* *techniques in operations research and  management science...*

*No longer the approach of  "last resort"!*

❑ **Not a very old technique:**

❖ **World War II, '40s**
  ➢ *"Monte Carlo"* simulation: originated with the work on the atomic bomb. Used to simulate bombing raids. Given the security code name "Monte-Carlo"
  ➢ Still widely used today for certain problems which are not analytically solvable (for example: complex multiple integrals, optimization problems, etc.)

❖ **Late '50s, early '60s**
  ➢ Computers improve
  ➢ First languages introduced: SIMSCRIPT, GPSS (IBM)
  ➢ Simulation viewed at the tool of "last resort"

# Simulations: Brief History

❖ **Late '60s, early '70s**
- ➤ Primary computers were mainframes: accessibility and interaction was limited
- ➤ GASP IV introduced by Pritsker.  Triggered a wave of diverse applications.  Significant in the evolution of simulation.

❖ **Late '70s, early '80s**
- ➤ SLAM introduced in 1979 by Pritsker and Pegden.
- ➤ Models more credible because of sophisticated tools.
- ➤ SIMAN introduced in 1982 by Pegden.  First language to run on both a mainframe as well as a microcomputer.

# Simulations: Brief History

❖ **Late '80s through present**

➢ Powerful PCs

➢ Languages are very sophisticated (market almost saturated)

➢ Major advancement: graphics. Models can now animated.

# What can we Simulate?

*Almost anything can and almost everything has…*

❖ **Applications**

- ✓ *PHYSICAL SCIENCES:* Simulations of materials, processes, etc.
- ✓ *COMPUTER SYSTEMS:* hardware components, software, systems, networks, data base management, information processing, etc..
- ✓ *MANUFACTURING:* material handling systems, assembly lines, automated production facilities, inventory control systems, plant layout, etc..
- ✓ *BUSINESS:* stock and commodity analysis, pricing policies, marketing strategies, cash flow analysis, forecasting, etc..
- ✓ *GOVERNMENT:* military weapons and their use, military tactics, population forecasting, land use, health care, delivery, fire protection, criminal justice, traffic control, etc..

*And the list goes on and on…*

# Advantages of Simulations

❖ **Greatest strength: Its ability to answer** <span style="color:red">**"what if" questions**</span>...

➢ Can be used to study existing systems without disrupting the ongoing operations.

➢ Proposed systems can be "tested" before committing resources.

➢ Allows us to control time.

➢ Allows us to identify bottlenecks.

➢ Allows us to gain insight into which variables are most

➢ Important to system performance.

# More Advantages of Simulations ...

❑  When mathematical *analysis methods are not available*, simulation may be the only investigation tool

❑  When mathematical analysis methods are available, but are so complex that simulation may provide a simpler solution

❑  Allows *comparisons* of alternative designs or alternative operating policies

❑  Allows time compression or expansion

# Drawbacks of Simulations

➢ Model building is an art as well as a science. The *quality of the analysis depends on the quality of the model* and the skill of the modeler. Remember: "Garbage In → Garbage Out" (GIGO)

➢ Simulation results are sometimes *hard to interpret*.

➢ Simulation analysis can be *time consuming* and expensive.

➢ Should not be used when an analytical method would provide for quicker results.

➢ Often expensive and time consuming to develop

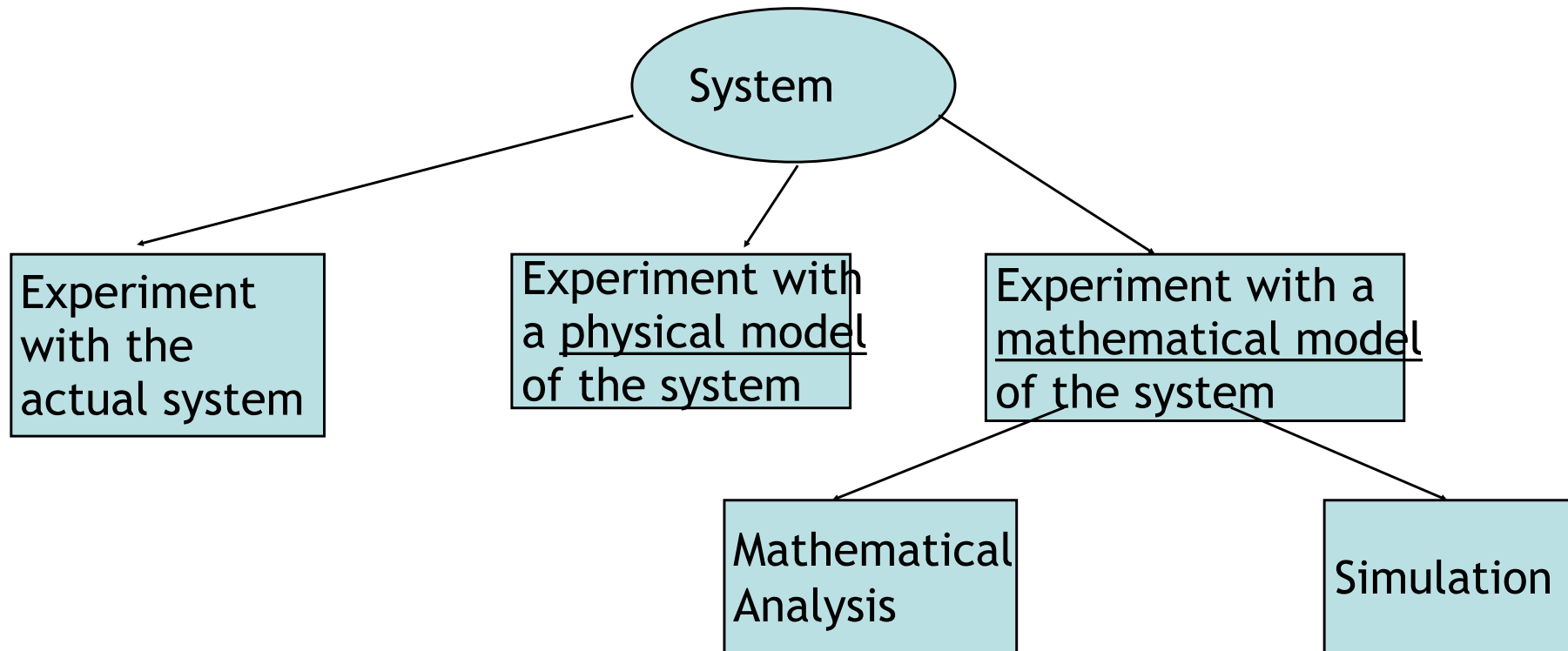➢ An *invalid model* may result with confidence in wrong results.

# Any Questions Till Now?

❖ **Why and How to Study a System**

➢ Measure/estimate performance
➢ Improve operation
➢ Prepare for failures

# Usage of Models



ACTUAL SYSTEM
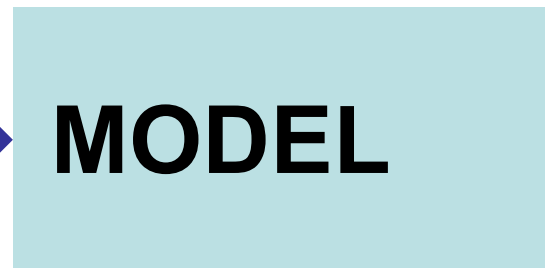
**Operating Policies**

• **Single queue, parallel servers**

• **FIFO**

(X)

**Input Parameters**

• **No of servers**

• **Inter-arrival Time Distribution**

• **Service Time Distributions**

**MODEL**

(Y)

**Output Parameters**

• **Waiting Times**

• **System Size**

• **Utilizations**

$$Y = f(X)$$

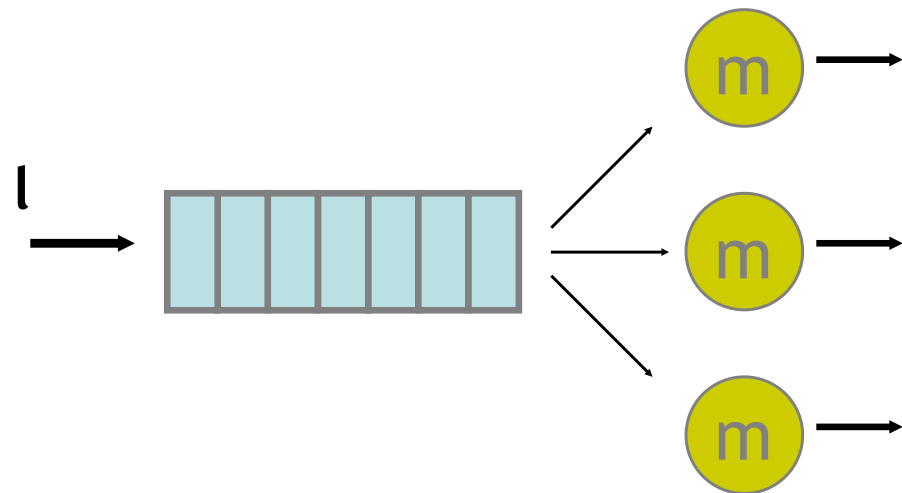Numerical Simulations: A Short Introduction

# Stochastic Models

❖ **Modeling of Stochastic Systems**

- Randomness or uncertainty is inherent
- Example: Bank with customers and tellers



ACTUAL SYSTEM



QUEUEING MODEL

# How to Simulate

✓ **By hand**
  **Buffon Needle and Cross Experiments (see Kelton et al.)**

✓ **Spreadsheets**

✓ **Programming in General Purpose Languages**
  ➢ **Java**

✓ **Simulation Languages**
  ➢ **SIMAN**

✓ **Simulation Packages: e.g. MATLAB, Arena**

**Issue: Modeling Flexibility vs. Ease of Use**

# Methodology of Simulations

**A) Problem Formulation**

- A statement of the problem
  - the problem is clearly understood by the simulation analyst
  - the formulation is clearly understood by the client.

**B) Setting of Objectives and Project Plan**

- Determine the questions that are to be answered
- Identify scenarios to be investigated
- Decision criteria
- Determine the end-user
- Determine data requirements
- Determine hardware, software, & personnel requirements
- Prepare a time plan
- Cost plan and billing procedure

# Methodology of Simulations

❖ **Steps in a Simulation Study**



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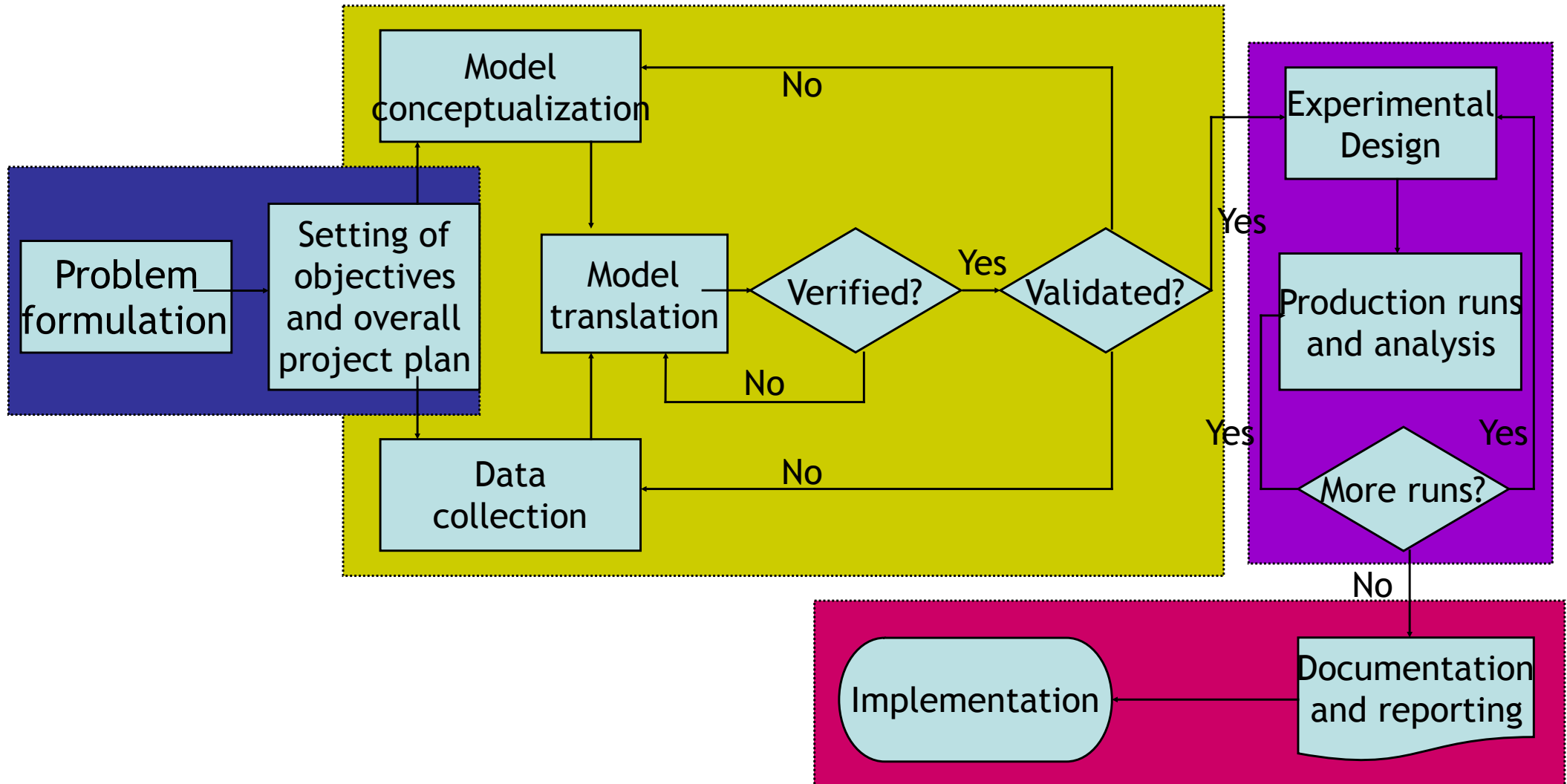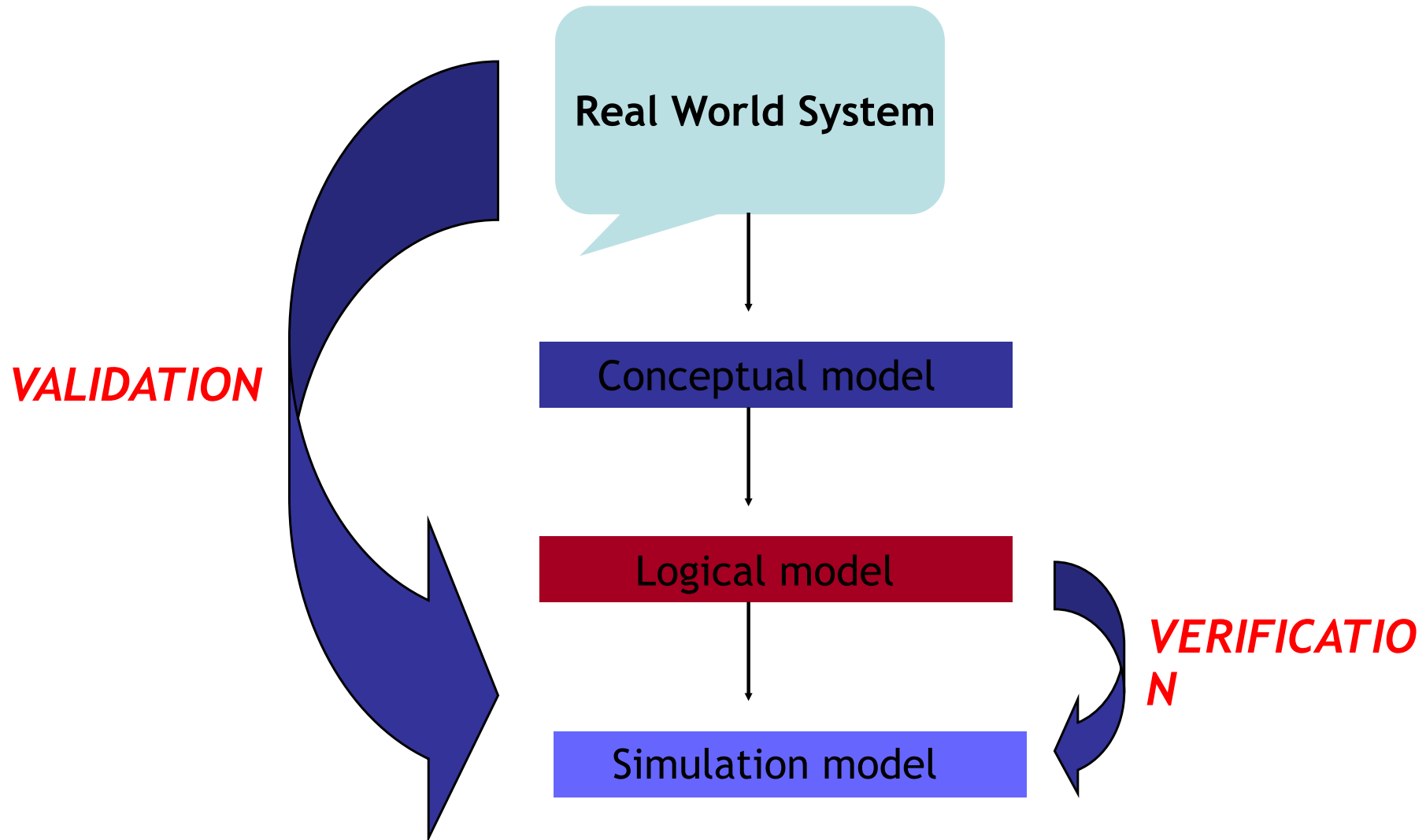
❖ **More or Less Detailed Models?**

❑ **Low levels** of detail may result in **lost of information** and goals cannot be accomplished

❑ High levels of detail require:
  ➢ more time and effort
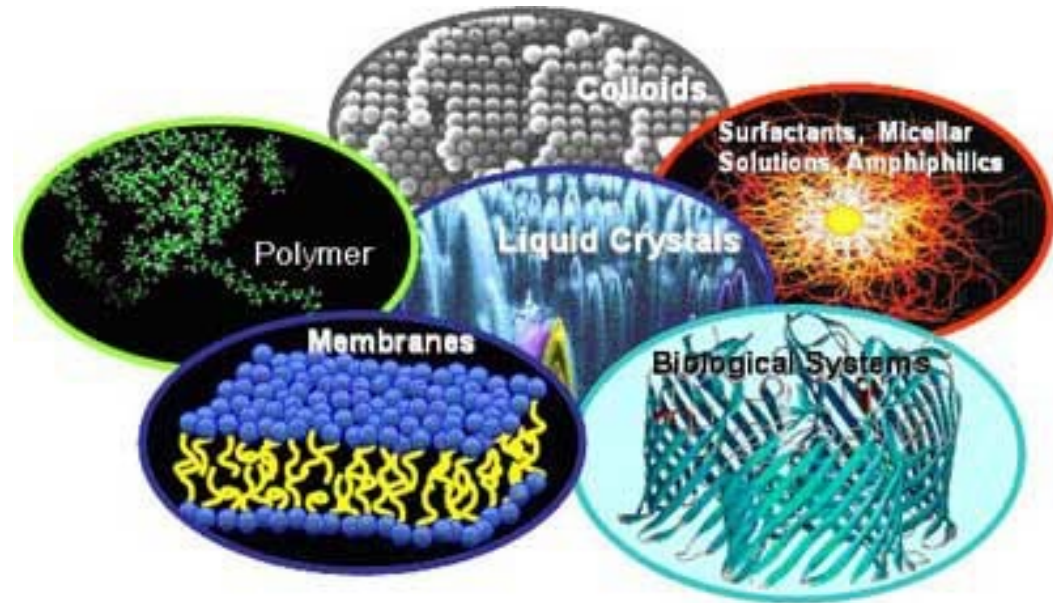  ➢ longer simulation runs
  ➢ more likely to contain errors

# Simulations: Analysis of Results

❖ Statistical tests for significance and ranking

❖ Point Estimation

❖ Confidence-Interval Estimation

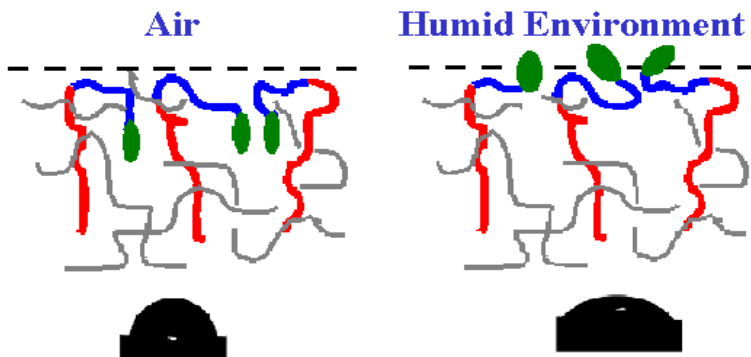❖ Interpretation of results

❖ More runs?

# Example: Simulations of Materials

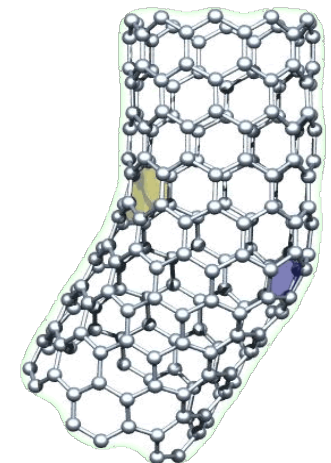❖ **Complex materials**



❑ **Applications**

➢ **Nanotechnology** (materials in nano-dimensions), **biotechnology** (drug release, ... etc)

➢ **Clever-responsive Materials**



➢ **Molecular Electronics, Carbon Nanotubes**



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# Complex Systems: Interdisciplinarity
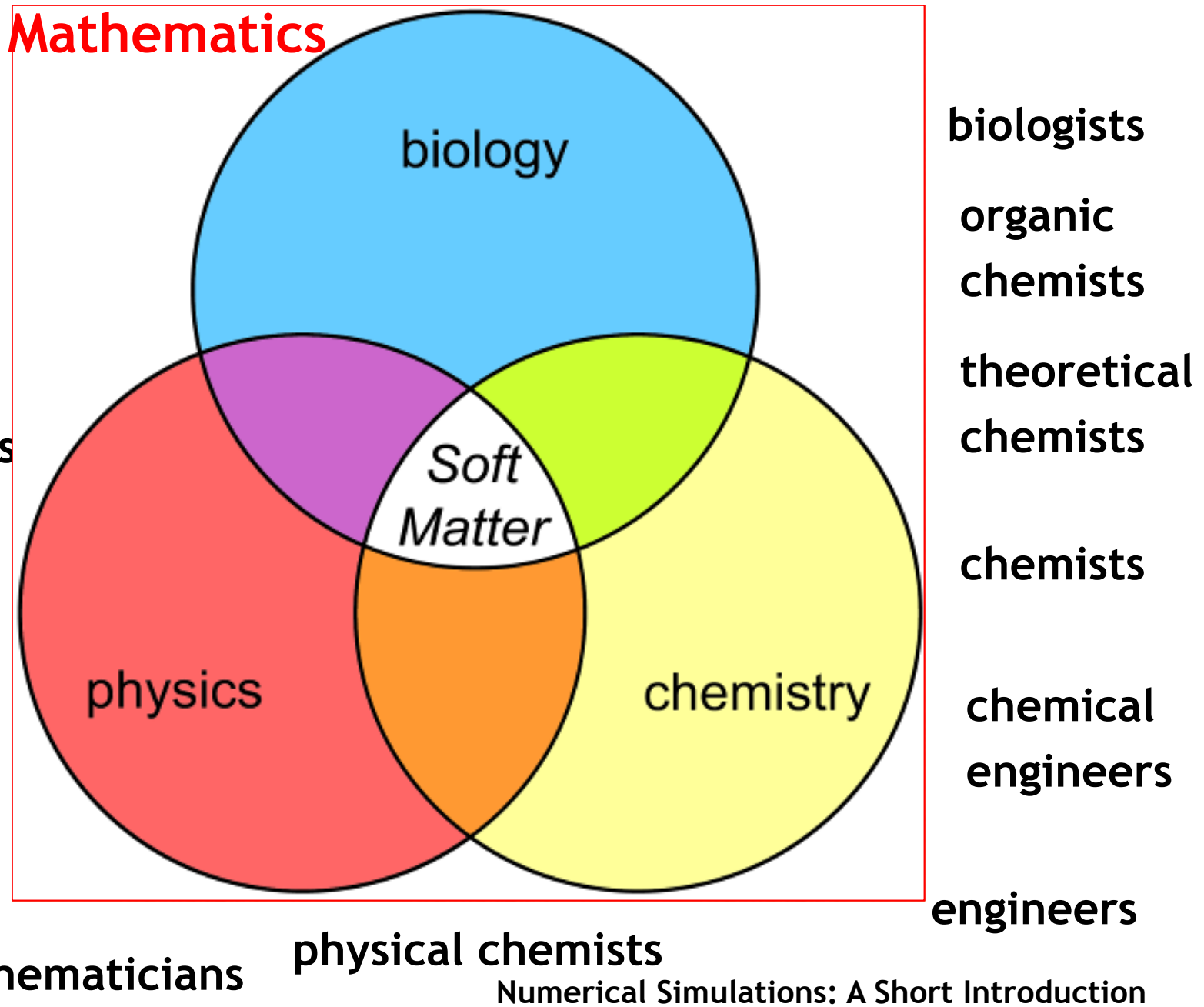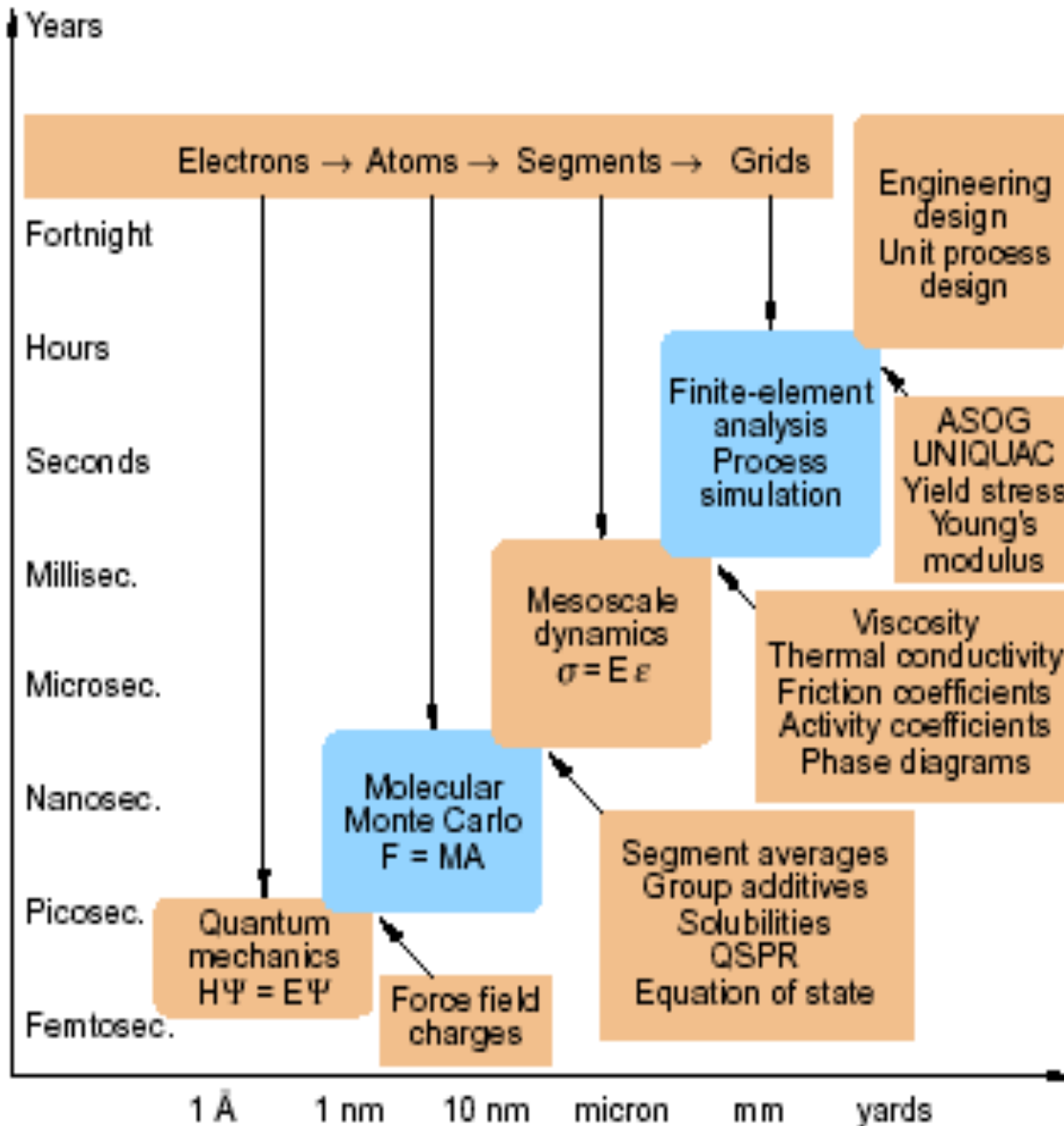


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❑ **Various Methods: Time vs Length**

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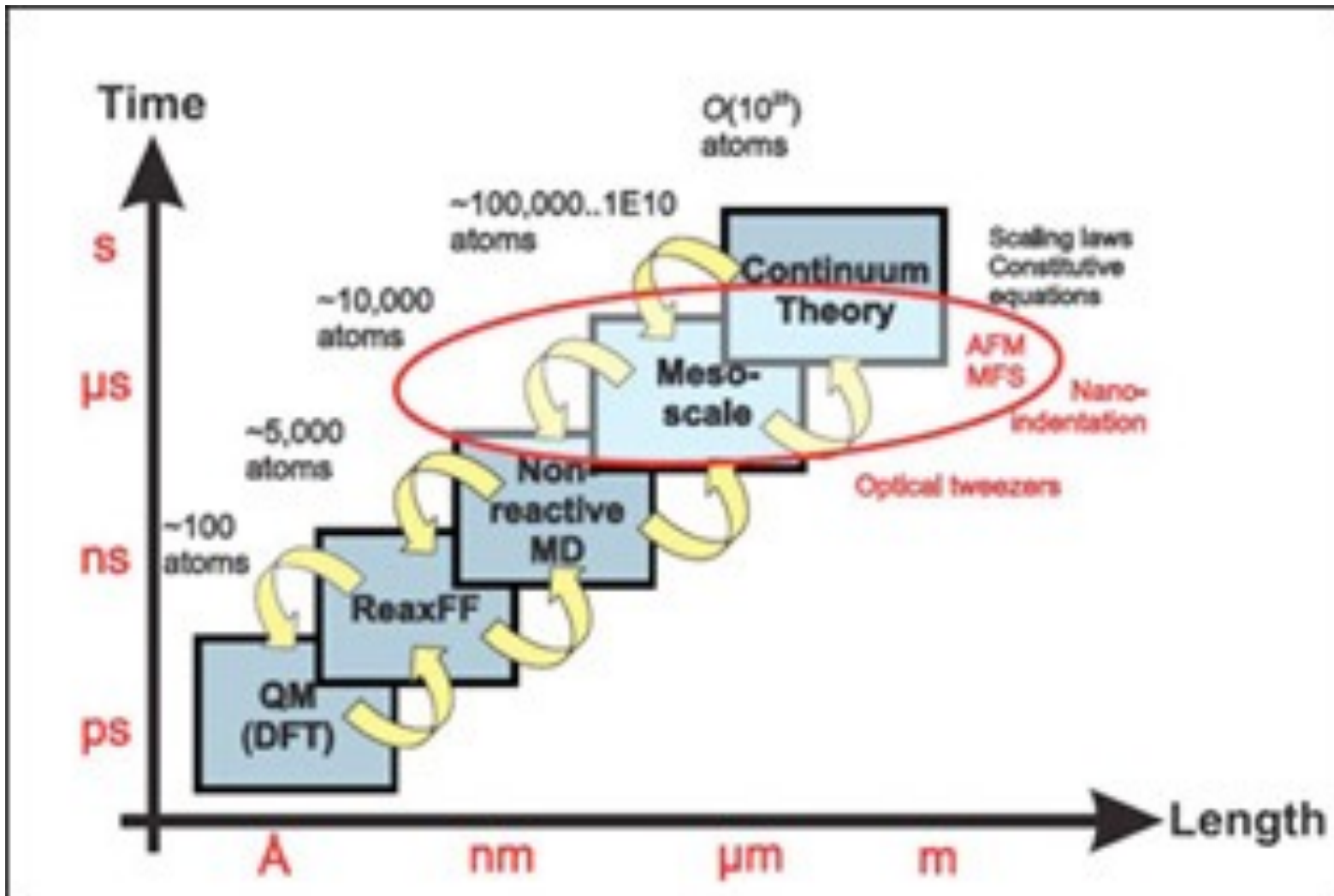
## What is Monte Carlo?

❑ **The famous casino place**





❑ **But also ….**

# Monte Carlo Methods

❑ **Monte Carlo numerical methods - Definition :**

> ❖ Any computational method which solves a problem by generating suitable random numbers and observing that fraction of the numbers obeying some property or properties. The method is useful for obtaining numerical solutions to problems which are too complicated to solve analytically.

✓ It was named by **S. Ulam**, who in 1946 became the first mathematician to dignify this approach with a name, in honor of a relative having a propensity to gamble (Hoffman 1998, p. 239). **Nicolas Metropolis** also made important contributions to the development of such methods.

❑ They are also called "**Monte Carlo Simulation**" or "**Stochastic Simulation**" methods.

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# Monte Carlo Methods

❑ **ENIAC Los Alamos (1945-1955), from Stanislaw Ulam:**

➢ The first thoughts and attempts I made to practice [the Monte Carlo Method] were suggested by a question which occurred to me in 1946 as I was convalescing from an illness and playing solitaires. The question was what are the chances that a Canfield solitaire laid out with 52 cards will come out successfully? After spending a lot of time trying to estimate them by pure combinatorial calculations, I wondered whether a more practical method than "abstract thinking" might not be to lay it out say one hundred times and simply observe and count the number of successful plays. This was already possible to envisage with the beginning of the new era of fast computers, and I immediately thought of problems of neutron diffusion and other questions of mathematical physics, and more generally how to change processes described by certain differential equations into an equivalent form interpretable as a succession of random operations. Later [in 1946], I described the idea to John von Neumann, and we began to plan actual calculations.

# Monte Carlo Methods

➢ Being secret, the work of von Neumann and Ulam required a code name. Von Neumann chose the name "Monte Carlo". The name is a reference to the Mote Carlo Casino in Monaco where Ulam's uncle would borrow money to gamble!



The Monte Carlo Casino

# Applications of Monte Carlo Algorithms

❖ **Natural sciences**: Statistical physics, chemistry, materials science, …

❖ **Engineering**,

❖ **Economics**,

❖ **Mathematics**: Applied Statistics,

❖ **Astrophysics**,

❖ **Environmental** models,

❖ Computational **Biology**, Biostatistics,

❖ **Neural network models**: modeling of brain,

❖ Many more …

# Stochastic vs Deterministic

✓ Monte Carlo is a stochastic simulation technique:

❑ **Deterministic system**: A system in which the later states of the system follow from, or are determined (exactly) by, the earlier ones.

  ➢ No randomness.

  ➢ A deterministic model always produce the same output from a given starting condition or initial state.

❑ **Stochastic system**: A system in which the later states of the system are <u>not</u> determined (exactly) by the earlier ones.

  ➢ Involve randomness.

  ➢ There are many possible future states, for a given starting condition.

# Stochastic vs Deterministic: Examples

❑ **Deterministic systems:** Classical mechanics, quantum mechanics, Navier – Stokes equations, … etc.

❑ **Stochastic systems**: Random walks, Brownian motion, stock market prices, biology (gene expression), … etc.

✓ **Note**: If a system is deterministic, this doesn't necessarily imply that later states of the system are **predictable** from a knowledge of the earlier ones. In this way, chaos is similar to a random system. For example, chaos has been termed "deterministic chaos" since, although it is governed by deterministic rules, its property of sensitive dependence on initial conditions makes a chaotic system, in practice, largely unpredictable.

# History of Monte Carlo Methods

❑ **(1733)** Buffon's needle problem.

❑ **(1812)** Laplace suggests using Buffon's needle experiment to estimate π.

❑ **(1946**) ENIAC (Electronic Numerical Integrator And Computer) built.

❑ **(1947)** John von Neuman and Stanislaw Ulam propose a computer simulation to solve the problem of neutron diffusion in fissionable material.

❑ **(1949)** Metropolis and Ulam paper (Journal of the American Statistical Association).

❑ **(1984)** Gibbs sampler technique (Geman & Geman).

❑ **From then onwards**: continuously growing interest of statisticians in Monte Carlo methods.

# A little bit of History: Buffon's Needle

❖ **First (?)** application of Monte Carlo methods: **Buffon's needle** (Buffon 1777)

" Suppose we have a floor made of parallel strips of wood, each the same width, and we drop a needle onto the floor. What is the probability that the needle will lie across a line between two strips?"

Georges-Louis Leclerc, Comte de Buffon
(7 September 1707 – 16 April 1788)
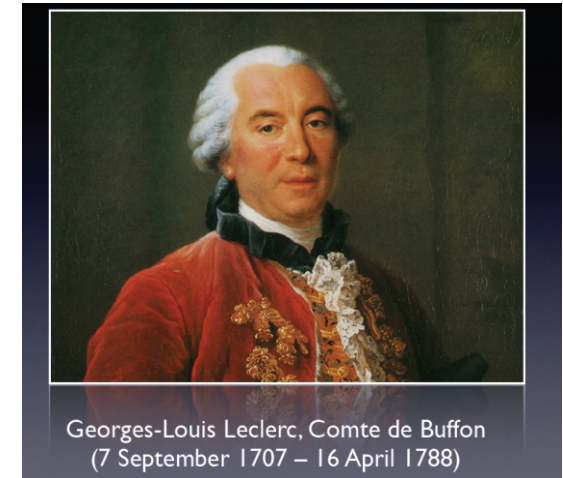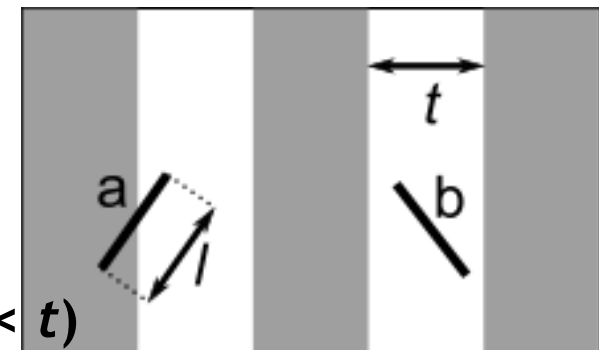
➢ Solution (short needle $l < t$

$$P = \frac{2l}{\pi t}$$

➢ **Home exercise:**

A) Derive the above solution (**short needle** $l < t$)

B) What is the solution for **large needle** ($l > t$)?

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# Buffon's Needle

❖ **Monte Carlo algorithm for the calculation of π:**

A. "Throw" randomly *n* needles.

B. Check how many of them cut a line (suppose *m*).

C. Compute probability $P_n$ through: $P_n = m/n$

$$\pi = \lim_{n \to \infty} \frac{2l}{P_n t}$$

# The Best of the 20th Century: Top 10 Algorithms

❖ Dongarra and Sullivan, Computing in Science and Engineering, 2000, SIAM News.

❑ "Great algorithms are the poetry of computation," says Francis Sullivan of the Institute for Defense Analyses' Center for Computing Sciences in Bowie, Maryland. He and Jack Dongarra of the University of Tennessee and Oak Ridge National Laboratory have put together a sampling that might have made Robert Frost beam with pride--had the poet been a computer jock.

❑ Their list of 10 algorithms having "the greatest influence on the development and practice of science and engineering in the 20th century" appears in the January/February issue of Computing in Science & Engineering. If you use a computer, some of these algorithms are no doubt crunching your data as you read this.

# The Best of the 20th Century: Top 10 Algorithms

**The drum roll, please:**

**1946: The Metropolis Algorithm for Monte Carlo.** Through the use of random processes, this algorithm offers an efficient way to stumble toward answers to problems that are too complicated to solve exactly.

**1947: Simplex Method for Linear Programming.** An elegant solution to a common problem in planning and decision-making.

**1950: Krylov Subspace Iteration Method.** A technique for rapidly solving the linear equations that abound in scientific computation.

**1951: The Decompositional Approach to Matrix Computations.** A suite of techniques for numerical linear algebra.

**1957: The Fortran Optimizing Compiler.** Turns high-level code into efficient computer-readable code.

**1959: QR Algorithm for Computing Eigenvalues.** Another crucial matrix operation made swift and practical.

**1962: Quicksort Algorithms for Sorting.** For the efficient handling of large databases.

**1965: Fast Fourier Transform.** Perhaps the most ubiquitous algorithm in use today, it breaks down waveforms (like sound) into periodic components.

**1977: Integer Relation Detection.** A fast method for spotting simple equations satisfied by collections of seemingly unrelated numbers.

**1987: Fast Multipole Method.** A breakthrough in dealing with the complexity of n-body calculations, applied in problems ranging from celestial mechanics to protein folding.

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