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

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What are Simulations?

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.”

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”!*
Simulations: Brief History

- 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 “what if” questions…**

➢ 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.
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 $\rightarrow$ 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

System

- Experiment with the actual system
- Experiment with a physical model of the system
- Experiment with a mathematical model of the system

Mathematical Analysis

Simulation
Usage of Models

Operating Policies
- Single queue, parallel servers
- FIFO

Input Parameters
- No of servers
- Inter-arrival Time Distribution
- Service Time Distributions

Output Parameters
- Waiting Times
- System Size
- Utilizations

\[ Y = f (X) \]
Modeling of Stochastic Systems

- Randomness or uncertainty is inherent
- Example: Bank with customers and tellers
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
Steps in a Simulation Study

- Problem formulation
- Setting of objectives and overall project plan
- Model conceptualization
- Model translation
- Data collection
- Implementation
- Experimental Design
- Production runs and analysis
- More runs?
- Documentation and reporting

- Verified?
- Validated?
- Yes
- No
- More runs?
- Yes
- No
Simulations: Levels of Detail

❖ 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
Numerical Simulations: A Short Introduction

Complex Systems: Interdisciplinarity

- biophysicists
- physicists
- surface scientists
- theoretical physicists
- materials scientists
- applied mathematicians
- physical chemists
- biologists
- organic chemists
- theoretical chemists
- chemists
- chemical engineers
- engineers
Simulations Across Length-Time Scales

- Various Methods: Time vs Length

- Electrons → Atoms → Segments → Grids
- Engineering design
  - Unit process design
- Finite-element analysis
  - Process simulation
  - ASOG
  - UNIQUAC
  - Yield stress
  - Young's modulus
- Mesoscale dynamics
  - $\sigma = E \varepsilon$
- Viscosity
  - Thermal conductivity
  - Friction coefficients
  - Activity coefficients
  - Phase diagrams
- Molecular Monte Carlo
  - $F = MA$
- Quantum mechanics
  - $H \Psi = E \Psi$
- Force field charges
- Segment averages
  - Group additives
  - Solubilities
  - QSAR
  - Equation of state

- Time scales:
  - Years
  - Fortnight
  - Hours
  - Seconds
  - Milliseconds
  - Microseconds
  - Nanoseconds
  - Picoseconds
  - Femtoseconds

- Distance scales:
  - 1 Å
  - 1 nm
  - 10 nm
  - Micron
  - Millimeter
  - Yard
Various Methods: Time vs Length
Example: Monte Carlo Simulations

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.
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!
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 ...**
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 not 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


- **(1812)** Laplace suggests using Buffon's needle experiment to estimate $\pi$.


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


- **(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?”

➢ 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 ($l > t$)?
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


- "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.


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


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.


Bibliography

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