Stochastic Simulation Part I.B - WWII Code Name - Monte Carlo





The Monte Carlo Method: at the origins - a computing method for complex multiple integrals in high dimensions...

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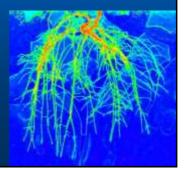
Simulations Deterministic vs. Stochastic

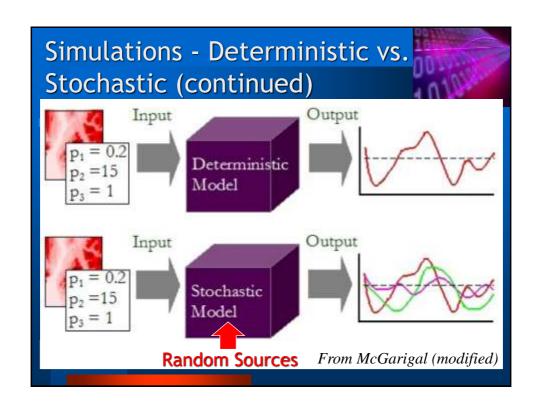


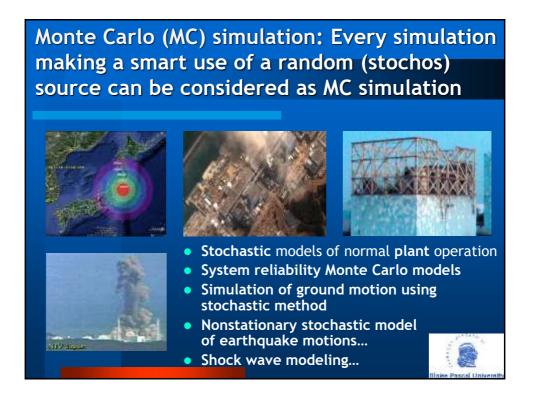
- Deterministic simulation: the output of the model is precisely determined by its structure and its parameter values
- Stochastic modeling : use of a random source
 - New scientific barriers to break are sometimes behind our best deterministic models
 - The assessment of stochastic parallel simulations is tough and this domain is less studied











In various domains

We still need to increase reliability...



n the 1990s Mulhouse FRANCE

electronic automated commercial blane, Automatic Analytical and deterministic models are very fast and can be preferred in many cases

BUT: they can be imprecise in some conditions

- Monte Carlo (MC) simulations help increasing model precisions with spatial constraints but they can be very slow
- In many industries stochastic models are more widely used for risk assessment (and to take into account rare & random events
- Quantitative risk analysis can be improved with Monte Carlo simulations

landing test with no pilot, no eletro-mechanic controls or cables

Pharmaceutical Industry & Drug discovery

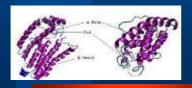
Ex: problems with the Mediator drug in France (and with more than 200 other drugs)



Example of Improvements:

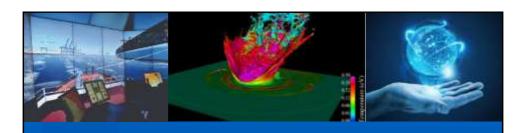
- Multi-scale stochastic drug release model
- Stochastic model for the origin and treatment of tumors containing drug-resistant cells
- Comparison of stochastic models to to predict the influence of drug distribution, enzyme heterogeneity...

• ...









When possible, mathematical models have to be preferred

However most complex real world systems with stochastic elements cannot be accurately described by a mathematical model that can be evaluated analytically.

Monte Carlo Methods is a solution...

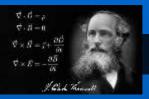
- Monte Carlo is another name for statistical random sampling methods of great importance to physics and computer science
- Applications of Monte Carlo Method
 - Evaluating integrals of arbitrary functions Predicting future values of stocks
 - Solving partial differential equations
 - Sharpening satellite images
 - Modeling cell populations
 - Finding approximate solutions to NP-hard problems
 - Financial applications (MC & Quasi Monte Carlo...)

History of Science



- In 1738, Swiss physicist and mathematician Daniel Bernoulli published Hydrodynamica which laid the basis for the kinetic theory of gases
- A great numbers of molecules moving in all directions (random directions...)
- Their impact on a surface causes the gas pressure that we feel, and that what we experience as heat is simply the kinetic energy of their motion.

History of Science (continued)



- In 1859, Scottish physicist James Clerk Maxwell formulated the distribution of molecular velocities, which gave the proportion of molecules having a certain velocity in a specific range.
- This was the first-ever statistical law in physics.
- Maxwell used a simple thought experiment: particles must move independently of any chosen coordinates, hence the only possible distribution of velocities must be normal in each coordinate.

1864, Ludwig Boltzmann S = k log W

- S, the Entropy can be seen as the measure of the disorder level at a microscopic level.
- k is the Boltzmann constant and W (Wahrscheinlichkeit, « probability » in German) being the number of possible microstates for a macrostate of a closed thermodynamical system.
- The higher the Entropy, the lesser will be the organization of the elements inside a system.
- The 2nd thermodynamic principle states that with 'real' transformation, the Entropy (disorder) increases. This process is irreversible (non reversibility of physical phenomenon) – 1st principle: conservation of Energy

History of Monte Carlo Method (1/2)

- Boltzmann is considered as the father of statistical physics. He was defending the existence of atomes, thus validating the « Démocrite hypothesis » stating that material things can be considered as a set of indivisible things.
- Credit for inventing the Monte Carlo method is shared by Stanislaw Ulam, John von Neuman and Nicholas Metropolis.
- Ulam, a Polish born mathematician, worked for John von Neumann on the Manhattan Project.
- In a thought experiment, Ulam designed the basis of the Monte Carlo method while pondering the probabilities of winning a card game of solitaire.
- Less funny: Ulam is known for designing the hydrogen bomb with Edward Teller in 1951.

History of Monte Carlo Method (2/2)



- Ulam, von Neuman, and Metropolis developed algorithms for computer implementations, as well as exploring means of transforming non-random problems into random forms that would facilitate their solution via statistical sampling.
- This work transformed statistical sampling from a mathematical curiosity to a formal method applicable to a wide variety of problems.
- It was Metropolis who named the new method after the casinos of Monte Carlo.
- Ulam and Metropolis published their paper in 1949 :
- "The Monte Carlo Method" in *Journal of the American Statistical Association*, 44 (247), 335-341, in 1949.

Finally what is a Monte Carlo method?

The name Monte Carlo method refers to any method that makes use of random numbers and statistical sampling:

- ✓ Simulation of natural phenomena
- ✓ Simulation of experimental apparatus
- ✓ Numerical analysis for complex integration purposes (eg. In multiple dimensions)
- ✓ And so many other applications...

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