Chapter

Applying Monte Carlo Simulation in New Tech

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Abstract

Monte Carlo in Monaco is given to the theory for mathematics, whose simulation process involves generating chance variables and exhibiting random behaviours in nature. This simulation is a powerful statistical analysis tool and widely used in both non-engineering fields and engineering fields for new perspectives. This simulation has been applied to diverse problems ranging from the simulation of complex physical phenomena such as atom collisions, to the simulation of river boundary layers as meanders and Dow Jones forecasting. It can deal with many random variables, various distribution types and highly nonlinear engineering models, while Monte Carlo is also suitable for solving complex engineering problems in two areas which are varying randomly. Monte Carlo simulation is given as an application for hydrogen energy potential determination.

Keywords: Monte Carlo method, renewable energy, hydrogen potential

1. Introduction

Monte Carlo simulation, or probability simulation, is a technique used to understand the impact of risk and uncertainty in natural occurrences, project management, cost and other forecasting models [1]. You must make certain assumptions—for any model that plans ahead for the future—when you develop a forecasting model. In this research, there might be assumptions about the future shape of river curvatures which is called as river meanders. These are projections into the future, and the best you can do is to estimate the expected value. What the actual value will be you cannot know with certainty, but based on historical data, or expertise in the field, or past experience, you can draw an estimate value. It contains some inherent uncertainty and risk, because it is an estimate of an unknown value.

The Monte Carlo simulation performs random sampling and conducts a large number of experiments on computer, which is different from a physical experiment, At the first step, experimental statistical properties (model values) are given, and results for the model outputs are calculated with a computer program. According to the calculation procedure, the input random variables are distributed randomly. The output Y variables are given as a function of x in formula $Y = g(x)$, where this function is called as performance function. After collecting the necessary input values from each experiment carried out in this manner, a set of samples of output variable Y are available for the statistical analysis, which estimates the characteristics of the output variable Y. In **Figure 1,** the flowing

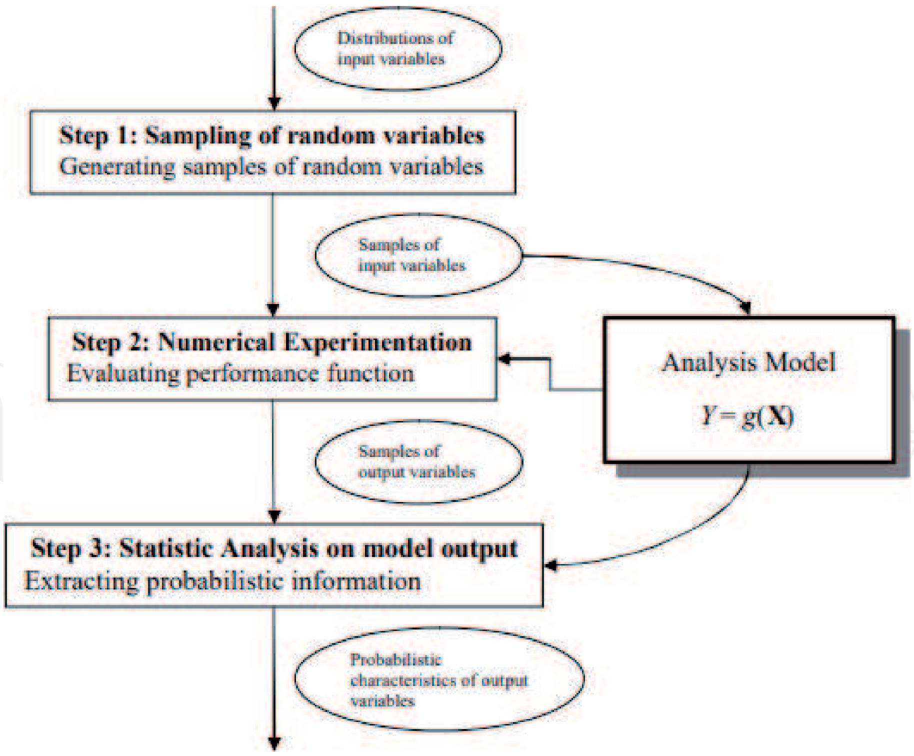

Figure 1.
Monte Carlo simulation [4].

computer chart is given as an example where the three steps are required in the simulation process:

Step 1: Sampling on random input variables X.

Step 2: Evaluating model output Y.

Step 3: Performing statistical analysis on the model output.

The discussion about the choosing of independent random variables will be given. But, the Monte Carlo simulation is applicable for dependent variables where it is needed to follow the three steps [2].

Monte Carlo methods generally follow the following steps:

1. Determining the statistical properties of possible inputs.

2. Generating many sets of possible inputs that follow the above properties.

3. Performing a deterministic calculation with these sets.

4. Analysing statistically the results.

The error on the results typically decreases as $1/\sqrt{N}$ [3].

2. Application

The Monte Carlo simulation is applied for determination of hydrogen energy potential where hydrogen can be used as a save energy without any pollution control like fossil fuels. The atomic construction of hydrogen consists of only one proton and one electron, which can be found in the universe easily. In the universe, hydrogen does not occur naturally as a gas on Earth, as it is always combined with other elements in our environment.

On the Earth, hydrogen can be found in organic compounds as hydrocarbons which can be used as gasoline, natural gas, earth gas and methanol or propane and with a heat separation procedure, it can be converted into reforming procedure. With electrolysis, hydrogen is separated from water into its component of oxygen where we can use this process for electrical energy. In sea boundary layer, some algae and bacteria, using sunlight as their energy source, even give off hydrogen under certain conditions. Hydrogen fuel is used by NASA as a fuel for space shuttles.

In praxis, hydrogen and oxygen combine in a fuel cell to produce electricity, heat and water where they are often compared with batteries for converting the chemical reaction into usable electric power. As long as fuel (hydrogen) is supplied, the fuel cell will produce electricity, never losing its charge.

For buildings, and as an electrical power source for electric motors propelling vehicles, fuel cells are new innovation for converting heat and electricity.

Hydrogen is a best energy carrier that is used by consumers in different ways. Other innovative energy sources, like the Sun and bioenergy, cannot produce energy all the time in the future where they could, for example, produce electric energy and hydrogen, which can be stored until it is needed. In the hydrogen generation, it can also be transported (like electricity) to locations where it is needed.

In scientific research, this simulation (Monte Carlo) is a new technique in science which forms random variables as input results for risk assessment or uncertainty of a certain system.

In new application on the basis of probability distributions such as normal, log normal, etc., the random variables or inputs are modelled, where different iterations or simulations are run for generating paths, and the outcome is arrived at by using suitable numerical computations.

In the application of Monte Carlo simulation for an exact solution, the hydrogen energy potential problem is solved by Monte Carlo simulation, which is used in a dynamic complex system that needs to be analysed, which is a probabilistic method for modelling risk in a system.

The Monte Carlo method is used also in physical science, statistics, artificial intelligence and robotics. In the example of the determination of hydrogen energy potential, the Monte Carlo simulation gives as a result a probabilistic estimate of uncertainty. But it is a useful tool for approximation of realty which gives never deterministic results.

The Monte Carlo simulation technique was observed in innovation extensively for modelling uncertain situations like hydrogen energy potential determination in renewable energy systems [5].

It is difficult to predict the real situation with absolute precision and accuracy, which can be attributed to the different parameters that can impact the outcome of a course of action. The Monte Carlo simulation can give all possible results for a new decision. It can thereby help us take improvements of a solution for a difficult situation under uncertainty. The probabilities of outcomes can be easily discussed by decision-makers.

For instance, the Monte Carlo simulation can be used to compute the value at risk of a portfolio where this method tries to predict the worst return expected from a portfolio, given a certain confidence interval for a specified time period.

3. Results

In description of Monte Carlo simulation, this model can be easily calculated using the random value. A typical Monte Carlo simulation program can easily calculate the model verification by counting indefinitely, where each time they use different randomly selected evaluations.

As the result, the Monte Carlo simulation program is a very important program that was used also by Einstein's group in Manhattan Program for atomic bomb energy determination.

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4. Description of program or function

Super Monte Carlo simulation program for nuclear and radiation process (SuperMC), a general, intelligent, accurate and precise simulation software system for the nuclear design and safety evaluation of nuclear systems, is designated to support the comprehensive neutronics calculation, taking the radiation transport as the core and including the depletion, radiation source term/dose/biohazard, material activation and transmutation, etc. [6]. It supports multi-physics coupling calculation including thermo-hydraulics, structural mechanics, chemistry, biology, etc. The main technical features include hybrid MC-deterministic methods and the adoption of advanced information technologies, while the main usability features include automatic modelling of geometry and physics, visualisation and virtual simulation and cloud computing services.

The latest version of SuperMC can accomplish the transport calculation of n, γ and can be applied for criticality and shielding design of reactors as well as analysis in medical physics.

SuperMC has been verified and validated by more than 2000 benchmark models and experiments, such as International Criticality Safety Benchmark Evaluation Project (ICSBEP), Shielding Integral Benchmark Archive and Database (SINBAD) and the comprehensive applications from the reactors including fusion reactor (ITER benchmark model, FDS-II), fast reactor (BN600, IAEA-ADS), PWR (BEAVRS, HM, TCA) and International Reactor Physics Experiment Evaluation Project (IRPhEP), etc. SuperMC greatly speeds up the neutronics analysis, especially for complicated problems. Based on this program, detailed and accurate nuclear analysis models can be created, and accurate nuclear analysis can be performed as well.

5. Methods

The methods used are the following:

- Monte Carlo transport methods of neutron and photon with series of novel acceleration methods for transport calculation.

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- Automatic CAD-based geometry modelling method with geometry decomposing algorithm and model reuse technique [7–11].
- 4D whole process intelligent and visualised analysis method including data visualisation mixed with calculation geometries.

6. Restrictions on the complexity of the problem

The energy range is 1.0e-11~150 MeV for neutron and 1 keV~1GeV for photon.

7. Typical running time

The running time is dependent on the complexity of problem.

8. Unusual features of the program

The unusual features are the following:

- CAD-based automatic geometry and physics modelling with high efficiency and precision.
- Efficient particle transport calculation based on particle uniformity and location anticipation.
- Multi-dimensional and multi-style intelligent visualisation analysis.
- Intelligent automation modelling, efficient computation and visualisation analysis based on cloud computing.

9. Related or auxiliary programs

MPICH2-1.4.1 is one of the related or auxiliary programs.

10. Status

Package ID	Status date	Status
IAEA1437/01	07-JUL-2016	Tested at NEADB

11. Hardware requirements

The following are the hardware requirements for the program:

Bottommost PC hardware configuration:
CPU: Dual-Core 1.5 GHZ
Memory: 512 MB
Hard disk space: 3 GB

Recommended hardware configuration:
CPU: Dual-Core 3.0 GHZ
Memory: 4 GB
Hard disk space: 10 GB

12. Programming language(s) used

No specified programming language is used.

13. Software requirements

SuperMC can run on Windows XP 32-bit, Windows 7 32/64-bit and Linux CentOS 5.4/6.6.

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