Advances in Simulation: The Interplay of Inspiration, Intuition, Abstraction, and Experimentation

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Introduction

Our focus is on how advances in simulation are driven by the continuous interplay of the following:

- **inspiration**, which may be motivated by sheer curiosity as well as specific theoretical or practical problems;

- **intuition**, which may guide the search for a problem solution or lead to new discoveries when reasoning alone is insufficient to ensure continued progress;

- **abstraction**, which encompasses the modeling and analysis techniques required to build a simulation model, design experiments using that model, and draw appropriate conclusions from the observed results; and

- **experimentation**, which is computer based and thus differs fundamentally from other empirical scientific work because of the efficiency improvements that are achievable using Monte Carlo methods.

The slides for this talk are available via [www.ise.ncsu.edu/jwilson/wsc11tos.pdf](http://www.ise.ncsu.edu/jwilson/wsc11tos.pdf).
William Sealy Gosset (1876–1937), trained in mathematics and chemistry, was a brewer with Arthur Guinness, Son & Co. Ltd.; and he made numerous contributions to statistical methodology *in his spare time*. 
The Beginning of “Scientific Brewing” at Guinness

Source: www.guinness.com
Gosset’s Early Work at Guinness

Hired as a staff scientist by Guinness in 1899, Gosset was faced with the problem of maintaining consistent quality of Guinness’s ale and stout based on data collected under the following conditions:

- small sample sizes arising from the need to run short series of experiments; and
- measurements that are not independent.

Gosset was working in quality control 25 years before the appearance of the Shewhart chart.

Gosset arranged to spend 1906–1907 studying under Karl Pearson at University College London, but he quickly discovered that Pearson’s large-sample statistical methods were inadequate for Guinness’s problems.
Gosset’s Approach to Small-Sample Process Control

To estimate the mean $\mu$ of a normal population based on a random sample \{\(X_i : i = 1, \ldots, n\)\} with sample size \(n\) in the range \(4 \leq n \leq 10\), he proceeded as follows:

(a) He calculated the sample mean and variance,

\[
\bar{X} = \frac{1}{n} \sum_{i=1}^{n} X_i \quad \text{and} \quad S^2 = \frac{1}{n} \sum_{i=1}^{n} (X_i - \bar{X})^2. \tag{1}
\]

(b) He derived the first four moments of \(S^2\), and he showed that these moments of \(S^2\) match exactly those of a Pearson type III distribution (now known as a gamma distribution); then he guessed that \(S^2\) has this distribution when the \{\(X_i\)\} are normal, and he calculated the distribution’s parameters.
(c) He showed that if the \( \{X_i\} \) are sampled from a symmetric distribution, then
- the statistics \( |\bar{X} - \mu| \) and \( S \) are uncorrelated; and
- the statistics \( (\bar{X} - \mu)^2 \) and \( S^2 \) are also uncorrelated.

(Gosset’s argument for the first result is flawed.)

(d) Since the normal distribution is symmetric about its mean, Gosset guessed that in random samples from a normal distribution, \( |\bar{X} - \mu| \) and \( S^2 \) must be independent random variables.
Gosset’s Approach to SPC (Cont’d)

Gosset used his results (a)–(d) to show that the statistic

\[ Z = \frac{\bar{X} - \mu}{S} \]  

(2)

based on a random sample of size \( n \) from a normal distribution with mean \( \mu \) has a probability density function of the form

\[ f(z) \propto \frac{1}{(1 + z^2)^{n/2}} ; \]  

(3)

and from (3), he computed tables of selected percentage points of the distribution of \( Z \) for sample sizes in the range \( 4 \leq n \leq 10 \).
To validate his results, Gosset conducted a precomputer simulation experiment by randomly sampling from a population of left middle finger lengths of 3,000 habitual British criminals, measured to the nearest 1/8 inch by Scotland Yard.

- These measurements were written on 3,000 pieces of cardboard, thoroughly shuffled, and drawn at random to yield a randomly ordered list of the entire population.

- Each consecutive set of 4 measurements from this list was taken as a sample of size $n = 4$, so that there were 750 such samples.
For each sample of size 4, Equations (1)–(2) were used to compute the corresponding $Z$-statistic; and a frequency polygon of the resulting 750 $Z$-values was superimposed on the density (3) with $n = 4$ as shown below.

**Diagram IV.** Comparison of the theoretical frequency curve $y = \frac{1500}{\pi} \left(1 + \frac{x^2}{\pi^2}\right)^{-3}$, with an actual sample of 750 cases.
Guinness allowed Gosset to publish his results, provided he used a pseudonym and their data was not used. The Managing Director of Guinness suggested the pseudonym “Student.”

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**No. 1**

**BIOMETRIKA.**

**THE PROBABLE ERROR OF A MEAN.**

**BY STUDENT.**
Final Thoughts on the Discovery of Student’s $t$-Distribution

In 1915 R. A. Fisher published a rigorous derivation of the probability density function of $Z$; and in 1925 Fisher reformulated $Z$ as Student’s $t$-statistic,

$$t = Z \sqrt{n-1}.$$ 

In 1992 E. L. Lehmann (University of California, Berkeley) made the following statement about Student’s 1908 paper (emphasis added):

> It took both Gosset and Fisher to make the $t$-test into the tool it has become and to begin the development of small-sample theory. But **what remains true without question is Student’s paper is one of the seminal contributions to 20th century statistics.**

This inaugural application of simulation to statistical process control is a ground-breaking example of the synergy of *intuition, abstraction*, and *simulation-based experimentation* in the discovery of the exact solution to what is now regarded as a classical industrial-engineering problem.
Final Thoughts on the Discovery of Student’s $t$-Distribution (Cont’d)

As for \textit{inspiration}, E. S. Pearson (University College London) closes the book “\textit{Student}”: A Statistical Biography of William Sealy Gosset with the following statement (emphasis added):

\begin{quote}
The development of the theory of small samples may well have brought financial rewards for Guinness, but Gosset’s extension of existing theory arose from the sheer intellectual attraction of the problem. \ldots\ A brief reflection on the life and work of this remarkable man is enough to make clear his commitment to scientific advance often quite distant from the work of the brewery, and his invariable wish to help friends in circumstances where the consequences for his career were non-existent.
\end{quote}
Aftermath: Gosset Became Head Brewer in London

Source: www.guinness.com
Stanisław Ulam (1909–1984) was a Polish-American mathematician who worked on the Manhattan Project and originated the Teller-Ulam design of thermonuclear weapons.
Ulam’s Epiphany

Ulam was fond of card games; and in 1946 while recovering from an illness and playing solitaire, he considered methods for calculating the probability that a Canfield solitaire laid out with 52 cards will come out successfully.

Because of the difficulty of a purely combinatorial approach, Ulam envisioned a computer simulation–based method for estimating this quantity.
Ulam’s Epiphany (Cont’d)

In 1946 Ulam performed detailed calculations showing that Edward Teller’s initial design for the hydrogen bomb would not work.

With the 1946 debut of ENIAC, the first general-purpose electronic computer, Ulam realized that computer simulation could estimate effectively the intractable multivariate integrals arising in the design of a workable hydrogen bomb.
Using Monte Carlo Methods to Design the Hydrogen Bomb

Ulam proposed an alternative design for the hydrogen bomb that he and Teller ultimately perfected and patented.

Ulam convinced John von Neumann and Nicholas Metropolis to work with him on developing the “Monte Carlo” (i.e., computer simulation–based) methods required to implement the Teller-Ulam design for thermonuclear weapons:

(a) The “middle-square” method for generating pseudorandom numbers;

(b) The acceptance-rejection method for random sampling from general (nonuniform) distributions;

(c) The solution of particle-diffusion problems by simulating the sample paths of a large ensemble of individual particles using (a) and (b); and

(d) The methods of Russian roulette and splitting to improve the efficiency of the simulation-based solution (c) of particle-diffusion problems.
John von Neumann and Nicholas Metropolis
Postscript on the Term “Monte Carlo”

Metropolis coined the term “Monte Carlo,” explaining that

\[\ldots\] Stan had an uncle who would borrow money from relatives because he “just had to go to Monte Carlo.” The name seems to have endured.

Apparently the only archival documentation on the genesis of this term is the following:

Gian-Carlo Rota on Ulam’s Powers of Inspiration, Intuition, Abstraction, and Experimentation

Source:

On Ulam’s inspiration and intuition—

... [his] contradictory traits in behavior: deep intuition and impatience with detail, playful inventiveness and dislike of prolonged work.

On Ulam’s collaboration with von Neumann—

From their free play of ideas came some of the great advances in applied mathematics of our day: the Monte Carlo method, mathematical experiments on the computer, cellular automata, simulated growth patterns.
On Ulam’s physical intuition—

After watching Fermi and Feynman at the blackboard, he discovered that he too had a knack for accurately estimating physical quantities by doing simple calculations with orders of magnitude. In fact he turned out to be better at that game than just about anyone around him.

It is hard to overstate how rare such an ability is . . . .

On Ulam’s professional achievements (emphasis added)—

Stan did his best work in fields where no one dared to tread, where he would be sure of having the first shot, free from all fear of having been anticipated. He used to brag about being lucky. But the source of his luck was his boundless intellectual courage, which let him see an interesting possibility where everyone else could only see a blur.
General Simulation Program (GSP): The First General-Purpose Simulation Platform

Originally conceived by Tocher while in his bath during Christmas 1957, the General Steelplant Simulation (GSP) was designed to handle the operation of steel plants using the open-hearth, electric-arc, or Bessemer-converter technologies.

Created in 1958, GSP consisted of a set of routines recognized by Tocher as necessary for any simulation platform:

- Model initialization;
- Time and state advance; and
- Report Generation.

Tocher envisioned the simulation’s principal components as “machines”—

- Cycling through states such as *busy*, *idle*, *unavailable*, *failed*, etc.; and
- Making transitions between states based on the simulation’s current time or the machine’s current state (or both).
Tocher’s Three-Phase Method for Simulation Time Advance

The state of each machine evolves over time in three phases:

A Advancing time to the next scheduled event that is “bound to occur” and that may change the machine’s state (called a “B-event”);
B Processing the associated B-event; and
C Attempting to process: (i) each “conditional” event (called a “C-event”) that occurs when a prespecified condition on the machine’s state is satisfied, and (ii) any additional events triggered by the C-event (i).
Wheel Charts and Activity Cycle Diagrams

K. D. Tocher: Simulation Pioneer and Polymath

Tocher sought a simple, expressive graphical representation (i.e., a flow diagram) of the cycle of state transitions that:

- Focuses on the machines in the system (i.e., the major pieces of equipment); and
- Represents state transitions that are costly (e.g., transitions between the states busy, idle, unavailable, failed, etc.).

Tocher’s Activity Cycle Diagram (Wheel Chart)—

- Has been adapted by academics and practitioners in UK; and
- Has had a major conceptual role in several simulation languages.
Activity Cycle Diagram of the Steelmaking Process

Innovative Features of GSP

As GSP was being developed in 1958, it became clear that the program provided a framework for a general-purpose simulation platform; and thus its full name was changed to General Simulation Program.

GSP incorporated some features that were far ahead of their time and thus not widely recognized or used, even within the United Steel Companies:

- The concept of block structure;
- The concept of objects; and
- Facilities for real-time, open-loop control of a plant using a discrete-event or combined discrete-continuous simulation driven by semiautomatic real-time collection of data on the plant’s performance.
Innovative Features of GSP (Cont’d)

GSP-2, GSP-3, and GSP-4 were released in 1964, 1967, and 1976, respectively.

- GSP-3 was implemented on an Elliott 503 computer that was delivered without an operating system.
- To develop GSP-3 on the Elliott 503 computer, Tocher designed and led the development of an operating system for that machine.
- In 1972 GSP-3 was ported to IBM System/360 computers and to ICL computers.

Key reference for GSP:

Innovative Features of GSP (Cont’d)

Innovative Features of GSP (Cont’d)

- Tocher designed his model for real-time, open-loop control of the temperature, chemical composition, and weight of the steel produced in each “blow” (or “heat”) of the acid Bessemer process.

- In the course of developing this simulation, Tocher had to formulate an empirical mathematical model of the total amount of oxygen available for oxidizing the bath reactants as a function of the mass of carbon and molten metal in the bath; and thus he made a significant discovery in metallurgy.

Key reference for Tocher’s simulation model of the acid Bessemer process:

Summary of Tocher’s Professional Contributions

K. D. Tocher’s work spanned the fields of simulation, statistics, operations research, computer science, and systems engineering.

- He contributed extensively to statistical theory, methodology, and applications;
- He made major contributions to the Monte Carlo method for distribution-sampling experiments;
- He worked on the design of digital computer hardware and software;
- He wrote the first textbook on simulation,
  

- He developed GSP, the first general-purpose simulation platform; and
- He made ground-breaking applications of computer-based planning systems for large-scale systems engineering.

K. D. Tocher was indeed a polymath of the first order and a pioneer in the field of computer simulation.
The Role of Inspiration and Intuition in Scientific Discovery

Key references:


Although both Poincaré and Hadamard are concerned primarily with discovery in mathematics, they discuss the discovery process in a broad diversity of scientific and nonscientific disciplines, including the arts.
Henri Poincaré and Jacques Hadamard
Steps in Scientific Discovery: Preparation

1. **Preparation:** preliminary, sharply focused action of the conscious requiring “severe tenseness of mind” and often multiple failed attempts to solve the problem at hand.

Hadamard (1945, pp. 43–44) on preparation—

   Newton’s discovery of universal attraction . . . [required] tenacious continuity of attention, “a consented, a voluntary faithfulness to an idea.”
Tchaikovsky on Preparation and Inspiration

Peter Ilich Tchaikovsky (1878) on preparation as a prerequisite to inspiration (emphasis added)—

Do not believe those who try to persuade you that composition is only a cold exercise of the intellect. **The only music capable of moving and touching us is that which flows from the depths of a composer’s soul when he is stirred by inspiration.** There is no doubt that even the greatest musical geniuses have sometimes worked without inspiration. **This guest does not always respond to the first invitation. We must always work, and a self-respecting artist must not fold his hands on the pretext that he is not in the mood.** If we wait for the mood, without endeavouring to meet it half-way, we easily become indolent and apathetic. We must be patient, and believe that inspiration will come to those who can master their disinclination. A few days ago I told you I was working every day without any real inspiration.
Had I given way to my disinclination, undoubtedly I should have drifted into a long period of idleness. But my patience and faith did not fail me, and to-day I felt that inexplicable glow of inspiration of which I told you; thanks to which I know beforehand that whatever I write to-day will have power to make an impression, and to touch the hearts of those who hear it. I hope you will not think I am indulging in self-laudation, if I tell you that I very seldom suffer from this disinclination to work. I believe the reason for this is that I am naturally patient. I have learnt to master myself, and I am glad I have not followed in the steps of some of my Russian colleagues, who have no self-confidence and are so impatient that at the least difficulty they are ready to throw up the sponge. This is why, in spite of great gifts, they accomplish so little, and that in an amateur way.
2. **Incubation**: turning the problem over to the unconscious to try all promising combinations of ideas for solving the problem at hand.

Poincaré (1914, pp. 61–62) on his atomic model of unconscious work (emphasis added)—

> Perhaps we must look for the explanation in that period of preliminary conscious work which always precedes all fruitful unconscious work. . . . [L]et us represent the future elements of our combinations as something resembling Epicurus’s hooked atoms. When the mind is in complete repose these atoms are immovable; they are, so to speak, attached to the wall. . . .

On the other hand, *during a period of apparent repose, but of unconscious work, some of them are detached from the wall and set in motion*. They plough through space in all directions, like a swarm of gnats, for instance, or, if we prefer a more learned comparison, like the gaseous molecules in the kinetic theory of gases. *Their mutual collisions may then produce new combinations.*
What is the part to be played by the preliminary conscious work? Clearly it is to liberate some of these atoms, to detach them from the wall and set them in motion. We think we have accomplished nothing, when we have stirred up the elements in a thousand different ways to try to arrange them, and have not succeeded in finding a satisfactory arrangement. But after this agitation imparted to them by our will, they do not return to their original repose, but continue to circulate freely.

Now our will did not select them at random, but in pursuit of a perfectly definite aim. Those it has liberated are not, therefore, chance atoms; they are those from which we may reasonably expect the desired solution. The liberated atoms will then experience collisions, either with each other, or with the atoms that have remained stationary, which they will run against in their course. ...
3. **Illumination**: a sudden flash of insight coming after a period of intense conscious preparation and a latency period in which the unconscious has done its work.

Poincaré (1914, pp. 54–55) on illumination (emphasis added)—

Thereupon I left for Mont-Valérien, where I had to serve my time in the army, and so my mind was preoccupied with very different matters. *One day, as I was crossing the street, the solution of the difficulty which had brought me to a standstill came to me all at once.* I did not try to fathom it immediately, and it was only after my service was finished that I returned to the question. I had all the elements, and had only to assemble and arrange them. Accordingly I composed my definitive treatise at a sitting and without any difficulty.
Other examples of illumination:

- K. D. Tocher’s vision for GSP while taking a bath during Christmas 1957; and

- Alan Pritsker’s sudden insight into the solution of the central problem in his dissertation research while playing with his cat; see

4. **Intervention of consciousness:** the insights provided by the unconscious are summoned into consciousness to be worked out completely in two stages.

   (a) **Precise Expression:** providing a formal written statement of the results using standard terminology and symbolism.

   Auguste Rodin (as quoted by Delacroix (1939)) on precise expression—

   Till the end of his task, it is necessary for him [the sculptor] to maintain energetically, in the full light of his consciousness, his global idea, so as to reconduct unceasingly to it and closely connect with it the smallest details of his work. And this cannot be done without a severe strain of thought.
(b) **Detailed Verification**: providing a rigorous justification of the results, and deducing their immediate consequences.

Poincaré (1914, p. 56) on detailed verification (emphasis added)—

*I have spoken of the feeling of absolute certainty which accompanies the inspiration*; in the cases quoted this feeling was not deceptive, and more often than not this will be the case. But we must beware of thinking that this is a rule without exceptions. *Often the feeling deceives us without being any less distinct on that account, and we only detect it when we attempt to establish the demonstration.*
(c) **Discovery of Links to Other Work:** finding the connections between the precisely stated and verified result and other problems, and then using the newly established result to make progress in solving those other problems.

Hadamard (1945, pp. 62–63) on the discovery of links to other work (emphasis added)—

> After a first stage of research has been brought to an end, the following one requires a new impulse, which can be originated and directed only when our consciousness takes account of the first precise result. . . .

> . . . *It most often happens that such a result needs to be digested, or to say it differently, to be classed in our fringe-consciousness, so as to be “ready for use.”* Then it can easily and rapidly find its place in the synthetic scheme of deduction.
Intuition and the Unconscious

A prominent example of such intuition in simulation research—Bruce Schmeiser’s intuition on the advantages of the simulation analysis method of overlapping batch means; see


Twenty-five years elapsed before this intuition was formalized in Theorem 2 of the following article:

Another prominent example of intuition in simulation research—Lee Schruben’s intuition on the advantages of the simulation analysis method of standardized time series; see


The ground-breaking work of Meketon and Schmeiser (1984) and Schruben (1983) has spawned much follow-up research on simulation analysis methods—and all this work has ultimately led back to Student’s $t$-statistic.
Key references on scientific discovery that is *focused on* simulation or *based on* simulation as a research tool:


Abstraction in Simulation: Modeling and Analysis

Abstraction encompasses both simulation modeling and the simulation analysis required to do the following:

- Build a model;
- Design experiments using that model; and
- Draw appropriate conclusions from the observed results.
Simulation-based experimentation differs fundamentally from all other types of empirical scientific work by the large potential efficiency improvements that are achievable because we have complete control of the experimental conditions under which each alternative scenario is simulated.

This control of the experimental conditions can be exploited using several Monte Carlo methods, especially the following:

- The method of importance sampling as discussed in

The methods of common random numbers and antithetic variates as detailed in Sections 15.2 and 16.6 of:


and in Section 3.2 of:

The discussions of paired-comparison experiments by Schriber (1991) and Box, Hunter, and Hunter (2005) lead us back to where we began—Student’s $t$-distribution and Student’s seminal 1908 paper.
Conclusions

Advances in simulation are driven by the continuous interplay of the following:

- Our sources of inspiration—both internal and external—for the discovery of solutions to practical problems as well as the theory and methodology required to attack those problems;

- The intuition that we acquire from careful experimentation with well-designed simulation models, from intense scrutiny of the results, and from allowing the unconscious to work on the results; and

- The conscious follow-up work in which the emerging flashes of insight into the problem at hand are expressed precisely, verified completely, and connected to other simulation work.
Thank You

Questions?