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Title: Visualizing the Distribution of Converged MCNP Tally Means with a Quincunx Machine

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Visualizing the Distribution of Converged MCNP Tally Means with a Quincunx Machine

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Los Alamos National Laboratory

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Acknowledgements

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- Tony Zukaitis (LANL XCP-3) for introducing us to the Galton Board (2019)
- Mark Hebner (Four Pines Publishing) and Philip Poissant (Poissant Design Associates Inc.) for
  - designing and relentlessly refining a Galton Board,
  - many interesting and informative discussions about these STEM.org-authenticated Galton Boards
  - allowing a prototype of their latest Galton Board to be used in this presentation, and
  - providing the galtonboard.com bead-flow video (Robert Bray)
- Colin Josey (LANL XCP-3) for discussions on eigenvalue convergence

Outline

Statistical Definitions

- True precise tally mean $$E(x) = \int x\, f(x) \mathrm{d}x$$
  - x is the tally random variable
  - $f(x)$ is the tally history score probability density function
- Estimated precise tally mean $$\overline{x} = \frac{1}{H} \sum_{h=1}^{H} x_h$$
  - H is the number of independent and identically distributed histories
- True population variance $$\sigma^2 = \int (x - E(x))^2 f(x) \mathrm{d}x = E(x^2) - E^2(x)$$
- Estimated sample variance $$S^2 = \frac{H}{H-1} \left(\left[\frac{1}{H} \sum_{h=1}^{H} x_h^2 \right] - \overline{x}^2 \right)$$
- True variance of the mean $$\sigma_{\overline{x}}^2 = \sigma^2 / H$$
- Estimated variance of the mean $$S_{\overline{x}}^2 = S^2 / H$$
- Estimated standard deviation of the mean $$S_{\overline{x}} = S / \sqrt{H}$$

The Central Limit Theorem (CLT)

- The distribution of the sum of H independent and identically distributed random variables approaches a normal distribution as H approaches infinity where the mean and variance must exist (i.e., be finite).

$$P\left\{\alpha \le \frac{\overline{x} - E(x)}{\sigma_{\overline{x}}} \le \beta\right\} \to \frac{1}{\sqrt{2\pi}} \int_{\alpha}^{\beta} \exp\left(\frac{-t^2}{2}\right) \mathrm{d}t \tag{1}$$

- Typical confidence intervals:

$$P\{\overline{x} - 1\sigma_{\overline{x}} < E(x) < \overline{x} + 1\sigma_{\overline{x}}\} \approx 0.683$$

$$P\{\overline{x} - 2\sigma_{\overline{x}} < E(x) < \overline{x} + 2\sigma_{\overline{x}}\} \approx 0.955$$

$$P\{\overline{x} - 3\sigma_{\overline{x}} < E(x) < \overline{x} + 3\sigma_{\overline{x}}\} \approx 0.997$$

- MCNP has statistical tests to assess convergence (H is large)

Definition: MCNP Tally Result and Confidence Interval

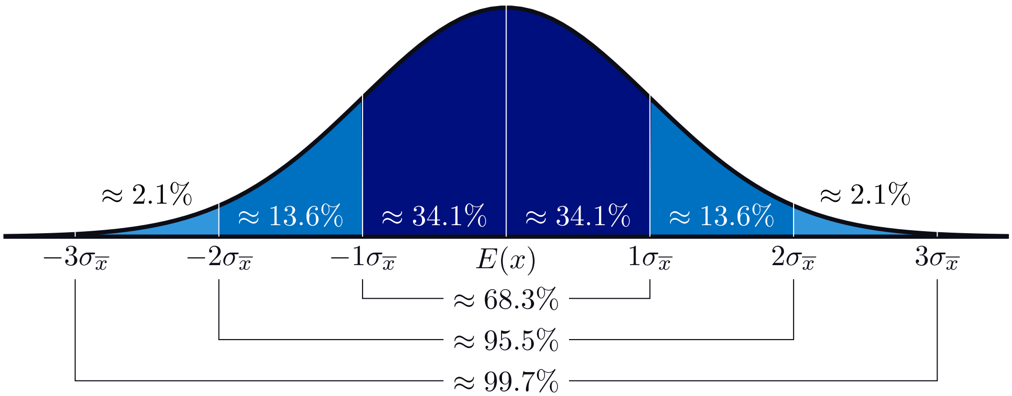
- The goal of an MCNP tally is to determine $E(x)$
- A converged MCNP tally result has two requirements:
  - $f(x)$ is completely sampled (MCNP Print Table 161)
  - First 2 moments of $f(x)$ exist so $\overline{x} \sim E(x)$ and $S_{\overline{x}} \sim \sigma_{\overline{x}}$
- An MCNP tally result is comprised of two parts:
  - The estimated mean, $\overline{x}$
  - The estimated standard deviation of the mean, $S_{\overline{x}}$
- Provided: estimated mean and the estimated relative error ($S_{\overline{x}}/\overline{x}$)

A *converged* MCNP tally confidence interval, characterized by its precision, is a range of tally values constructed from the MCNP tally result that is expected to include $E(x)$ at a specified confidence level (i.e., some particular fraction of the time).

- The MCNP confidence interval is based on the normal distribution

$$\mathcal{N}(x, E(x), \sigma_{\overline{x}}) = \frac{1}{\sigma_{\overline{x}}\sqrt{2\pi}} \exp\left(\frac{-(x - E(x))^2}{2\sigma_{\overline{x}}^2}\right) \tag{2}$$

Probability Density Function for a Normal Distribution



- Plot of $\mathcal{N}(x, E(x), \sigma_{\overline{x}})$ versus x for a normal distribution with mean of $E(x)$
- The Central Limit Theorem states $\overline{x} \sim \mathcal{N}(x, E(x), \sigma_{\overline{x}})$ as $H \to \infty$
- An MCNP tally mean $\overline{x}$ in the dark blue range is most probable
  - $\overline{x}$ in the dark blue range with $\pm 1 S_{\overline{x}}$ confidence interval will include $E(x)$
  - $\overline{x}$ outside the dark blue range will NOT include $E(x)$ at the $1 S_{\overline{x}}$ level

An Example MCNP Tally for a Purely Absorbing Slab

- Probability of transmission:

$$\exp(-\Sigma_t s) = \exp(-\ln(2)) = 1/2$$

- Score of 1 when transmitted, 0 otherwise:

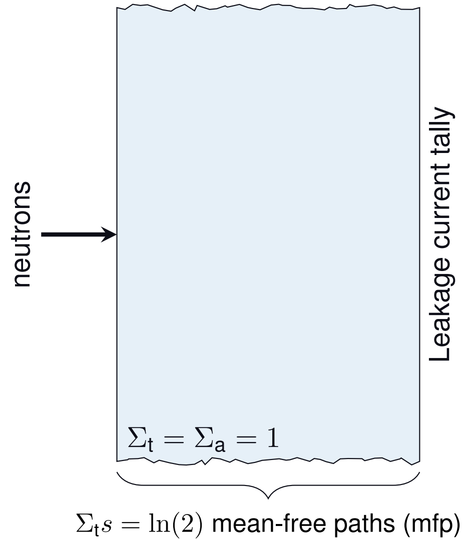
$$f(x) = \frac{\delta(0-x)}{2} + \frac{\delta(1-x)}{2},$$

$$E(x^n) = \int x^n f(x) \mathrm{d}x = 1/2,$$

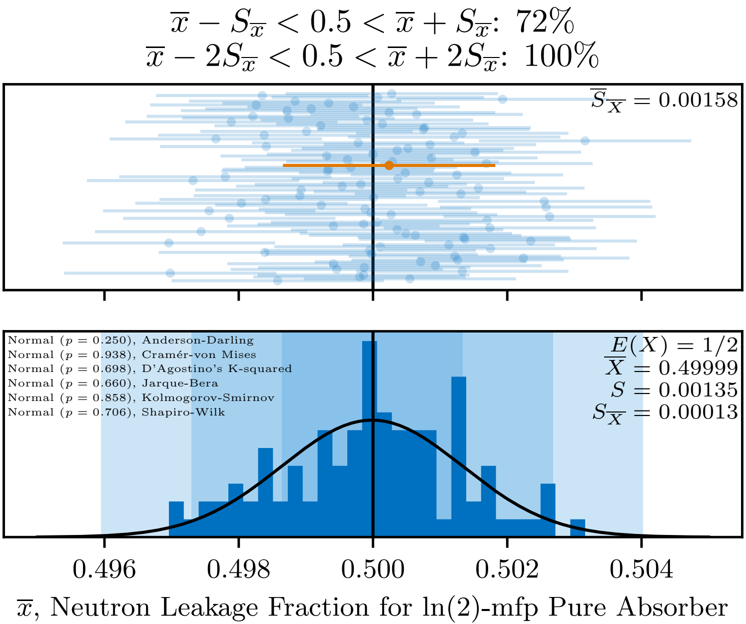
$$\sigma = \sqrt{E(x^2) - E^2(x)} = \sqrt{1/4} = 1/2$$

- For 100,000 histories:

$$\sigma_{\overline{x}} = \frac{\sigma}{\sqrt{H}} = \frac{1}{2\sqrt{10^5}} \approx 0.00158$$



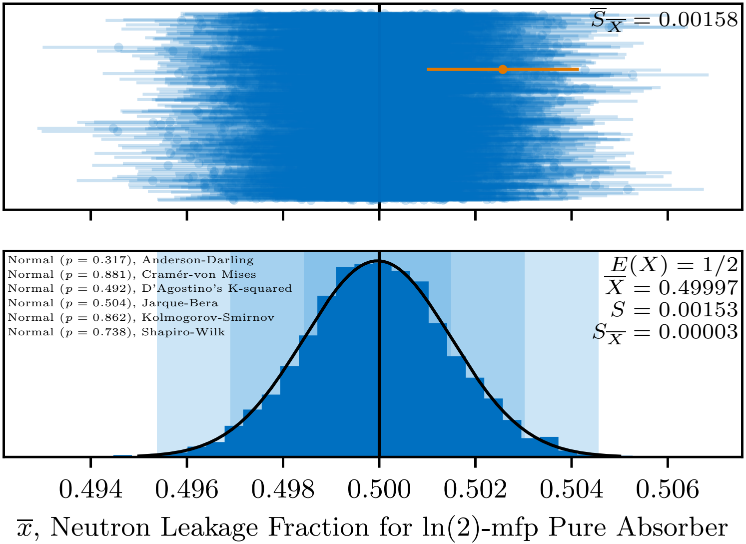
100 Converged Tally Means and Confidence Intervals



Similar to k-eigenvalue plots in [1, 2].
The probability p values > 0.05 fail to reject the null hypothesis
that these data are normally distributed, which suggests that they are.

3,000 Converged Tally Means and Confidence Intervals

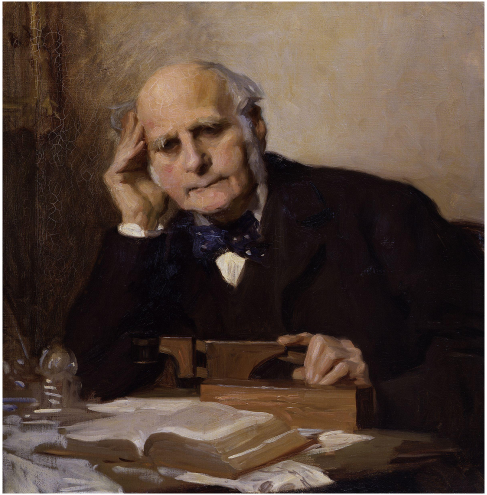
$$\overline{x} - S_{\overline{x}} < 0.5 < \overline{x} + S_{\overline{x}}: \ 70\%$$
$$\overline{x} - 2S_{\overline{x}} < 0.5 < \overline{x} + 2S_{\overline{x}}: \ 96\%$$



Similar to k-eigenvalue plots in [1, 2].
The probability p values > 0.05 fail to reject the null hypothesis
that these data are normally distributed, which suggests that they are.

First Animated Device Showing the Normal Distribution

- British scientist Sir Francis Galton (1822–1911) was a statistician, anthropologist, sociologist, psychologist, geographer, and meteorologist
- He studied the characteristics of human populations
- He saw that his data was in a normal distribution
- He invented the quincunx (⚄) in 1873 to demonstrate the Central Limit Theorem
- He was fascinated by the animated demonstration of "order out of chaos"



Sir Francis Galton by Charles Wellington Furse, 1903

Image from: https://en.wikipedia.org/wiki/Francis_Galton.

Galton's Quincunx Design Inspired by a Bagatelle Board

- This version of a bagatelle board is called Rocks of Scilly (c. 1810)
- Bagatelle board balls fall through a series of pins in a quincunx (⚄) pattern with bins at the bottom
  - Ball starts on the right-hand side and is shot upward with a plunger
  - Similar to a modern pinball machine
- This bagatelle board could be considered an early quincunx machine

Original Quincunx Designs by Sir Francis Galton (1889)

- The bead source is at the top and the “tally” bins are at the bottom
- Pins are in a quincunx pattern
  - Pips on the five side of the die: ⚄
- Each bead produces a random walk through the pins to a “tally” bin
- Demonstrates “order out of chaos”
- The “quincunx” today is called a Galton Board
- Mimics an MCNP calculation with a particle source, a random walk, and tally bins

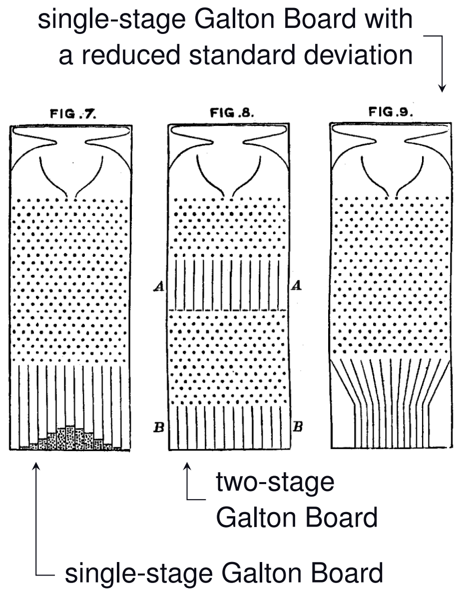
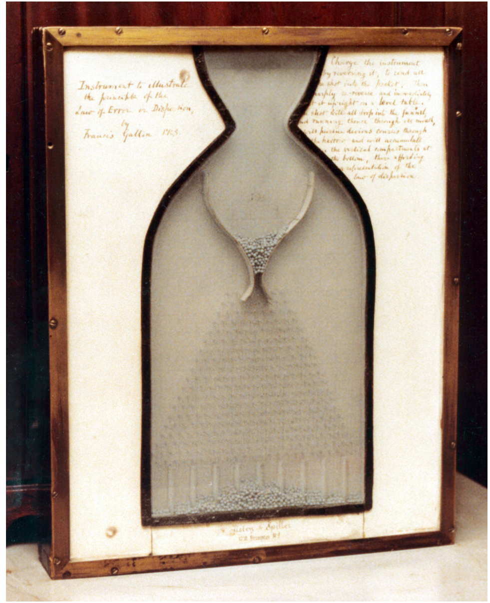


Image from [4, p. 89].

An Original Quincunx (a.k.a Galton Board) (1893)

- The bead (“charge of shot”) reservoir is at the top
- 19 rows of a quincunx-pattern pins
- “The shot passes through the funnel and scamper deviously down through the pins in a curious and interesting way; each of them darting a step to the right or left, as the case may be, every time it strikes a pin.”
- “The outline of the columns of shot that accumulate in the bins approximates to the Curve of Frequency, and is closely of the same shape however often the experiment is repeated.”



Galton’s handwritten instructions in upper right

Image from https://www.galtonboard.com.

Mathematics of the Galton Board Bead Flow

- A binomial distribution is a discrete probability distribution that defines the number of successes from n Bernoulli trials
- The bead flow is a physical model of the binomial distribution

$$\Pr(k; n, p) = \binom{n}{k} p^k (1-p)^{n-k} \tag{3}$$

where

$$\text{Binomial coefficients} = \binom{n}{k} = \frac{n!}{k!(n-k)!} \tag{4}$$

where

n number of left-right experiments (Bernoulli trials),
p probability of success (right),
$1-p$ probability of failure (left),
k number of successes (right, 0 to n)

Mathematics of the Galton Board Bead Flow, cont.

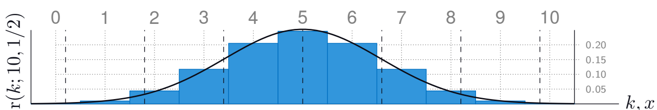
- n Galton Board rows perform n Bernoulli trials (no skipped rows)
- For the Galton board, $p = 1/2$ (like a coin flip)
- The binomial distribution for the Galton board:

$$\Pr(k; n, {}^1\!/\!_2) = \frac{n!}{2^n k!(n-k)!} = \binom{n}{k} \frac{1}{2^n} \tag{5}$$

- De Moivre-Laplace theorem

$$\mathcal{N}\left(x, \frac{n}{2}, \frac{\sqrt{n}}{2}\right) \sim \Pr(k; n, {}^1\!/\!_2) \ , \ \ n \geq 10 \tag{6}$$

$$Z_{\text{max}}(n) = \frac{n + 1/2 - n/2}{\sqrt{n}/2} = \frac{n+1}{\sqrt{n}} \tag{7}$$



Binomial distribution for $n = 10$ and $p = 1/2$

$\mathcal{N}(x, 5, \sqrt{10}/2)$: $E(x) = 5$, $\sigma = 1.58$

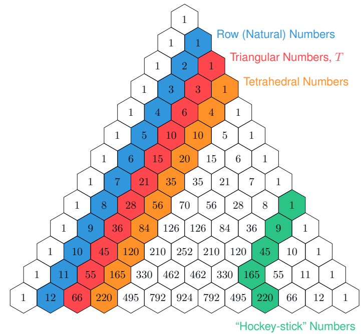
↑ $Z_{\text{max}}(10) \approx 3.48$

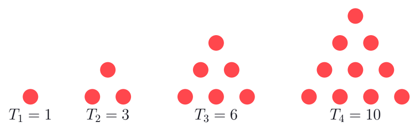
Pascal's Triangle Defines the Number of Random Walks

- Pascal's triangle is an array of binomial coefficients (unnormed binomial distribution)

$$C(n,k) = C_k^n = \binom{n}{k} = \frac{n!}{k!(n-k)!} \qquad (8)$$

- Each value is the sum of the above two values
- The kth entry of the nth Pascal's triangle row (blue) is the number of paths a bead can take to reach that location after n Bernoulli trials
- Probability of reaching the kth location of the nth Pascal triangle row = $\Pr(k; n, {}^1\!/_2)$
- The total number of possible random walks for n Galton Board rows is 2^n





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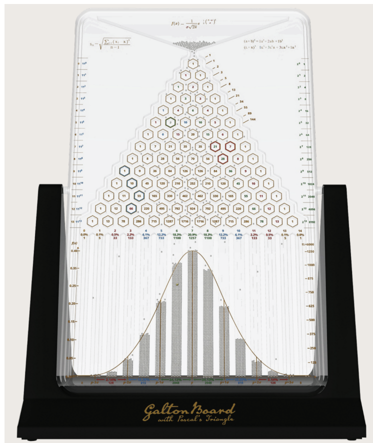
Modern Day Galton Boards

- A few physical and many digital Galton Boards exist today
- Desktop sized for a real hands-on experience
- Easy to use, with thousands of beads, and complete documentation
- High-quality engineering and relatively inexpensive ($50)

12 rows of round pins
Unrestricted flow of 3000 beads to 28 tally bins
$3.375'' \times 5.5''$



Prototype: 14 rows of hex pins
Restricted (Pascal's triangle) flow of 6000 beads to 15 tally bins
$6.75'' \times 11''$

$5.5/3.375 = 11/6.75 = 1.\overline{629}\ldots \approx \varphi$ (the "Golden Ratio", 1.618034).

What Does "Order Out of Chaos" Look Like?

- A Galton Board's binomial distribution bead flow is chaotic
- Small Galton Board video of constrained bead flow
  - $Z_{\text{max}}(12) \approx 3.75$
  - Observed ≈ 1.8
  - $BDM = 3.75/1.8 \approx 2$
- Large Galton Board demonstration of constrained bead flow
  - $Z_{\text{max}}(14) \approx 4.01$
  - Observed ≈ 4
  - $BDM = 4.01/4 \approx 1$
- Small Galton Board bead flow is more chaotic ($BDM \approx 2$)

Click picture for 1 minute video courtesy of galtonboard.com [5].
BDM is Bead Distribution Metric: ratio of Z_{max} to the observed number of standard deviations at the edge of Pascal's triangle.

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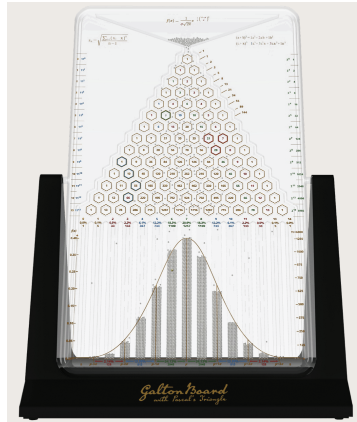
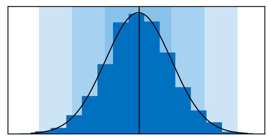
Visualizing the Distribution of Converged MCNP Tally Means With a Galton Board

- One bead's random walk and result represents one converged MCNP tally mean $\overline{x}$
- Many beads represent many independent MCNP tally means
- Converged MCNP tally means are normally distributed (CLT)
- Galton Board bead random walks form a normal distribution (CLT)
- Galton Board flip shows 3000/6000 converged MCNP tally means
- One gold bead is present to follow its behavior (one $\overline{x}$)

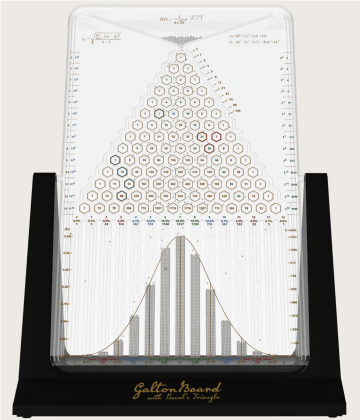


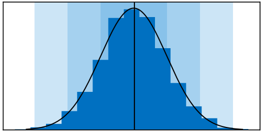


Summary of Visualizing Converged MCNP Tally Means

- Reviewed statistical concepts, normal distribution, and CLT
- Examined the statistical behavior of a simple MCNP tally
- Introduced Galton, his quincunx, and “order out of chaos”
- Discussed binomial distributions and Pascal’s Triangle
- Used modern Galton Boards to visualize converged MCNP $\overline{x}$s
  - Beads (and $\overline{x}$s) are normally distributed according to the CLT
  - One bead’s random walk and result represents one converged MCNP $\overline{x}$
  - Know distribution of beads, but not a bead location (gold bead)
  - Must form an $\overline{x}$ confidence interval to “find” $E(x)$
- A quincunx machine is a great tool to visualize the formation and distribution of converged MCNP tally means
  - ...and will be used in MCNP class demonstrations

Questions?





If you were to develop a Galton Board coin, how would you do so to have a normal distribution in your pocket?

Engineering a Galton Board Coin

Click picture for 34 minute video [6].

Backup Slides

References

[1] T. J. Urbatsch, R. A. Forster, R. E. Prael, and R. J. Beckman, “Estimation and Interpretation of k_{eff} Confidence Intervals in MCNP,” Los Alamos National Laboratory, Los Alamos, NM, USA, Tech. Rep. LA-12658 / UC-910, Nov. 1995. URL: https://mcnp.lanl.gov/pdf_files/la-12658.pdf

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[4] F. Galton, *Natural Inheritance*. Macmillan and Co., 1889.

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[6] Philip Poissant, “The Galton Board: an Industrial Engineering Story,” MathEd Forum, The Fields Institute for Research in Mathematical Sciences, University of Toronto, Ontario, Canada, Sep. 2018.
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Abstract

Visualizing what a collection of independent, converged (normally distributed) MCNP tally means looks like is interesting, informative, and reinforces the need for creating a confidence interval from an MCNP tally result. The first successful dynamic animated visualization technique for the normal distribution was invented by British Scientist Sir Francis Galton in 1873 to illustrate the results of his studies of human populations. He devised a quincunx machine or Galton Board, as it is known today, to demonstrate "order out of chaos" (the Central Limit Theorem) using beads that cascade down a wall of pins arranged in a quincunx pattern. The beads are collected in "tally" bins at the bottom. The resulting binomial distribution of beads, defined by Pascal's triangle, is a good discrete approximation to the continuous normal distribution in the Central Limit Theorem. To visualize one converged MCNP tally mean using a Galton Board, define one bead, its random walk through the Galton Board, and scoring in a "tally" bin as representing that one tally mean. The accumulation of many beads, which represents many independent MCNP tally means, simulates the normal distribution of these converged MCNP tally means. Today, major design improvements have been made to the original Galton Board that facilitate ease of use, increased number of beads, bead flow reproducibility, and the statistical understanding of the importance and implications of the bell-shaped curve. Two modern Galton Boards with slightly different bead flow patterns are presented and used to visualize and interpret the distribution of "converged MCNP tally means" in much the same way Galton did. These Galton Boards will be used in MCNP Class instructions and demonstrations.