NE 155
Introduction to Numerical Simulations in Radiation Transport
Lecture 31: Introduction to Monte Carlo

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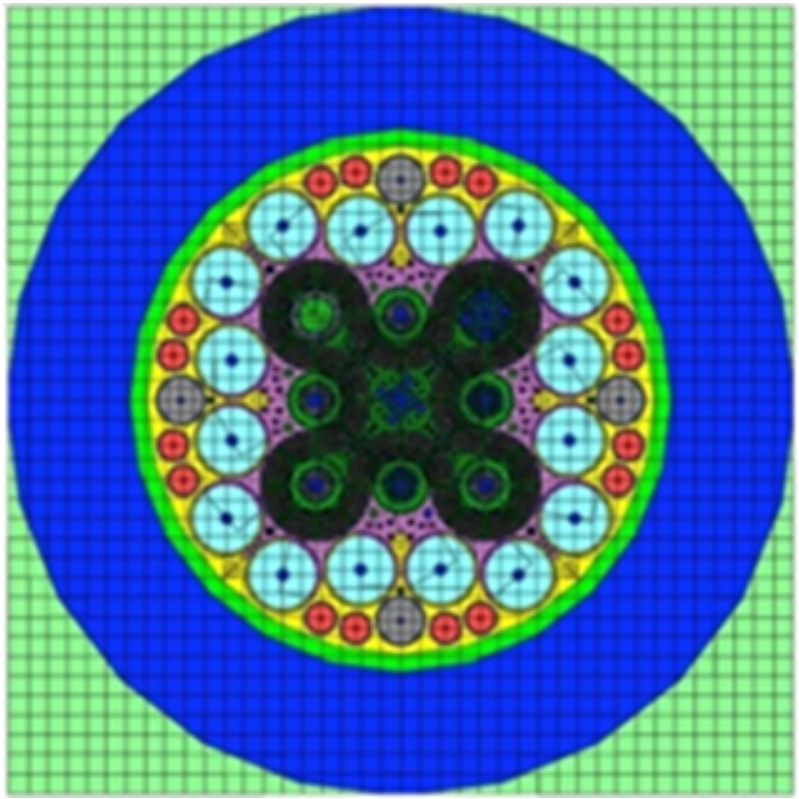
April 7, 2017

Learning Objectives

1. Define Monte Carlo simulation
2. Understand the history of Monte Carlo methods
3. Justify the choice of Monte Carlo for radiation transport
4. Understand the mathematical validity of Monte Carlo for radiation transport



Notes derived from Jasmina Vujic and Paul Wilson

What is Monte Carlo?

- The use of *random processes* to determine a *statistically-expected* solution to a problem

- Random processes can fulfill two roles:
  - Statistical approximation to mathematical equations
  - Statistical approximations to physical processes

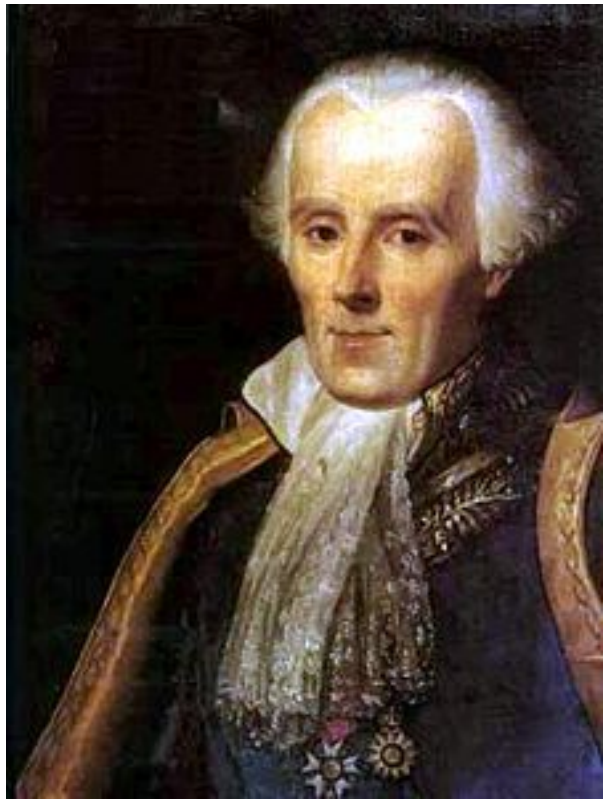
- Construct a random process for a problem,
- Carry out a numerical simulation by N-fold sampling from a random # sequence

Historical Perspective

- Comte du Buffon (1777): needle tossing experiment to calculate π
- Laplace (1786): random points in a rectangle to calculate π
- Lord Kelvin (1901): used random sampling to aid in evaluating time integrals associated with kinetic theory of gases
- Fermi (1930): was among the first to use random sampling methods to study neutron moderation while still in Rome, Italy
- 1947: Fermi, von Neumann, Frankel, Metropolis, Ulam, and others developed computer-oriented Monte Carlo method at Los Alamos to trace neutrons through fissionable materials; coined the term "Monte Carlo"
- Berger (1963): first complete coupled electron-photon transport code

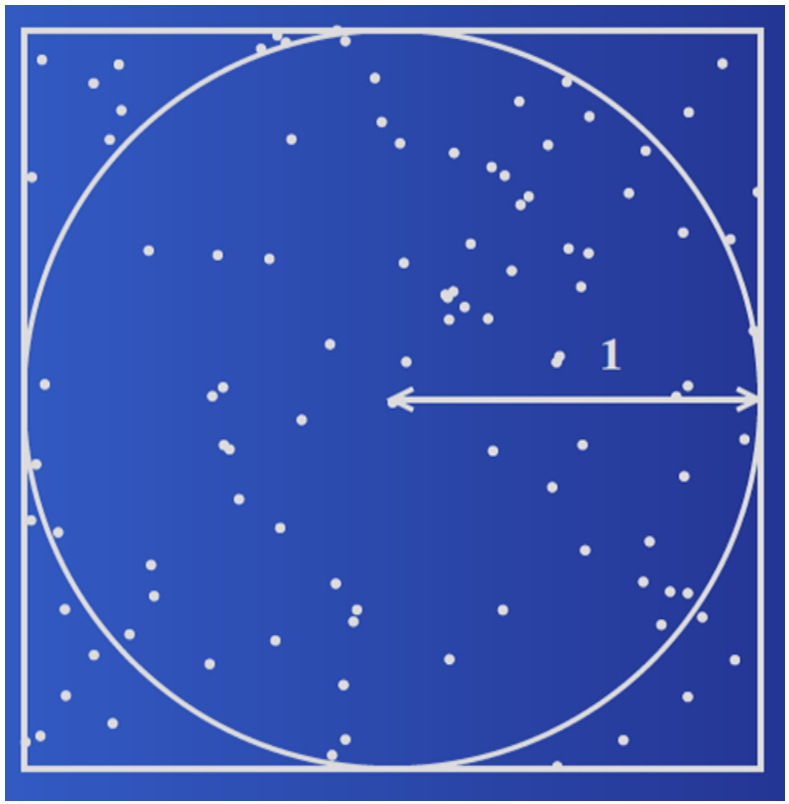
Evaluate π by Random Sampling

- Pierre-Simon Laplace
- Born: 23 March 1749
- Died: 5 March 1827 (aged 77)
- Nationality and Residence: France
- Fields: Astronomy and Mathematics
- Institutions: Ecole Militaire; Alma mater: University of Caen



Marquis Pierre-Simon de Laplace, "Theorie Analytique des Probabilities, Livre 2", *Ouvres Completes de Laplace*, de L'Academie des Sciences, Paris, **7**, part 2, 356-366 (1786).

Evaluate π by Random Sampling



- Area of square, $A_s = 4$
- Area of circle, $A_c = \pi$
- Fraction of random points in circle

$$p = \frac{A_c}{A_s} = \frac{\pi}{4}$$

- Random points = N
- Random points in circle = N_c, $\therefore$

$$p = \frac{N_c}{N}\ ; \quad \pi = \frac{4N_c}{N}$$

Manhattan Project

- The first human engineered nuclear detonation, the Trinity Test in New Mexico.
- Active: 1942–1945
- Branch: U.S. Army Corps of Engineers
- Monte Carlo Pioneers:
  - Enrico Fermi,
  - Stanislaw Ulam,
  - John von Neumann,
  - Robert Richtmeyer,
  - Nicholas Metropolis

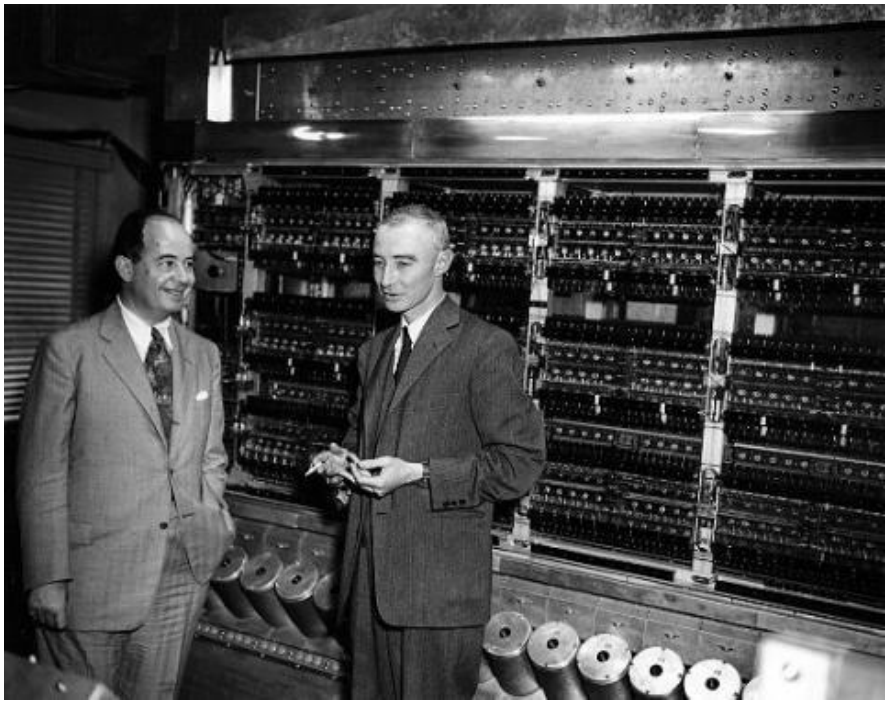


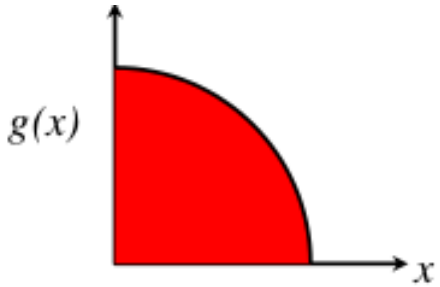
Figure 1: Oppenheimer, von Neumann, MANIAC

Nicholas Metropolis, S. Ulam. "The Monte Carlo Method," *Journal of the American Statistical Association*, **44**, No. 247, 335-341 (Sep. 1949).

General Purpose MC Codes

- MCNP: developed at LANL, distributed via RSICC, http://rsicc.ornl.gov
- Geant4: developed by a large collaboration in the HEP community, http://geant4.web.cern.ch/geant4/
- EGSnrc: developed at NRC (Canada), http://www.irs.inms.nrc.ca/EGSnrc/EGSnrc.html
- SERPENT: Developed by Dr. Jaakko Leppanen, VTT, Finland, http://montecarlo.vtt.fi/
- Shift: developed at ORNL, distributed via RSICC, http://rsicc.ornl.gov

Evaluate π by Random Sampling (math)



$$g(x) = \sqrt{1 - x^2} \qquad G = \int_0^1 g(x)dx = \frac{\pi}{4}$$

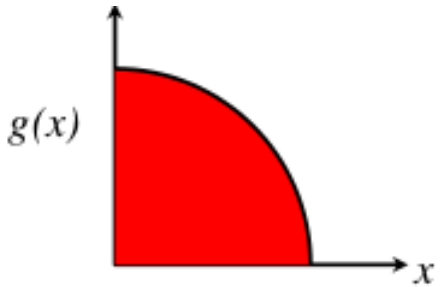
$$G = \int_0^1 g(x)dx = (1 - 0)\overline{g(x)}$$

Determine $\overline{g(x)}$ by random sampling:

for $k = 1, \ldots, N$, choose $\hat{x}_k$ randomly on the interval $(0, 1)$,

$$\overline{g(x)} \equiv \frac{1}{N}\sum_{k=1}^{N} g(\hat{x}_k) = \frac{1}{N}\sqrt{1 - \hat{x}_k^2}$$

Evaluate π by Random Sampling (physics)



$$g(x) = \sqrt{1 - x^2} \qquad G = \int_0^1 g(x)dx = \frac{\pi}{4}$$

G = area under curve,
= fraction of unit square under curve

for $k = 1, \ldots, N$, chose $\hat{x}_k, \hat{y}_k$ randomly on the interval $[0, 1]$,

m_N = # of times in N trials that $\hat{x}_k^2 + \hat{y}_k^2 \leq 1$,

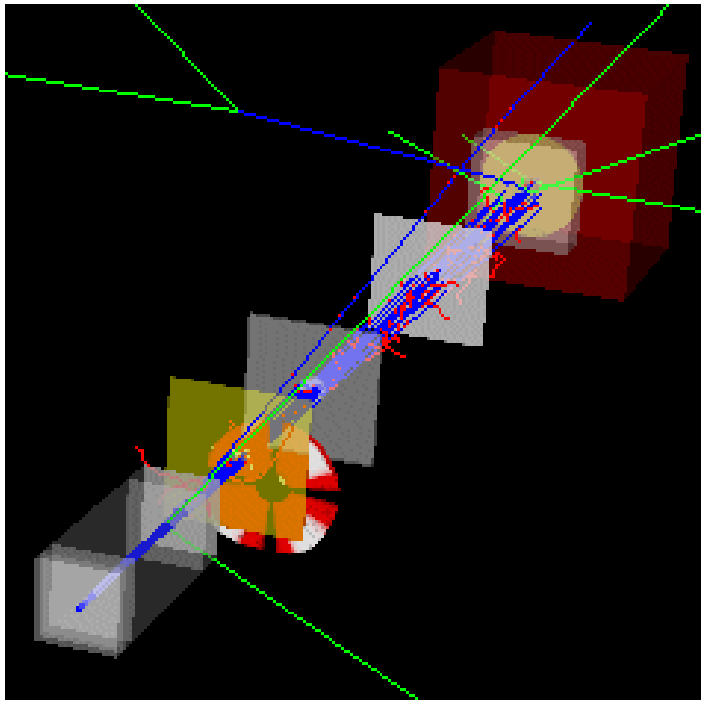
$$G = \frac{m_N}{N}$$

Why/When Monte Carlo?

- Applications that are mathematically equivalent to *integration over many dimensions*
  - Analytic integration may be impossible
  - Deterministic numerical integration may be slow and/or require error prone approximations
- However, statistically accurate results can require **significant computer time**
- Fortunately, Monte Carlo and parallel computing go well together
- and we also have Variance Reduction methods

MC is Used in Many Fields

- High Energy Physics
  Many nucleon interactions
- Process Engineering
  Combine uncertainties in many variables
- Financial sector
  Prices and rates of return for many objects
- Risk Analysis
  Many individual contributions to risk



What is MC Radiation Transport?

Simulate many independent particles in a system

- Treat each physical process as a *probabilistic process*
- *Randomly sample* each process using an independent stream of random numbers
- Follow each particle from birth until it no longer matters
- Accumulate the contributions of each particle to find the statistically-expected mean behavior and variance

Mathematical Validity

- Consider particles with a phase space describing position, $\vec{r}$, and velocity, $\vec{v}$
- A neutral particle can be transmitted from one position to another at a constant velocity

$$T(\vec{r}\,' \rightarrow \vec{r}, \vec{v})$$

- A particle can undergo a collision at a single position that changes its velocity

$$C(\vec{r}, \vec{v}\,' \rightarrow \vec{v})$$

Contributions After 0 Collisions

- Consider a particle born from a source described by

$$Q(\vec{r}\,', \vec{v}\,')$$

- This particle will contribute to the flux at $(\vec{r}, \vec{v})$ before any collisions

$$\psi_0(\vec{r}, \vec{v}) = \int_{\vec{r}\,'} Q(\vec{r}\,', \vec{v}\,') T(\vec{r}\,' \rightarrow \vec{r}, \vec{v}) d\vec{r}\,'$$

Contributions After 1 Collision

- The uncollided particles, $\psi_0(\vec{r}\,', \vec{v}\,')$, could undergo 1 collision and then be transmitted to the point $(\vec{r}, \vec{v})$

$$\psi_1(\vec{r}, \vec{v}) = \underbrace{\int_{\vec{r}\,'} \left[\underbrace{\int_{\vec{v}\,'} \psi_0(\vec{r}\,', \vec{v}\,') C(\vec{r}\,', \vec{v}\,' \rightarrow \vec{v}) d\vec{v}\,'}_{collision} \right] T(\vec{r}\,' \rightarrow \vec{r}, \vec{v}) d\vec{r}\,'}_{transmission}$$

Contributions After k Collisions

- Particles that have undergone k collisions, $\psi_k(\vec{r}\,', \vec{v}\,')$, could undergo another collision and then be transmitted to the point $(\vec{r}, \vec{v})$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \underbrace{\int_{\vec{r}\,'} \left[\underbrace{\int_{\vec{v}\,'} \psi_k(\vec{r}\,', \vec{v}\,') C(\vec{r}\,', \vec{v}\,' \rightarrow \vec{v}) d\vec{v}\,'}_{collision} \right] T(\vec{r}\,' \rightarrow \vec{r}, \vec{v}) d\vec{r}\,'}_{transmission}$$

Combine Collision and Transmission Kernels

$$\vec{p} = (\vec{r}, \vec{v}) \quad \text{and}$$
$$R(\vec{p}\,' \to \vec{p}) \equiv C(\vec{r}\,', \vec{v}\,' \to \vec{v}) T(\vec{r}\,' \to \vec{r}, \vec{v})$$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \int_{\vec{p}_k} \psi_k(\vec{p}_k) R(\vec{p}_k \to \vec{p}_{k+1}) d\vec{p}_k$$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \int_{\vec{p}_k} \left[\int_{\vec{p}_{k-1}} \psi_{k-1}(\vec{p}_{k-1}) R(\vec{p}_{k-1} \to \vec{p}_k) d\vec{p}_{k-1} \right] R(\vec{p}_k \to \vec{p}_{k+1}) d\vec{p}_k$$

$$\ldots \text{and so on} \ldots$$

$$\psi_{k+1}(\vec{r}, \vec{v}) = \int_{\vec{p}_k} \int_{\vec{p}_{k-1}} \cdots \int_{\vec{p}_0} \psi_0(\vec{p}_0) R(\vec{p}_0 \to \vec{p}_1) d\vec{p}_0 \cdots$$
$$\psi_{k-1}(\vec{p}_{k-1}) R(\vec{p}_{k-1} \to \vec{p}_k) d\vec{p}_{k-1} R(\vec{p}_k \to \vec{p}_{k+1}) d\vec{p}_k$$

Sum Over All Collisions

$$\psi(\vec{p}) = \sum_{k=0}^{\infty} \psi_k(\vec{p})$$

Arriving at the *integral form* of the transport equation

$$\psi(\vec{r},\vec{v}) = \int_{\vec{r}\,'} \left[\int_{\vec{v}\,'} \psi(\vec{r}\,',\vec{v}\,') C(\vec{r}\,',\vec{v}\,' \rightarrow \vec{v}) d\vec{v}\,' \right] T(\vec{r}\,' \rightarrow \vec{r},\vec{v}) d\vec{r}\,'$$

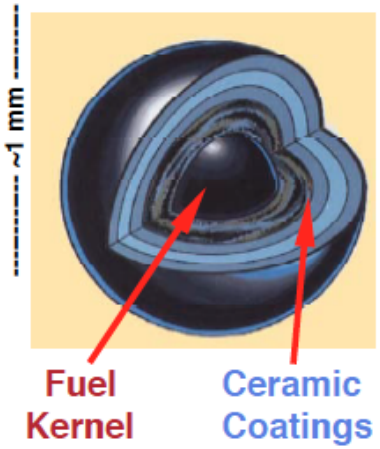
Mathematical Validity

$$\Psi_k(\vec{p}) = \int \int \cdots \int \Psi_0(\vec{p}_0) R(\vec{p}_0 \to \vec{p}_1) R(\vec{p}_1 \to \vec{p}_2) \cdots R(\vec{p}_{k-1} \to \vec{p}_k) d\vec{p}_0 d\vec{p}_1 \cdots d\vec{p}_{k-1}$$

- Integration over many variables
- Generate a "history"
  (sequence of states $\vec{p}_0, \vec{p}_1, \ldots, \vec{p}_k$)
  - Randomly sample from source: $\Psi_0(\vec{p}_0)$
  - Randomly sample for each of k transitions: $R(\vec{p}_{k-1} \to \vec{p}_k)$
- Average for result A by averaging of M histories

$$\langle A \rangle = \int A(\vec{p}) \Psi(\vec{p}) d\vec{p} = \frac{1}{M} \sum_{m=1}^{M} \left[\sum_{k=1}^{\infty} A(\vec{p}_{k,m}) \Psi(\vec{p}_{k,m}) \right]$$

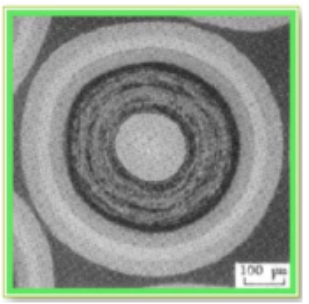
Can Model Very Complex Things

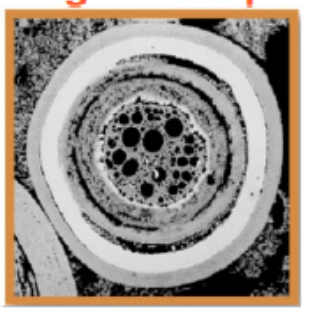


TRISO Fuel Particles:

- Fission product gases trapped within coatings
- Coatings remain intact, even with high T & burnup

Fuel concept is same for block or pebble bed



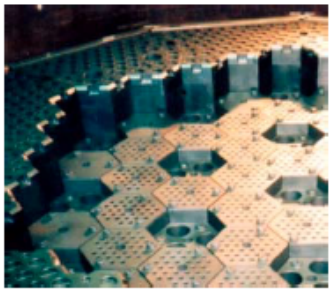


(From General Atomics)

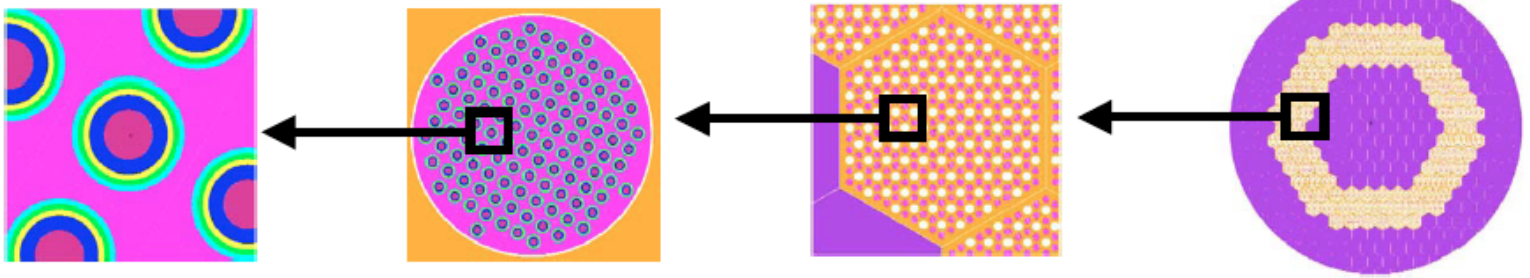
PARTICLES

COMPACTS

FUEL BLOCK



CORE



Accurate & explicit modeling at multiple levels