

NE 155

**Introduction to Numerical Simulations in
Radiation Transport**

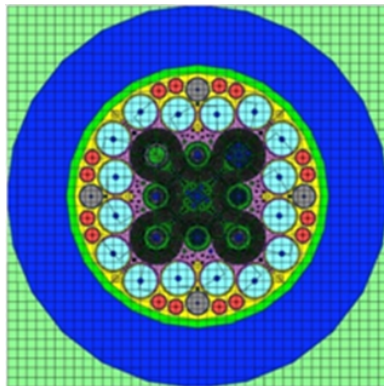
Introduction to Monte Carlo

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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

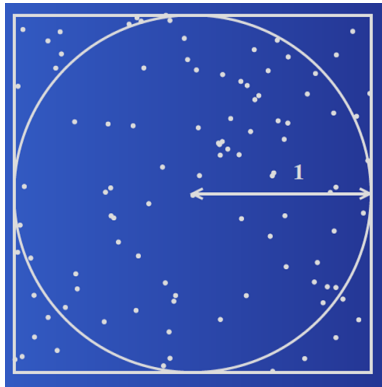
EVALUATE π BY RANDOM SAMPLING

- 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 Probabilites,
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

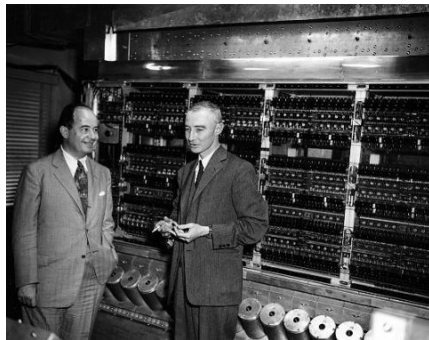


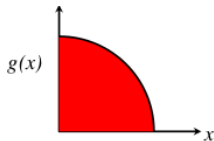
Figure 1: Oppenheimer, von Neumann, MANIAC

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)



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

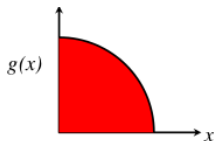
$$G = \int_0^1 g(x) dx = (1 - 0) \overline{g(x)}$$

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

for $k = 1, \dots, N$, 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)



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

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

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

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

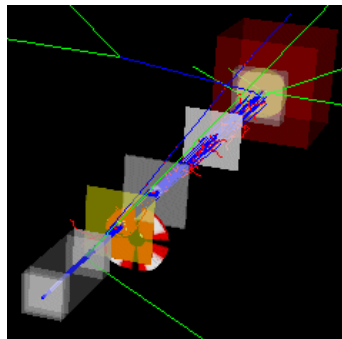
$$G = \frac{m_N}{N}$$

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})

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

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})

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

COMBINE COLLISION AND TRANSMISSION KERNELS

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

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

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

... and so on ...

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

SUM OVER ALL COLLISIONS

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

Arriving at the *integral form* of the transport equation

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

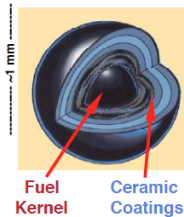
MATHEMATICAL VALIDITY

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

- Integration over many variables
- Generate a “history”
(sequence of states $\vec{p}_0, \vec{p}_1, \dots, \vec{p}_k$)
 - Randomly sample from source: $\Psi_0(\vec{p}_0)$
 - Randomly sample for each of k transitions: $R(\vec{p}_{k-1} \rightarrow \vec{p}_k)$
- 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

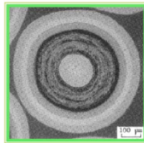


TRISO Fuel Particles:

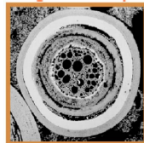
- Fission product gases trapped within coatings
- Coatings remain intact, even with high T & burnup

Fuel concept is same for block or pebble bed

Fresh Fuel



High Burnup



(From General Atomics)



PARTICLES



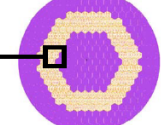
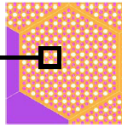
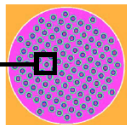
COMPACTS



FUEL BLOCK



CORE



Accurate & explicit modeling at multiple levels