NE 155/255
Numerical Simulations in Radiation Transport
Introduction to Monte Carlo

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Learning Objectives

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

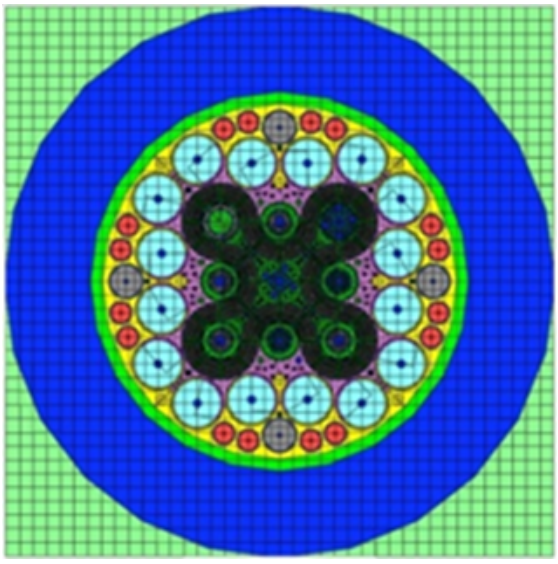


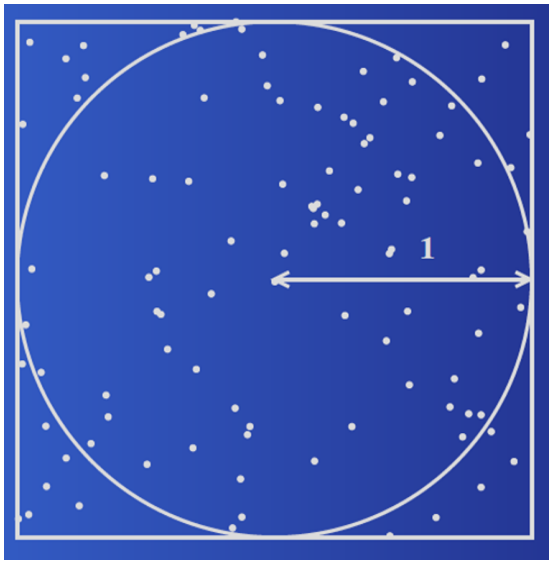
Figure 1: ATR reactor geometry

Notes derived from Rachel Slaybaugh, Jasmina Vujic, and Paul Wilson.

What are Monte Carlo methods?

- 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 number sequence

Evaluate π by Random Sampling



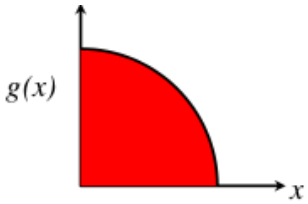
- Area of square, $A_s = 4$
- Area of circle, $A_c = \pi$
- Fraction of random points in circle

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

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

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

Evaluate π by Random Sampling (math)



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

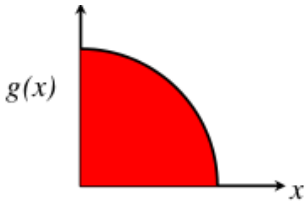
$$G = \int_0^1 g(x)dx = (1 - 0)\overline{g(x)}$$

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 $\hat{x}_k^2 + \hat{y}_k^2 \leq 1$,

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

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

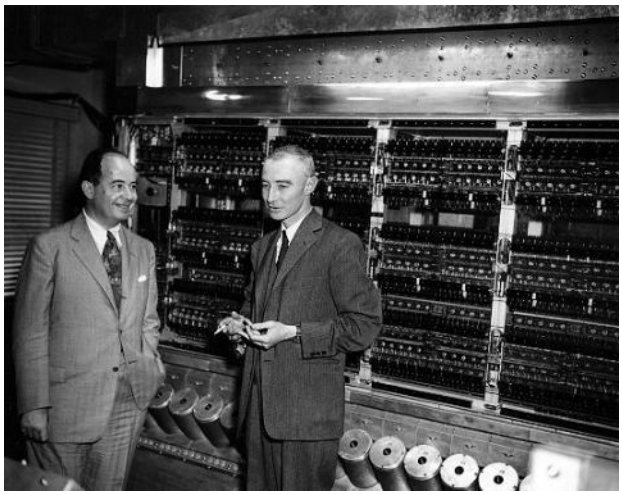


Figure 2: Oppenheimer, von Neumann, MANIAC

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/
- OpenMC: originally developed at MIT, https://docs.openmc.org/en/stable/
- Serpent: Developed by Dr. Jaakko Leppanen, VTT, Finland, http://montecarlo.vtt.fi/
- Shift: developed at ORNL, distributed via RSICC, http://rsicc.ornl.gov
- Mercury: developed at LLNL, https://wci.llnl.gov/simulation/computer-codes/mercury

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
- We also have Variance Reduction methods

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

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

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

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

Combine Collision and Transmission Kernels

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

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

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

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

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

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

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

- 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

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