

1 Learning Objectives

1. Be able to define what a Monte-Carlo (MC) simulation is
2. Be able to justify the choice of MC for radiation transport
3. Be able to identify and explain the major components of MC radiation transport methods
4. Provide examples of probabilistic representations of physics
5. Distinguish between a PDF and CDF
6. Distinguish between a discrete PDF (CDF) and continuous PDF (CDF)
7. Describe the goal of random sampling
8. Identify and implement the best random sampling technique for a given distribution

What is Monte Carlo?

Monte Carlo methods employ the use of random processes to determine a statistically-expected solution to a problem. These random processes can fulfill two roles:

- Statistical approximation to mathematical equations
- Statistical approximations to physical processes

The basic concept for a MC simulation is to construct a random process for a problem and carry out a numerical simulation by N-fold sampling from a random number sequence. These processes have been used extensively for hundreds of years to solve complicated problems of the time:

- 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

MC is applicable to applications that are mathematically equivalent to *integration over many dimensions*. This can be useful when

- Analytic integration is impossible
- Deterministic numerical integration is slow and/or requires error prone approximations.

The relatively straightforward approach of MC methods, combined with the fact that they easily simulation non-deterministic processes has led them to be used in a wide variety of fields:

- High energy physics: many nucleon interactions
- Process engineering: Combine uncertainties in many variables
- Financial sector: Prices and rates of return for many objects (simulate many possible futures given trends and uncertainty)
- Risk analysis: Many individual probabilistic contributes to risk

However, MC methods often require significant computer time to general statistically significant results. This can be overcome with parallel computing since MC methods are “embarrassingly parallelizable”. Additionally, variance reduction (VR) methods have been developed that can be used to improve statistics with fewer particles. Finally, hybrid methods have been developed that use deterministic methods to accelerate MC calculations. We will explore all of this over the next couple of lessons.

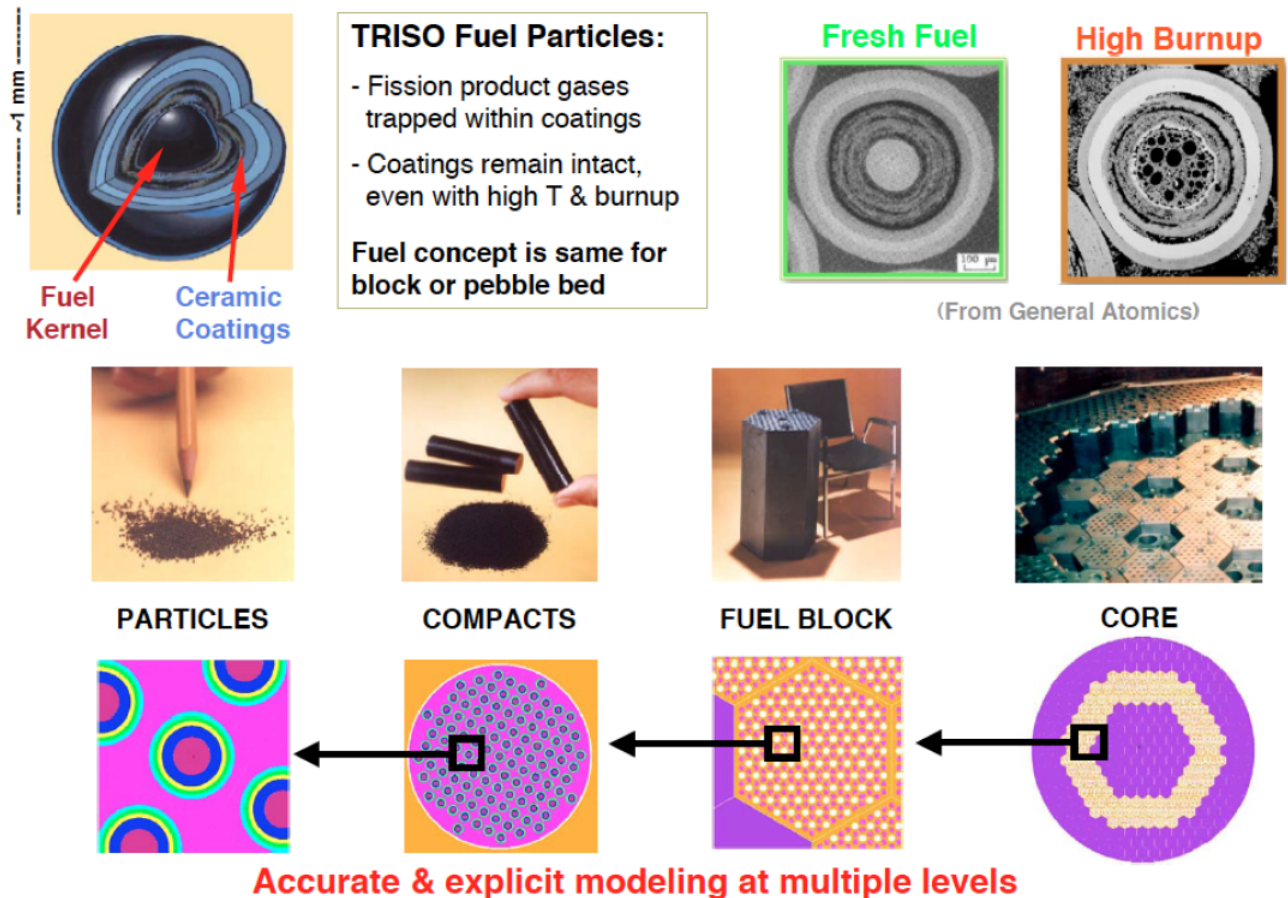
For now, let us explore the earliest use of MC to evaluate π using the iPython notebook.

What is MC Radiation Transport?

MC transport works by simulating many independent particles in a system. For radiation transport, this works well as most of the physical processes that affect source generation and transport can be described as probabilistic events. The basic formulation of a MC transport method is to

- 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

Unlike deterministic approaches, MC methods can readily model very complex things such as pebble bed reactors. Why?



Is it worth considering

- Is the independence assumption valid for all radiation transport?
- If not, where does the independence assumption cause problems?
- Are there radiation transport mechanisms that are deterministic instead of probabilistic?

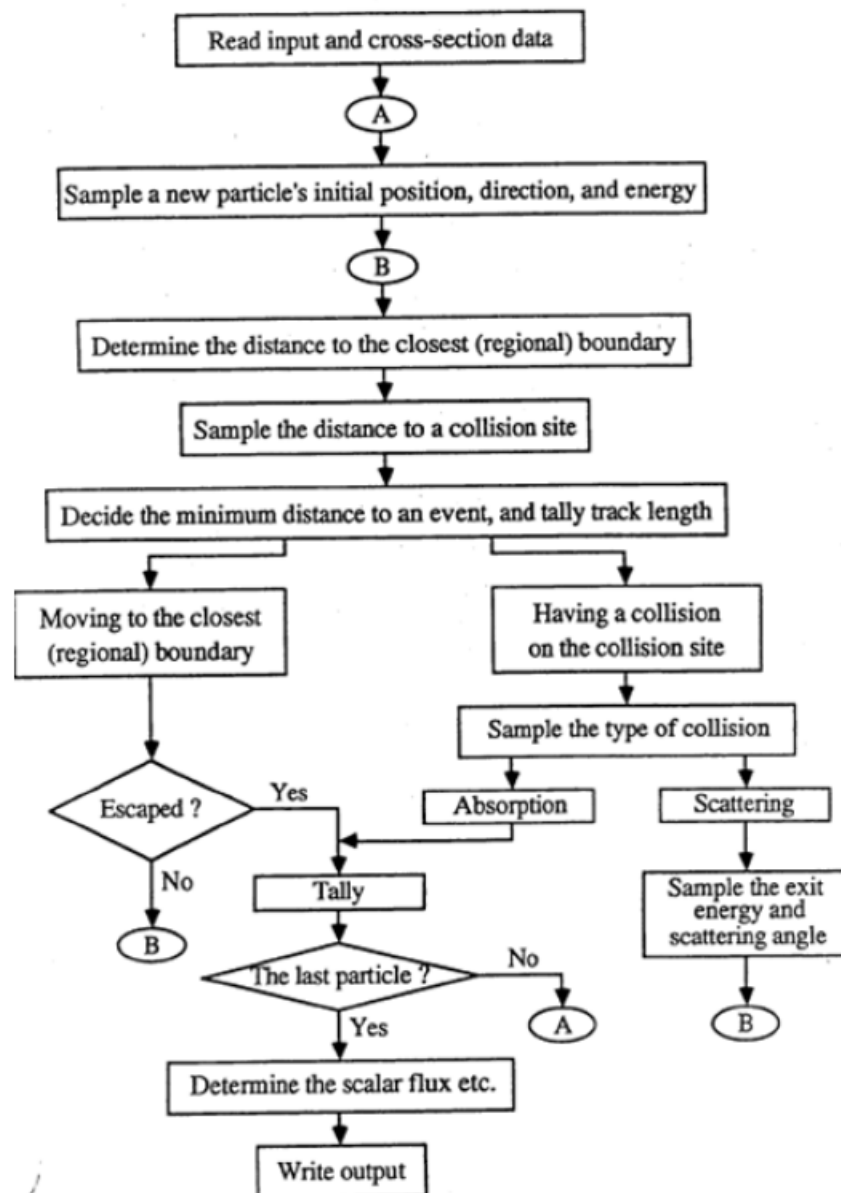
Major Components of a MC Algorithm

There are several common components of a MC algorithm that apply across any implementation considered:

- PDFs: the physical/mathematical system must be described by a set of pdfs.
- Random number generator: a source of random #s uniformly distributed on the unit interval.
- Sampling rule: prescription for sampling the pdf (given having random #s)

- Scoring: the outcomes must be accumulated/tallied for quantities of interest
- Error estimation: an estimate of the statistical error (variance) of the solution
- Variance Reduction: methods for reducing the variance and computation time simultaneously
- Parallelization: efficient use of computers

For radiation transport, and example simple algorithm, using these components might be formulated as:



General Purpose MC Codes

MC is the most common radiation transport method used across a wide range of applications. A non-inclusive list of common MC codes include:

- 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>
- Mercury: developed at LLNL, <https://wci.llnl.gov/simulation/computer-codes/mercury>

Physics as Probability

Various radiation related physical phenomena can be represented by probability distributions:

- Photon emission energy: Each possible energy has a different probability (intensity)
- Scattering cross-sections: Each possible scattering angle has a different probability as a function of the energy
- Transmission through a medium: Probability of reaching a particular position depends on the cross-section
- Radioactive decay: Each decay event is probabilistic based on probability of individual atoms to tunnel through energy barriers

To implement MC, we must quantify the underlying probability distributions for the outcome of each physical event. We can then estimate the statistical moments of these distributions to get our physical answers. Let's start by exploring probability density functions (PDFs) in more detail.

PDFs and CDFs

In the MC simulation, all variables, x , have a Probability Density Function (PDF), $p(x)$, with the following characteristics:

Continuous:

$$\begin{aligned} p\{a \leq x \leq b\} &= \int_a^b p(x)dx \\ p(x) &\geq 0 \\ \int_{-\infty}^{\infty} p(x)dx &= 1 \end{aligned}$$

Discrete:

$$\begin{aligned} p(x = x_k) &= p_k \equiv p(x_k) \\ k &= 1, \dots, N \\ p_k &\geq 0 \\ \sum_{k=1}^N p_k &= 1 \end{aligned}$$

The PDF represents the *collective behavior* of the system. All PDFs, $p(x)$, have an associated Cumulative Distribution Function (CDF), $P(x)$, with the following properties:

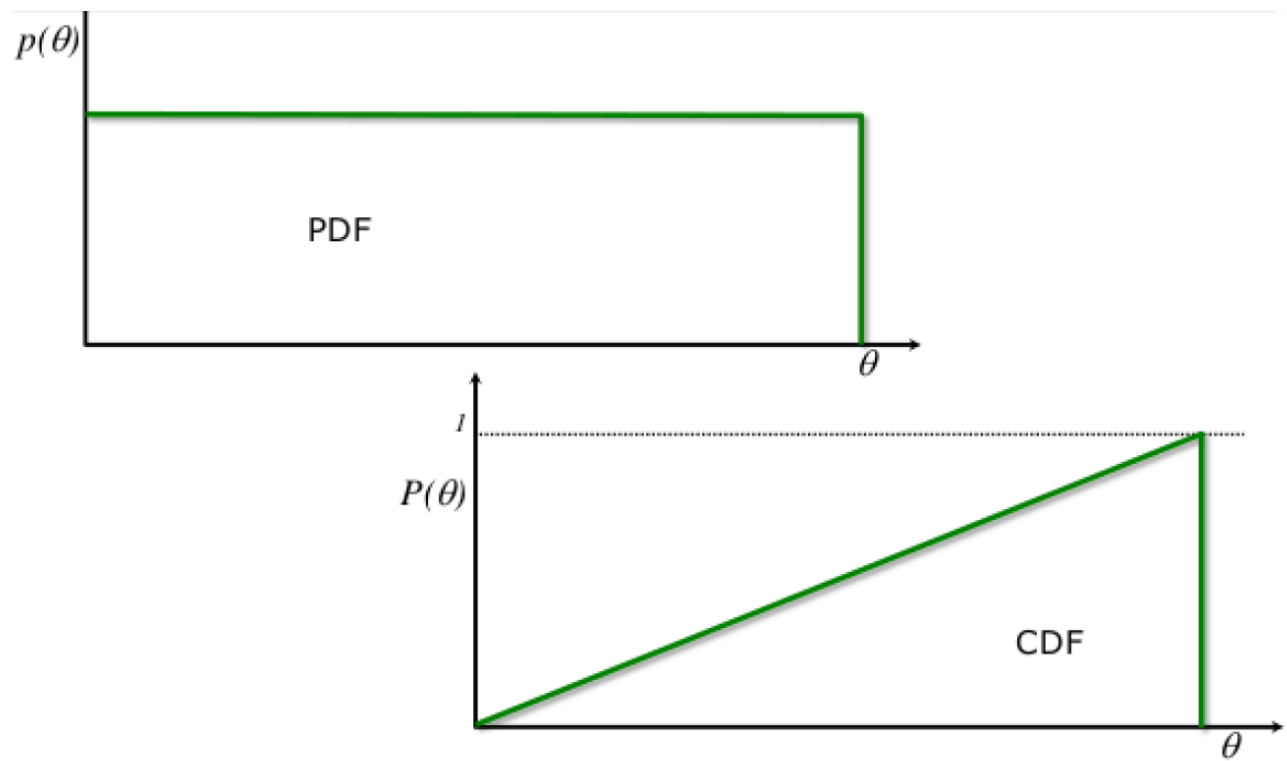
Continuous:

$$\begin{aligned} p\{x' \leq x\} &= P(x) = \int_{-\infty}^x p(x')dx' \\ P(-\infty) &= 0, \quad P(\infty) = 1 \\ 0 &\leq P(x) \leq 1 \\ \frac{dP(x)}{dx} &\geq 0 \end{aligned}$$

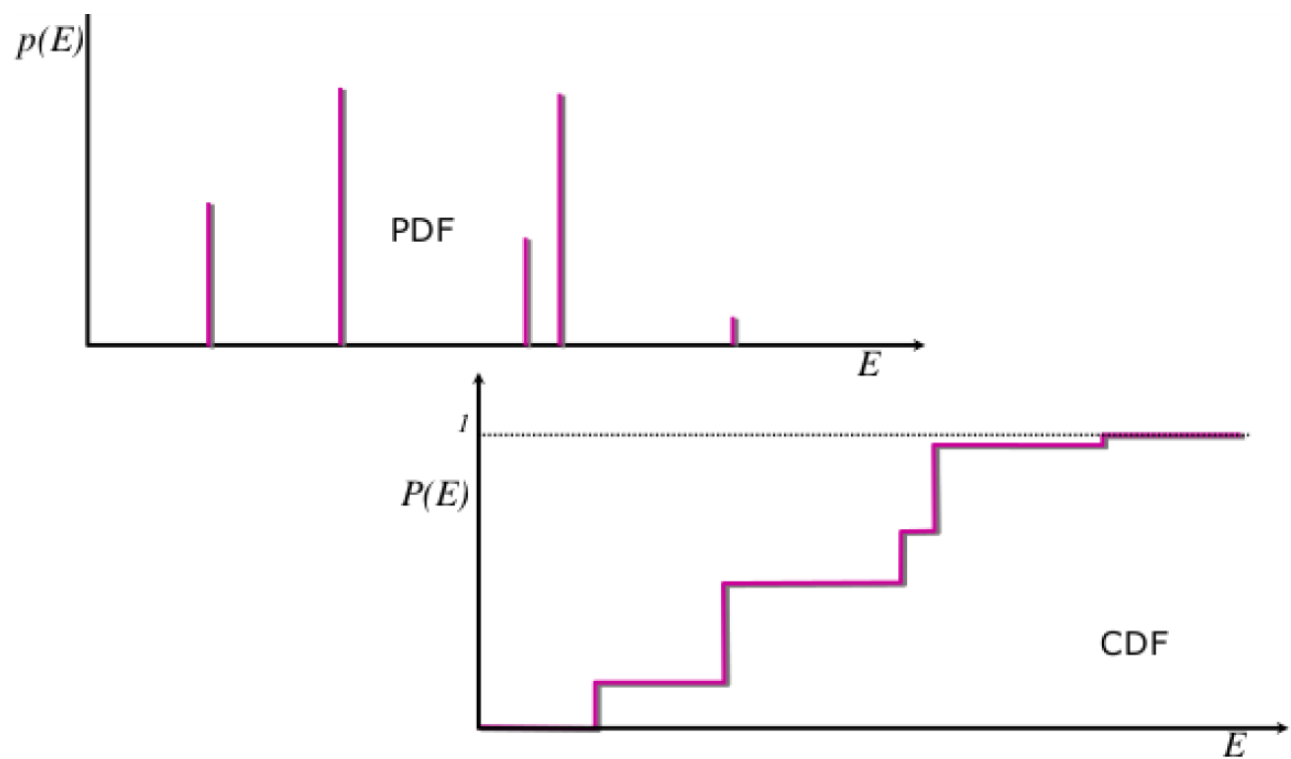
Discrete:

$$\begin{aligned} pP\{x' \leq x\} &= P_k \equiv P(x_k) = \sum_{j=1}^k p_j \\ k &= 1, \dots, N \\ P_0 &= 0, \quad P_N = 1 \\ 0 &\leq P_k \leq 1 \\ P_k &\geq P_{k-1} \end{aligned}$$

To demonstrate, consider a uniform probability distribution:



Or a discrete probability distribution:



Sampling Techniques

Random sampling uses uniformly distributed random variables to choose a value for a variable according to its PDF. The implementations can vary based on the form of the data and the physics process being modeled. Some sampling techniques are

- *Basic* sampling techniques
 - Direct discrete sampling
 - Continuous discrete sampling
 - Rejection sampling
- *Advanced* sampling techniques
 - Histogram
 - Piecewise linear
 - Alias sampling
 - Advanced continuous PDFs

Several of these will be explored in the Sampling iPython notebook